U.S. DEPARTMENT OF ENERGY | Office of Science

Virtual Townhall: Artificial Intelligence Research for High Energy Physics

DE-FOA-0002705

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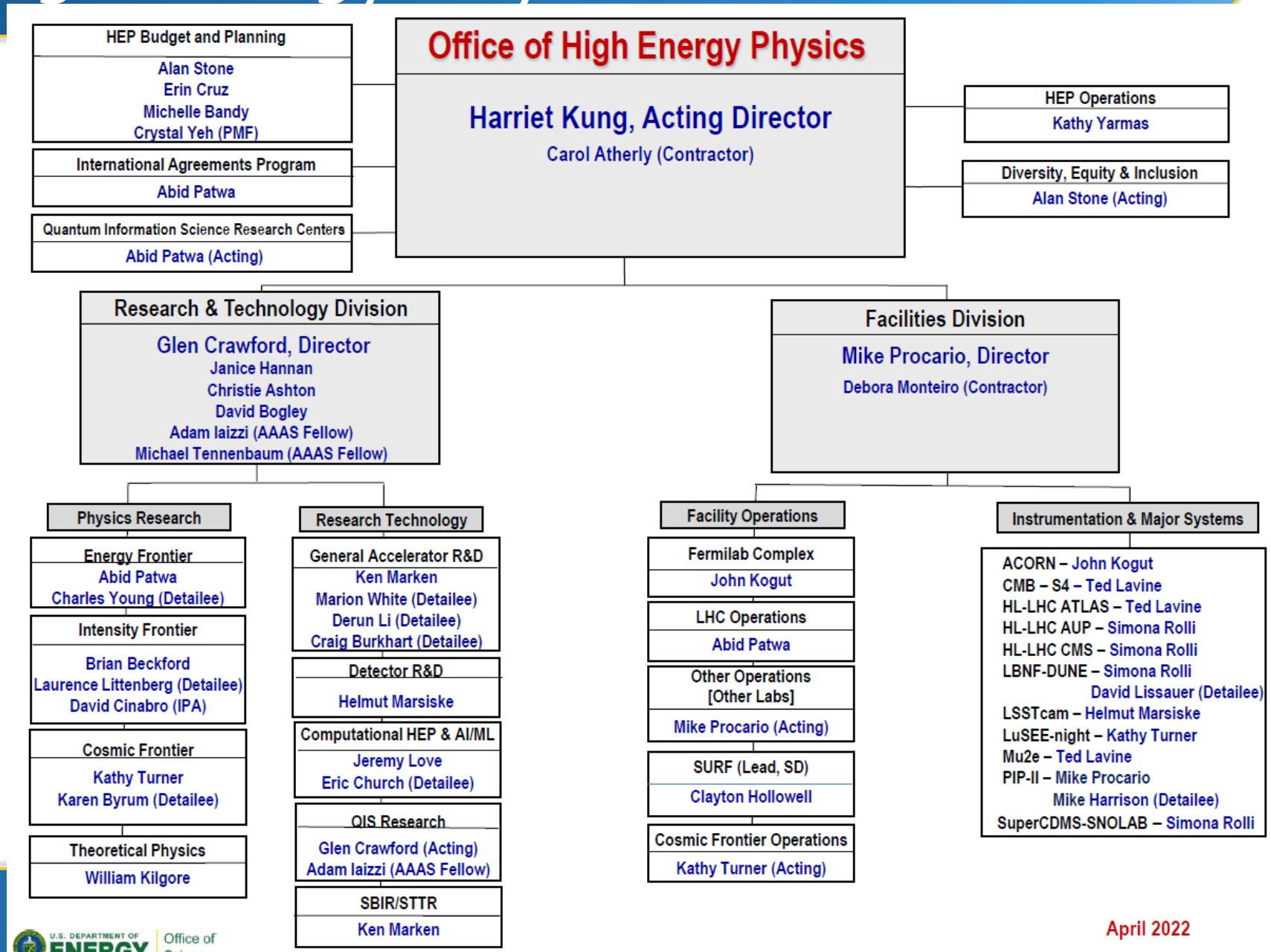
Welcome

- Welcome to the Artificial Intelligence Research for High Energy Physics FOA Virtual Townhall (DE-FOA-0002705)
  - This is a new HEP FOA in support of the DOE SC AI Initiative
- This meeting is to provide some context and clarification for the FOA, and to answer questions
- Please use the "raise hand" feature in zoom to indicate you would like to ask a question
  - Please keep questions general and concise
    - Please avoid specifics of research topics or teaming arrangements to be proposed as part of a question

