Artificial Intelligence for Nuclear Physics

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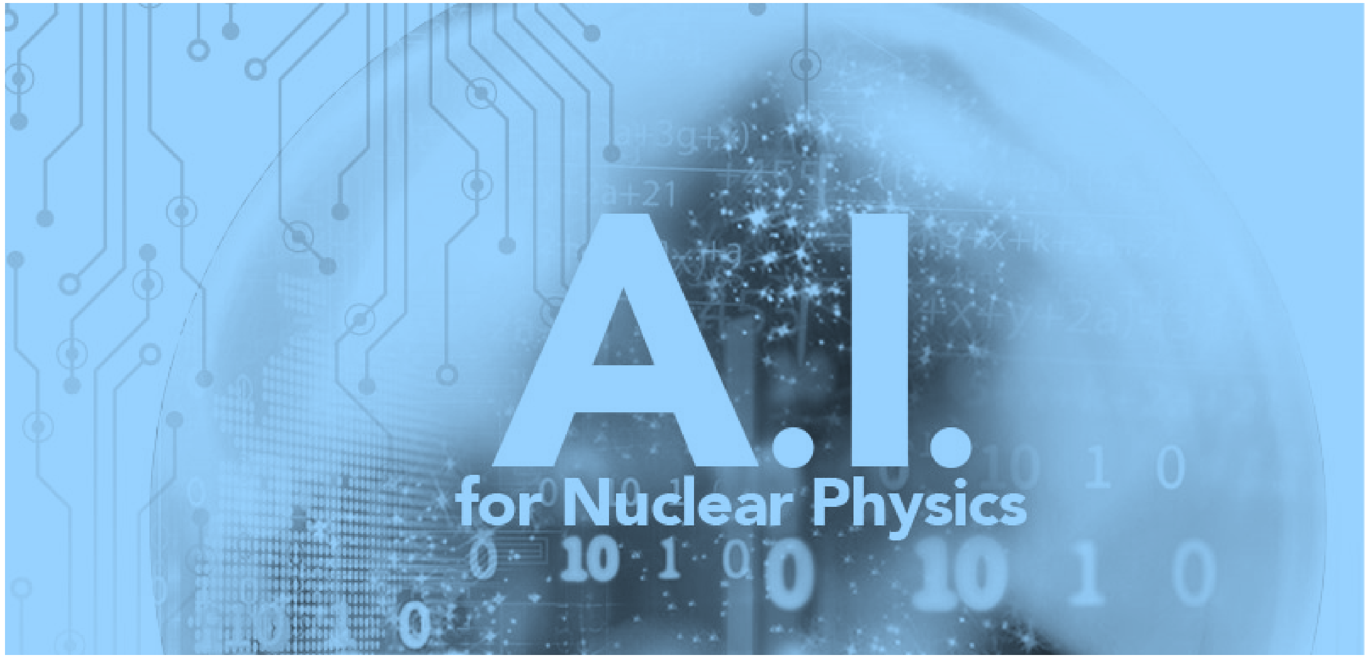


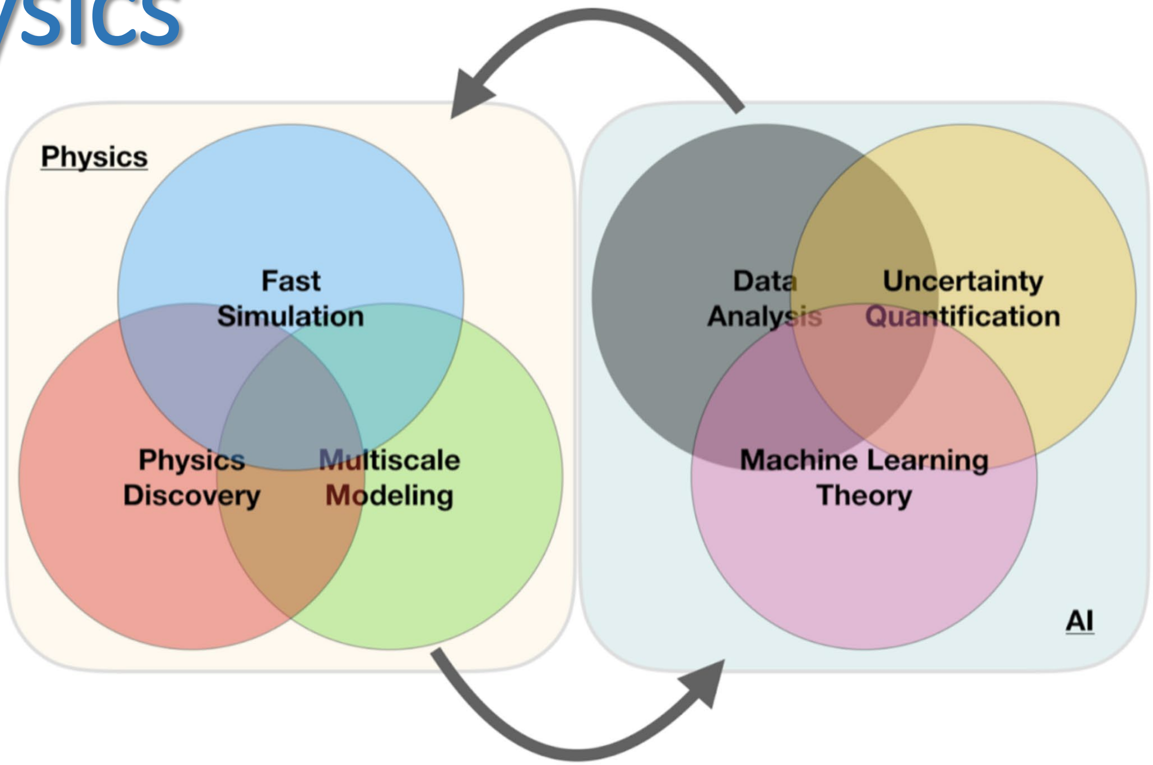
IUPAP Nuclear Science Symposium and
IUPAP WG.9 Annual General Meeting

14-15 June 2022
SURA HQ, Washington DC

Outline

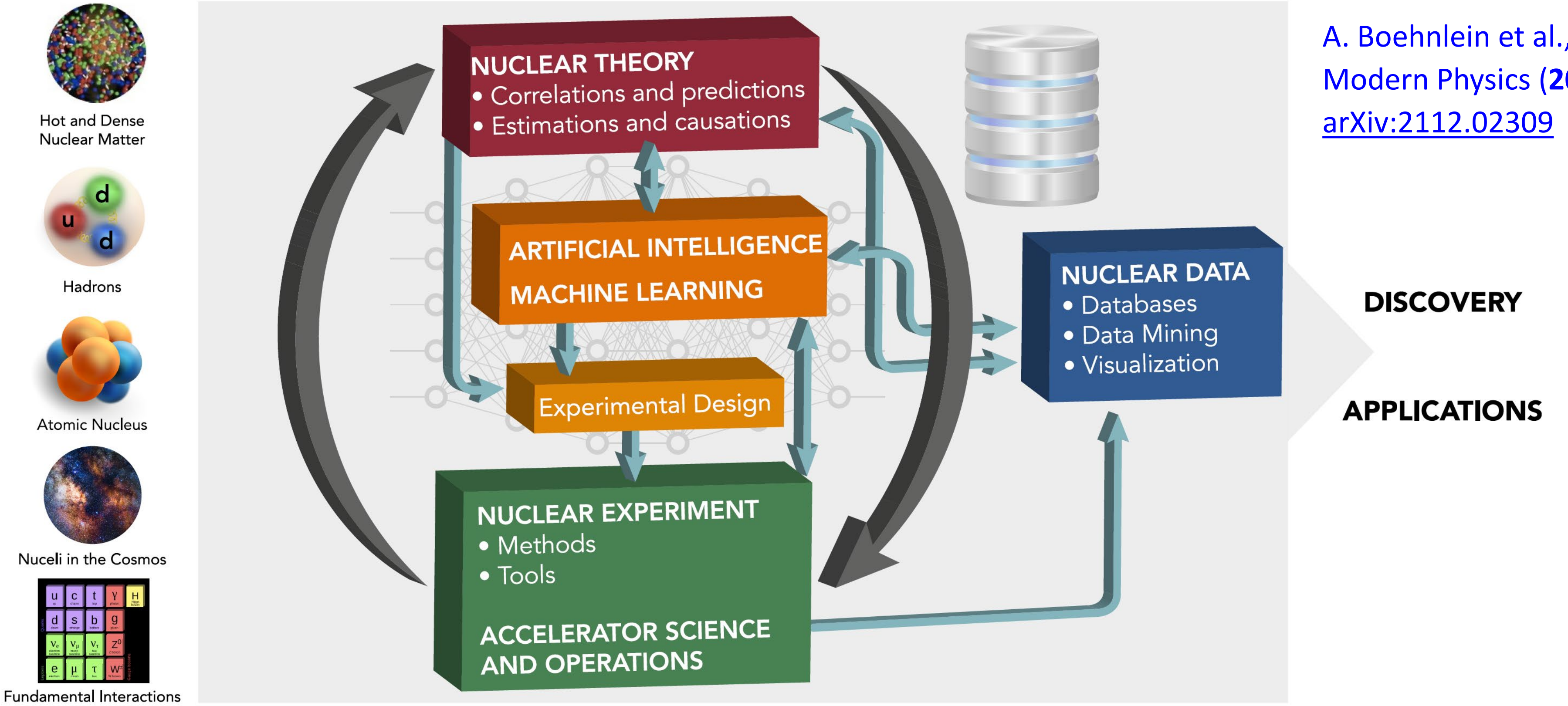
- Introduction and context
- Activities including community identified communalities and needs
- Areas of active research
  - Nuclear theory
  - Experimental methods
  - Accelerator technology
  - Nuclear data
- Educational activities
- Observations and Outlook

A simple perspective on the interface between AI and Physics



- ❑ Statistics, data science, and AI/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.
- ❑ Recent advances in AI capabilities are being applied to advance scientific discovery in the physical sciences *(Carleo et al. RMP **91** (**2019**) 045002; Deiana et al. (**2021**), arXiv:2110.13041).*

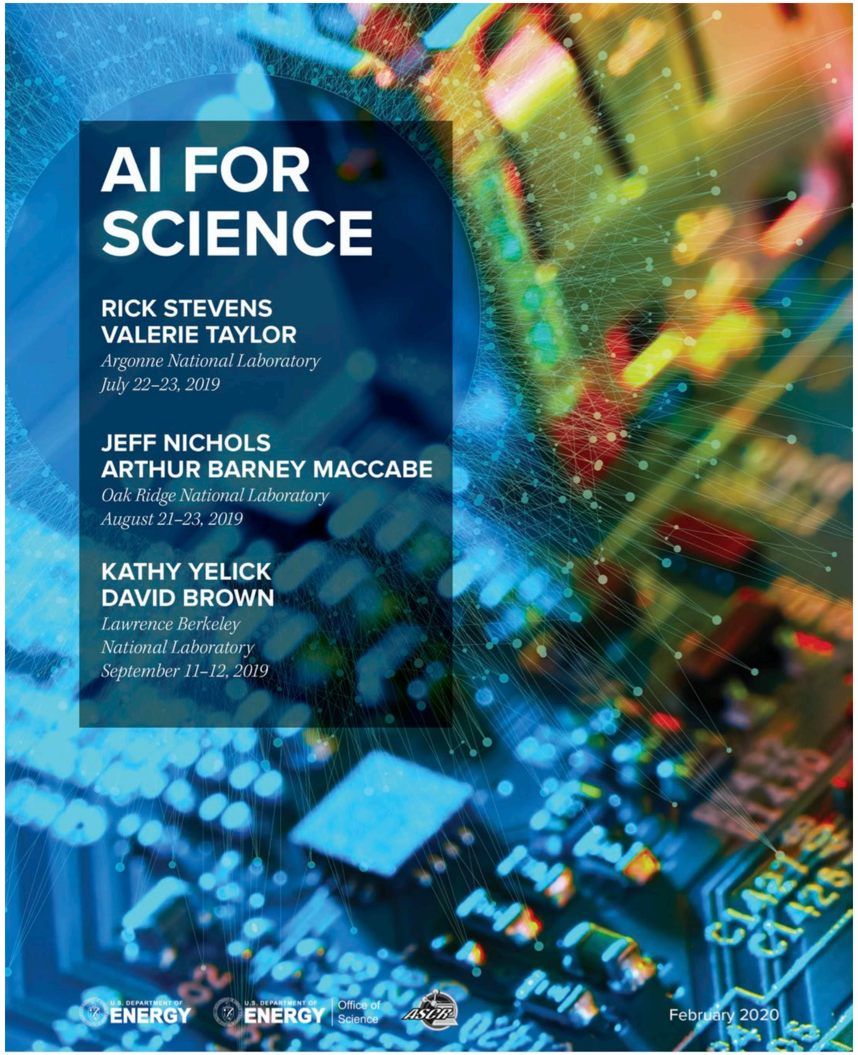
Introduction: AI in Nuclear Physics



A. Boehnlein et al., Review of Modern Physics (**2022**), **in press**, arXiv:2112.02309

- ❑ **Nuclear physics covers 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.
- ❑ The broad aims of nuclear physics as a field corresponds to a highly distributed scientific enterprise. **These efforts, utilizing arrays of data types across size and energy scales, create a perfect environment for applications of AI/ML**

