NP Artificial Intelligence Principal Investigators Exchange Meeting

December 05, 2023

Manouchehr Farkhondeh
DOE Office of Science, Nuclear Physics Program

U.S. DEPARTMENT OF ENERGY

Outline:

- This Meeting
- Overview of DOE-SC and NP AI/ML initiative
- FY2020 Data, AI and ML Lab call and awards
- FY2021 Data Analytics AI/ML FOA and awards
- FY2023 Data, AI and ML FOA and Lab call
- PIER Plan Requirement for all FY2023 and beyond FOAs
- Communications and Presentation Guidelines

DOE SC Statement of Commitment

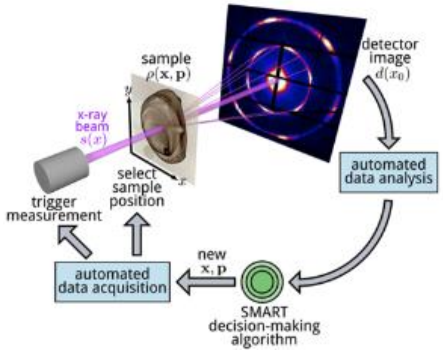
- *The DOE SC Diversity, Equity and Inclusion webpage:*
- *https://science.energy.gov/sc-2/research-and-conduct-policies/diversity-equity-and-inclusion/*
- *"The DOE Office of Science (SC) is fully committed to fostering safe, diverse, equitable, and inclusive work, research, and funding environments that value mutual respect and personal integrity. Effective stewardship and promotion of diverse and inclusive workplaces that value and celebrate a diversity of people, ideas, cultures, and educational backgrounds is foundational to delivering on the SC mission. The scientific community engaged in SC-sponsored activities is expected to be respectful, ethical, and professional.*
- *The DOE SC does not tolerate discrimination or harassment of any kind, including sexual or non-sexual harassment, bullying, intimidation, violence, threats of violence, retaliation, or other disruptive behavior in the federal workplace, including DOE field site offices, or at national laboratories, scientific user facilities, academic institutions, other institutions that we fund, or other locations where activities that we support are carried out…"*

- *If you are subject to or witness harassment or discrimination, please contact any of the NP PM present or our Division Director. You can also visit the following:*

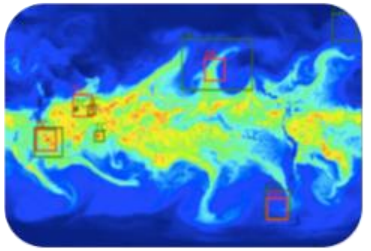
  How to Report a Complaint | U.S. DOE Office of Science (SC) (osti.gov)

Artificial Intelligence in the Office of Science

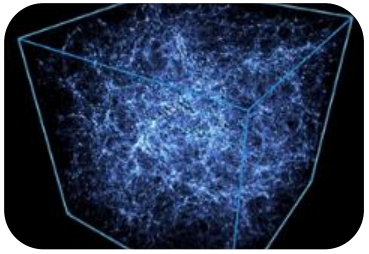
- **AI for User Facilities and Advanced Technology**
  - Optimize design of experiments and operations
  - Enable real-time analysis and integrated workflows
  - Predict and mitigate instrument and facility down time
  - Increase particle beam availability to users through optimization of beam tuning and risk reduction in accelerator machine protection
  - Create Self-driving instruments and experiments
- **AI for Science**
  - Accelerate scientific discovery through federated learning to gather broader insight via shared datasets
  - Develop surrogate models for expensive or time constrained experiments
  - Make sense of multi-modal, noisy data
  - Reduce time for complex scientific instrument calibration
- **AI Tools**
  - Incorporate uncertainty quantification and domain-knowledge
  - Increase robustness, interpretability and repeatability
  - Develop new storage and archival tools to make data FAIR (Findable, Accessible, Interoperable, and Reusable)
  - Develop privacy-preserving algorithms for use of AI in edge devices and to support biopreparedness research efforts