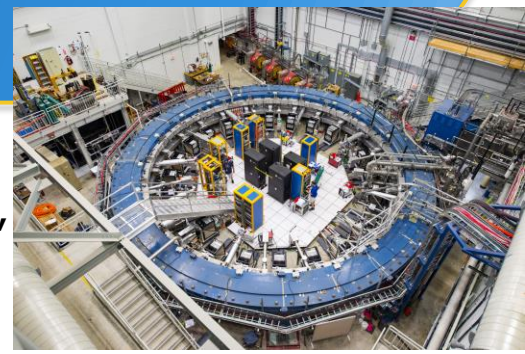
DOE Office of High Energy Physics

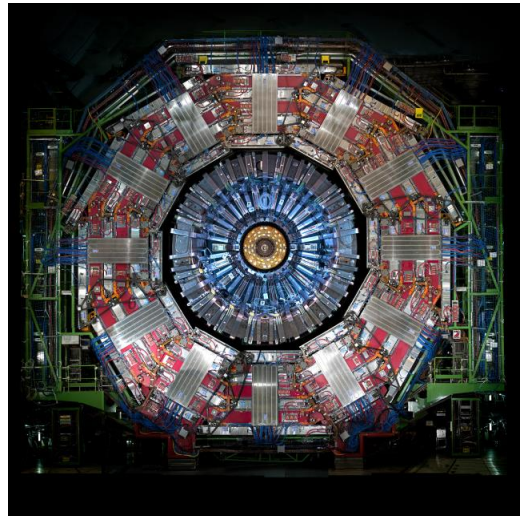
- HEP underpins and advances the DOE missions and objectives through a balanced portfolio of scientific **research**, facilities' **operations** and **projects**, and by the development of **key technologies** and **trained person-power** needed to work at the cutting edge of science



High Energy Physics Research Program

- The mission of the HEP program is to **understand how the universe works** at its most fundamental level by **discovering the elementary constituents of matter and energy**, probing the interactions between them, and **exploring the basic nature of space and time**.
- Experimental Science and Technology R&D is "mission-driven":
  - Develops and supports a specific portfolio of projects. **Emphasis is placed on supporting science collaborations in all stages; conducting experiments; and seeking the best possible science results**.
  - Makes **significant, coherent contributions to facilities/experiments** selected for the program, including project management.
  - Supports **R&D that will advance the state-of-the-art in particle accelerators and detectors**, which will lead to new, more capable facilities.
  - Supports **R&D to enable new and transformative capabilities in QIS, AI/ML**, and crosscutting technology areas
- Theory supports activities that **provide the vision** and the mathematical framework for understanding and **extending our knowledge** of particles, forces, space-time, and the universe.
- **HEP supports ~85% of the U.S. particle physics (in $)**, incl. **~all national labs**
- Priorities are set by the P5 report.





DOE SC AI Initiative

- The President has placed a high priority on ensuring continued U.S. leadership in AI research and development
  - Lead the world in the development of trustworthy AI and prepare the future U.S. workforce for the integration of AI systems across all sectors of economy and society.
- Broad interest in AI is being driven by the accumulation of large datasets and growing computational capacity for processing
  - Machine Learning (ML) is included when appropriate as tool to derive insights from these large datasets
- DOE SC is looking to support AI research that maximizes the scientific impact
  - Further the scientific mission beyond what is currently possible
  - Develop new or improved methods of analyzing datasets to extract information
  - Develop tools to broaden participation among interested communities

Current HEP AI Program

- Particle Physics has a long history of being early adopters of AI/ML to do great science
  - A few examples from the past of today's popular topics:
    - Study of electron-photon separation and sensitivity improvement of $H \rightarrow \gamma\gamma$ searches at D0, using a NN from 1989.
    - Study of a VLSI NN computational accelerator for CDF electron isolation trigger based on the Intel ETANN (Electrically Trainable Analog Neural Network) processor, in 1992.
    - Starting in 1995 events of the HERA H1 experiment were processed by a NN hardware trigger with a 5kHz event rate running on Xilinx FPGAs.
- In recognition of this history, HEP supports AI/ML research activities through two paths
  - **Programmatic AI/ML** – integrated/embedded in the frontier programs. Applications of primarily ML techniques to improve HEP results within a given frontier.
    - Supported through the University and Lab comparative review process
  - **Core AI/ML** – research into AI/ML topics from an HEP perspective and blue-sky R&D necessary to enable future HEP breakthroughs across frontiers
- Snapshot of Core AI/ML programs:
  - Early Career Awards across HEP frontiers with significant AI/ML component
  - Machine Learning Across the Frontiers – Computational HEP program to develop ML applications for HEP
  - Exa.TrkX – Computational HEP program to use Exascale computing to perform track reconstruction for HL-LHC
  - AI for Scientific User Facilities – projects to develop AI systems that can improve online facility operations
  - **New FOA seeking to grow the Core AI/ML program**