Context: AI for Science – what's next after Exascale



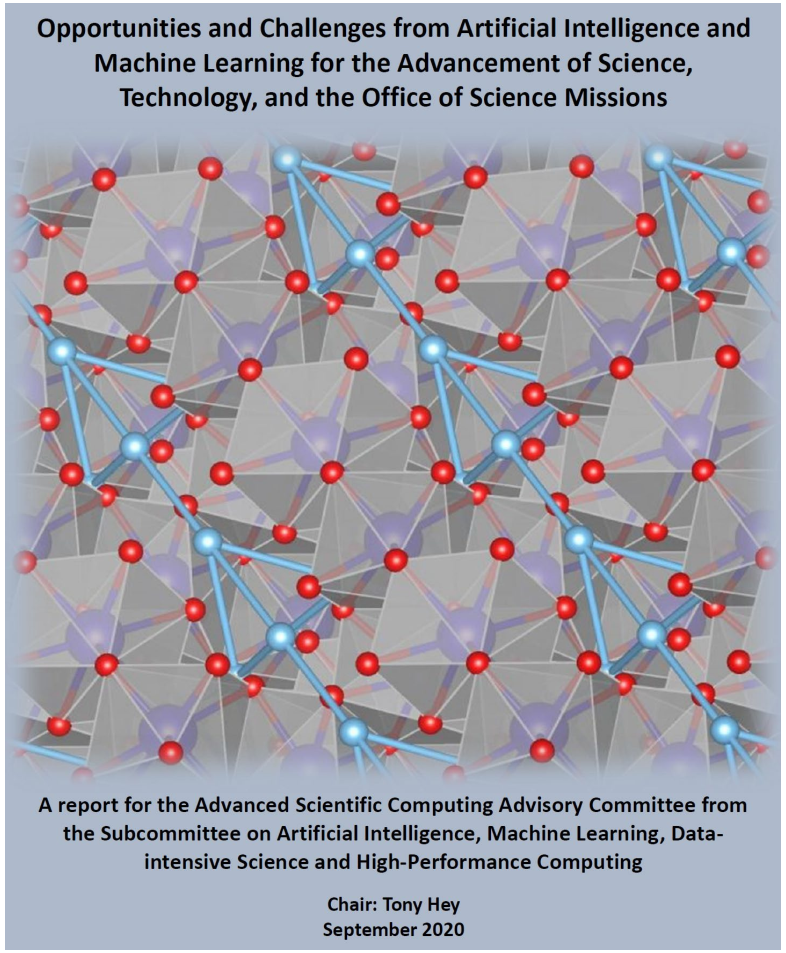
- Over 1,000 scientists participated in four town halls during the summer of 2019
- Research Opportunities in AI
  - Biology, Chemistry, Materials,
  - Climate, Physics, Energy, Cosmology
  - Mathematics and Foundations
  - Data Life Cycle
  - Software Infrastructure
  - Hardware for AI
  - Integration with Scientific Facilities
- Modeled after the Exascale Series in 2007

https://www.anl.gov/ai-for-science-report

AI in Nuclear Physics – Grand Challenges

- **Harness the physics program of the Electron-Ion Collider (EIC)**
  - AI/ML will help guarantee maximum science output from the EIC
- **Realize the science potential of FRIB**
  - A variety of AI/ML tools will be developed to address specific needs including beam generation, event characterization, detector response, experiment optimization and data analysis
- **Event Reconstruction in Nuclear Physics**
  - AI techniques for reconstruction of tracks in time projection chambers at FRIB, and for heavy ion collisions
- **Improve Tracking Algorithms**
  - AI/ML to significantly improve tracking at all NP accelerator facilities
- **Particle Identification**
  - AI/ML to complement existing Monte Carlo methods for PID
  - Gamma-Ray Energy Tracking Array (GRETA): AI/ML to reconstruct the path of multiple gamma rays from measured interaction positions and deposited energies

Context: 2020 ASCAC Subcommittee on: ‘AI/ML, Data-intensive Science and High-Performance Computing’ (Subcommittee on ‘AI for Science’)



https://science.osti.gov/ascr/ascac/Meetings/202009

Components needed for successful AI in Science Initiative

Application-specific solutions based on hardware/software/algorithm co-design

Research in AI algorithms and foundations

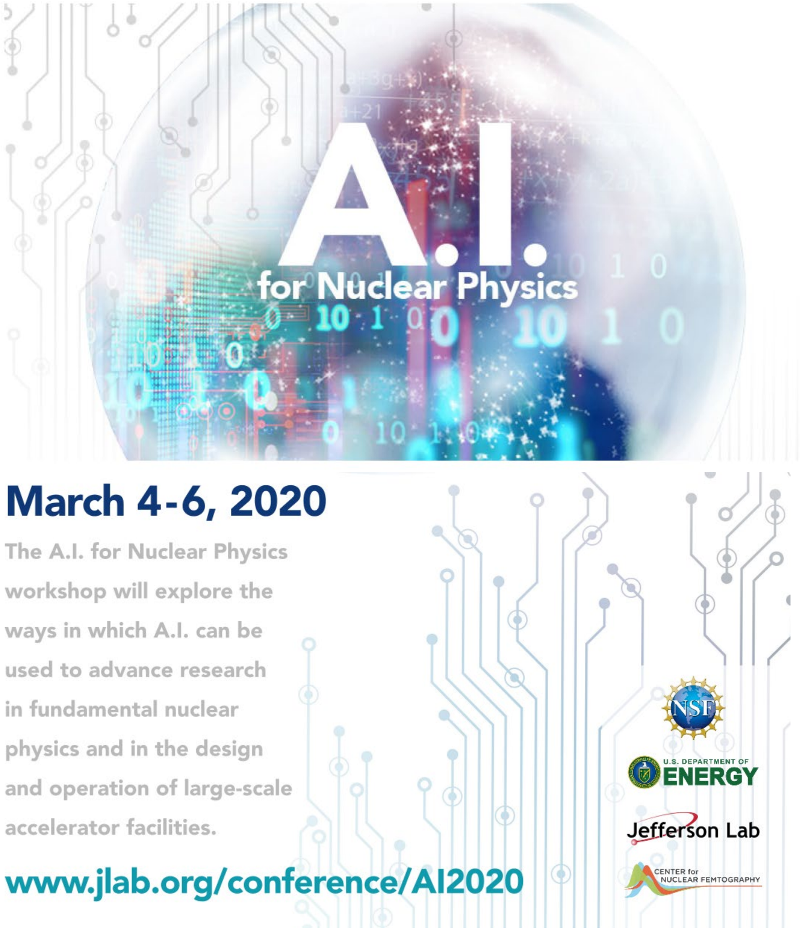
Development of AI software infrastructure

AI-specific computing architectures and hardware

Successful integration of these components will require

1. A **full partnership between all areas of the Office of Science**
2. Engagement of the National Laboratories and their user facilities
3. Involvement of the university and private industry research community
4. Mechanisms for collaborative projects with agencies such as the NSF, NIH, NIST and DOD
5. Collaboration with expert organizations from similarly minded countries
6. An organized process for dissemination to the scientific community

Activities in Nuclear Physics: 2020 AI for NP Workshop



- ❑ 3 day workshop with 180 attendees with plenary breakout format
- ❑ 1 day pre-meeting ‘hackathon’
- ❑ 8 Break out groups to address aspects of Theory, Experiment, and Accelerator
- ❑ The results were summarized in a report containing an assessment of ongoing efforts

[P. Bedaque et al., Eur.Phys.J.A 57 (2021) 3, 100]

- Also summary of the breakout session and additional topical areas (relativistic heavy Ions, Project 8, NEXT and Wanda) not present at the workshop
- Identified need for workforce development and education and a need for cross disciplinary collaborations.

Based on this and many subsequent activities:
Tremendous interest in AI/ML in the Nuclear Physics Community

A.I. for NP: Priority Research Directions

- **Game Changers in Nuclear Theory**
  - LQCD: sign problem, extraction of physical observables, propagator inversion
  - Global QCD analysis
  - Identifying rare events
  - Microscopic description of nuclear fission, origin of the elements, quantified computation of heavy nuclei, correlations and emergent phenomena, spectroscopic quality nuclear density functional, neutron star and dense matter EOS
- **Holistic approach to experimentation – expert systems to increase scientific output**
  - Intelligently combine disparate data sources
  - Real time analysis and feedback
- **Experiment Design not limited by computation**
  - Data compactification, sophisticated triggers, and fast online analysis
- **Improving simulation and Analysis**
  - Use AI/ML to improve the sensitivity of current instruments and accuracy of data
  - Decrease simulation and analysis time
- **Accelerator Design and operations**

A.I. for NP: Community Identified Needs and Communalities

- **Need for workforce development**
  - Educational activities
  - Need for broader community
  - Need for collaboration
- **Need for problem-specific tools**
  - NP applications are unique in that they are often aimed at accelerating calculation, e.g.,
    - Evaluation of models where one can use AI techniques to identify the most promising calculative pathways
    - Simulations where AI-determined parameterizations can be used to circumvent performance limiting elements
- **Enabling infrastructure for AI in NP**
  - Need for standardized frameworks
  - Need for comprehensive data management
  - Need for adequate computing resources
- **Need for uncertainty quantification**

Areas of Active Research in AI/ML in NP

- Invited article for Review of Modern Physics A. Boehnlein et al. (**2022**) **in press**, arXiv:2112.02309

- Focuses on recent application of AI/ML in NP covering topics in:
  - Nuclear Theory
  - Experimental Methods
  - Accelerator Technology
  - Nuclear Data

Artificial Intelligence and Machine Learning in Nuclear Physics

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CONTENTS

AI/ML in Nuclear Theory and Lattice QCD

Topics in Low-Energy, Medium-Energy, High-Energy Nuclear Theory and Lattice QCD

- **Properties of heavy nuclei and nuclear density functions theory**
  - Crucial for understanding rare isotopes
- **Nuclear Properties - Nuclear Shell Model**
  - Improve the predictive power of nuclear models – model residuals
- **Discovering nucleonic correlations and emergent phenomena**
  - Discover correlations in calculations of nuclear wave functions that use underlying forces
- **Nuclear femtography – parton distribution functions**
  - Global feature extraction from (large) datasets
- **Neutron star and dense matter equation of state**
  - Deduce nuclear matter equation of state from intermediate-energy heavy-ion collisions data
  - **Phase transitions and estimators for correlation functions**
- **Ensemble generation in lattice QCD**
  - Scalability, compact variables, sign problem

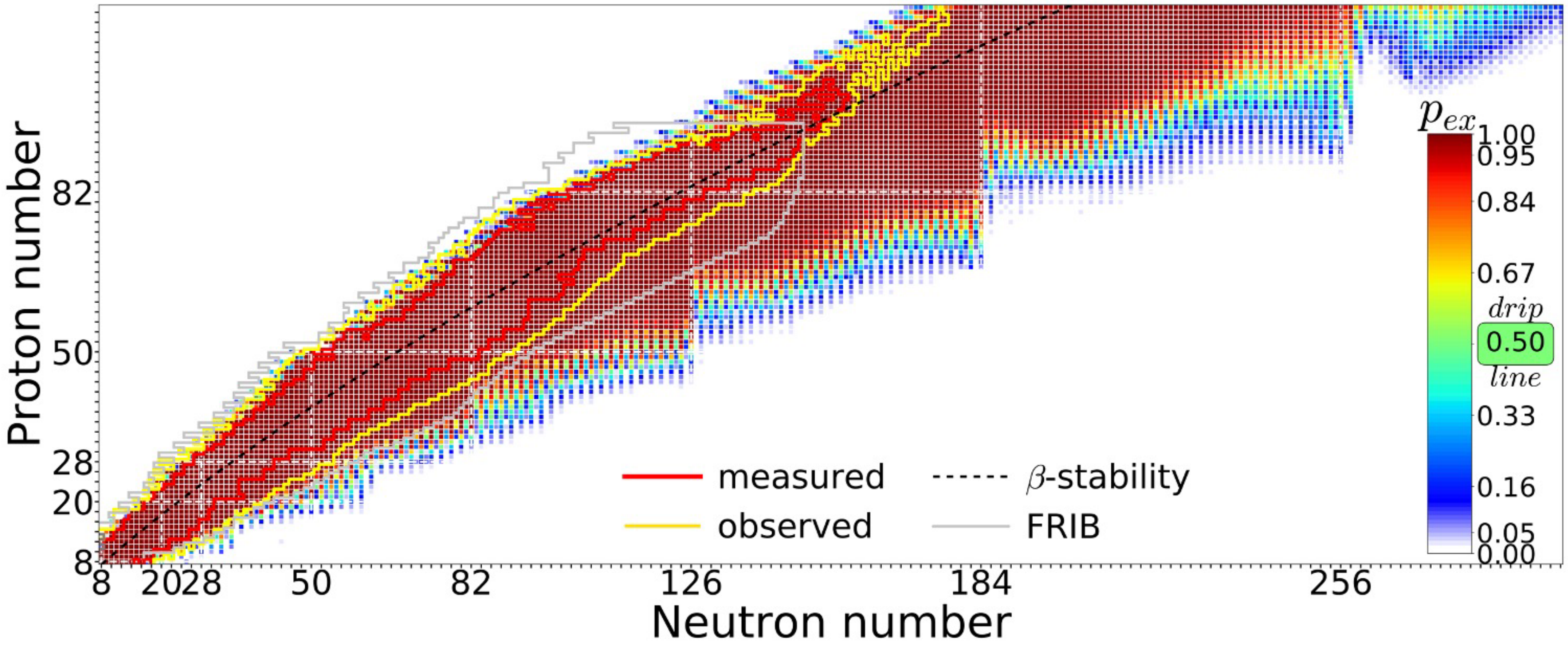
Nuclear Theory Examples

- **Example 1: Bayesian Model Averaging to Quantify Limits of the nuclear landscape**

Constrained density functional theory calculations in multidimensional collective spaces with Bayesian Model Averaging

