OVERVIEW ON MACHINE LEARNING AND ARTIFICIAL INTELLIGENCE

IN LOW-ENERGY NUCLEAR PHYSICS

NSAC TOWN HALL MEETING
ARGONNE NATIONAL LABORATORY
15 NOVEMBER 2022

MICHELLE KUCHERA
DAVIDSON COLLEGE

No mention of machine learning or artificial intelligence in 2015 Long Range Plan

three-family picture of the Standard Model. The fourth experiment, which lies at the heart of modern cosmology and particle physics, involves the search for the neutron electric dipole moment (nEDM). This experiment would improve sensitivity by two orders of magnitude over the best existing searches for CP violation beyond the Standard Model, as needed to account for the baryon asymmetry of the universe.

The ultracold neutron (UCN) facility at Los Alamos National Lab is the only currently operating UCN source in North America and provides UCN densities comparable to the world's other sources (located in Europe and Japan). Following the ongoing successful UCNA experiment on the neutron beta decay asymmetry, the facility will host the neutron lifetime measurement UCNτ, detector development for the Nab and UCNB experiments, the applied nuclear physics experiment UCNS, and neutron guide and storage cell development. A more precise determination of the neutron decay lifetime can be used to determine the CKM matrix element V_{ud} with high precision in a fashion that is relatively free of theoretical uncertainties. Complementary precision studies using decays of rare isotopes are being carried out at ANL using ion and atom traps.

The Fermilab Muon Campus is being developed to host two high-priority approved experiments that will challenge the Standard Model. While primary support comes from DOE-HEP, many nuclear physics groups and international partners are playing leading roles in these interdisciplinary experiments. The Muon g-2 Experiment will measure the anomalous magnetic moment of the muon to the unprecedented precision of 140 parts per billion. The result will either confirm or refute a long-standing discrepancy between the Standard Model and the previous measurement. The Mu2e Experiment will study the low-energy (essentially forbidden) process of coherent conversion of a muon to an electron from an atomically bound muonic atom. The goal is a four orders of magnitude improvement in the limit of this charged-lepton-violating process, with single event sensitivity approaching 1 part in 10^{17}.

ADVANCED TECHNOLOGIES

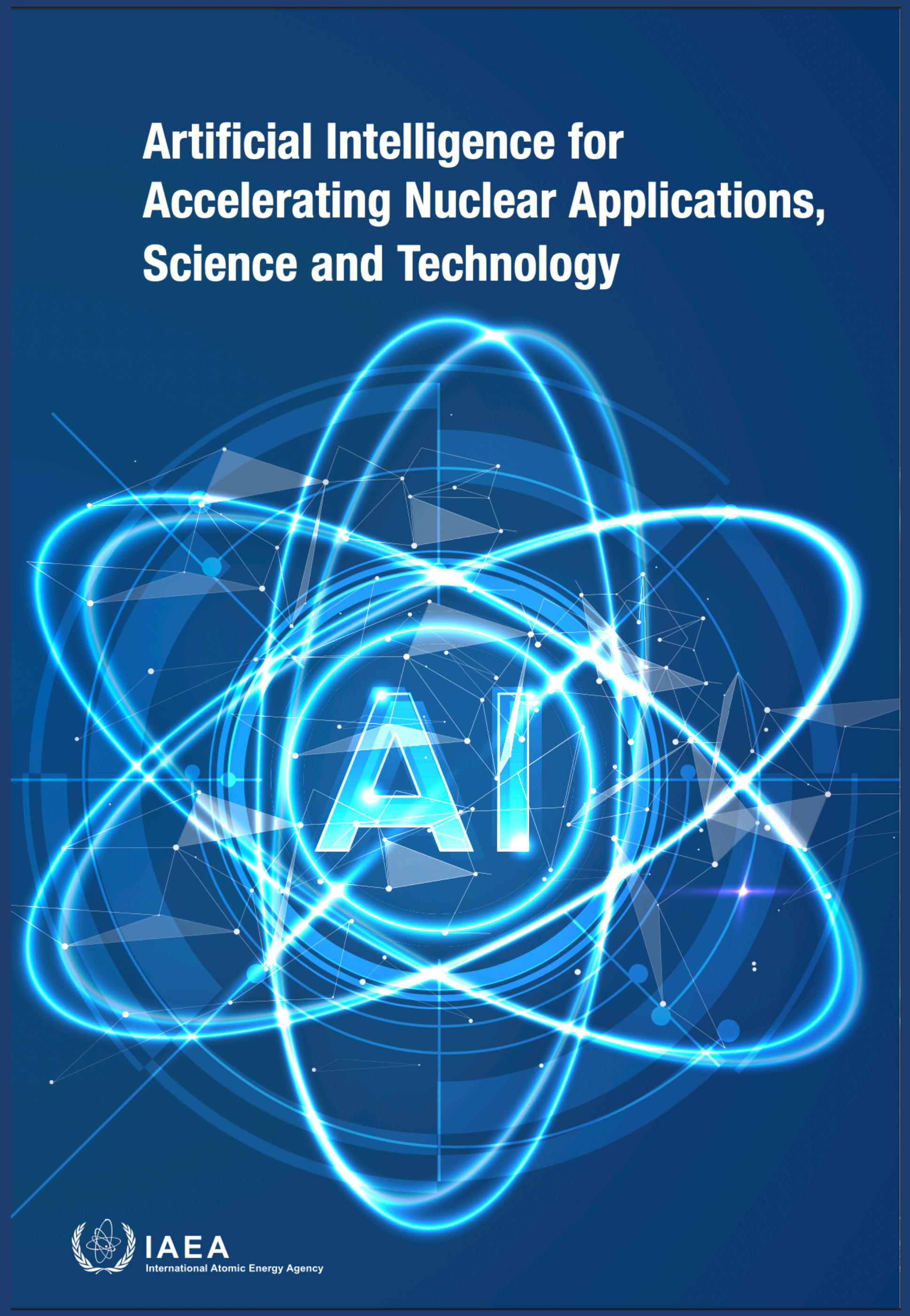
Advanced Computing

Computation now plays an essential role in every area of nuclear physics research (Sidebar 7.3). Nuclear physicists exploit available computational resources, ranging from leadership-class capability computing resources, such as Titan at OLCF and Mira at ALCF, through capacity (mid-scale) computing resources, such as Edison at the National Energy Research Scientific Computing Center (NERSC) and USQCD hardware at JLab, BNL, and Fermilab, as well as university clusters and small local clusters and workstations. The capability resources are allocated in programs such as INCITE and ALCC through peer-reviewed proposals in competition with other areas of science. Nuclear physics has obtained an approximately constant fraction (12%) of the national resources during the last several years. Access to capacity computing resources at NERSC and through the XSEDE program is also obtained through a proposal process. In addition, the USQCD project operates its own capacity computers, supported jointly by the DOE Offices of Nuclear Physics and High Energy Physics. In addition to the homogeneous machines it operates in the form of clusters and a Blue-Gene/Q, USQCD has invested in heterogeneous machines, primarily those accelerated with nVidia Graphics Processing Units (GPUs). GPU machines, through the development of very efficient software, have proven to be effective in many aspects of LQCD calculations.

Ten years ago, the capability, capacity, and local clusters were essentially of the same architecture, comprised of multiple homogeneous compute cores embedded in a fast communication fabric. Today, and into the future, the architectures are heterogeneous and diverse in nature. The limits of CMOS technology and the resulting failure to track Moore's Law, along with the power requirements of such technologies, make it necessary to embrace heterogeneous architectures. Two machine architectures are being pursued to deliver exascale computing resources within the next 10 years. One architecture is IBM Power-9 processors with Nvidia Volta GPUs being procured for Lawrence Livermore National Laboratory and Oak Ridge National Laboratory. The other is based on the evolution of Intel Xeon-Phi accelerators and will be deployed at Argonne National Laboratory as well as in the next NERSC machine.