AI Research for HEP Scope

- Seeking to support new research distinct from currently funded work, or consolidation of existing research being carried out at multiple institutions
  - The thrusts of this FOA are distinct from, but complimentary to, university and lab comparative review core research programs
- Request applications primarily targeting one of three topic areas:
  - **AI for HEP** – AI research that furthers HEP priorities of pursuing the P5 science drivers
  - **HEP for AI** – AI research that makes use of unique aspects of the HEP (datasets, theory, etc.) to improve understanding of the theoretical capabilities and limitations of fundamental AI techniques
  - **HEP AI Ecosystem** – Production of open datasets, software ecosystems, or access to shared computing resources that enable broad democratic participation in AI research for HEP
    - Including democratic participation from historically underserved communities
- In the **AI for HEP** thrust, proposals are sought for innovative applications of AI tools and techniques or demonstration and development of new capabilities not currently available to HEP researchers
  - Applications that **go well beyond** Programmatic AI/ML research are especially encouraged

AI Research for HEP FOA

- This solicitation provides up to a total of **$10M over 3 years** ($3.3M/year).
  - As few as 2 and up to 50 projects may be supported
  - Expect to support approximately 3 multi-institution proposals and 10 seed proposals
    - Will be determined by the composition of meritorious proposals received
- Eligible Institutions: universities/colleges, DOE National Labs through two distinct paths
  - Multi-institution team proposals led by DOE National Labs
    - Anticipated award size of $500k – $750k per year
  - Single-institution "seed" proposals from universities/colleges
    - Anticipated award size of $50k – $75k per year
- Letters of Intent are optional but encouraged – LoI deadline is **April 21, 2022 at 5pm EST**
  - We do not anticipate encouraging or discouraging LoIs
- Application deadline is **May 24th, 2022 at 11:59 EST**
- Priority support is intended for research with hardware a lower priority
  - Proposals are asked to estimate computing resources needed and identify how those needs will be met
    - **Modest** computing time at NERSC may be possible for some successful projects

Application Paths

- Multi-institution team applications **must be led by a DOE National Lab**
  - Single application submitted by the lead lab
    - Subawards to other DOE National Labs, colleges, universities, or other eligible institutions as appropriate **without restriction or requirement**
  - Lead-PI from the lead lab is **expected to charge 25%** of their effort to the award
    - The lead-PI **may not appear** as a senior investigator or key personnel on any other application
  - DOE National Labs may submit up to four (4) multi-institution applications
    - DOE National Labs **may not** submit single-institution "seed" applications
  - Project narrative limited to **20 pages or less**.
- Single-institution "seed" applications **must be submitted by** eligible institutions such as **a university or college**
  - May contain multiple PIs from that institution
  - Each institution may submit up to four (4) single-institution applications
    - Regardless of participation as subawardee in multi-institution applications
  - Project narrative limited to **5 pages or less**.

Guidance on Paths

- Multi-institution teams:
  - Broad ambitious research requiring multiple institutions to address multi-faceted questions of scientific inquiry
    - Particularly when these challenges can be factorized across team members and institutions
- Seed applications:
  - Exploratory investigations and smaller scale studies of feasibility
    - Researchers or institutions new to either AI or HEP research
    - Establishing the feasibility of blue-sky research from experienced PIs or institutions
      - Proposals in either of these categories **are equally valid and encouraged**
- In both paths **multi-disciplinary efforts are encouraged** when appropriate for the proposed work
  - Partnerships across HEP frontiers and with non-HEP AI/ML experts
- Given the expected number of awards and the level of interest in this FOA, the review process is expected to be extremely competitive
  - As always, the focus should be on submitting high quality proposals not on quantity
    - Institutions are allowed to submit up to four applications, but are not required to do so

