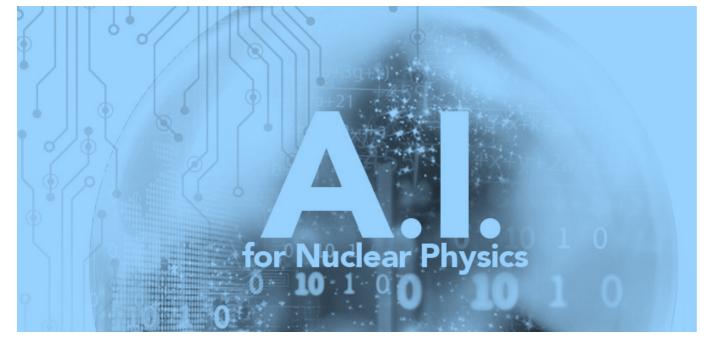
Artificial Intelligence for Nuclear Physics

Tanja Horn



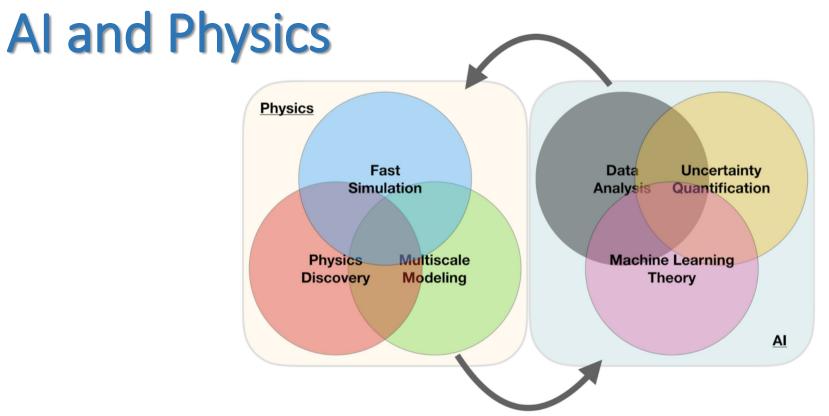




Outline

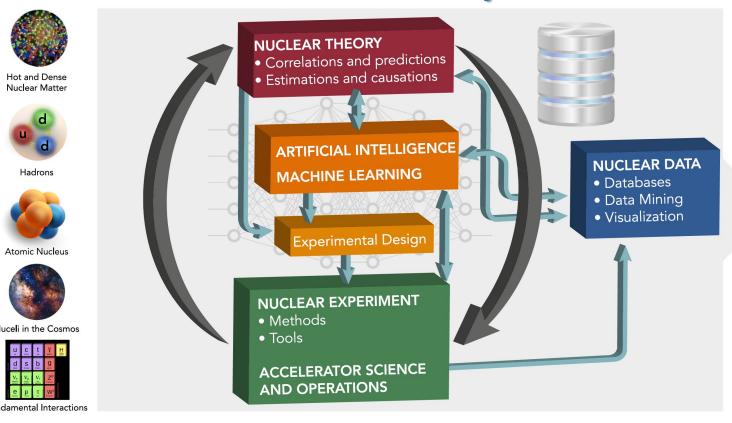
Introduction and context		
Activities including community identified communalities and needs		
Areas of active research		
0	Nuclear theory	
0	Experimental methods	
0	Accelerator technology	
0	Nuclear data	
Educational activities		
Observations and Outlook		

A simple perspective on the interface between



- ☐ 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



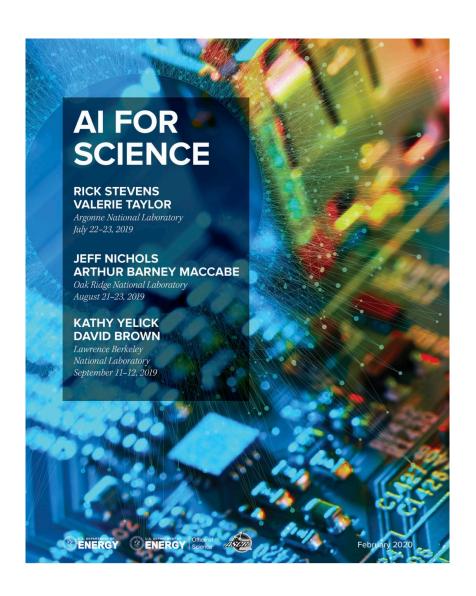
A. Boehnlein et al., Review of Modern Physics Review of Modern Physics 94 (**2022**) 3, 031003; arXiv:2112.02309