Significant software development is required to exploit these two quite different architectures. Supported through the SciDAC program and in collaboration with the SciDAC Institutes, nuclear physicists collaborate to port and to optimize the performance of the code bases on these platforms. As an example, the Chroma

No mention of machine learning or artificial intelligence in 2015 Long Range Plan



Reaching for the Horizon

The 2015 Long Range Plan for Nuclear Science

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Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence (IJCAI-21)
Survey Track

A Survey of Machine Learning-Based Physics Event Generation

Yasir Alanazi[1], Nobuo Sato[2], Pawel Ambrozewicz[2], Astrid Hiller-Blin[2], Wally Melnitchouk[2], Marco Battaglieri[2], Tianbo Liu[3] and Yaohang Li[1]
[1]Department of Computer Science, Old Dominion University, Norfolk, Virginia 23529, USA
[2]Jefferson Lab, Newport News, Virginia 23606, USA
[3]Key Laboratory of Particle Physics and Particle Irradiation (MOE), Institute of Frontier and Interdisciplinary Science, Shandong Univ
yalan001@odu.edu, {nsato, pawel, ahblin, wr
yaohang@

International Journal of Modern Physics A

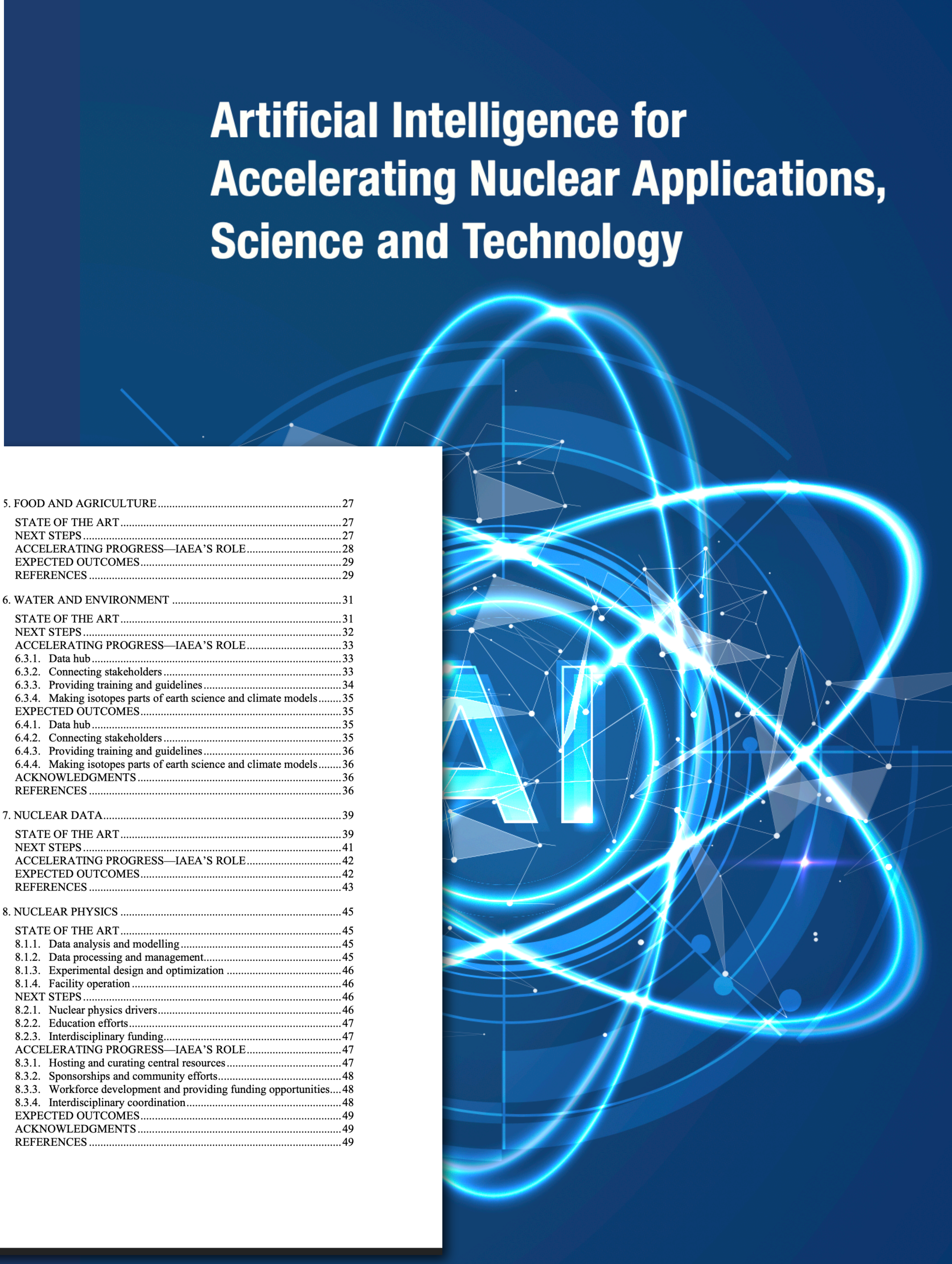
A Review on Machine Learning for Neutrino Experiments

Fernanda Psihas
Neutrino Division, Fermi National Accelerator Laboratory
Batavia, Illinois, United States of America
psihas@fnal.gov

Micah Groh
Department of Physics, Indiana University
Bloomington, IN, United States of America
mcgroh@iu.edu

Christopher Tunnell
Department of Physics and Astronomy, RICE University
Houston, Texas, United States of America
tunnell@rice.edu

Karl Warburton
Department of Physics and Astronomy, Iowa State University
Ames, Iowa, United States of America
karlwarb@iastate.edu



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Rev. Mod. Phys. 94, 031003 – Published 8 September 2022

OUTLINE

Research Highlights

- low-energy uses underrepresented in this meeting

Looking forward

- promising research avenues
- research needs in our field

Enabling advancement

- educational efforts
- interdisciplinary collaboration

HIGHLIGHTS

Day 1 (Monday, November 14, 2022) *Registration and coffee/refreshments will be available from 7:30 (APS Conference Center)*			
Plenary Session 1 *Chair: Rebecca Surman (Notre Dame)* *Held in the APS Conference Center (Bldg. 402) Auditorium*			
Time (CST)	Presentation	Speaker	Duration
08:05-08:15	Welcome and logistics	Rebecca Surman (Notre Dame)	10
08:15-08:30	Charge and LRP process	Gail Dodge (ODU)	15
08:30-09:00	Predictive theory of nuclei and their interactions	Thomas Papenbrock (UTK)	30
09:00-09:30	Experimental studies of nuclei - Structure and reactions	Heather Crawford (LBNL)	30
09:30-10:00	Theory for nuclear astrophysics	Gail McLaughlin (NSCU)	30
10:00-10:30	Nuclear astrophysics experiments	Kelly Chipps (ORNL)	30

Plenary Session 3 *Chair: Grigory Rogachev (TAMU)* *Held in the APS Conference Center (Bldg. 402) Auditorium*			
13:30-13:55	Fostering a culture of belonging in the low-energy nuclear physics community	Warren Rogers (IWU)	25
13:55-14:20	Training the next generation of nuclear scientists	Shelly Lesher (UW-La Crosse)	25
14:20-14:45	Quantum computing and simulations for nuclear physics	Dean Lee (FRIB)	25
14:45-15:10	Challenges, opportunities, and priorities for nuclear data	Libby McCutchan (BNL)	25
15:10-15:35	Broader applications of nuclear science and technology (remotely from London)	Graham Peaslee (ND)	25
15:35-16:00	Isotope production and harvesting	Sherry Yennello (TAMU)	25

Active learning:

Generate first subset of training data

Train model

Identify new training examples

Repeat


PHYSICAL REVIEW LETTERS

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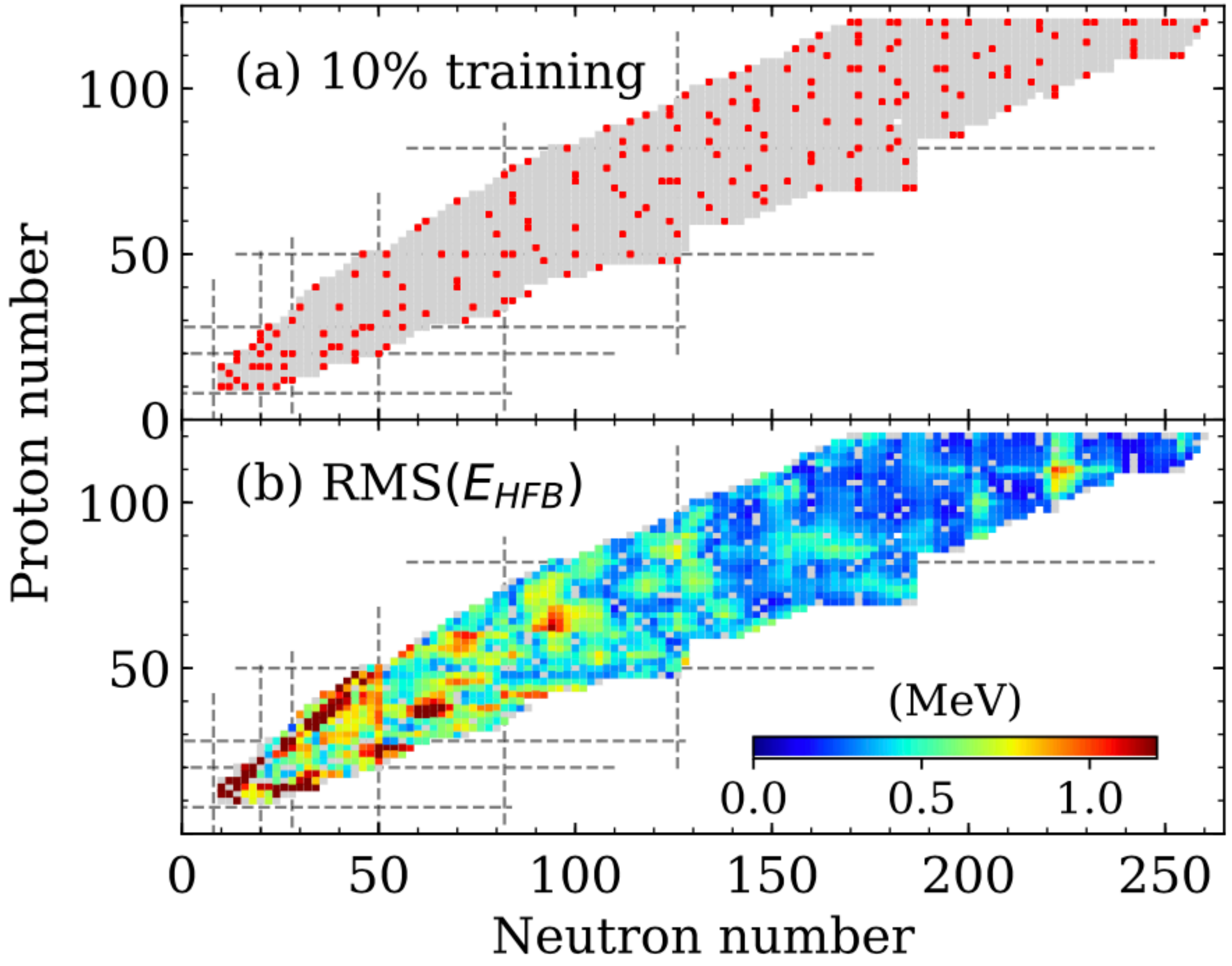
Editors' Suggestion

Taming Nuclear Complexity with a Committee of Multilayer Neural Networks

Raphaël-David Lasseri, David Regnier, Jean-Paul Ebran, and Antonin Penon

Phys. Rev. Lett. **124**, 162502 – Published 20 April 2020



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machine learning

Journal or book title: Nuclear Instruments and Methods in Physics Research ...

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Research article

Comparative pulse shape discrimination study for Ca(Br, I)$_2$ scintillators using machine learning and conventional methods

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 23 October 2022, ...

M. Yoshino, T. Iida, ... A. Yoshikawa

Research article

Experimental tests of Gamma-ray Localization Aided with Machine-learning (GLAM) capabilities

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 3 June 2022, ...

Matthew Durbin, Ryan Sheatsley, ... Azaree Lintereur

Research article

Implementation of a machine learning technique for estimating gamma direction using a coaxial High Purity Germanium detector

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 30 June 2022, ...

R. W. Gladen, T. J. Harvey, ... V. A. Chirayath

Estimation of uranium concentration in ore samples with machine learning methods on HPGe gamma-ray spectra

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 16 March 2022, ...

P. G. Allinei, N. Pérot, ... R. Goupillou

Research article

Machine learning based event classification for the energy-differential measurement of the ^{nat}C(n,p) and ^{nat}C(n,d) reactions

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 6 April 2022, ...

P. Žugec, M. Barbagallo, ... E. Chiaveri

Research article • *Open access*

Machine learning for beam dynamics studies at the CERN Large Hadron Collider

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 16 September 2020, ...

P. Arpaia, G. Azzopardi, ... J. Wenninger

View PDF

Research article

Fast muon tracking with machine learning implemented in FPGA

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 10 October 2022, ...

Chang Sun, Takumi Nakajima, ... Makoto Tomoto

Research article

Classical and machine learning methods for event reconstruction in NeuLAND

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 19 July 2021, ...

Jan Mayer, Konstanze Boretzky, ... Andreas Zilges

Research article

Particle identification and analysis in the SciCRT using machine learning tools

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 8 April 2021, ...

R. Garcia, M. Anzorena, ... Y. Nakamura

Research article

Machine Learning aided 3D-position reconstruction in large LaCl3 crystals

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 16 March 2021, ...

J. Balibrea-Correa, J. Lerendegui-Marco, ... C. Domingo-Pardo

Short communication

Imaging particle collision data for event classification using machine learning

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 9 April 2019, ...

S. V. Chekanov

Research article

Improvement of machine learning enhanced genetic algorithm for nonlinear beam dynamics optimization

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 5 September 2019, ...

Jinyu Wan, Paul Chu, ... Yongjun Li

Research article

Machine learning methods for track classification in the AT-TPC

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 14 June 2019, ...

M. P. Kuchera, R. Ramanujan, ... Ruiming Chen

ML IN LOW-ENERGY EXPERIMENTS

M.P. Kuchera, R. Ramanujan, J.Z. Taylor et al. — Nuclear Inst. and Methods in Physics Research, A 940 (2019) 156–167