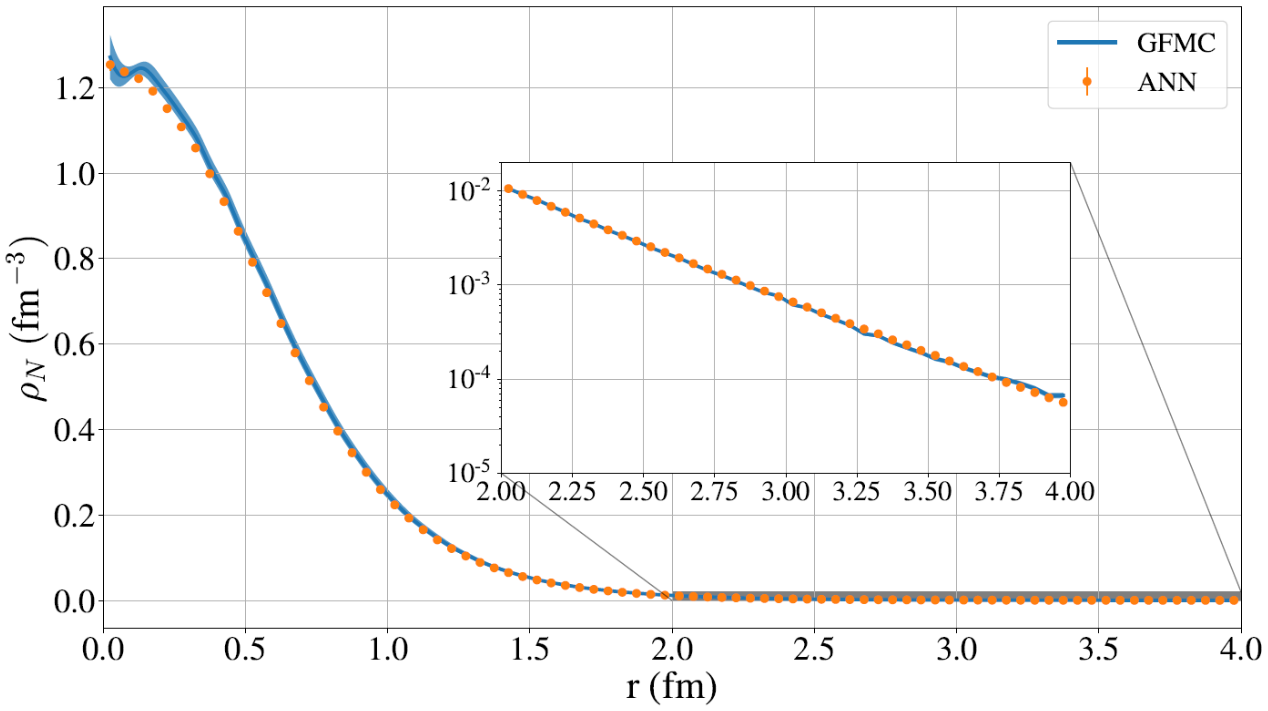
L. Neufcourt et al., PRL **122** (**2019**) 062502
L. Neufcourt et al,, Phys, Rev, C **101** (**2020**) 014319
V. Kejzlar et al., J. Phys. G **47** (**2020**) 094001

L. Neufcourt et al., Phys. Rev. C **101** (**2020**) 044307



Nuclear Theory Examples

- ❑ **Example 2: Many body-variational calculations with ANN**



Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of light nuclei with up to six nucleons

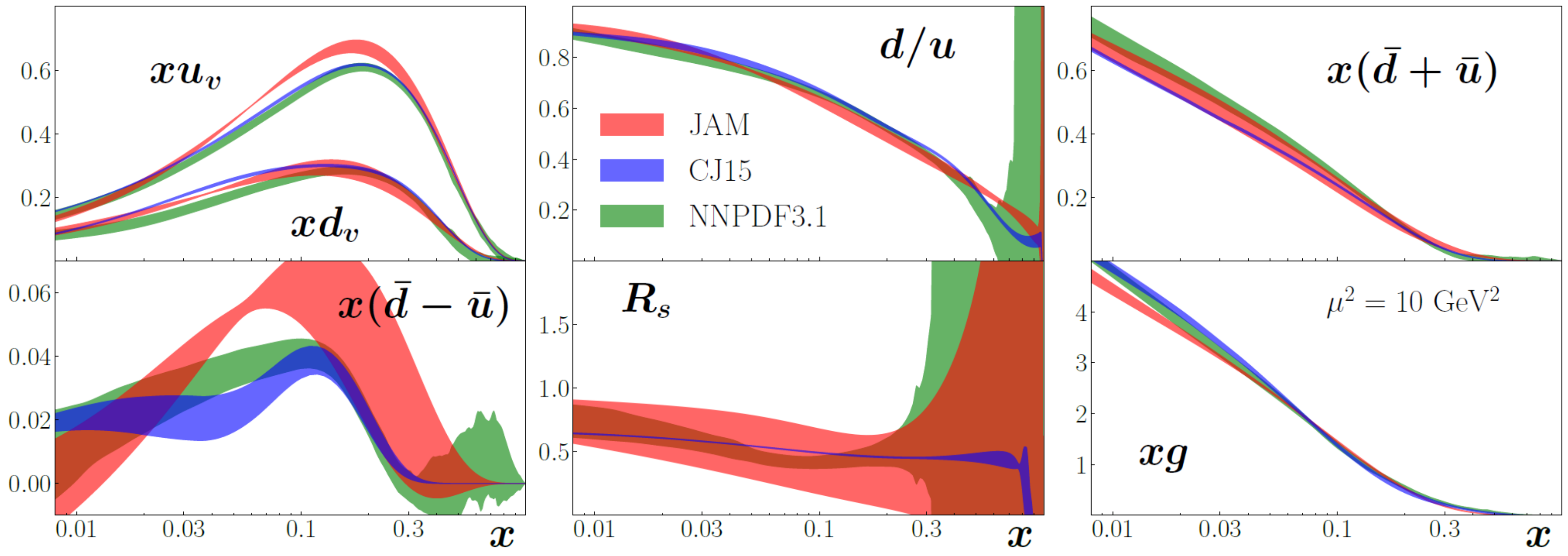
C. Adams et al., Phys. Rev. Lett. **127** (**2021**) 022502

Nuclear Theory Examples

❑ Example 3: Monte Carlo approach for Bayesian inference

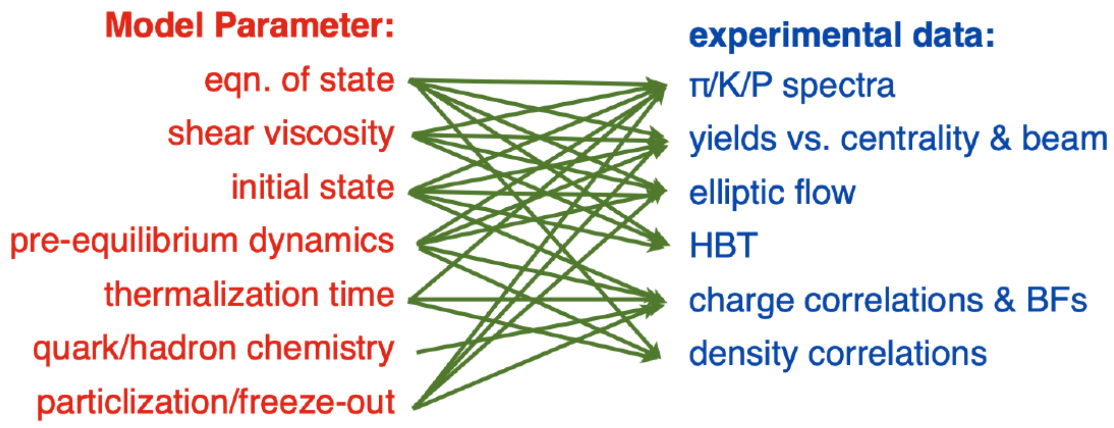
Simultaneous extraction of a variety of Quantum Correlation Functions for nuclear femtography

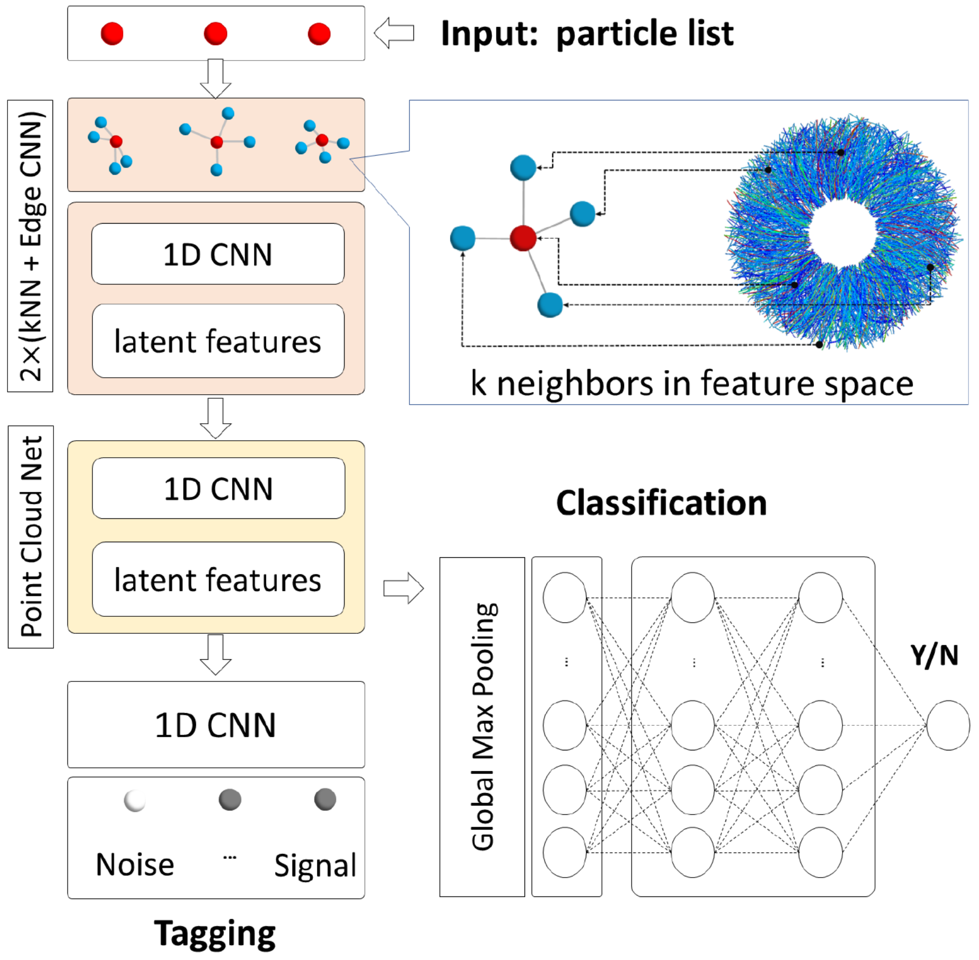
J.J. Ethier et al., PRL **119** (**2017**) 13, 132001; Moffat et al., (**2021**) arXiv:2101.04664; Sato et al., PRD **101** (**2020**) 7, 074020



Nuclear Theory Examples

- ❑ **Example 4: Bayesian analysis to constrain model parameters**





Generative models to approximate model output
ANN help to reveal correlations hidden in high-dimensional data

Lattice QCD Examples

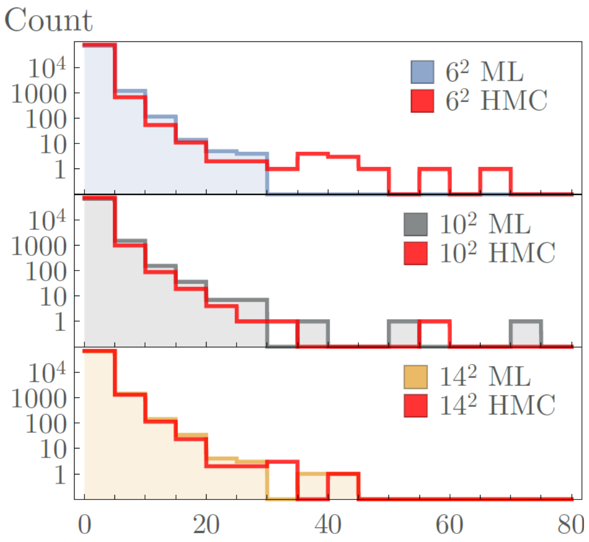
❑ **Example 1: Field configurations and properties**

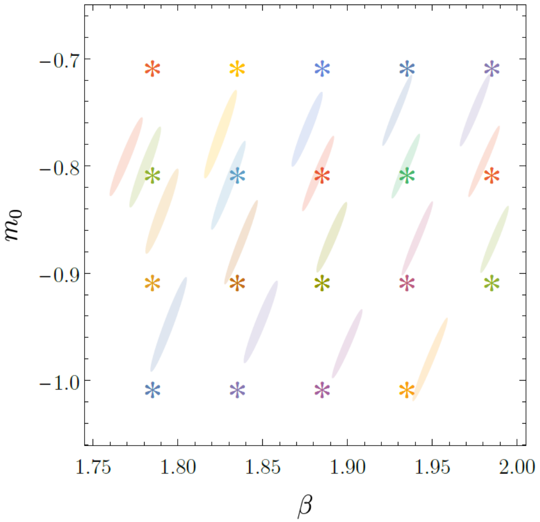
Towards elimination of critical slowing down in MCMC for scalar ϕ^4 theory – construct normalizing flows via ANN

NN to predict lattice action parameters from field configurations

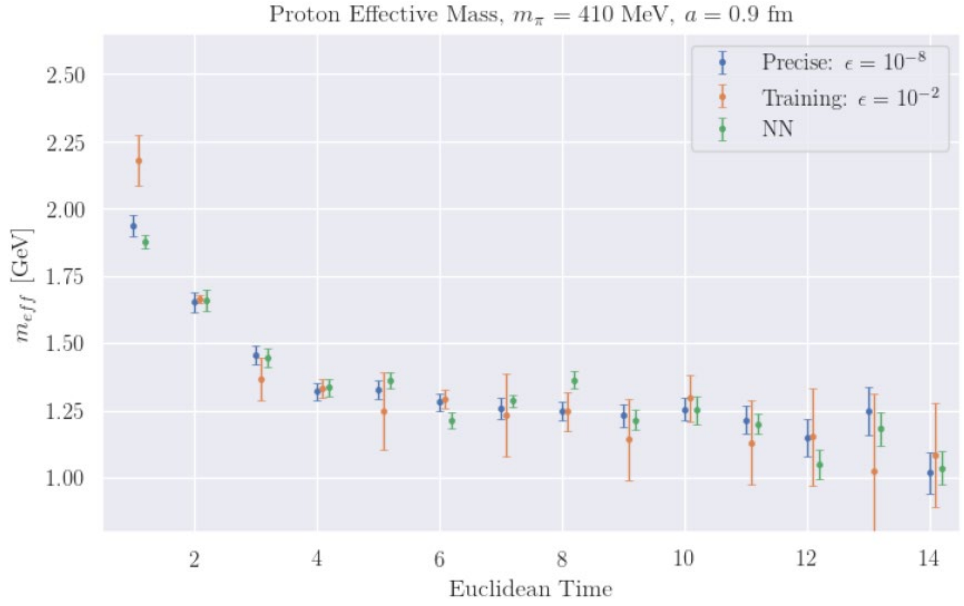
P. E.Shanahan et al., Phys. Rev. D **97** (2018) 094506