Autonomous experiments



Deep learning for extreme weather events



Analyze relationship between 10 billion galaxies in LSST

U.S. DEPARTMENT OF ENERGY

Overview of AI/ML initiative

- Artificial Intelligence (AI) represents a paradigm shift for scientific high-performance computing. DOE and the Office of Science (SC) recognize the power that AI will have to accelerate progress in scientific research and missions by developing new data analysis tools and integrating data focused approaches with our physics-based computer simulations.
- AI is one of the **current initiatives for SC** with focused efforts and fundings.
- Nuclear Physics (NP) — NP has been supporting applications of artificial neural networks in the analysis of nuclear physics data for decades. Current and planned NP facilities and scientific instrumentation face a variety of technical challenges in simulations, control, data acquisition, and analysis.
  - *January 2020: A roundtable NP meeting of experts was convened to discuss AI/ML techniques focused on improving efficiencies of accelerator and detector operations.*
  - *March 2020: An NP community workshop at TJNAF considered priority research opportunities in AI/ML.*
- In FY2020 NP participated in a three SC program offices (BES,HEP and NP) Lab only funding opportunity call in Data science and AI/ML for SC accelerator and detector facilities.
- NP has published an NP only funding opportunity (FOA) in FY2021 and one for FY2023-24 funding.
- An SC AI/ML working group with representation from all five SC Programs meets bi-weekly to discuss developments and coordination. I represent NP in this working group.

NP Lab AI-ML proposals Lab-20-2261

- *This was a SC Laboratory call from BES, HEP and NP allowing 2 proposals per user facilities.*
- *NP received 3 proposals in accelerators and 2 in experiments and detectors, a total of 5 Proposals*

PI Name	SC Lab	Proposal Title	FY 2020 Award ($K)	Total Award ($K)
David Lawrence	TJNAF	A.I. Assisted Experiment Control and Calibration		
Christopher Tennant	TJNAF	AI for Improved SRF Operation at CEBAF		
Brahim Mustapha	ANL	Use of Artificial Intelligence to Optimize Accelerator Operations and Improve Machine Performance		
		Total ($K)	**1,000**	**3,000**

- *Funding in Year-1 came from accelerator R&D base funds (total of $1M / year).*
- *These were 3 –year awards, FY20-22 funding*
- *Last three talks today are on these award works*

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NP AI/ML FOA DE-FOA-0002490

FY2021

Today's first 6 talks are on awards for this FOA

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**

Awards: NP AI/ML FY2021 DE-FOA-0002490 (subject of this meeting)

	Awards for NP FY2021 FOA on Data Analytics and … SC_FOA_0002490		
Award #	**Institution**	**Proposal Title**	**Principal Investigator**
1	MIT NJIT FNAL LANL	Intelligent experiments through real-time AI: Fast Data Processing and Autonomous Detector Control for sPHENIX and future EIC detectors Lead Institution	Roland, Gunther Yu, Dantong Tran, Nhan Liu, Ming Xiong
2	UNC	Deep Learning for Germanium-Based Neutrinoless Double Beta Decay Searches	Gruszko, Julieta
3	LBNL	Machine Learning Optimization Upstream and Downstream of the Accelerator: The Cases of VENUS and GRETA	Crawford, Heather
4	LLNL UC, Riverside LBNL	AI-driven detector design for the EIC Lead Institution	Angerami, Aaron Arratia, Miguel Nachman, Benjamin
5	ANL- ATLAS	Autonomous Optimization of the Secondary Beam Production and Delivery at the ATLAS In-Flight Facility	Hoffman, Calem
6	ANL-ATLAS	Modern Data Analytics for the Large Gamma-Ray Spectrometers: GRETINA/GRETA and Gammasphere via Machine Learning and Optimization	Carpenter, Michael
		Total 2-year Awards ($k)	**5,680**

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NP AI/ML FOA DE-FOA-0002875
FY2023

- *FOA: DE-FOA-0002875*
- *Issue Date: Nov 9, 2022*
- *Proposals due: Jan 11, 2023*
- *No LOIs or preapplications*

DEPARTMENT OF ENERGY (DOE)
OFFICE OF SCIENCE (SC)
NUCLEAR PHYSICS (NP)

ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING FOR AUTONOMOUS OPTIMIZATION AND CONTROL OF ACCELERATORS AND DETECTORS

FUNDING OPPORTUNITY ANNOUNCEMENT (FOA) NUMBER:
DE-FOA-0002875

FOA TYPE: INITIAL
CFDA NUMBER: 81.049

FOA Issue Date:	November 9, 2022
Submission Deadline for Applications:	January 11, 2023, at 11:59 PM Eastern Time

FY 2023 NP AI/ML FOA- P1

General approach: Application of AI/ML tools and methods for **experiments, simulation, theory and accelerator operation to expand scientific outreach**

Technical areas and scope for FY2023 FOA

- Efficiently extract critical and strategic information from large complex data sets,
- Address the challenges of autonomous control and experimentation,
- Efficiency of operation of accelerators and scientific instruments,
- AI for data reduction of large experimental data.