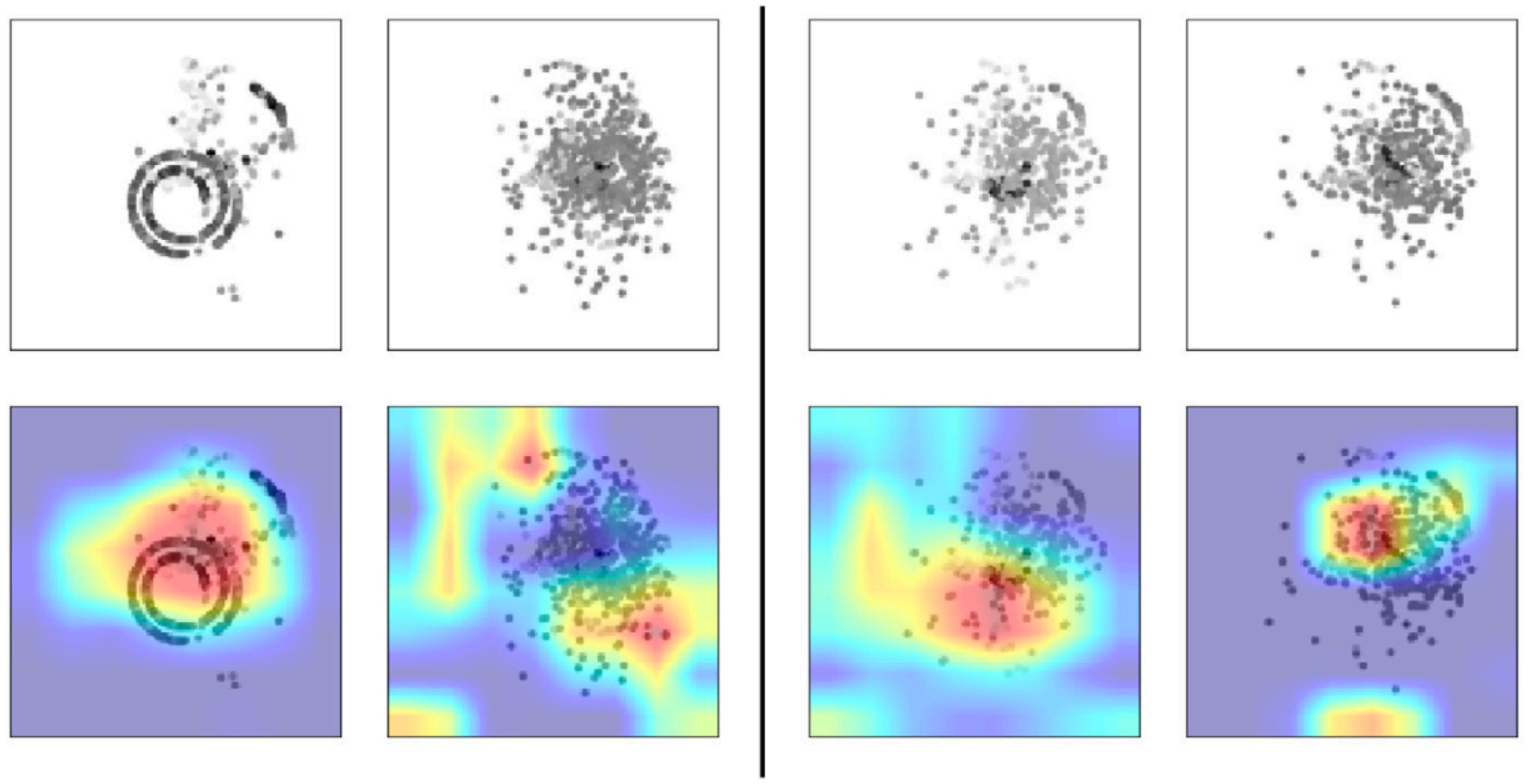

Fig. 12. Sample visual explanations of the CNN's classification decisions on experimental data. The top row shows the input images. The heatmaps on the bottom row indicate the regions of the respective images that the model paid particular attention to when making its classification decisions. Areas shaded in red correspond to pixels that were weighted more heavily in the decision, while areas shaded in blue were weighted less. From left-to-right, these examples constitute cases where the model correctly labeled a proton event, correctly labeled a non-proton event, mistook a proton event for a non-proton event, and mistook a non-proton event for a proton event. We note that the model focuses on regions of the point cloud that display structure when correctly identifying proton events. Its "attention" is more diffuse in the other scenarios. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Nuclear Inst. and Methods in Physics Research, A 940 (2019) 156–167

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

Machine learning methods for track classification in the AT-TPC

M.P. Kuchera [a,*], R. Ramanujan [b], J.Z. Taylor [a], R.R. Strauss [b], D. Bazin [c], J. Bradt [c], Ruiming Chen [a]

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment

Volume 1010, 11 September 2021, 165461

Unsupervised learning for identifying events in active target experiments

R. Solli [a, b], D. Bazin [c], M. Hjorth-Jensen [c, d], M.P. Kuchera [e], R.R. Strauss [f, g]

Show more

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https://doi.org/10.1016/j.nima.2021.165461

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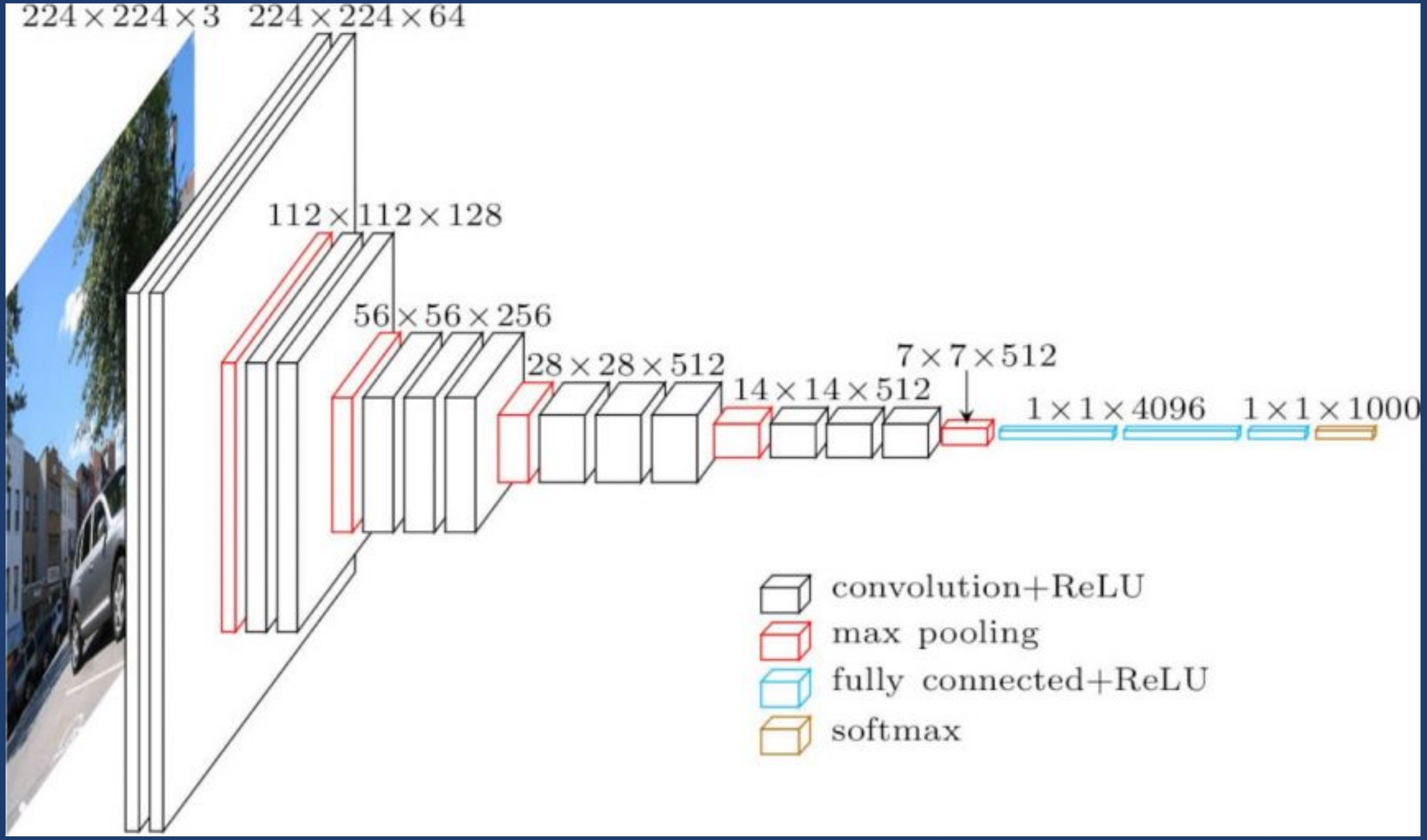


LOOKING FORWARD:

- NUCLEAR DATA
- UNCERTAINTY QUANTIFICATION
- UNIQUELY STRUCTURED DATA
- REALTIME SYSTEMS

IMPACT OF AI FOR NUCLEAR SCIENCE

MORE HIGH-QUALITY DATA

IMPROVED BEAM QUALITY

DATA STANDARDS

ACCELERATION OF SCIENTIFIC DISCOVERY

REPRODUCIBILITY

INCREASED BEAMTIME / MORE EXPERIMENTS

WORKFORCE DEVELOPMENT

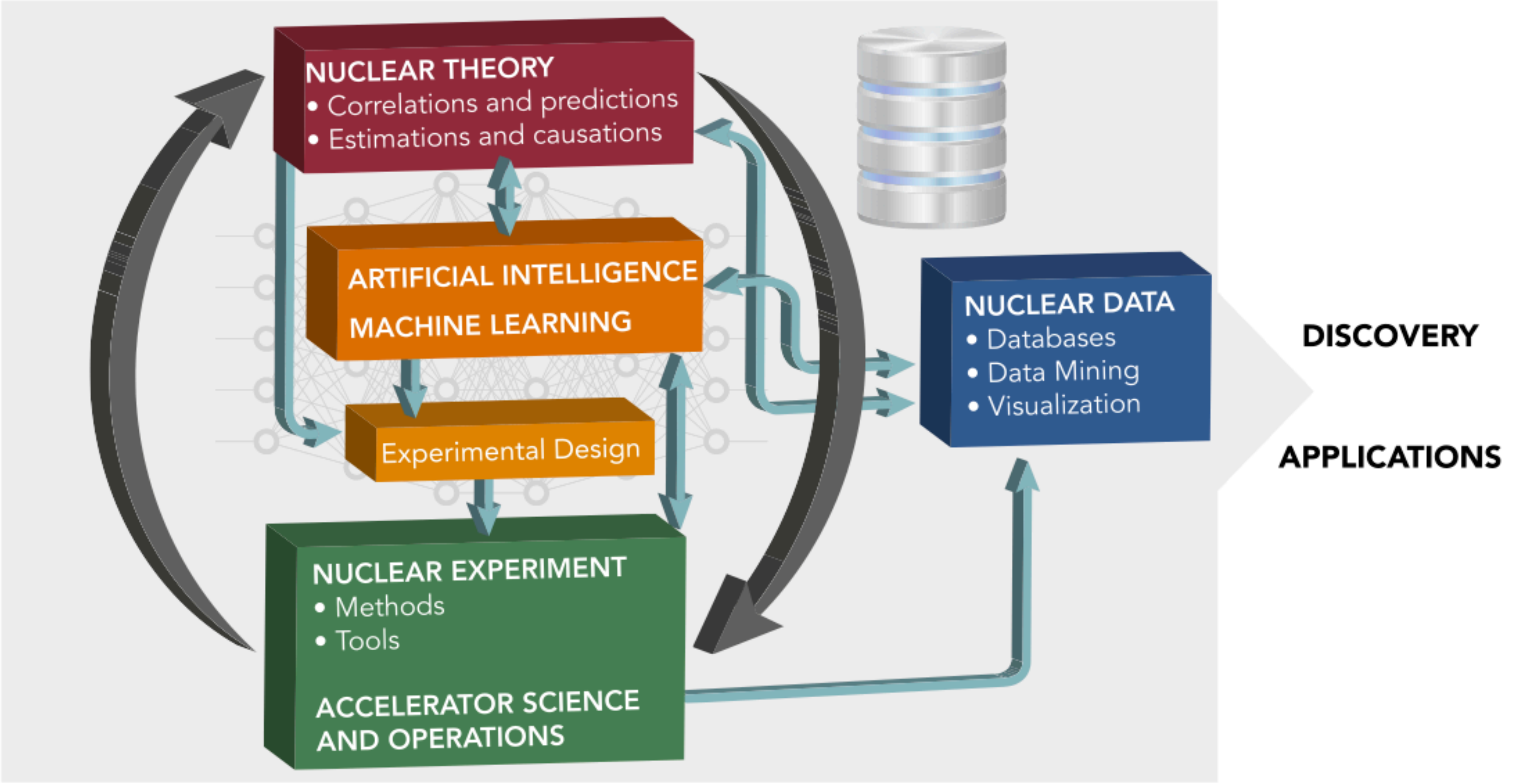
CROSS-CUTTING NEEDS

Nuclear Science Drivers

- Realtime systems
- Uncertainty quantification in AI

Education Efforts

- AI focused summer schools and workshops



Interdisciplinary collaboration and funding

- Interdisciplinary positions
- Research and development
- Production and deployment

IAEA TECHNICAL MEETING ON AI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NUCLEAR DATA
• Databases
• Data Mining
• Visualization
DISCOVERY
APPLICATIONS

NUCLEAR DATA

COURTESY C. MORSE, BNL (DNP 2022)

NNDC: new database format

- 2023 release for ENSDF
- JSON based
- python API
- enables ML

```python
# Initialize API
api = ensdfAPI(ipAddress="127.0.0.1", port=5001)

# Get all ground state halflives
values_dict = api.filterByGroundStateHalfLife()

# Create dataframe and add log scale column
dataframe = plot.createViewDataFrame(values_dict)
dataframe["halflife_log"] = np.log2(dataframe["halfLife"])

# Label plot
plot.configuration.setAxisTitle("x", "log<sub>10</sub>(t<sub>1/2</sub> [s])")
plot.configuration.setAxisTitle("y", "Counts")

# Plot as a histogram
figure=plot.createHistogram(dataframe, "halflife_log")

plot.showFigure(figure)
```

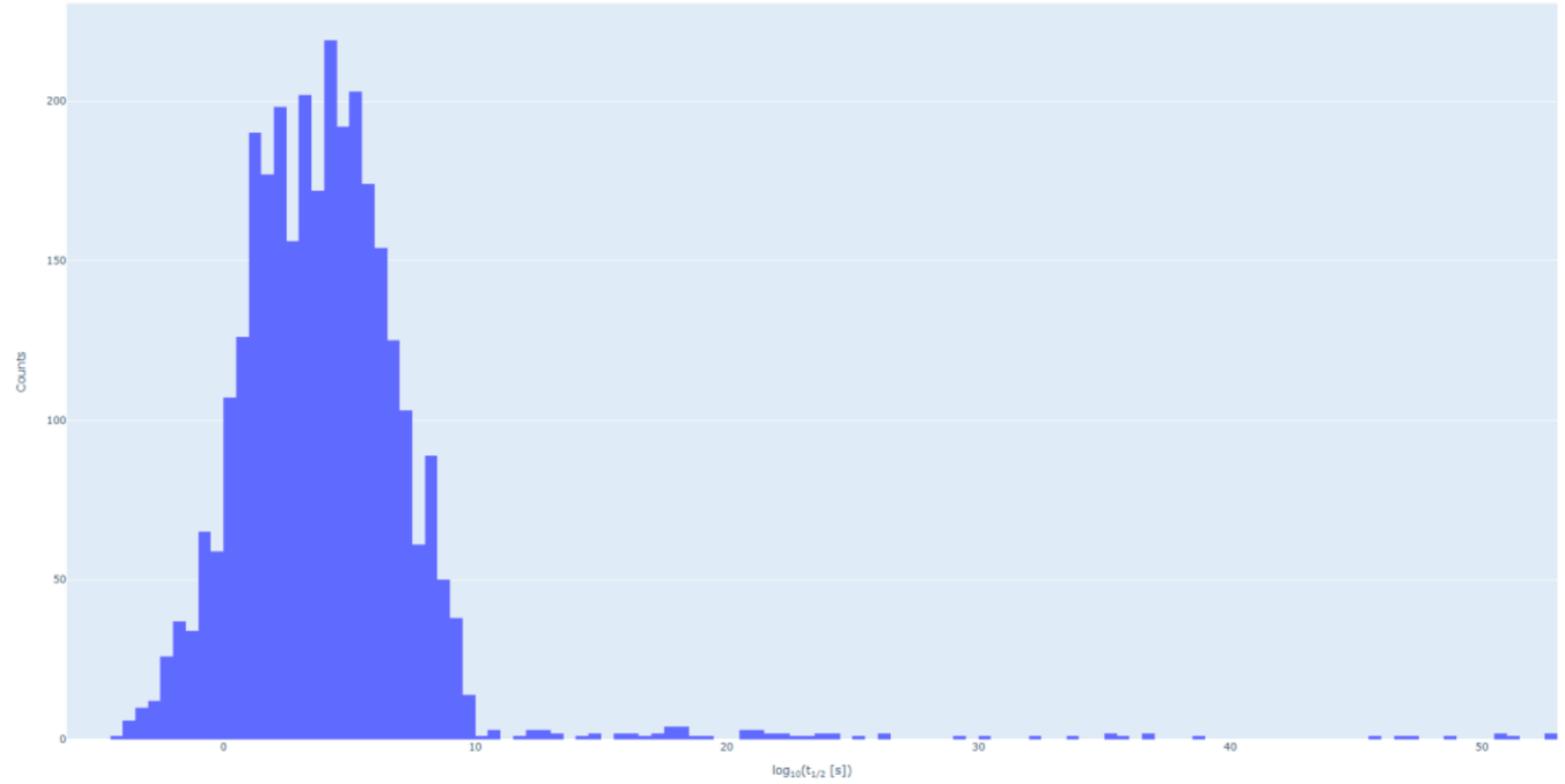

Image courtesy of Donnie Mason


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NUCLEAR THEORY: UNCERTAINTY QUANTIFICATION

Mach. Learn.: Sci. Technol. **2** (2021) 015002 https://doi.org/10.1088/2632-2153/aba6f3