DISCOVERY

APPLICATIONS

- □ 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: Al for Science – what's next after Exascale



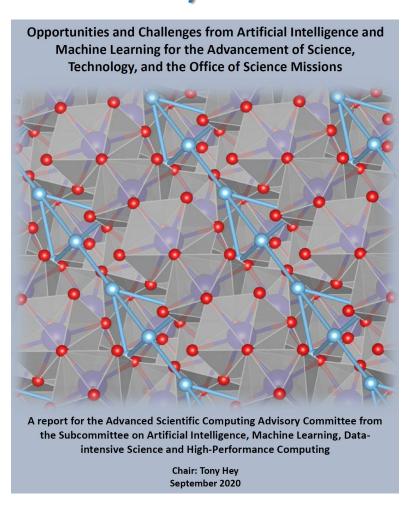
- Over 1,000 scientists participated in four town halls during the summer of 2019
- Research Opportunities in Al
 - Biology, Chemistry, Materials,
 - Climate, Physics, Energy, Cosmology
 - Mathematics and Foundations
 - Data Life Cycle
 - Software Infrastructure
 - Hardware for Al
 - Integration with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

Al 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
 - ➤ Al 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 'Al for Science')



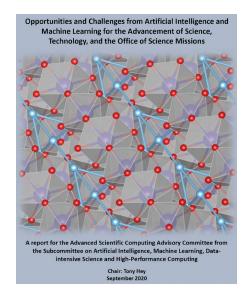
The Charge Letter:

- ☐ The letter sets the context of the challenge to the subcommittee:
 - Artificial Intelligence and Machine Learning (AI/ML) have the potential for providing new insights and even new discoveries from this data, including the correlation of experimental and computational data.
 - However, the technical aspects of "AI/ML for Science" may be more challenging than currently envisioned. Over the last few years, several workshops and subcommittee reports have identified and enumerated the scientific opportunities and some challenges from the intersection of AI/ML with data-intensive science and high performance computing.
- ☐ The letter requires the sub-committee deliver a report that:
 - Assesses the opportunities and challenges from Artificial Intelligence and Machine Learning for the advancement of science, technology, and Office of Science missions.
 - Identifies strategies that ASCR can use, in coordination with the other SC programs, to address the challenges and deliver on the opportunities.
 - Notes that, due to the cross-cutting nature of this effort, in assembling this subcommittee, we need to include members of, and recommendations from the other Office of Science Federal Advisory Committees, as well as Industry and other Federal experts.

2020 ASCAC Subcommittee on: 'Al for Science'

Advances expected from use of AI/ML in Science

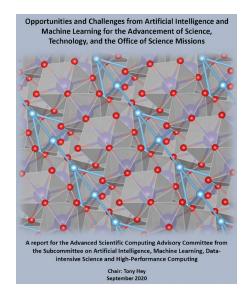
- Accelerate the design, discovery, and evaluation of new materials
- Advance the development of new hardware and software systems, instruments and simulation data streams
- Identify new science and theories revealed as a result of increasingly high-bandwidth instrument data streams
- Improve experiments by inserting inference capabilities in control and analysis loops
- Enable the design, evaluation, autonomous operation, and optimization of complex systems from light sources and accelerators to instrumented detectors and HPC data centers
- Advance the development of self-driving laboratories and scientific workflows
- Increase the capabilities of exascale and future supercomputers by capitalizing on AI surrogates
- Automate the large-scale creation of "FAIR" (Findable, Accessible, Interoperable, Reusable) data



2020 ASCAC Subcommittee on: 'Al for Science'

Recommendations

- #1 Creation of a 10-year AI for Science Initiative
- #2 Structure of an SC AI for Science Initiative
 - Al-enabled applications
 - Al algorithms and foundational research
 - Al software infrastructure
 - New hardware technologies for AI
- **#3 An Instrument-to-Edge Initiative**
- #4 Training, focusing, and retention of AI/ML workforce
- **#5 Inter-Agency Collaboration**
- #6 International Collaboration



