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NOFO Artificial Intelligence and Machine Learning Applied to Nuclear Science and Technology

Notice of Funding Opportunity (NOFO) Number:
DE-FOA-0003458

NOFO Type: INITIAL
CFDA Number: 81.049

NOFO Issue Date:	Date: October 15, 2024
Submission Deadline for Letters of Intent:	Date:November 14, 2024 at 5:00 PM ET A Letter of Intent is required. Letters of Intent must be submitted by an authorized institutional representative.
Letter of Intent Response Date	Date: December 5, 2024 at 11:59 PM ET
Submission Deadline for Applications:	Date: January 14, 2025 at 11:59 PM ET

Funding Details

Expected total available funding	Up to $22 million in current and outyears
Expected number of awards	10-15
Expected dollar amount of individual awards	$200,000 -$3,500,000
Expected award project period	Two years

Internal PSA deadline: 4th of November

Template for PSA expression of interest - https://docs.google.com/presentation/d/12la6t6ph1IfKtWNwkzvDNL-ihWxtbkchdO51nD3LesY/edit?usp=sharing

For internal NSD understanding / support - please contact: nsd-advanced-computing-wg@lbl.gov

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D. Limitations on Submissions

Applicant institutions are limited to **no more than three letters of intent per institution as the lead applicant of a multi-institutional team or as the sole applicant.**

20% PI

Applicant institutions are limited to **no more than three applications per institution as the lead applicant of a multi-institutional team or as the sole applicant.** Lead PIs are expected to budget at least 20% of their time to the applications on which they are named.

There is no limitation to the number of applications on which an institution appears as a subrecipient for which the institution is not the lead.

DOE will consider the latest received submissions to be the institution's intended submissions.

- Letters of intent in excess of the limited number of submissions may be discouraged.
- Applications in excess of the limited number of submissions may be declined without review.

LIMITATIONS ON PI

The PI on a letter of intent, or application may also be listed as a senior or key personnel, including in any role on a proposed subaward, on an unlimited number of separate submissions.

Internal PSA deadline: 4th of November

Template for PSA expression of interest - https://docs.google.com/presentation/d/12la6t6ph1IfKtWNwkzvDNL-ihWxtbkchdO51nD3LesY/edit?usp=sharing

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A. Purpose

The DOE SC program in Nuclear Physics (NP) hereby announces its interest in receiving applications for research and development (R&D) efforts directed at artificial intelligence (AI) and machine learning (ML) for autonomous optimization and control of accelerators and detectors of relevance to current or next generation NP accelerator facilities and scientific instrumentation, as well as applications applying AI/ML to advance nuclear physics computations.

Current and planned NP facilities and scientific instrumentation face a variety of technical challenges in theory, simulations, control, data acquisition, and data analysis. AI methods and techniques promise to address these challenges and shorten the timeline for experimental and computational discovery.

Key takeaways: - focus on

- Autonomous control - facilities and instrumentation
- Applications to advance NP computations
- Extraction of critical information from large data sets - data-driven discovery

Most facilities mentioned in the NOFO (including 88", FRIB, EIC, RHIC, LHC, KATRIN)

NP has been supporting applications of artificial neural networks in the analysis of nuclear physics data for decades. That foundation in the use of ML techniques is revolutionizing how extremely large and information-rich data sets are interpreted, greatly increasing the discovery potential of present and future experiments at NP facilities and future machines, such as the EIC. Additionally, NP is supporting technical developments at the intersections between real-time ML and control, and the optimization of accelerator systems and detector design using AI models. Future "intelligent" experiments will seek to incorporate next generation AI hardware and electronics into detector systems.

NP is supporting .. intersections between real-time ML and control, and the optimization of accelerator systems and detector design using AI models... "intelligent" experiments … next generation AI hardware and electronics into detector systems.

The approach for this NOFO is to support the development and application of AI/ML in all research areas of NP to expand and accelerate scientific reach and discovery. Opportunities include AI to address challenges in autonomous control, efficiency of operation of accelerators and scientific instruments, digital twinning for future colliders, efficient extraction of critical information from large complex data sets and enabling data-driven discovery of new physics. Major areas of research may include, for example:

- Efficient extraction of critical and strategic information from large complex data sets:
- Development and implementation of digital twins for future colliders;
- Efforts to address the challenges of autonomous control and experimentation,
- Efficient operation of accelerators and scientific instruments,
- Deployment of AI for reduction of large and/or complex experimental data,
- Development of software to enable data-driven discovery of new physics

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- **Efficient extraction of critical and strategic information from large complex data sets:** Address how advanced AI models and data analytics can extract robust and meaningful information from the increasingly vast and complex data now being produced at the NP user facilities and by major experimental groups. AI techniques and foundational models have the potential to significantly reduce the effort to process and analyze the data to obtain the desired physical information. In addition, AI and data analytics can help unmask the complexity hidden in problems in high-dimensional spaces (multi-modal measurements, many experimental variables, etc.) by finding connections elusive to human observations. NP also seeks proposals that can lead to AI/ML applications that can be used by scientists in other areas of physics.