MACHINE LEARNING Science and Technology

PAPER

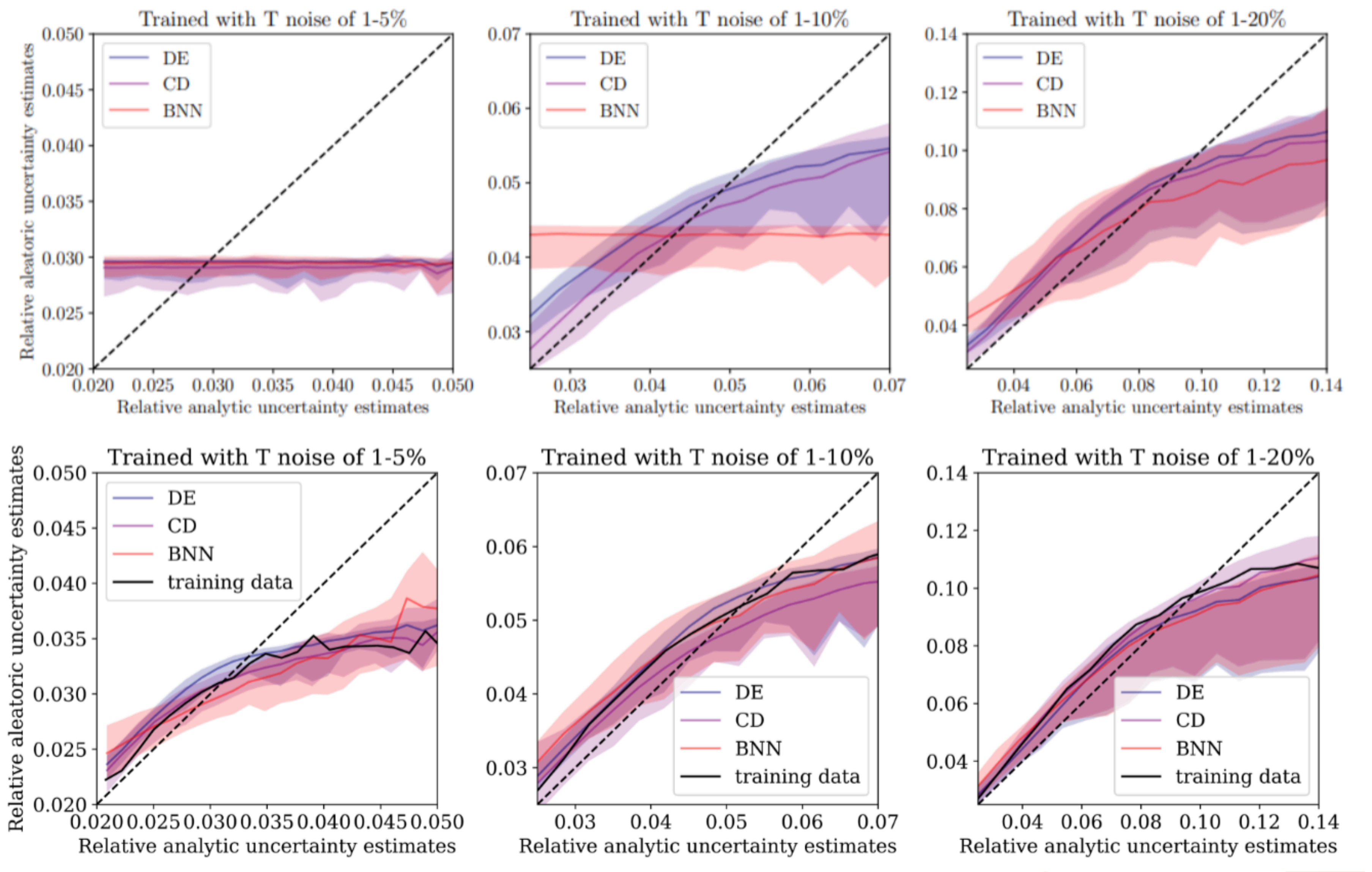
Deeply uncertain: comparing methods of uncertainty quantification in deep learning algorithms

João Caldeira[1] and Brian Nord[1,2,3]

1 Fermi National Accelerator Laboratory, P.O. Box 500, Batavia, IL 60510, United States of America
2 Kavli Institute for Cosmological Physics, University of Chicago, Chicago, IL 60637, United States of America
3 Department of Astronomy and Astrophysics, University of Chicago, Chicago, IL 60637, United States of America

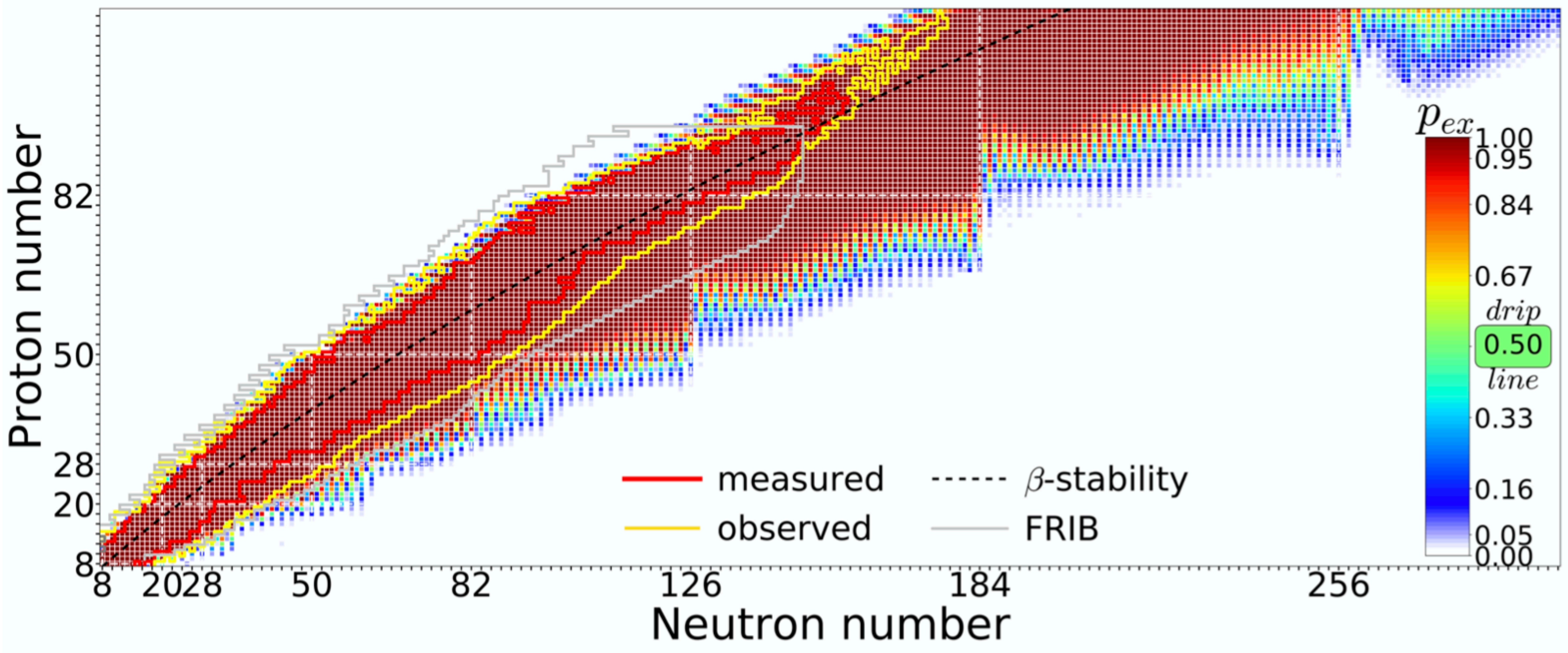
E-mail: caldeira@fnal.gov

Keywords: uncertainty quantification, neural networks, Bayesian inference, ensemble of neural networks



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

probability of existence



PLOTS COURTESY B. KRONHEIM, UMD

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UNIQUE CHALLENGES / OPPORTUNITIES IN LE-NP

- uniquely structured data
- “multimessenger” data sources
- distributed systems

STEPS TOWARDS WIDESPREAD CAPABILITIES

- data standards
- open source code
- following best practices
    + standards
    + documentation
    + fully-working examples
- collaboration with AI scientists

BIG-PICTURE ADVANCEMENTS IN AI

Large models trained on massive amounts of data

- large language models
- image-based models
- image-text pairs
- transformer models

RECENT DISRUPTORS IN AI RESEARCH

Would require:

- (more) open access, data sharing
- computational resources (GPUs)
- easy interface with packages
- collaboration

ENABLING ADVANCEMENT OF OUR SCIENCE WITH AI/ML

- EDUCATION EFFORTS
- INTERDISCIPLINARY COLLABORATIONS

EDUCATION EFFORTS

Pipeline: students enter graduate school with strong computational skills

PICUP

PARTNERSHIP FOR INTEGRATION OF COMPUTATION INTO UNDERGRADUATE PHYSICS

J-TUPP

JOINT TASK FORCE ON UNDERGRADUATE PHYSICS PROGRAMS

"Both graduates and their employers report that preparation for positions available to those with physics training could be significantly improved. Studies of physics graduates conclude that their technical skills should be expanded to address a wider and deeper knowledge of computational analysis tools..."