M.S. Albergo et al., Phys. Rev. D **100** (2019) no.3 034515





❑ **Example 2: Speed up Hadron Correlator Computation**



Boosted Decision Trees and ANNs to reduce the cost of iterative solvers for quark propagator by relating solutions to the system computed at different precision

Enormous increase in efficiency of the computation

G. Pederiva et al., "Machine Learning Algorithms for Hadron Correlators from Lattice QCD", 2020, Work in progress

Experimental Methods

- **Near Term: Improved analysis, simulations, and AI-driven detector design**
  - Improved sensitivity
  - Faster Analysis → faster scientific output
  - Accelerate simulations – ML for event generators
  - Detector Design – AI helps steering the design (and eventually fine-tune) and can capture hidden correlations among design parameters
- **Long Term:**
  - Holistic approach to experimentation
  - Standardized data formats
  - Experiment design not limited by computation

Experimental Methods Examples: Reconstruction and Analysis

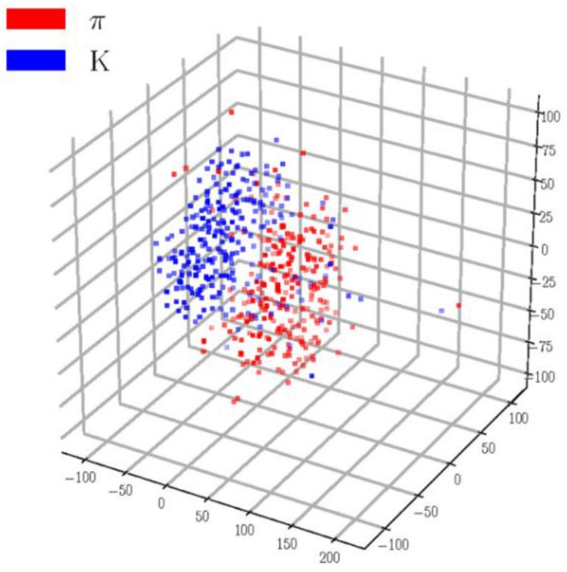
- **Example 1: Particle Identification with Cherenkov Detectors**
  - Identify charged particles by detected hit pattern
  - Recent custom architecture combines VAE, CNN and ANN achieving a fast and accurate reconstruction with capability for deeply learning the detector response

C. Fanelli, JINST 15 **(2020)** 02, C02012

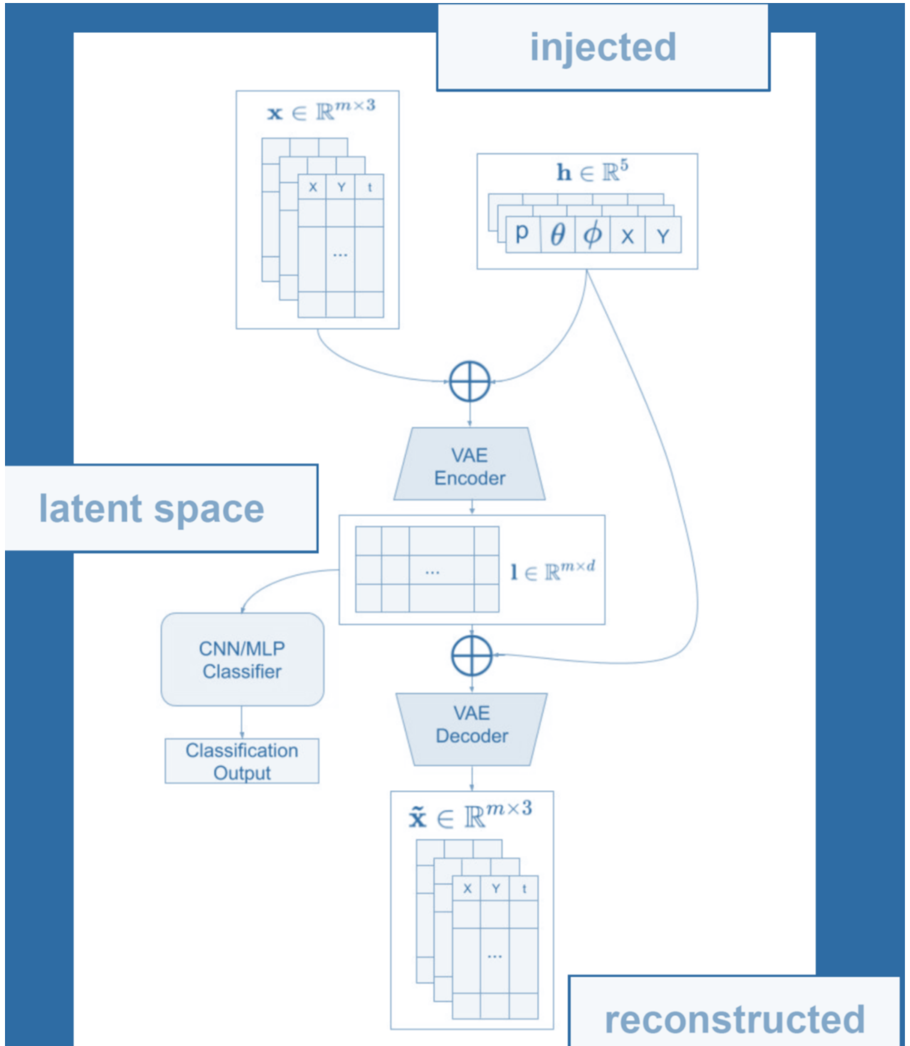
C. Fanelli and J. Pomponi Mach. Learn.:Sci. Technol. **(2020)** 1, 015010

D. Derkach et al., NIMA 952 **(2020)** 161804

A. Maevskiy et al. J. Phys. Conf. Ser. (**2020**) 1525, 012097



Features extracted by CNN

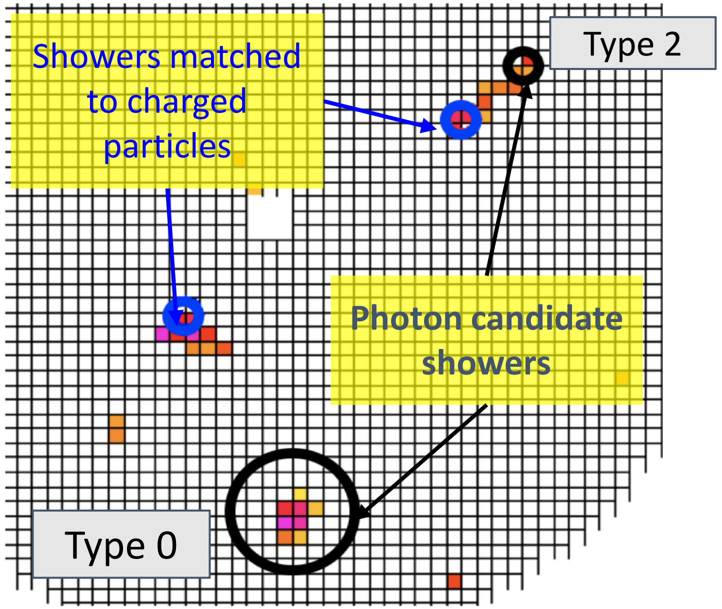


DeepRICH architecture

Experimental Methods Examples: Reconstruction and Analysis

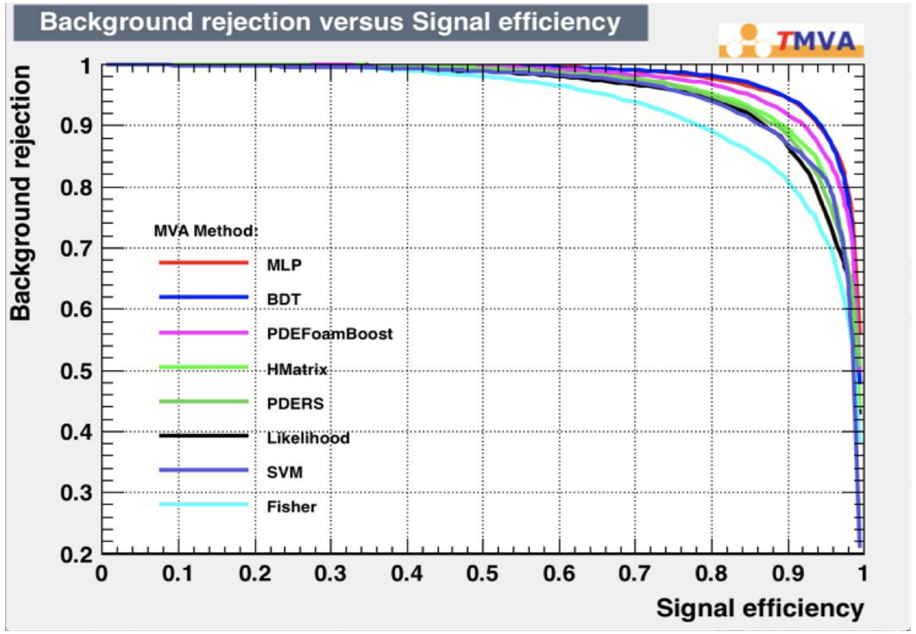
❑ Example 2: Boosted Decision Trees to Search for Exotic Mesons in GlueX

- ➢ Isolate events of interest from a disproportionately large background
- ➢ These ANN-based algorithms have the potential to offer vast improvements in both signal selection efficiency and purity over more traditional techniques.



Radius of the circle proportional to the energy of the shower≈

R. Barsotti and M.R. Shepherd **(2020)** *JINST* **15** P05021

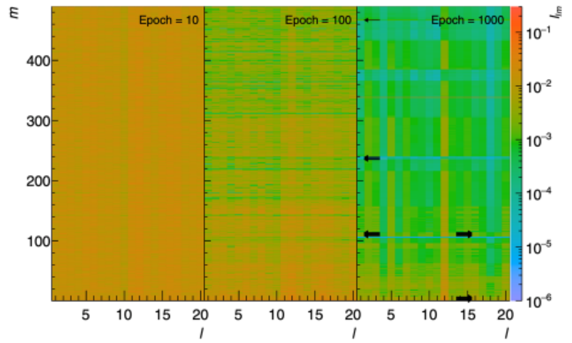


Experimental Methods Examples: Reconstruction and Analysis

- **Example 3: automated (ML driven) design of observables**
  - NN to discover new observables that are sensitive to jet quenching and parton splitting
  - Discovery of theoretical models via automated analysis

- Previous: Finding most sensitive observables to a model parameters

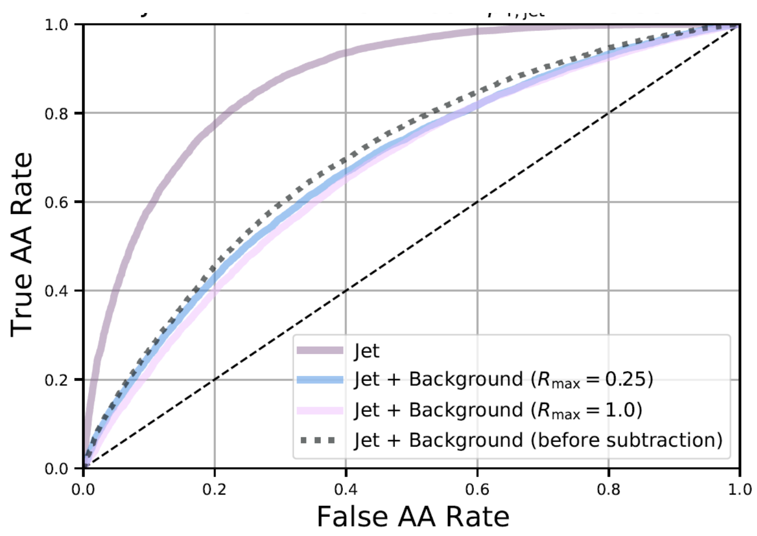
Lai; 1810.00835



- Current focus (from a longer list): How much information is contained in high-energy particle collisions and jets?

Extract knowledge on complex processes (e.g. jet quenching) directly from data - human understandable result (!)
→ new guidance to experiment(s)
→ critical input for theory

Lai, Mulligan, Ploskon, Ringer (**2021**) arXiv:2111.14589



Next challenge?
→ Hadronization
- Long standing problem
- Impact in both NP and HEP
- Guidance for EIC experiments

Experimental Methods Examples: Reconstruction and Analysis

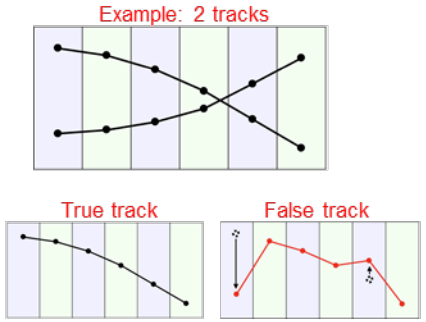
❑ Example 4: Charged Particle Tracking

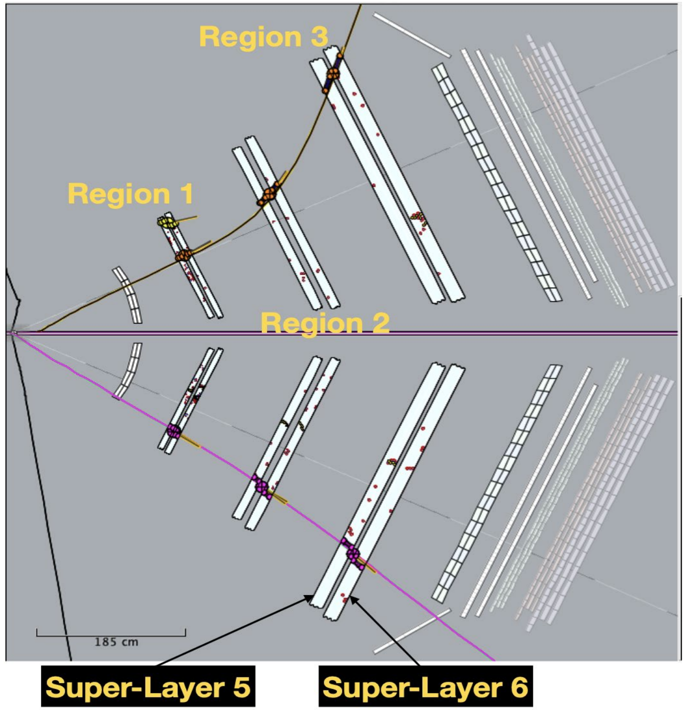
- ➢ ANN and Deep Learning in the CLAS12 workflow provides a 6 times faster track reconstruction speed.
- ➢ Selection of the correct seed results in improved tracking efficiency and recovery of missing tracks with accuracy of >99.8%.