Application context and NP Major Projects

- Any proposed work that is not part of a current NP project including EIC can be submitted to this FOA.
- AI/ML for EIC application can be carefully drafted to ensure they would not overlap with approved EIC project scope. However, they can be related to enhancing scientific output of the EIC project.
- The above is also true about other major NP projects in Fundamental Symmetry or any other programmatic research areas of NP (Medium Energy, Heavy Ion, Nuclear Structure and nuclear astrophysics, etc.).

FY 2023 NP AI/ML FOA – P2

- ***Solicitation S&T Scope:***
  - *Research focused on data for autonomous optimization and control of accelerators and detectors relevant to current- or next-generation NP accelerator facilities.*
  - *Research on technical developments at the intersections between real-time machine learning and the control and optimization of accelerator systems operation and detector design using AI models*
- ***Program Planning/Context:***
  - *Impart an acceleration of experimental and computational discovery by applying AI methods and techniques to address technical challenges in simulations, theory, control, data acquisition and analysis for NP accelerators and scientific instruments.*
  - *Provides support consistent with FY 2023 budget language for targeted investments to develop cutting-edge techniques based on AI of relevance to nuclear science research and accelerator facility operations.*
- ***Application Requirements:***
  - **Eligibility:** Universities/colleges, non-profit/ small business as collaborators, DOE/NNSA laboratories only;
  - **Award size/duration**: Up to $1M/year; up to 2-year awards
  - **Funding by Fiscal Year**: FY 2023 ~$8M, FY 2024 up to $8M - subject to budget appropriation
  - **Preproposals:** No Preproposals or Letters of Intent are required

NP AI/ML FY2023 DE-FOA-0002875 Statistics

U.S. DEPARTMENT OF ENERGY

Applications and Awards

A total of 15 independent awards

Institutions	# of Applications	# of Awards	Fraction (#)	Requests (K$)	Award (K$)	Fraction (%)
Laboratories	22	8	36%	-	9,600	
Universities	16	7	44%	-	6,400	
Totals	**38**	**15**	**39%**	**47,200**	**16,000**	**34**

Application/Award Types

Type of Proposal	Submitted	Awarded	Fraction (%)
Collaborative	16	7	44
Single PI	22	8	36
Totals	**38**	**15**	39.4

Application/Award Topics (note the diverse areas)

Proposal Topic	Submitted	Awarded	Fraction (%)
Accelerator	11	4	50
Detectors	8	4	50
Experiments + EIC	15	5	33
Theory	4	2	50
Totals	**38**	**15**	39.4

NP AI/ML FY2023 DE-FOA-0002875 Awards List-P1

Collaborations identified with same color rows. No significance to the choice of colors.

Award #	Topic Subj.	Institution	Project Title	PI and Co-PI
1	**Detector, SPHENIX**	**LANL** FNAL Georgia Tech MIT NJIT, NJ ORNL	**Intelligent Experiments Through Real-time AI: Fast Data Processing and Autonomous Detector Control for sPHENIX and Future EIC Detectors**	**Liu, Ming** Tran, Nhan Hao, Cong Roland, Gunther Yu, Dantong Schambach, Jo
2	**Accelerator**	**MSU** LANL	**Online Autonomous Tuning of the FRIB Accelerator Using Machine Learning**	**Ostroumov, Peter** Scheinker, Alexander
3	Detector ML	MSU	Machine Learning for Time Projection Chambers at FRIB	Wrede, Christopher
4	Experiment, LE	ANL	Modern Data Analytics for the Large Gamma-Ray Spectrometers: GRETINA/GRETA and Gammasphere via Machine Learning and Optimization - RENEWAL	Carpenter, Michael
5	Experiment, LE	VSU, Petersburg, VA **HBU**	Neural network classifier for analyzing measurements of fast neutrons for invariant mass spectroscopy	Redpath, Thomas