2020 ASCAC Subcommittee on: 'Al for Science'

Components needed for successful AI in Science Initiative

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

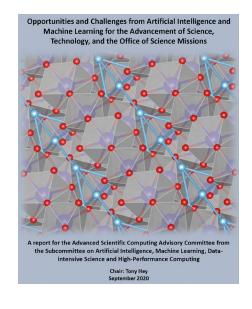
Research in AI algorithms and foundations

Development of AI software infrastructure

Al-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: Al for NP Workshops



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 Al-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

Activities in Nuclear Physics: AI for NP Workshops

Computational Nuclear Physics and AI/ML Workshop



6-7 September, 2022 / SURA headquarters

Organized by:

Alessandro Lovato – Joe Carlson (LANL), Phiala Shanahan (MIT), Bronson Messer (ORNL) Witold Nazarewicz (FRIB/MSU), Amber Boehnlein (JLab), Peter Petreczky (BNL) Robert Edwards (JLab), David Dean (JLab)

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

Workshop Resolution

- High Performance Computing (HPC) is essential to advance NP on the experimental and theory frontiers. Increased investments in computational NP will facilitate discovery and capitalize on previous progress. Thus, we recommend a target program to ensure the utilization of ever-evolving HPC hardware via software and algorithmic development, which includes taking advantage of novel capabilities offered by AI/ML
- ☐ The key elements are:
 - Strengthen and expand programs and partnerships to support immediate needs in HPC and AI/ML, and also to target development of emerging technologies and other opportunities
 - Take full advantage of exciting possibilities offered by new hardware and software and AI/ML within the NP community through educational and training activities
 - Establish programs to support cutting-edge developments of a multi-disciplinary workforce and cross disciplinary collaborations in HPC and AI/ML
 - Expand access to computational hardware through dedicated and HPC resources

Example of recent AI/ML Awards in NP

DEPARTMENT OF ENERGY OFFICE OF SCIENCE NUCLEAR PHYSICS



DATA ANALYTICS FOR AUTONOMOUS OPTIMIZATION AND CONTROL OF ACCELERATORS AND DETECTORS

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER: DE-FOA-0002490

ANNOUNCEMENT TYPE: INITIAL CFDA NUMBER: 81.049

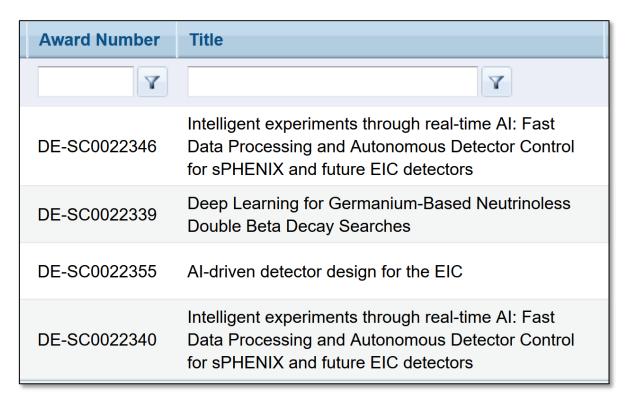
FOA Issue Date: DATE: March 16, 2021
Submission Deadline for Applications: DATE: April 30, 2021, 11:59 PM Eastern
Time

<u>Tremendous interest and activity in</u>

AI/ML in the Nuclear Physics Community

Three main goals:

- ☐ Efficiently extract critical and strategic information from large data sets
- ☐ Address the challenges of autonomous control and experimentation
- ☐ Efficiency of operation of accelerators and scientific instruments



Areas of Active Research in AI/ML in NP

- ☐ Invited article for Review of Modern Physics 94 (2022) 3, 031003 Boehnlein et al.
- ☐ 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

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

Thomas Jefferson National Accelerator Facility,

12000 Jefferson Avenue,

Newport News, Virginia,

Cristiano Fanelli

Laboratory for Nuclear Science, Massachusetts Institute of Technology, Cambridge, MA 02139,