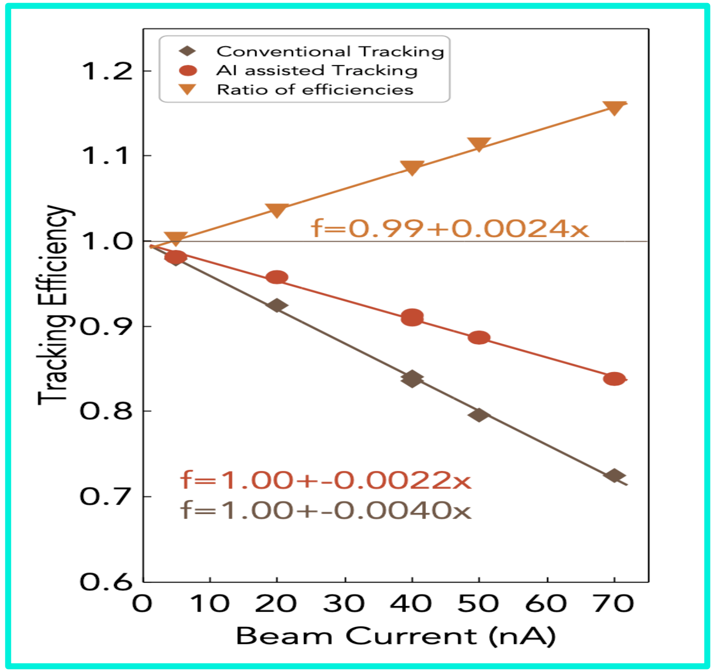
G. Gavalian, et al., (***2020***) *arXiv:2008.12860*

Charged particles tracked using DCs inside toroidal field:

- Each sector has 3 regions
- Each region has 2 Super-Layers
- Super-Layer has 6 layers
- Each Layer has 112 wires





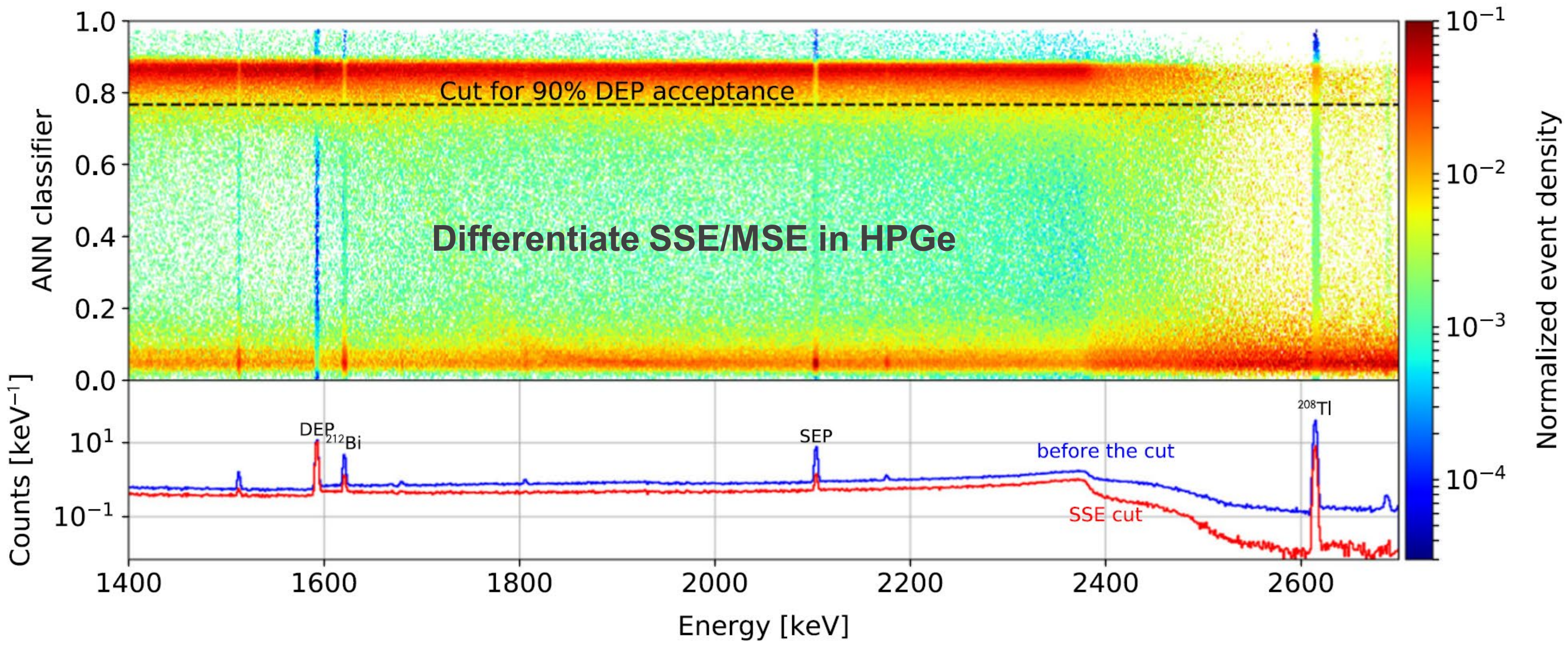


Experimental Methods Examples: Reconstruction and Analysis

- **Example 5: Event and signal classification**

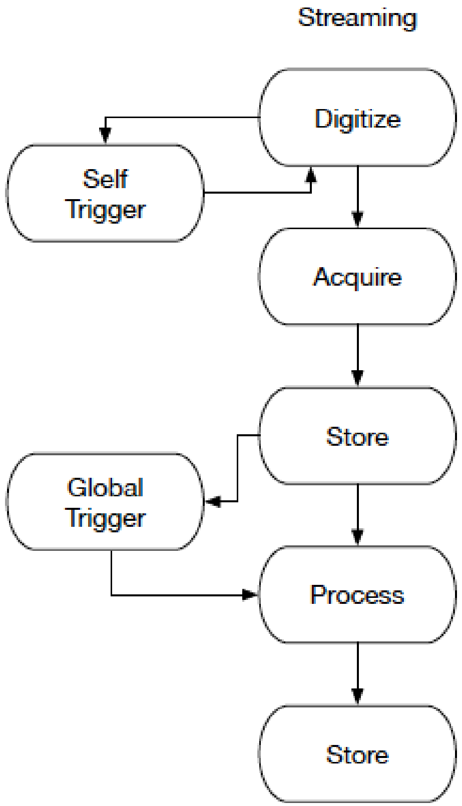
  - Deep ANN and CNN allow to differentiate physics signal types from backgrounds

A. Jany et al., Eur. Phys. J. C (**2021**) 81:38



Experimental Methods Examples: Streaming Readout

Read out detector data in continuous parallel streams that are encoded with information about when and where the data were taken



- ❑ All channels can be part of "the trigger", no bias
- ❑ Simplification of readout: No custom trigger hardware and firmware to implement & debug
- ❑ Enables sophisticated tagging/filtering algorithms
- ❑ Allows use of high-level programming languages
- ❑ Ease of scalability
- ❑ Takes advantage of emerging technologies
  - **Allows use of available AI/ML tools**
  - **Allows use of heterogeneous computing**
- ❑ Allows rapid turnaround of physics data

Many high-luminosity experments adopt the SRO scheme: LHCb, ALICE, AMBER, CBM, TPEX, sPHENIX, STAR, EIC, SOLID, BDX, CLAS12, …

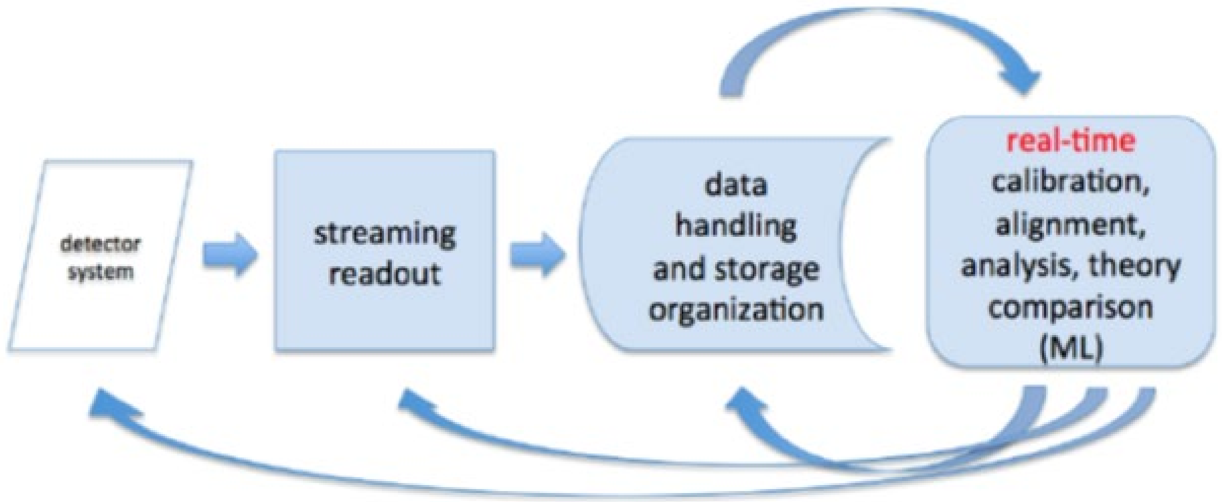
Streaming Readout – Grand Challenges

Develop a proof of concept of quasi-instantaneous high-level nuclear physics analysis based on modern statistics from a self-calibrating matrix of detector raw data synchronized to a reference time, without intermediate data storage requirements with production systems developed for analysis

Key Elements

- Streaming
- Calibration/ML
- Distributed Computing
- Heterogeneous
- Statistical Methods

Integrated whole-experiment model

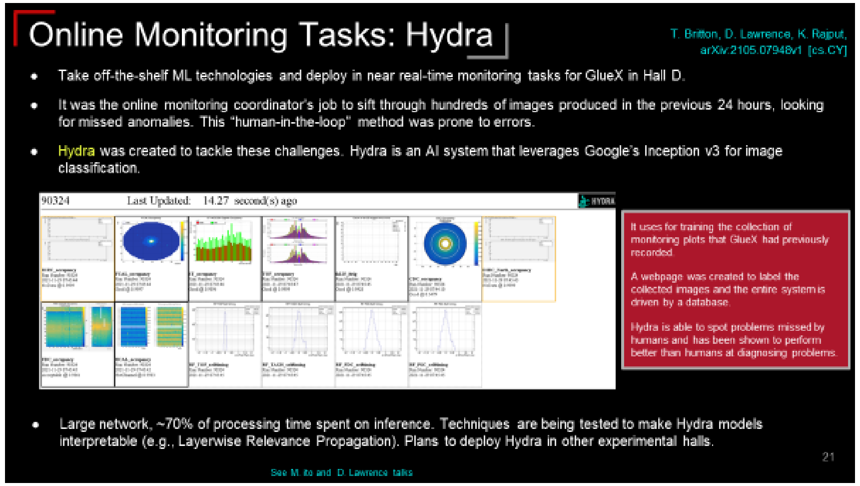


Many high-luminosity experments adopt the SRO scheme: LHCb, ALICE, AMBER, CBM, TPEX, sPHENIX, STAR, EIC, SOLID, BDX, CLAS12, …

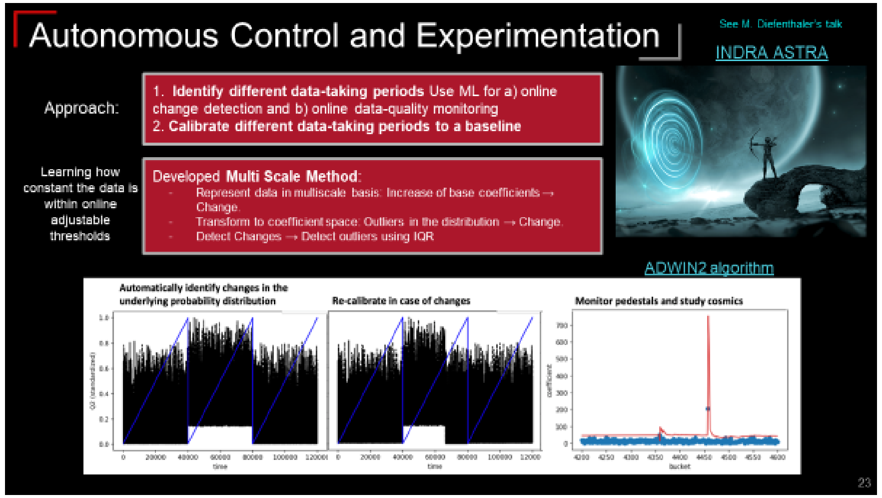
Adapted from A. Boehnlein, R. Ent, R. Yoshida, “Grand Challenge in Readout and Analysis for Femtoscale Science (2018)