NP AI/ML FY2023 DE-FOA-0002875 Awards List-P2

6	**Experiment AI**	**LBNL** Duke U Wayne SU, MI	**New approaches to Bayesian uncertainty quantification for Nuclear Science**	**Jacobs, Peter** Mak, Simon Shen, Chun
7	**Theory ML**	**MSU** ANL **FNAL** FSU Ohio S U Columbus Ohio U, Athens ORNL UNC, Chapel Hill UTK	**STREAMLINE Collaboration: Machine Learning for Nuclear Many-Body Systems**	**Lee, Dean** Lovato, Alessandro Rocco, Noemi Piekarewicz, Jorge Furnstahl, Richard Drischler, Christian Hagen, Gaute Konig, Sebastian Papenbrock, Thomas
8	Accelerator AI Op	ANL	Use of artificial intelligence to optimize accelerator operations and improve machine performance	Mustapha, Brahim
9	**Theory, LQCD**	**UVA** MSU NMSU, New Mexico ODU Tufts U V Pol I, Blacksburg, VA	**EXCLAIM - EXCLusives via Artificial Intelligence and Machine learning**	**Liuti, Simonetta** Lin, Huey-Wen Sievert, Matthew Li, Yaohang Goldstein, Gary Boer, Marie

NP AI/ML FY2023 DE-FOA-0002875 Awards List-P3

10	Experiment ML	LBNL	Machine Learning Optimization: VENUS & GRETA	Crawford, Heather
11	Accelerator	TJNAF UVA subcon	Graph Learning for Efficient and Explainable Operation of Particle Accelerators	Tennant, Chris
12	Detector, FS	UNC, Chapel Hill	Interpretable Machine Learning for Germanium-Based Neutrinoless Double Beta Decay Searches	Gruszko, Julieta
13	**Accelerator Pol.**	**BNL** Cornell RPI, NY SLAC TJNAF	**Beam polarization increase in the BNL hadron injectors through physics-informed Bayesian Learning**	**Hoffstaetter, Georg** Hoffstaetter, Georg Wang, Yinan Edelen, Auralee Schram, Malachi
14	**Detector**	**W&M** BNL Cath U Duke U. TJNAF	**A Scalable and Distributed AI-assisted detector design for the EIC**	**Fanelli, Cristiano** Wenaus, Torre Horn, Tanja Vossen, Anselm G. Diefentahler, Markus
15	Experiment ME	TJNAF	AI/ML Optimized Polarization	Lawrence, David, Subcon with CMU and W&M
	$16 M Funding cut off line			

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A new Requirement for FY 2023 SC FOAs

- ***A new Requirement for all FY2023 and beyond SC FOA applications:***

  - *All new and renewal applications must provide a Promoting Inclusive and Equitable Research (PIER) Plan as an appendix to the research narrative.*

- As a result, a new criteria (PIER) is added to the four existing SC Merit Review criteria
  - *Scientific and/or Technical Merit of the Project;*
  - *Appropriateness of the Proposed Method or Approach;*
  - *Competency of Applicant's Personnel and Adequacy of Proposed Resources;*
  - *Reasonableness and Appropriateness of the Proposed Budget; and*
  - *Quality and Efficacy of the Promoting Inclusive and Equitable Research (PIER) Plan.*

  Link to SC website https://science.osti.gov/grants/Applicant-and-Awardee-Resources/PIER-Plans

- *PIER Criterion Questions:*
  - *Is the proposed Promoting Inclusive and Equitable Research (PIER) Plan suitable for the size and complexity of the proposed project and an integral component of the proposed project?*
  - *To what extent is the PIER plan likely to lead to participation of individuals from diverse backgrounds, including individuals historically underrepresented in the research community?*
  - *What aspects of the PIER plan are likely to contribute…*

(PIER) Plans- Page 2

- The complexity and detail of PIER Plans are expected to increase with the size of the research team and the number of personnel supported.
- Applicants are encouraged to consider focusing on areas, including but not limited to:
  - The composition of the project team and partnering institutions.
  - The research environment—cultivating respectful, professional and accessible environments.
  - Equitable and inclusive implementation of the research project.