J-TUPP Report: "Preparing Physics Students for the 21st Century Careers"

2023 Excellence in Physics Education Award Recipient

Citation:

"For developing an active, inclusive, and supportive community of physics educators dedicated to integrating computation into their instruction; creating, reviewing, and disseminating instructional materials; and generating knowledge of computation in physics curricula and of effective practices."

EDUCATION EFFORTS

Establish annual education efforts to build an AI literate workforce

INSTITUTE for NUCLEAR THEORY

Theory Alliance
FACILITY FOR RARE ISOTOPE BEAMS

ICTP
The Abdus Salam
International Centre for Theoretical Physics

IAEA
International Atomic Energy Agency
(Virtual Event) Workshop on Computational Nuclear Science and Engineering

FONDAZIONE BRUNO KESSLER

ECT*
EUROPEAN CENTRE FOR THEORETICAL STUDIES IN NUCLEAR PHYSICS AND RELATED AREAS

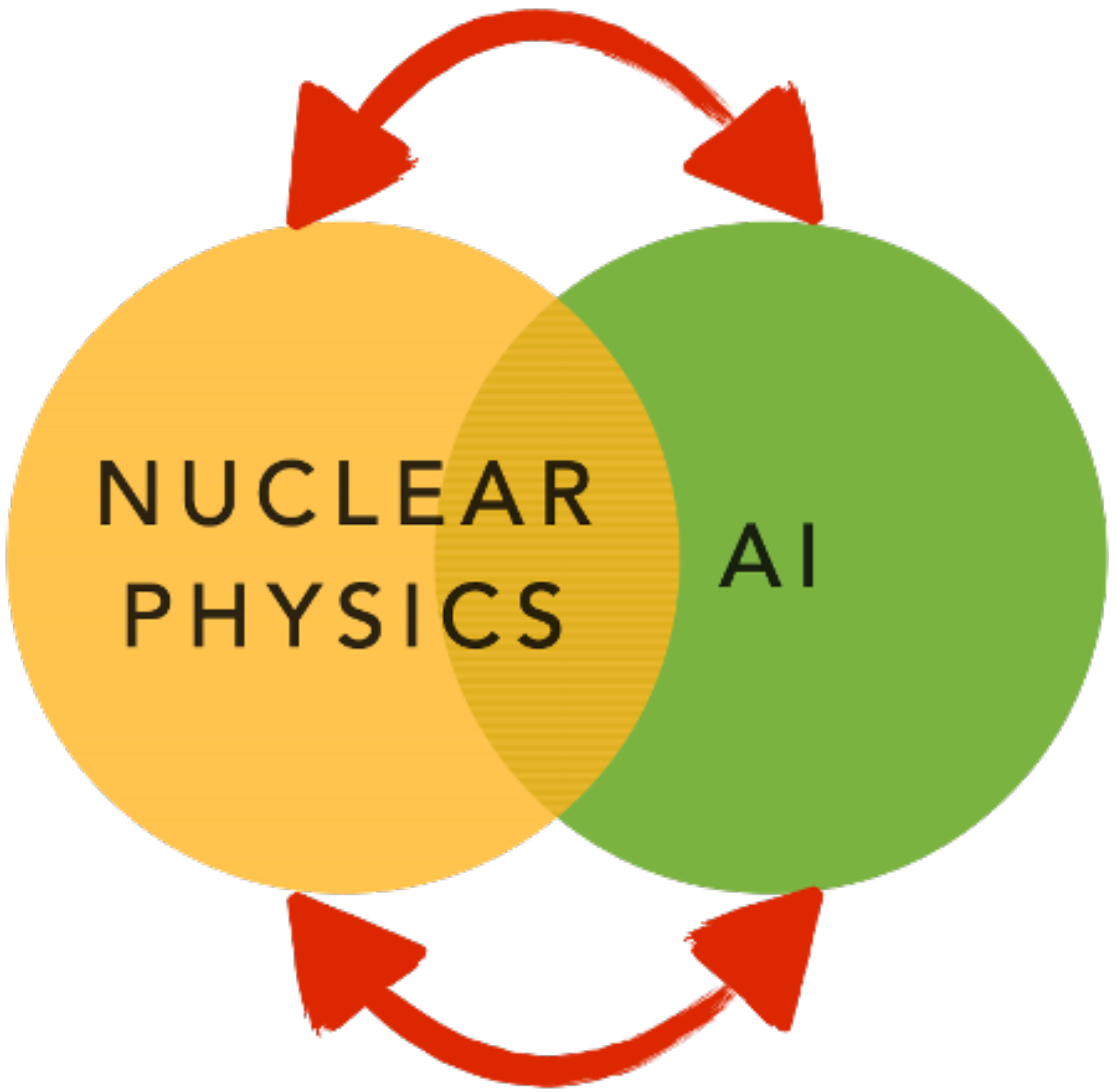
INTERDISCIPLINARY COLLABORATION AND FUNDING

Collaboration

- AI scientists
- Experts in adjacent fields

Funding

- Interdisciplinary positions
- Research and development
- Production and deployment



INTERDISCIPLINARY COLLABORATION

Engage meaningfully with the AI research community

TensorFlow

PyTorch

DeepMind

PHYSICAL REVIEW LETTERS **125,** 121601 (2020)

Equivariant Flow-Based Sampling for Lattice Gauge Theory

Gurtej Kanwar,[1] Michael S. Albergo,[2] Denis Boyda,[1] Kyle Cranmer,[2] Daniel C. Hackett,[1]
Sébastien Racanière,[3] Danilo Jimenez Rezende,[3] and Phiala E. Shanahan[1]
[1]*Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[2]*Center for Cosmology and Particle Physics, New York University, New York, New York 10003, USA*
[3]*DeepMind Technologies Limited, 5 New Street Square, London EC4A 3TW, United Kingdom*

INTERDISCIPLINARY COLLABORATION

Engage meaningfully with the AI research community

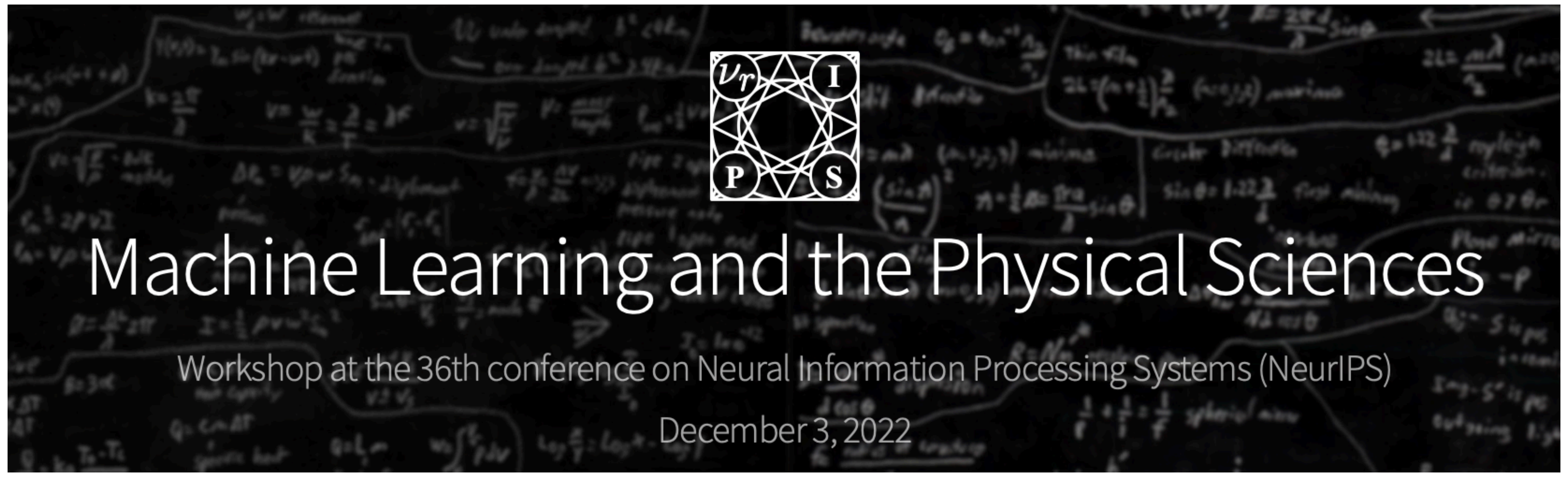
NEURAL INFORMATION PROCESSING SYSTEMS

Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence (IJCAI-21)
Survey Track