FOA Application Guidance

- There have been changes to DOE/SC FOAs for FY22. **Please read the FOA carefully** for details of specific requirements
  - Start preparing early.
    - Do not wait for a response to an LoI to begin preparation of the full application
  - Write a sensible well formatted and spell-checked COI list
    - Follow the **updated guidance** in the FOA for who should be included
  - Letters of support or recommendation are not allowed.
    - Letters from experimental collaborations, targeted by the proposed research, stating a willingness to perform routine necessary software maintenance after the award period are not considered letters of support.
      - Each application may include up to five (5) Letters of Collaboration.
  - **Do not wait until the deadline to submit applications.**

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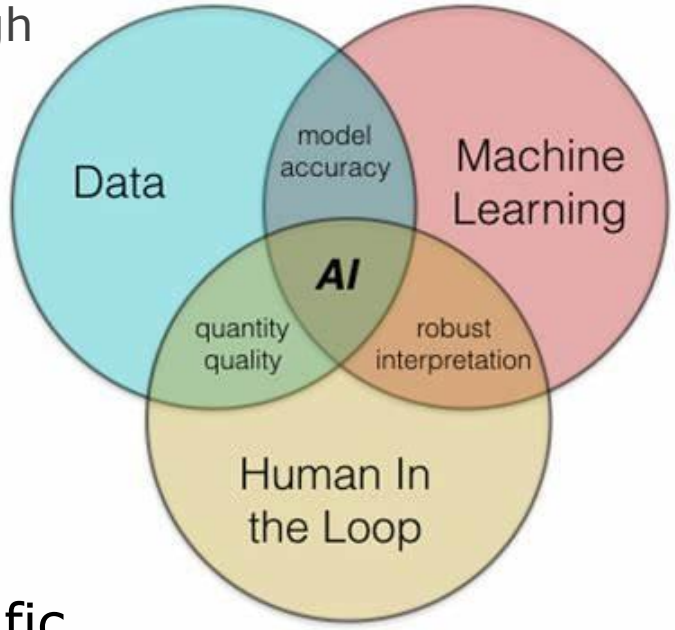
Questions?

AI/ML Definitions

- Machine Learning – Computational algorithms that are not rigidly programmed but have parameters learned from data. Anthropomorphized linear algebra. A tool.
  - Ex: Fitting parameters of a polynomial using MINUIT, or speed up of high fidelity simulation using ML-based digital twins or surrogate models
- Artificial Intelligence – Computational systems that respond to data and act, without human intervention, to achieve a goal and their development. A field of research.
  - Ex: An accelerator complex that tunes control parameters based on real-time sensor measurements to optimize efficiency, or research of uncertainty quantification techniques to more accurately determine the confidence of ML-based classifiers.



- These definitions provide some guidance for the kind of scientific effort required based on research topic.
  - ML – Cultivating training datasets and selecting, tuning, and training models to achieve good performance.
  - AI – Requires additional work on the autonomous aspects of the computational system, enhanced validation or improved understanding of techniques.
    - Work beyond training and optimizing algorithms to allow the computational system to interpret and act on results

Detailed FOA Scope

- **AI for HEP** – The scientific objectives and priorities for the field recommended by the High Energy Physics Advisory Panel (HEPAP) are detailed in its long-range strategic Particle Physics Project Prioritization Plan (P5).[4] Applications are sought that are well aligned with the HEP program priorities. AI research that advances the P5 science drivers, or development of new AI-based technologies that expand paths of investigation for HEP beyond what was considered in the P5 report are encouraged. Ambitious applications of AI benefitting multiple HEP programs or experiments coherently and which are of broad interest are especially sought, as are innovative applications that can deliver significant advances to HEP experimental reach or theoretical understanding.
- **HEP for AI** – This FOA also seeks to support research that makes use of unique aspects of HEP to improve the understanding of the theoretical capabilities and limitations of fundamental AI. Research into robust scientific ML, data intensive ML, ML-enhanced Modeling and Simulation, Uncertainty Quantification, and Physics Informed ML that exploits HEP theoretical understanding, experimental data, or simulations to provide insight into general AI/ML methods are encouraged. An example of a possible research topic in this area would be evaluation of various Physics Informed ML techniques compared to training more traditional networks.
- **HEP AI Ecosystem** – Proposed work toward production of open datasets, collaboration with industrial or national laboratory partners, as well as development of "ecosystem" software allowing for straightforward training and deployment of models is equally encouraged. Applications that address democratic access among all-sized institutions to computing resources and continued development and retention of the workforce for the products being developed are especially welcome. Examples of possible topics in this area would be curating HEP datasets for public access, or integration of modern ML software into standard HEP tools.