- **Development and implementation of digital twins for future colliders under design or considerations:** Digital twins and surrogate models have the potential to transform scientific research and all aspects of technical development of complex systems. A digital twin connects computational models with a physical counterpart to create a system dynamically updated through bidirectional data flows as conditions change in the physical system. Particle colliders such as RHIC, the Large Hadron Collider (LHC) and the EIC are complex accelerator systems that require fully optimized design and operation. Future colliders such as EIC must implement AI and ML in their design and operation. It would be very cost effective to develop a digital twin of a collider complex that includes the interaction region(s), and the beam complex with crab cavities for colliding beams suitable for conducting realistic virtual accelerator experiments aimed at optimizing design parameters. Capabilities of reading bidirectional data flows between collider instrumentation and it's digital twin is essential However, as stated by a 2023 National Academy of Sciences and Engineering study (https://www.nationalacademies.org/our-work/foundational-research-gaps-and-future-directions-for-digital-twins) many challenges remain before these applications can be fully realized. Digital twinning for colliders involves (a) modeling and simulation to create a virtual representation of a collider, and (b) Observations from the collider to inform and improve the virtual representation. Proposed work should clearly address challenges in creating a digital twin of a collider such as EIC and the method to tackle anticipated challenges.

- **Efforts to address the challenges of autonomous control and experimentation:** Incorporate use of AI to address the challenges in the real-time operation of large, complex NP user facilities and scientific instrumentation. AI based methods are needed to efficiently search large, complex parameter spaces in real time, and to predict the health and failure of instruments that operate at high power sources and experiments that run on these instruments. Such capabilities could dramatically reduce time for instrument calibration and facility downtime, improve facility performance, and maximize the productivity of the NP facilities and scientific instrumentation.

- **Efficient operation of accelerators and scientific instruments**: Increasing particle beam availability to users through the optimization of beam tuning, as well as the risk reduction in machine protection, will provide users with more opportunities to perform discovery science.

- **Deployment of AI for reduction of large and/or complex experimental data**: NP physics experiments generate huge volumes of data that would take a long time to go through for data analysis for one pass. AI methods are needed to increase the speed of data reduction beyond conventional methods used in data analysis for nuclear physics experiments.

- **Development of software to enable data-driven discovery of new physics:** In addition to the above topics, software development is needed for enabling data-driven discovery of new physics and exploration of new avenues in optimization, efficient surrogate models, data analytics, and inverse problems for accelerator and major detector operations and controls. The development of advanced design approaches using AI and machine learning to inform instrumentation development is also of interest. Finally, the integration of data-analytics-driven automated decision tree navigation capability into control systems is needed for existing NP-supported national user facilities, as well as into the design of the EIC.

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A note on applications and NP construction projects: Any proposed work that is not part of a current NP project scope can be submitted to this NOFO. Current NP project scope includes the approved Electron-Ion Collider (EIC). AI/ML methods related to the EIC need to be drafted to ensure they would not overlap with the approved EIC project scope. However, the methods can be related to enhancing scientific output of the EIC as a scientific user facility. The above is also true about other major NP projects in Fundamental Symmetries or other NP subprograms (Medium Energy, Heavy Ion, Nuclear Structure and Nuclear Astrophysics, etc.).

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Teaming Arrangements

Multi-Institutional Teams

SC uses two different mechanisms to support teams of multiple institutions.

COLLABORATIVE APPLICATIONS

Collaborative proposals **will not be accepted** under this NOFO.

SUBAWARDS[2]

Multi-institutional teams **must** submit one application from a designated lead institution with all other team members proposed as subrecipients.

DOE/National Nuclear Security Administration (NNSA) National Laboratories[3], if participating in a team led by another institution, must be proposed as subrecipients.

Note that the value of any such proposed subaward may be removed from any such prime award: DOE may make separate awards to Federally affiliated institutions.