Streaming Readout Examples

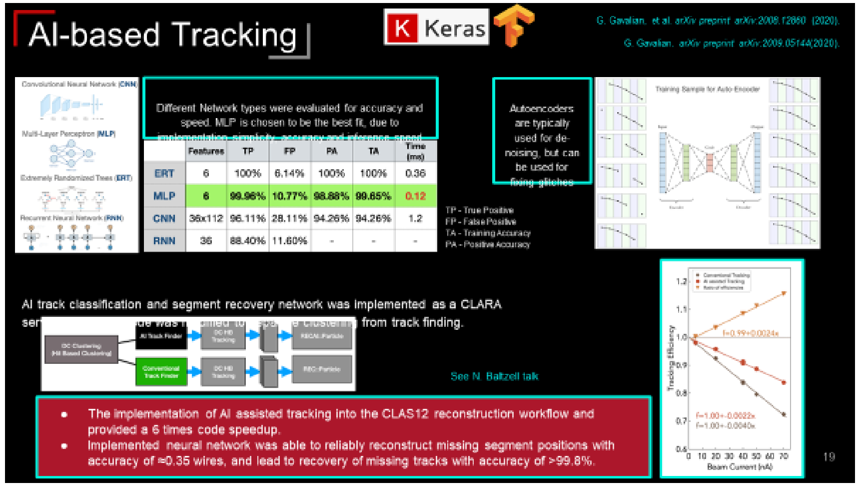
Automated Data Quality Monitoring



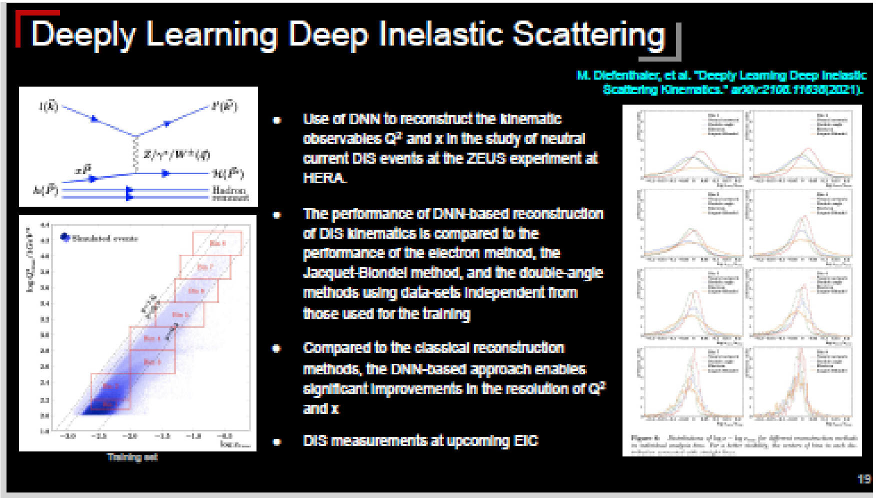
Automated Alignment and Calibrations



Event Reconstruction



Reconstruction of DIS Events

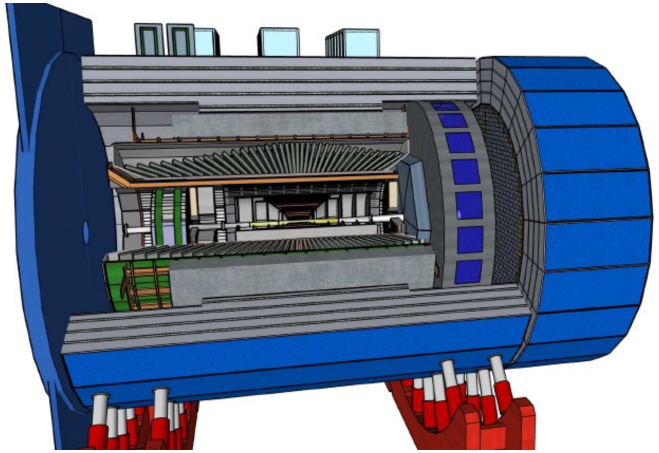


Using examples from C. Fanelli's presentation Crititical Path for the Compute-Detector Model for the EIC (**2021**)

Experimental Design: Design for Detector Systems

AI offers State Of The Art (SOTA) solutions to solve complex optimization problems in an efficient way

- Physics and detector simulations are critical for both initial design and optimization of complex subdetector systems in NP experiments
- Typically, full detector design is studied once the subsystem prototypes are ready - constraints from the full detector or outer layers are taken into consideration
- Need to use advanced simulations which are computationally expensive
- Many parameters (and multiples objective functions): curse of dimensionality - R. Bellman, Dyn. Program. Vol. 295 (1956)
- Entails establishing a procedural body of instructions – C. Fanelli et al. JINST 15.05 (2020): P05009
- The choice of a suitable algorithm is a challenge in itself (no free lunch theorem – D.H. Wolpert et al. 1997, Trans. Evol. Comp. 1, 67-82) and always requires some degree of customization
- Non-differentiable terms

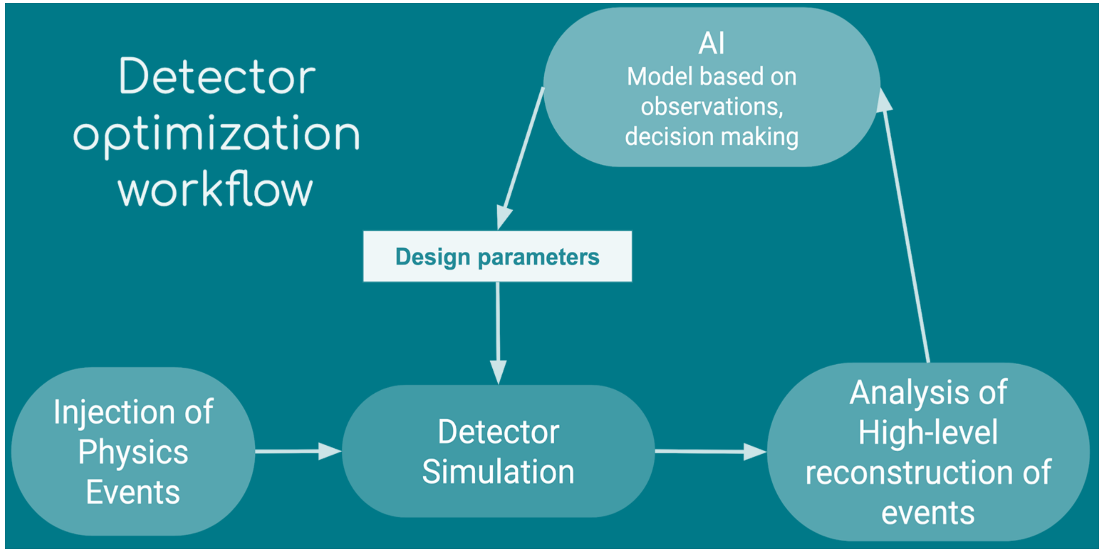


Example of a complex detector with many subsystems: the EIC Detector-1 reference design

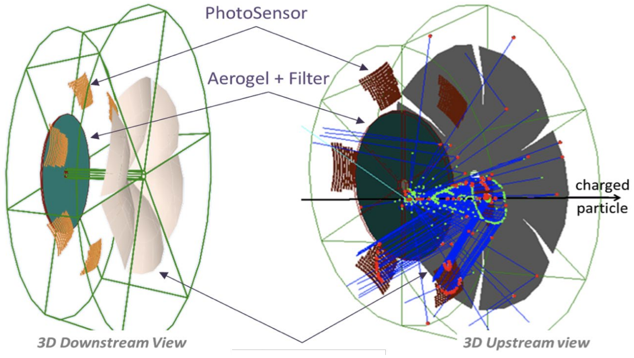
Experimental Design Examples: Design for Detector Systems

Example: Use A.I. to optimize the design during the R&D of large-scale detectors, i.e. simulating noisy and computationally expensive black-box functions

- Bayesian Optimization (BO), Evolutionary Algorithms (EA), etc
- Multi-objective optimization (MOO) in multi-dimensional design space

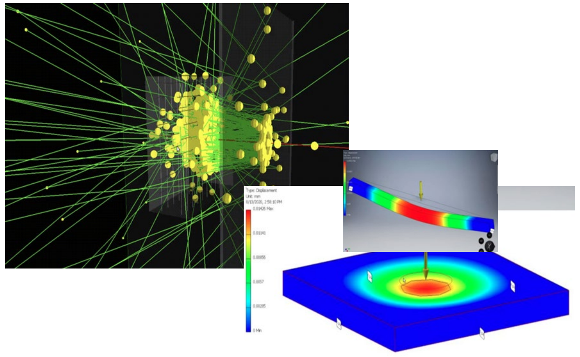


Dual-RICH @EIC: **First EIC paper using AI**, an automated, highly parallelized, self-consistent framework based on BO+ML to optimize the Geant simulation of the dual-RICH.



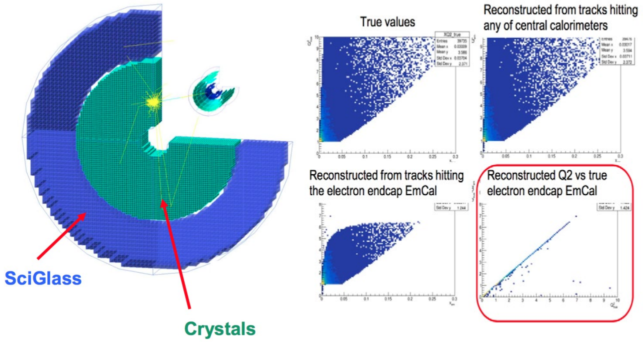
E. Cisbani, A. Del Dotto, C. Fanelli, M. Williams, …, T. Horn, et al **2020** JINST **15** P05009

R&D of novel composite aerogel+fibers: design with the AI optimizing **mechanical strength** and **resolution** using evolutionary MOO. Geant4 + Autodesk (gmsh+elmer)



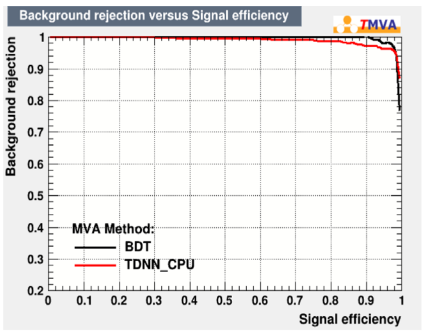
V. Berdnikov, J. Crafts, E. Cisbani, C. Fanelli, T.Horn , R.. Trotta

EIC Electron Endcap EM Calorimeter: Optimization of glass/crystal material selection with MOO to make decision on resolution (how it affects physics of interest), and crystal/glass cost optimization.



V. Berdnikov, M. Bondi', C. Fanelli, Y. Furletova, T.Horn, I. Larin, D. Romanov, R. Trotta

EIC Electron Hadron calorimeter: novel glass for hadron identification by Cherenkov/signal in the same material. May also be of interest for other multi-purpose detectors.

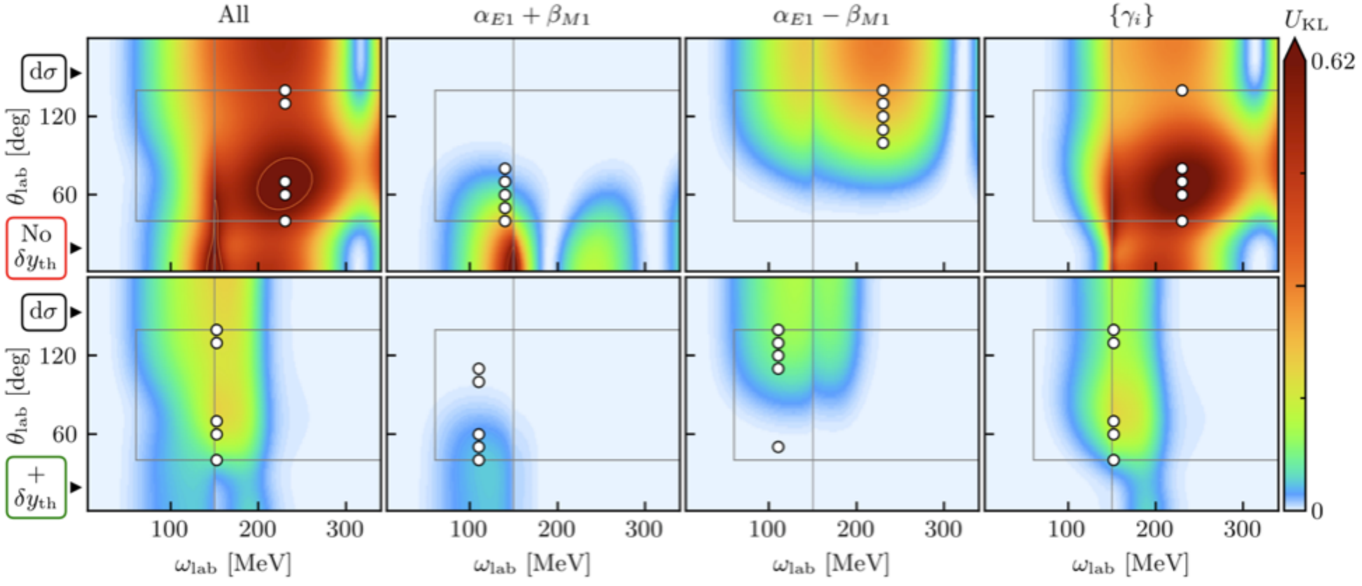


V. Berdnikov, C. Fanelli, T.Horn, P. Stepanov

Experimental Design Examples: Designing optimal experiments

Example: Proton Compton Scattering

- Bayesian experimental design provides a framework in which experiments can be designed using the best experimental and theoretical information available
- The utility function is designed to encode the goals of the experiment and the constraints inherent in carrying it out.
- Once the utility function and the possible designs have been specified, the optimal design is simply the scenario that maximizes the expected utility function over the domain of possible designs.



The expected utility of proton differential cross section measurements. The circles show the optimal design kinematics for five measurement points at the same energy but different angles.