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,

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Alan Poon and Xin-Nian Wang

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

CONTENTS

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

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

Scalability, compact variables, sign problem

☐ Ensemble generation in lattice QCD

Phase transitions and estimators for correlation functions

Nuclear Theory Examples

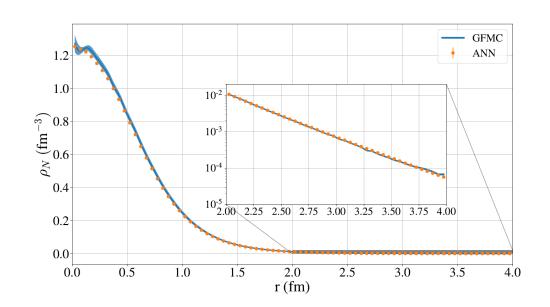
☐ Example 1: Bayesian Model Averaging to Quantify Limits of the nuclear landscape

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

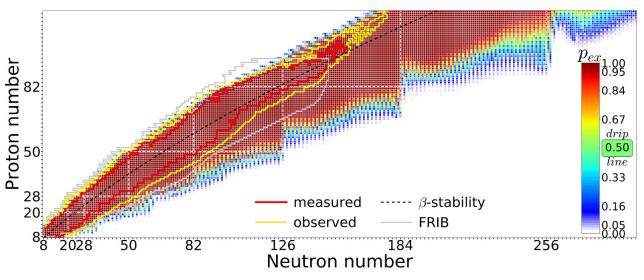
L. Neufcourt et al., PRL **122** (**2019**) 062502

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



☐ Example 2: Many body-variational calculations with ANN

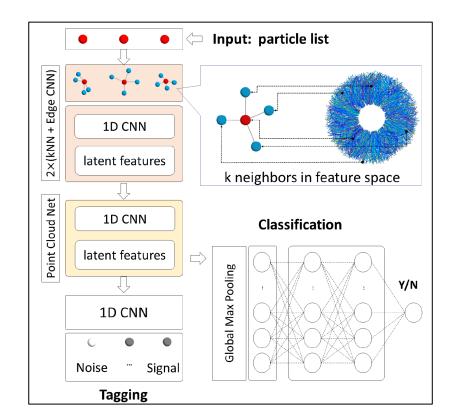
Demonstrated predictive power of ANNs for converged solutions of weakly converging simulations of light nuclei with up to six nucleons

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

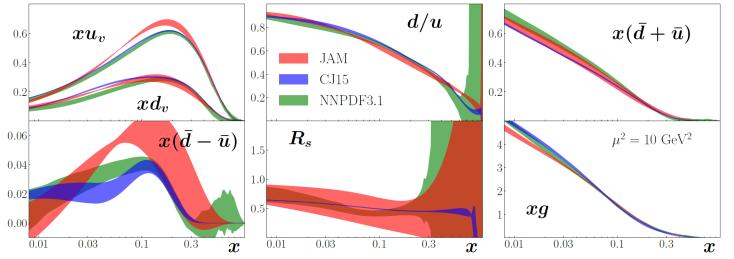
Nuclear Theory Examples

☐ 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



☐ Example 4: Bayesian analysis to constrain model parameters

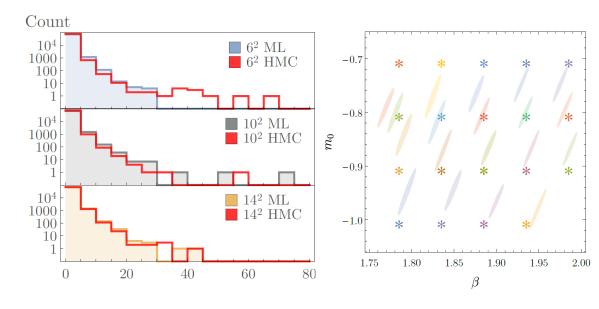
Generative models to approximate model output ANN help to reveal correlations hidden in high-dimensional data

Lattice QCD Examples

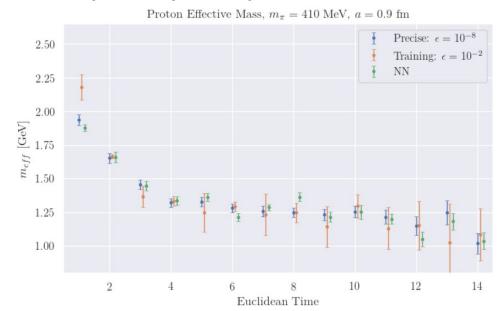
☐ Example 1: Field configurations and properties

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 Al-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) in multidimensional space and can capture hidden correlations among design parameters
- > Autonomous control and experimentation