A Survey of Machine Learning-Based Physics Event Generation

Yasir Alanazi[1], **Nobuo Sato**[2], **Pawel Ambrozewicz**[2], **Astrid Hiller-Blin**[2], **Wally Melnitchouk**[2], **Marco Battaglieri**[2], **Tianbo Liu**[3] and **Yaohang Li**[1]

[1]Department of Computer Science, Old Dominion University, Norfolk, Virginia 23529, USA
[2]Jefferson Lab, Newport News, Virginia 23606, USA
[3]Key Laboratory of Particle Physics and Particle Irradiation (MOE), Institute of Frontier and Interdisciplinary Science, Shandong University, Qingdao, Shandong 266237, China
yalan001@odu.edu, {nsato, pawel, ahblin, wmelnitc, battagli}@jlab.org, liutb@sdu.edu.cn, yaohang@cs.odu.edu



Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence (IJCAI-21)

Simulation of Electron-Proton Scattering Events by a Feature-Augmented and Transformed Generative Adversarial Network (FAT-GAN)

Yasir Alanazi[1], **Nobuo Sato**[2], **Tianbo Liu**[2], **Wally Melnitchouk**[2], **Pawel Ambrozewicz**[2], **Florian Hauenstein**[3], **Michelle P. Kuchera**[4], **Evan Pritchard**[4], **Michael Robertson**[5], **Ryan Strauss**[5], **Luisa Velasco**[6] and **Yaohang Li**[1]

ICLR International Conference On Learning Representations

IJCAI

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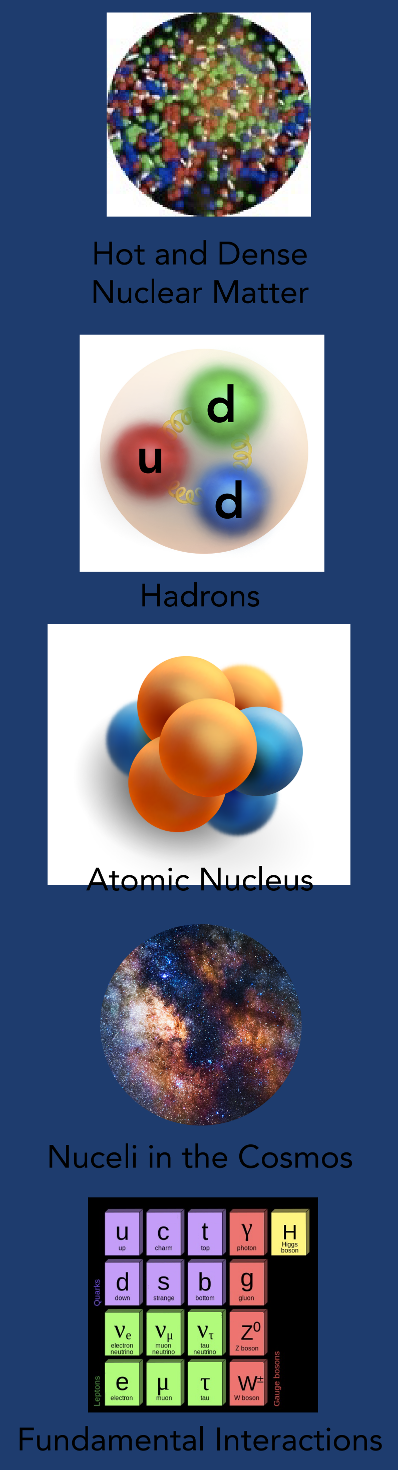
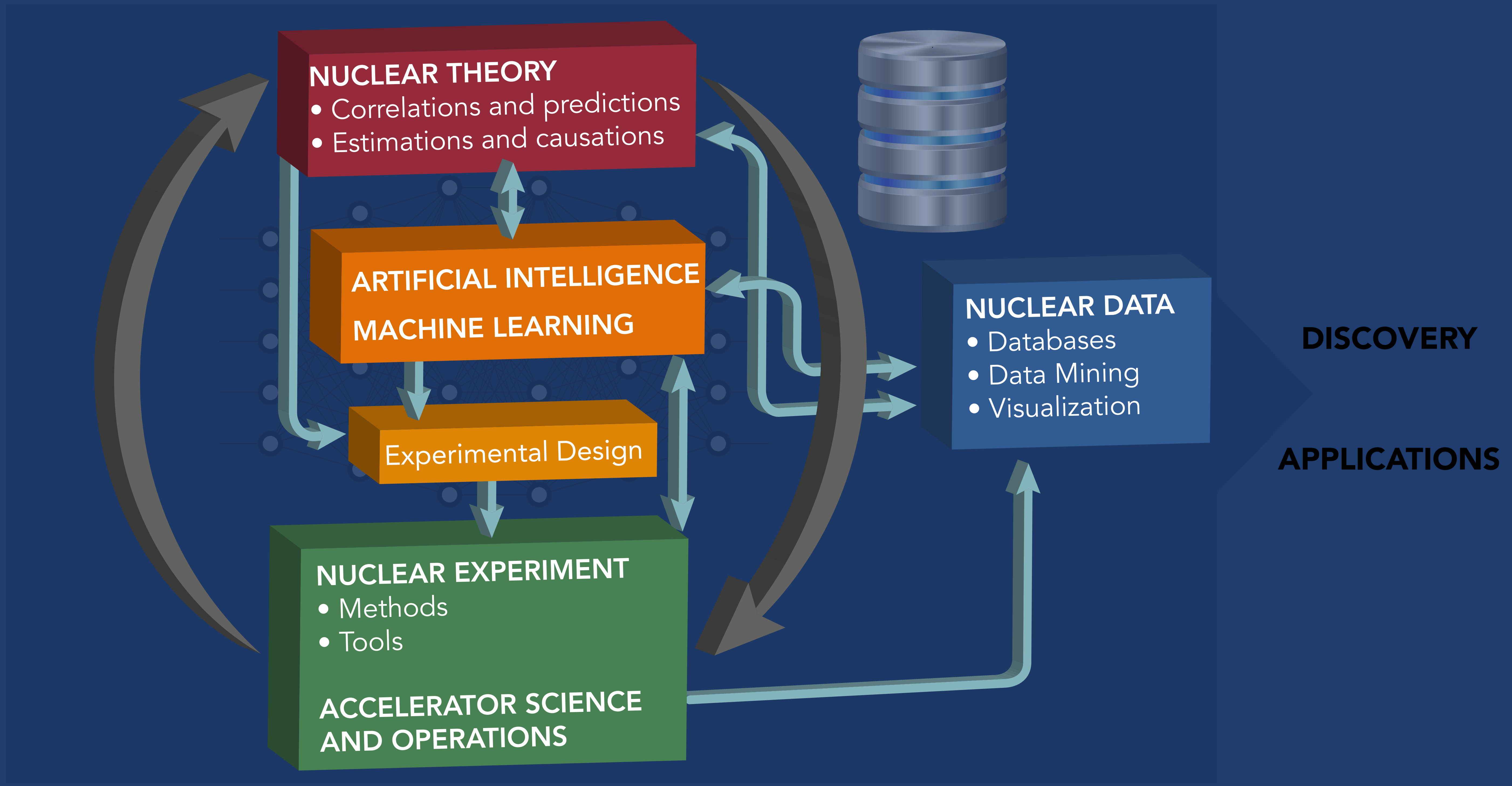
THANK YOU!


Hot and Dense
Nuclear Matter
Hadrons
Atomic Nucleus
Nuceli in the Cosmos
Fundamental Interactions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