J.A. Melendez, et al., EPJA 57, 81 (**2021**)

Control and Optimization of Complex Accelerators

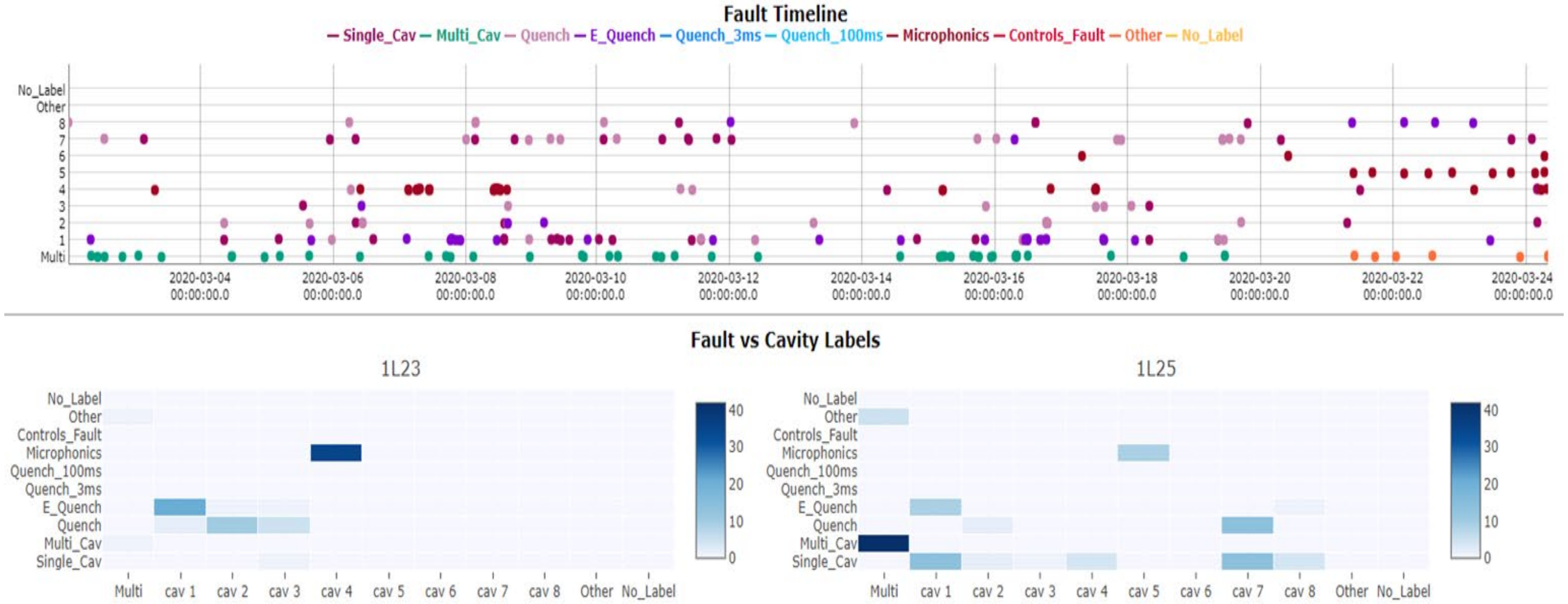
ML applications in accelerator facilities can provide data-driven digital models/twins for anomaly detection, design optimization tools, and real time operational control/tuning

- **Accelerator Science**
  - Optics and lattice design
  - Beam instrumentation design and optimization
  - Reinforcement learning for controls
- **Accelerator Operations**
  - Optics and lattice optimization
  - Target, charge stripper, collimation system
  - Anomaly detection and mitigation

Example 1: Superconducting RF Cavity Fault Classification

Anomaly detection and machine protection: ML-based solutions to challenges encountered in particle accelerators are yielding promising results.

- ML cavity identification and fault classification models have an accuracy of ~85% and 78%



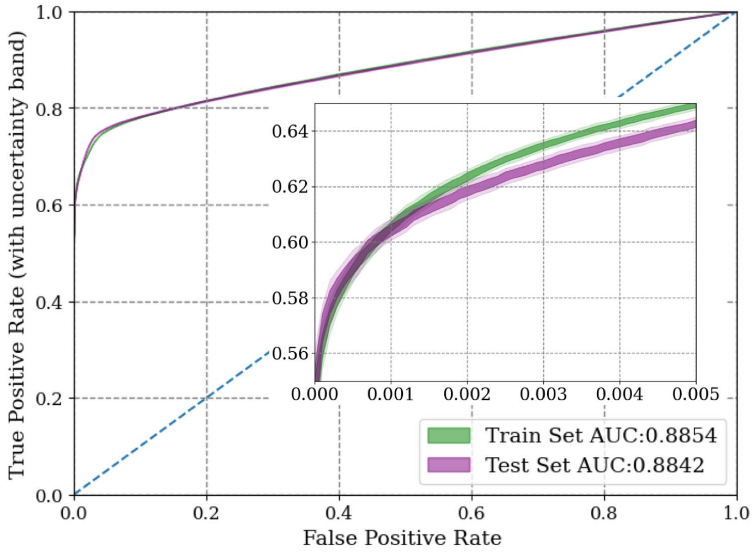
C. Tennant et al., Phys. Rev. Accel. Beams **23**, 114601 (**2020**)

Example 2: UQ for Accelerator Anomalies

Predict upcoming faults before they happen using a combination of uncertainty quantification and a deep Siamese architecture

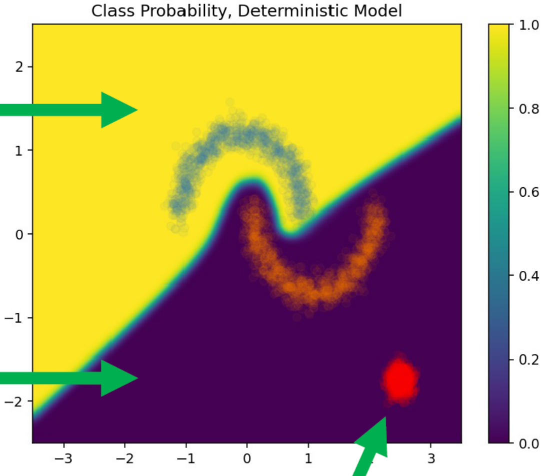
- ➢ Siamese model focuses on similarities between beam pulses
- ➢ GP layer provides an uncertainty estimate

Performance improved ~4x over previous published results



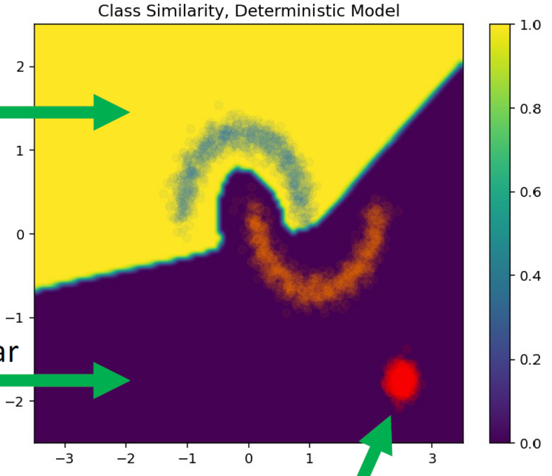
Class A

Class B



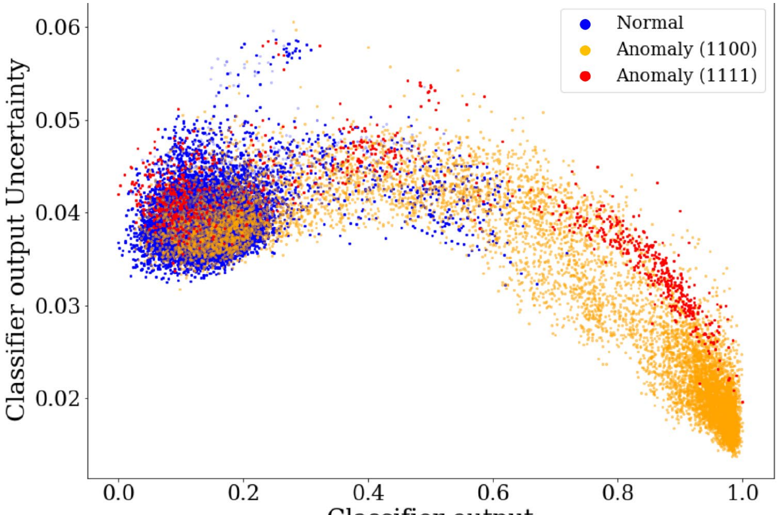
Similar

Not similar



Completely miss identified the out of domain sample.

Correctly identified as different from the reference data



W. Blokland, M. Schram, et al. (**2021**), arXiv:2110.12006

Adapted from M. Schram's presentation at the JLab Hall C meeting (2022)

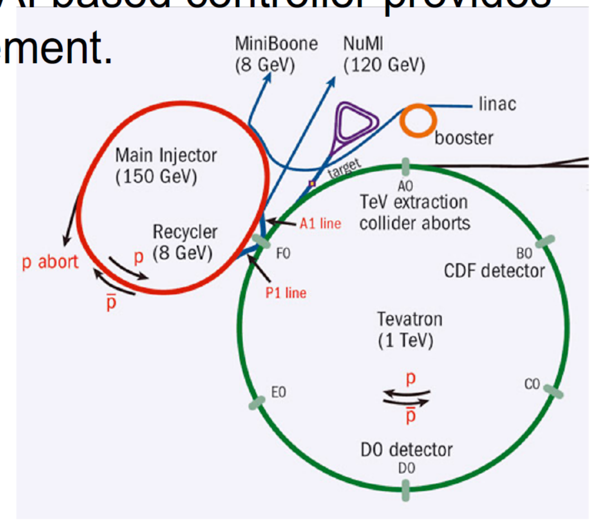
Example 3: ML-based surrogate models

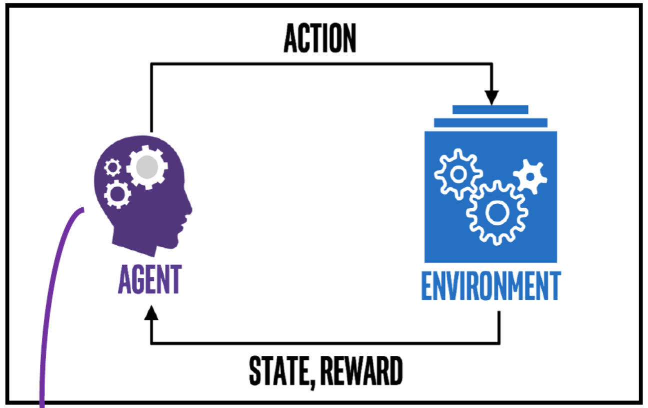
Intelligent Control: Reinforcement Learning for Accelerator Control at FNAL

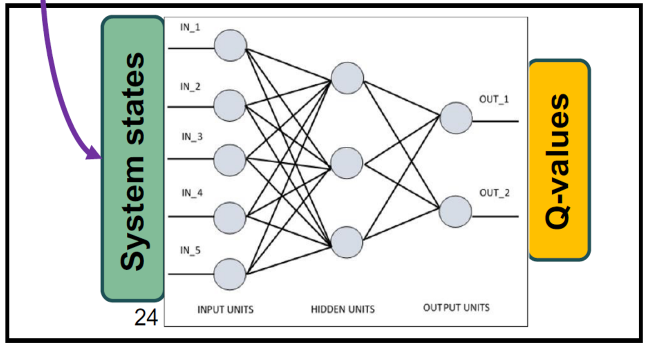
- Reduce beam losses in the FNAL booster by developing a ML model that provides an optimal set of actions for accelerator controls
- Surrogate model and reinforcement learning policy model online control system

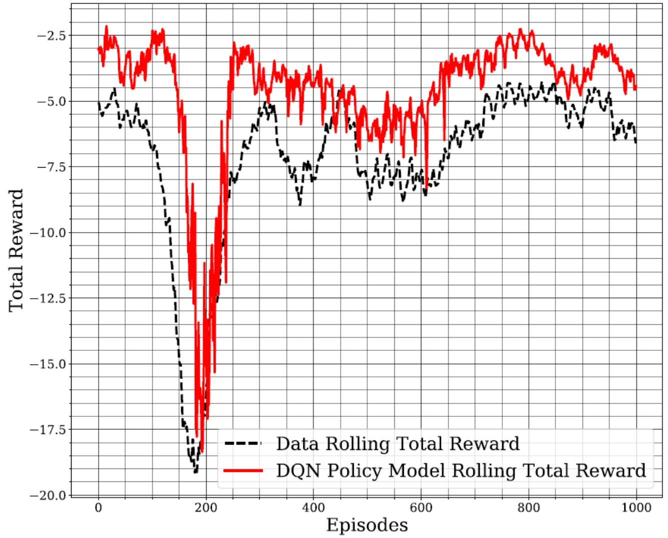
D. Kafkes, M. Schram (**2021**), arXiv:2105.12847

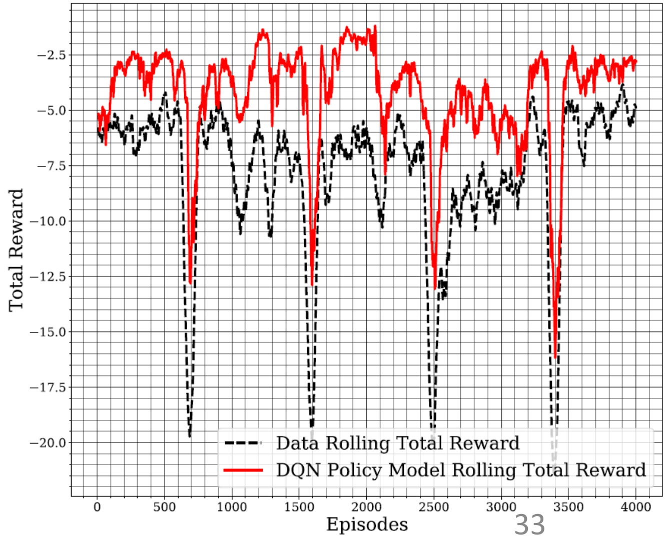
Results:
The current AI based controller provides ~2x improvement.