□Long Term:

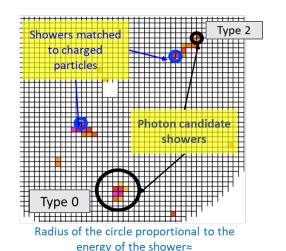
- ➤ Holistic approach to experimentation
- > Standardized data formats
- Experiment design not limited by computation

Experimental Methods Examples: Reconstruction and

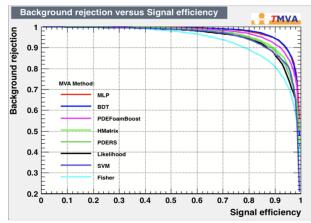
Analysis

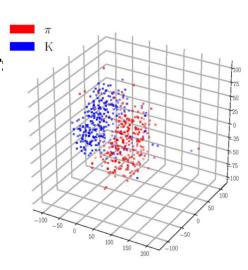
☐ Example 1: Particle Identification with Cherenkov Detector

- 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

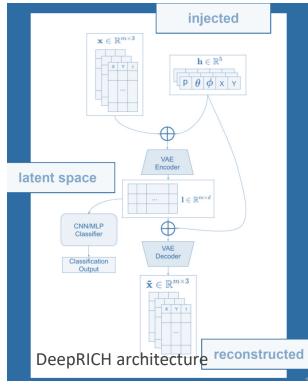












- ☐ Example 2: Boosted Decision Trees to Search for Exotic Mesons in GlueX
 - > Isolate small signal of from a large background
 - ➤ ANN-based algorithms have the potential to offer vast improvements in signal selection efficiency and purity over more traditional techniques. 20

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

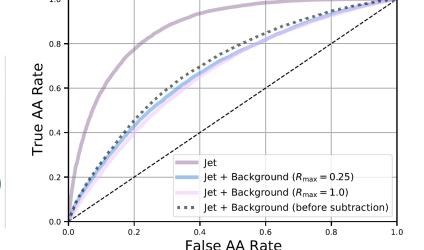
Lai, Mulligan, Ploskon, Ringer (2021) arXiv:2111.14589

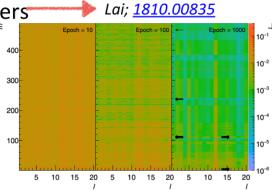
- > Discovery of theoretical models via automated analysis
 - Previous: Finding most sensitive observables to a model parameters
 - Current focus (from a longer list): How much information is contained in high-energy particle collisions and jets?



Extract knowledge on complex processes (e.g. jet quenching) directly from data - human understandable result (!)

- → new guidance to experiment(s)
- → critical input for theory





Next challenge?

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

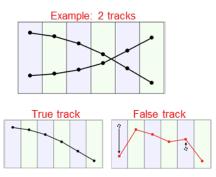
Experimental Methods Examples: Reconstruction and Analysis

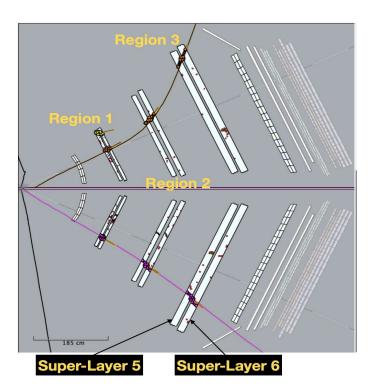
☐ Example 4: Charged Particle Tracking

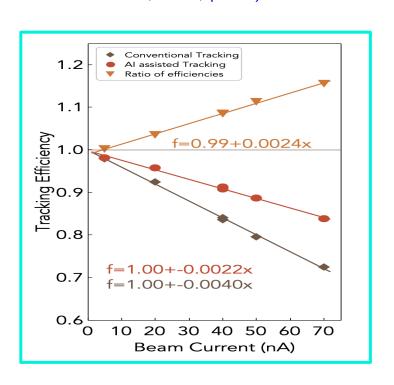
- > ANN and Deep Learning in the CLAS12 workflow provides a 6 times faster track reconstruction speed.
- > Selection of the correct seed results in improved tracking efficiency and recovery of missing tracks with accuracy of >99.8%.