Additional information and FAQs: https://science.osti.gov/grants/Applicant-and-Awardee-Resources/PIER-Plans and https://science.osti.gov/grants/Applicant-and-Awardee-Resources/PIER-Plans/Q-and-As

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Communications between NP and PI for AI/ML work

Two modes of communications between PIs and NP office: Quarterly reports and an annual meeting with all PI in one place.

- Quarterly Reports
  - PIs are asked to submit quarterly reports to NP in a “Small Project” format. Quarterly reports are reviewed by the Division (they are not just filed away). For FY2021 FOA awards Ms. Saryna Cameron has been requesting for these periodic reports.

- PI Exchange Meetings:
  - **AI/ML:** This is the first standalone annual NP AI/ML PI Exchange meeting, and we plan to have one yearly.

NP Matrix for Quarterly Report Review and PM Assessment.

Include brief and clear responses to these NP Matrix questions in your quarterly reports.

- *NP matrix for Quarterly Report and progress assessment.*
- *Make sure your quarterly reports addresses elements of this matrix for our evaluation*
- *Continue to use the NP "small Project" template Ms. Saryna Camron sends you.*

These questions are for the NP PM and your response are only part of the information I use to arrive at my own assessments.

1-		**PI's performance during the quarter**
	a	Progress made
	b	Milestones met
	c	Any breakthrough
2-		**Assessment of risk mitigation**
	a	Issue comunicated?
	b	appropriate mitigation strategies
3-		**Likelihood of achieving project goals**
	a	Will they meet cost and schedule
	b	Will they deliver the promised scope
4-		**Recommendation on need for action**
	a	Are there any actions you need to take in response to points above

PI Exchange Meeting, November 30, 2022

- Presentations on status of work by all Principal Investigators (PIs) who received awards
  - under FY 2021 FOA DE-FOA-0002490 for AI and Data Analytics
  - Under FY 2020 Lab call Lab-20-2261

- This is not a review, and no review panel is involved. Presentations will be made to NP Office Program Managers and Division Directors, and possibly a few PMs from HEP and BES Program Offices.

- To facilitate exchange of information between PIs and the NP Office and among PIs and institutions on all current NP AI/ML awards activities.

PI Meeting Presentation Guidelines:

Each presentation should include the following information:

- Description of the project and the current status;
- The main goal of the project for which you received the FY 2020- 22 AI/ML awards,
- A table showing annual budget and the total received to date (see below);
- A table showing major deliverables and schedule; and
- There will be no written report or follow up actions required for this meeting.
- Summary of expenditures by fiscal year (FY):
- All talks will be posted on PI Exchange meeting page on NP website.
- **35 min talks should allow 7 min for Q/A and 30 min talks 5 min for Q/A**