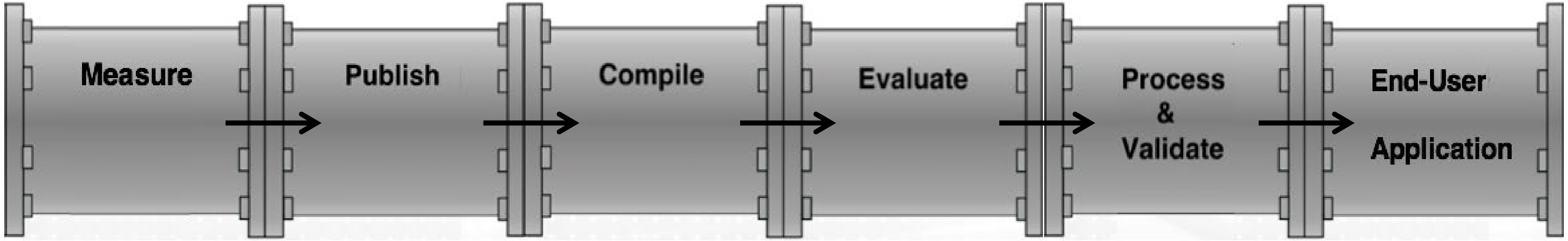


Adapted from M. Schram's presentation at the JLab Hall C meeting (2022)

AI in Nuclear Data

- ❑ Large potential of AI/ML algorithms to address critical Nuclear Data problems – already used for many tasks in the “nuclear data pipeline”

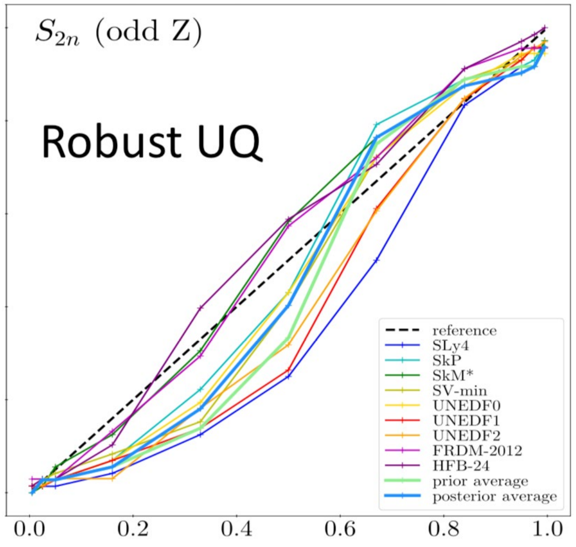
Example: Workshop on Applied Nuclear Data Activities (WANDA) in March 2020: https://conferences.lbl.gov/event/292/



- ❑ ML use anticipated to grow exponentially in nuclear data
  - offers new approaches to longstanding problems
  - TensorFlow and Pytorch libraries speed up ML utilization
  - Early-career researchers eager to use ML
- ❑ new trends include
  - **transforming workflows** with ML-based approaches
  - **“physics-aware” ML** models
  - **using ML to guide** experiments, theory, and evaluations

Examples AI in Nuclear Data

L. Neufcourt et al, PRL **122** (**2019**) 062502



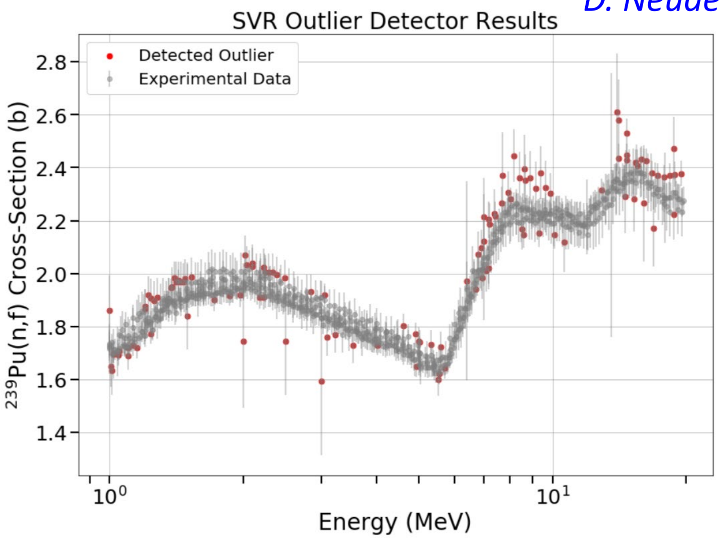
- **Example 1: Physics aware ML models**

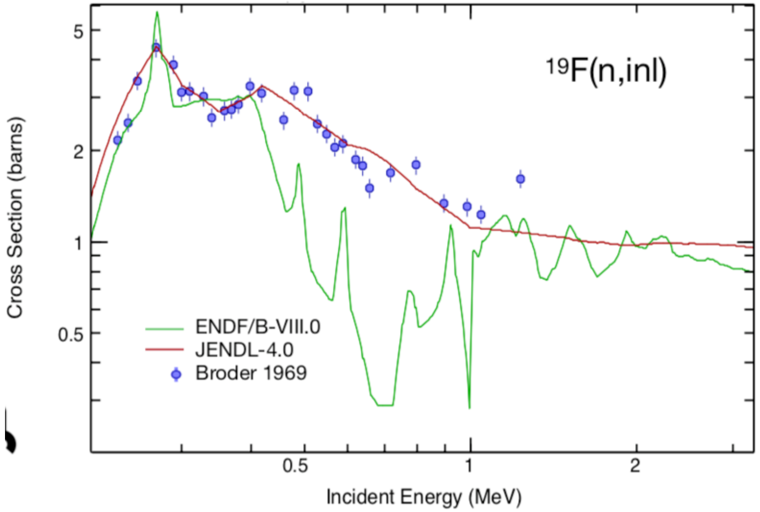
  Predict ground- and excited state energies from theory model; better predictions than traditional evaluation tools

- **Example 2: ML-guided search**

  Random forests were used to augment expert knowledge in pinpointing errors in nuclear data and benchmark experiments leading to bias in simulating criticality benchmarks, e.g., ML found ^{19}F(n,inl) missed by experts

D. Neudecker et al. Nucl. Data Sheets **167** (**2020**) 36





Educational Activities since 2019

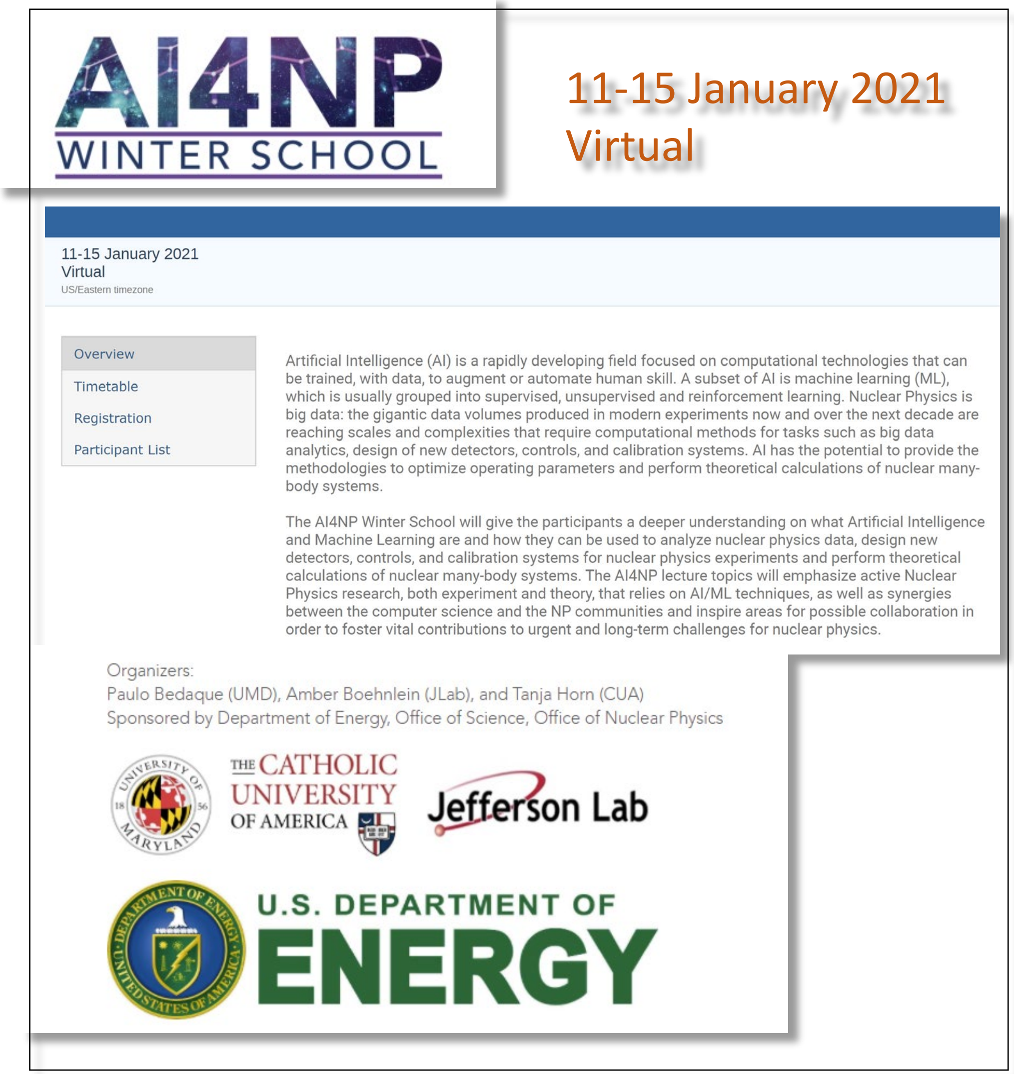
Please feel free to propose new schools and/or update the list here.

1. The FRIB-TA Summer School: Machine Learning Applied to Nuclear Physics, FRIB/NSCL (MSU)from May 20 to 23, 2019; organizers and teachers: Matthew Hirn (MSU), Morten Hjorth-Jensen (MSU) and Michelle Kuchera (Davidson)
2. Nuclear TALENT course Learning from Data: Bayesian Methods and Machine Learning, in York, UK, June 10-28, 2019; Teachers and organizers Christian Forssén, Chalmers University of Technology, Sweden, Dick Furnstahl, Ohio State University, USA, Daniel Phillips, Ohio University, USA
3. Nuclear TALENT School on Machine learning from 22 June 2020 to 03 July 2020. Teachers and organizers: Daniel Bazin (MSU), Morten Hjorth-Jensen (MSU), Michelle Kuchera (Davidson), Sean Liddick (MSU), Raghuram Ramanujan (Davidson)
4. Nuclear TALENT School on Machine learning from 19 July 2021 to 30 July 2021. Teachers and organizers: Daniel Bazin (MSU), Morten Hjorth-Jensen (MSU), Michelle Kuchera (Davidson), Sean Liddick (MSU), Raghuram Ramanujan (Davidson)
5. Intensive course on Machine Learning at FRIB/MSU, summer 2019; teacher Morten Hjorth-Jensen, MSU
6. Four two-week intensive course on Machine Learning for Nuclear Physics held at Ganil, France, 2019, 2020, 2021 and 2022. Teacher and organizer Morten Hjorth-Jensen (MSU)
7. AI4NP Winter School, 11-15 Jan 2021, (Virtual). Organizers Amber Boehnlein (JLAB), Paulo Bedaque (University of Maryland), Tanja Horn (Catholic University of America)
8. 2022?

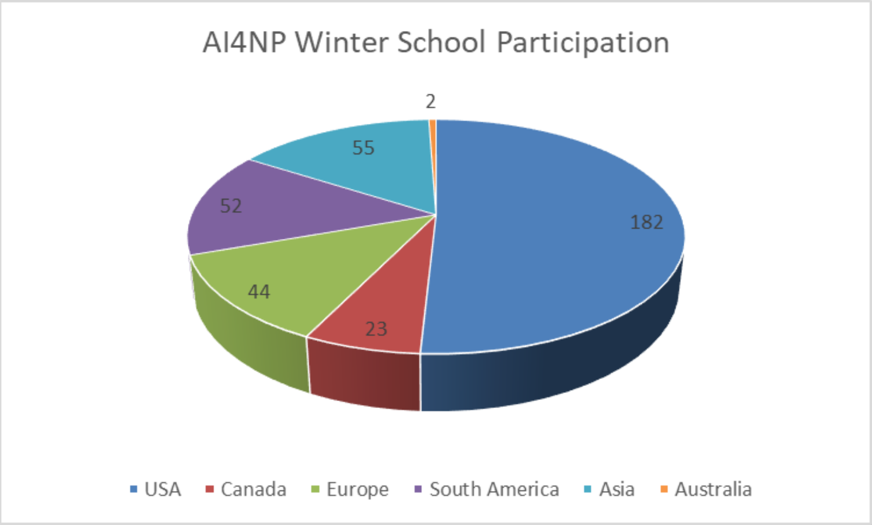
Adapted from M. Hjorth-Jensen’s presentation at KTH, Frontiers in Nuclear Structure Theory (May 2022)

Example: 2021 AI4NP Winter School

https://indico.jlab.org/event/409/overview



- ❑ 361 registered participants
  - ➢ Daily attendance ~100-200
  - ➢ Experience level ranging from absolute beginner to expert
- ❑ Four major lecture topics
  - ➢ Neural Networks and DL
  - ➢ Variational Monte Carlo and ML
  - ➢ Detector Design Optimizations
  - ➢ Data set feature extractions



Observations and Outlook

- ❑ The areas where NP research can benefit from AI/ML are ubiquitous, lots of ongoing activities
- ❑ NP researchers already have the talent and many of the tools required for this revolution – lots of ongoing activities
- ❑ NP addresses challenges that are not addressed in current technologies
- ❑ NP presents data sets that expose limitations of cutting edge methods
- ❑ To solve the many complex programs in the field and facilitate discoveries strong collaborations between NP, AI/ML/data science, and industry would be beneficial for all parties
- ❑ Education is key to increase the level of AI-literacy – research programs and curricula in AI/ML can help to attract students

Tremendous interest and activity in AI/ML in the Nuclear Physics Community