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



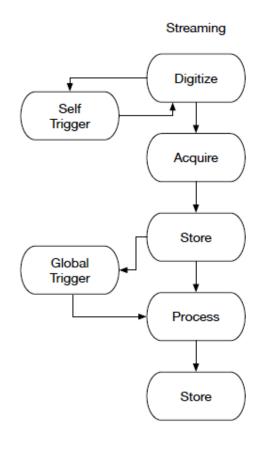




G. Gavalian, et al., (2020) arXiv:2008.12860

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 experiments adopt the SRO scheme: LHCb, ALICE, AMBER, CBM, TPEX, sPHENIX, STAR, EIC, SOLID, BDX, CLAS12, ...

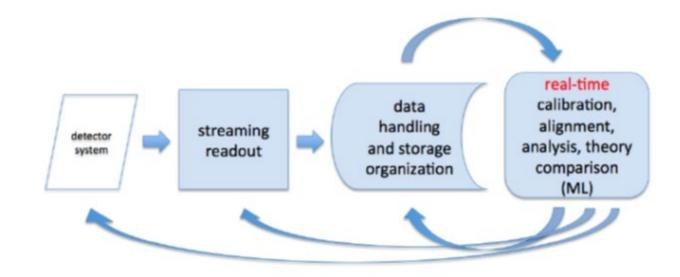
Streaming Readout – Grand Challenges

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

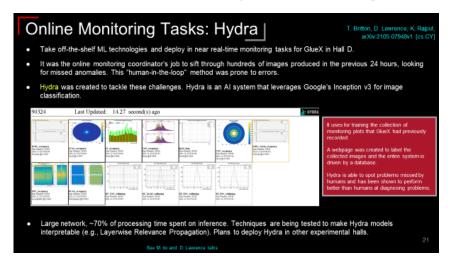
Integrated whole-experiment model



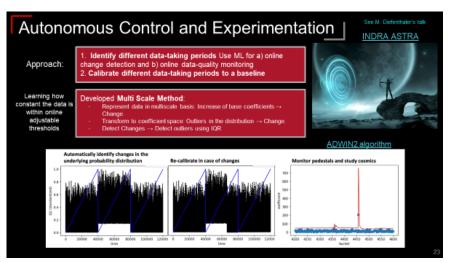
Many high-luminosity experiments adopt the SRO scheme: LHCb, ALICE, AMBER, CBM, TPEX, sPHENIX, STAR, EIC, SOLID, BDX, CLAS12, ...

Streaming Readout Examples

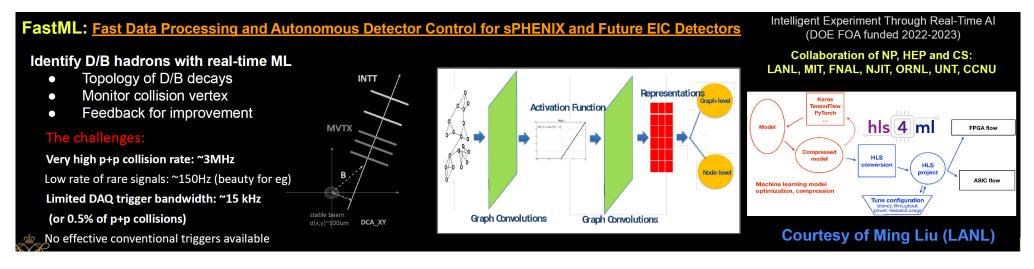
Automated Data Quality Monitoring



Automated Alignment and Calibrations



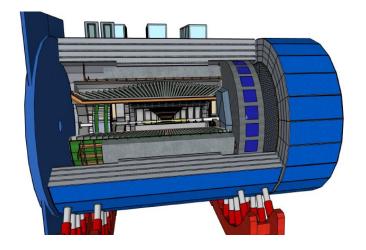
Autonomous Detector Control



Experimental Design: Design for Detector Systems

Al 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 Project Detector reference design