	Year 1	Year 2	Year 3	Totals
a) Funds allocated				
b) Actual costs to date				

U.S. DEPARTMENT OF ENERGY

FY2023 PI Meeting Agenda

#	Time (E.S.T)	Dur. (min)	Principal Investigator	Institution	R&D Area	Presentation Title	Speaker(s)
	AGENDA : 2023 NP AI-ML PI Exchange Meeting, Tuesday, December 5, In-Person						
	9:00	5	-	DOE NP	-	Introductory Remarks	**Mantica**
	9:05 AM	35	-	DOE NP	-	NP supported AI/ML	**Farkhondeh**
		FY2020 Lab call awards in LAB 20-2261: "Data, Artificial Intelligence and Machine Learning at DOE Scientific User Facilities					
1	9:40 AM	35	Lawrence, David	TJNAF	Detectors	A.I. Assisted Experiment Control and Calibration	**Lawrence**
2	10:15 AM	35	Tennant, Christopher	TJNAF	Accelerators	AI for Improved SRF Operation at CEBAF	**Tennant**
	10:50 AM	**20**	**Break**				
3	11:10 AM	35	Mustapha, Brahim	ANL	Accelerator	Use of Artificial Intelligence to Optimize Accelerator Operation	**Mustapha**
		FY2021 FOA and Lab call awards: DE-FOA-0002490 "Data Analytics for Autonomous Optimization and Control……"					
1	11:45 AM	35	**Liu, Ming Xiong** Roland, Gunther Yu, Dantong Tran, Nhan	**LANL** MIT NJIT FNAL	Detectors	Intelligent experiments through real-time AI: Fast Data Processing and Autonomous Detector Control for sPHENIX and future EIC	**Liu**
2	12:20 PM	35	Gruszko, Julieta	UNC	Detectors	Deep Learning for Germanium-Based Neutrinoless Double Beta Decay Searches	**Gruszko**
	12:55 PM	**85**	**Lunch**				
3	2:20 PM	35	Crawford, Heather	LBNL-88 inch	Accelerator	Machine Learning Optimization Upstream and Downstream of the Accelerator: The Cases of VENUS and GRETA	**Crawford /Todd**
4	2:55 PM	35	**Arratia, Miguel** Nachman, Benjamin Angerami, Aaron	**UC, Riverside** LBNL LLNL	Detectors	AI-driven detector design for the EIC	**Arratia**
	3:30 PM	**20**	**Break**				
5	3:50 PM	35	Hoffman, Calem	ANL- ATLAS	Accelerator	Autonomous Optimization of the Secondary Beam Production and Delivery at the ATLAS In-Flight Facility	**Hoffman**
6	4:25 PM	35	Carpenter, Michael	ANL-ATLAS	Detectors	Modern Data Analytics for the Large Gamma-Ray Spectrometers: GRETINA/GRETA and Gammasphere via Machine Learning and Optimization	**Carpenter**
	5:00 PM	5				**Closing Remarks**	
	5:05 PM		**Adjourn**				

Acknowledgements of Federal Support
For your award

Peer Reviewed Articles and Technical Papers

For peer reviewed and technical papers, the following acknowledgment of support is **required:**

- **For Financial Assistance (Grants, etc.):**

  Acknowledgment: "This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of [insert the sponsoring SC Program Office, e.g., Nuclear Physics], [Add any additional acknowledgements or information requested by the sponsoring SC Program Office] under Award Number(s) [Enter the award number(s)]."

  Example: "This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of **Nuclear Physics** under Award Number DE-SC-000yyy."

- **For National Lab awards:**

  Example: "This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office Nuclear Physics program under Award Number DE-SC-000zzz.

Here is the link on Acknowledgment:
https://science.osti.gov/Funding-Opportunities/Acknowledgements

BACKUP Slides

FY2021 FOA: Data, Artificial Intelligence and Machine Learning

Solicitation S&T Scope: ***DE-FOA-0002490;*** ***issue date: March 16, 2021***

Scope: The AI/ML for autonomous optimization and control of nuclear physics accelerators and detectors described in this FOA support efforts essential to developing leading core competencies and transformative technologies that significantly advance the state-of-the art AI and data analytics capabilities in accelerator science and nuclear physics research:

- Efficiently extract critical and strategic information from large complex data sets,
- Address the challenges of autonomous control and experimentation,
- Efficiency of operation of accelerators and scientific instruments,
- AI for data reduction of large experimental data.

Eligible Institutions: Universities/colleges, non-profit and small business as collaborators, DOE/NNSA laboratories only; New single- or multi-PI proposals.

Outcome of the FOA:

- Received 32 individual applications : 22 collaborative and single PI proposals
- A review panel helped NP **to select 6 R&D projects** (11 proposals)
- Total funding of $5.68M over 2 years.

SC AI Lab Call Lab-20-2261
(Also, topic of this Exchange meeting)

DEPARTMENT OF ENERGY
OFFICE OF SCIENCE
BASIC ENERGY SCIENCES
HIGH ENERGY PHYSICS
NUCLEAR PHYSICS

DATA, ARTIFICIAL INTELLIGENCE, AND MACHINE LEARNING AT DOE SCIENTIFIC USER FACILITIES

DOE NATIONAL LABORATORY PROGRAM ANNOUNCEMENT NUMBER: LAB 20-2261

ANNOUNCEMENT TYPE: INITIAL

Announcement Issue Date:	**March 9, 2020**
Submission Deadline for Proposals:	**May 1, 2020, at 5 PM Eastern Time**

NP AI/ML FY2023 DE-FOA-0002875 Statistics

Applications and Awards

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Application Topic			
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