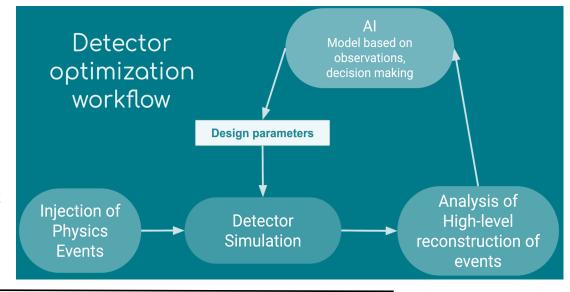
For details see: https://eic.ai/

Experimental Design Examples: Design for Detector

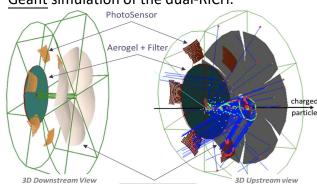
Systems

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

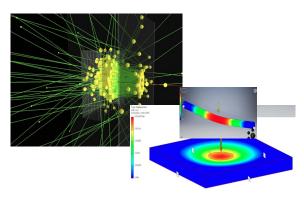


Dual-RICH @EIC: First EIC paper using AI, an automated, highly parallelized, self-consistent framework based on BO+ML to optimize the Geant simulation of the dual-RICH.



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

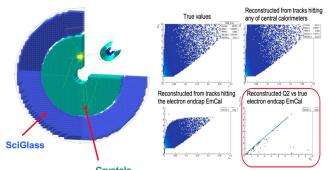
R&D of novel composite aerogel+fibers: design with the AI optimizing **mechanical strength** and **resolution** using evolutionary MOO. Geant4 + Autodesk (gmsh+elmer)



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

EIC Electron Endcap and barrel EM Calorimeter:

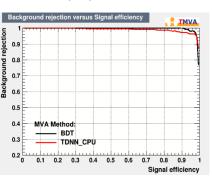
Optimization of glass/crystal material selection with MOO to make decision on resolution (how it affects physics of interest), and crystal/glass cost optimization.



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

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

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

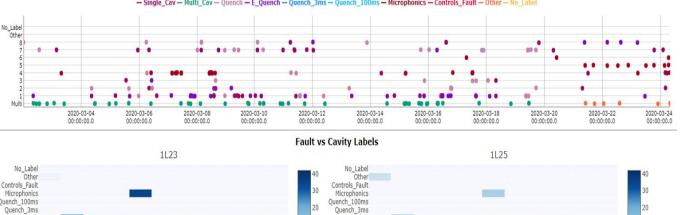
Control and Optimization of Complex Accelerators

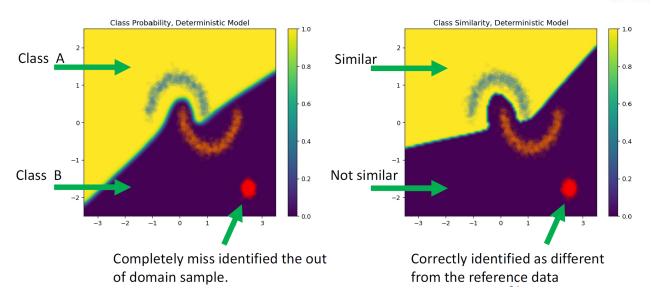
☐ Example 1: Superconducting RF Cavity Fault Classification

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

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%





☐ Example 2: **☐** Example 3: **☐** E

cay 2 cay 3 cay 4 cay 5 cay 6 cay 7 cay 8 Other No Label

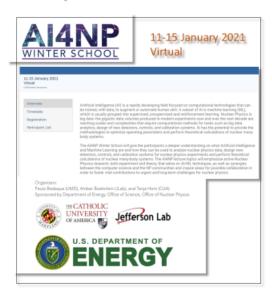
- Predict upcoming faults before they happen using a combination of uncertainty quantification and a deep Siamese architecture (focuses on similarities between beam pulses)
- Performance improved ~4x over previous published results

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) Liddick (MSU), Raghuram Ramanujan (Davidson)
- 4. Nuclear TALENT School on Machine learning from 19 July 202 organizers: Daniel Bazin (MSU), Morten Hjorth-Jensen (MSU) Liddick (MSU), Raghuram Ramanujan (Davidson)
- 5. Intensive course on Machine Learning at FRIB/MSU, summer
- 6. Four two-week intensive course on Machine Learning for Nucl 2020, 2021 and 2022. Teacher and organizer Morten Hjorth-Je
- 7. Al4NP Winter School, 11-15 Jan 2021, (Virtual). Organizers Ar (University of Maryland), Tanja Horn (Catholic University of Am
- 8. 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