DEPARTMENT OF ENERGY
OFFICE OF SCIENCE
ADVANCED SCIENTIFIC COMPUTING RESEARCH

FAIR DATA AND MODELS FOR ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING

DOE NATIONAL LABORATORY PROGRAM ANNOUNCEMENT NUMBER: LAB 20-2306

ANNOUNCEMENT TYPE: Initial

Announcement Issue Date:	**April 2, 2020**
Submission Deadline for Letter of Intent:	**April 17, 2020 at 5:00 PM Eastern Time** **A Letter of Intent is required**
Submission Deadline for Proposals:	**May 15, 2020 at 5:00 PM Eastern Time**

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REGISTRATIONS

A. DOE Office of Science Portfolio Analysis and Management System (PAMS)

The Department of Energy (DOE) Office of Science (SC) performs many functions for DOE national laboratory proposals in the Portfolio Analysis and Management System (PAMS), which is available at https://pamspublic.science.energy.gov.

You must register in PAMS to submit a pre-proposal, letter of intent, or DOE national laboratory proposal.

To access PAMS, you may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers.

Notifications sent from the Portfolio Analysis Management System (PAMS) will come from the PAMS email address <PAMS.Autoreply@science.doe.gov>. Please make sure your email server/software allows delivery of emails from the PAMS email address to yours.

Registering to PAMS is a two-step process; once you create an individual account, you must associate yourself with ("register to") your institution. Detailed steps are listed below.

1. CREATE PAMS ACCOUNT:

To register, click the "Create New PAMS Account" link on the website https://pamspublic.science.energy.gov/.
- Click the "No, I have never had an account" link and then the "Create Account" button.
- You will be prompted to enter your name and email address, create a username and password, and select a security question and answer. Once you have done this, click the "Save and Continue" button.
- On the next page, enter the required information (at least one phone number and your mailing address) and any optional information you wish to provide (e.g., FAX number, website, mailstop code, additional email addresses or phone numbers, Division/Department). Click the "Create Account" button.
- Read the user agreement and click the "Accept" button to indicate that you understand your responsibilities and agree to comply with the rules of behavior for PAMS.
- PAMS will take you the "Having Trouble Logging In?" page. (Note: If you reviewed for or were listed as PI on a prior submission to SC but have not previously created an account, you may already be linked to an institution in PAMS. If this is the case, PAMS will take you to the PAMS home page.)

2. REGISTER TO YOUR INSTITUTION:

- Click the link labeled "Option 2: I know my institution and I am here to register to the institution." (Note: If you previously created a PAMS account but did not register to an

institution at that time, you must click the Institutions tab and click the "Register to Institution" link.)
- PAMS will take you to the "Register to Institution" page.
- Type a word or phrase from your institution name in the field labeled, "Institution Name like," choose the radio button next to the item that best describes your role in the system, and click the "Search" button. A "like" search in PAMS returns results that contain the word or phrase you enter; you need not enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (Hint: If your institution has an acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may search for the acronym under "Institution Name like." Many institutions with acronyms are listed in PAMS with their acronyms in parentheses after their names.)
- Find your institution in the list that is returned by the search and click the "Actions" link in the Options column next to the institution name to obtain a dropdown list. Select "Add me to this institution" from the dropdown. PAMS will take you to the "Institutions – List" page.
- If you do not see your institution in the initial search results, you can search again by clicking the "Cancel" button, clicking the Option 2 link, and repeating the search.
- All DOE National Laboratories have established profiles in PAMS, so please keep searching until you find your laboratory.

For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this DOE National Laboratory Announcement should reference **LAB 20-2306.**

UPDATES AND REMINDERS

SC encourages you to register in all systems as soon as possible. You are also encouraged to submit letters of intent and proposals before the deadline.

DATA MANAGEMENT PLAN

The SC Statement on Digital Data Management, published at http://science.osti.gov/funding-opportunities/digital-data-management/, governs proposals submitted under this Announcement. Compliance is detailed in Section IV of this Announcement.

ACKNOWLEDGMENT OF FEDERAL SUPPORT

SC published guidance about how its support should be acknowledged is located at http://science.osti.gov/funding-opportunities/acknowledgements/.

AVOIDING ERRORS

The following advice is compiled from actual experiences of applicants for SC awards.
- Please ensure that the research narrative is comprised of one and only one Portable Document Format (PDF) file, including all appendices, when it is uploaded.
- When using the PAMS website at https://pamspublic.science.energy.gov, please avoid using the back-arrow button in your web browser to navigate.
- Please ensure that the proposal contains no personally identifiable information (PII).
- Please ensure that the budget is calculated using the applicable negotiated indirect cost and fringe benefit rates.

Checklist for Avoiding Common Errors:

Item	Issue
Page Limits	Strictly followed throughout application, including particular attention to: - Research Narrative - Appendix 2 Narrative, if any - Biosketches - Data Management Plan(s) (DMP's) - Letter(s) of Recommendation, if any
Personally Identifiable Information	None present in the application
Research Narrative	Composed of one PDF file including all appendices
Project Summary / Abstract	Name(s) of applicant, PI(s), PI's institutional affiliation(s), Co-Investigator(s), Co-Investigator's institutional affiliation(s)
DOE Cover Page	Follow instructions closely
Budget	Use current negotiated indirect cost and fringe benefit rates
Budget Justification (attached to budget)	Justify all requested costs
Biographical Sketches	Follow page limits strictly
Current and Pending Support	Ensure completeness, including brief abstract of scope of work for all items listed
Data Management Plans	- If referring to an experiment's DMP, describe the relationship to the proposed research - Include a DMP even if no experimental data is expected

Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

Technical/Scientific Program Contacts:
Dr. Laura Biven
301-903-5000
Laura.Biven@science.doe.gov

SUMMARY

The DOE SC program in Advanced Scientific Computing Research (ASCR) hereby announces its interest in making research data and artificial intelligence (AI) models findable, accessible, interoperable, and reusable (FAIR[1]) to facilitate the development of new AI applications in SC's congressionally authorized mission space, which includes the advancement of AI research and development. In particular, ASCR is interested in supporting FAIR benchmark data for AI; and FAIR frameworks for relating data and AI models.

For this Announcement, AI is inclusive of, for example, machine learning (ML), deep learning (DL), neural networks (NN), computer vision, and natural language processing (NLP). Data, in this context, are the digital artifacts used to generate AI models and/or employed in combination with AI models during inference. An AI model is an inference method that can be used to perform a "task," such as prediction, diagnosis, or classification. The model is developed using training data or other knowledge. An AI task is the inference activity performed by an artificially intelligent system

FAIR Benchmark Data:
Scientific data are different from other classes of data more typically used in AI research. Currently, algorithms developed for non-scientific data can perform poorly when applied to scientific data. The principal focus of this announcement topic is to close this gap by making scientific data publicly available to the AI community so that algorithms, tools, and techniques work for science. Further research and efforts are needed to expand critical capabilities that make unique scientific data open and FAIR (Findable, Accessible, Interoperable, and Reusable), provide sufficient metadata, provenance, and annotations to the AI community, and articulate challenge areas to focus the community on unique aspects of science data and open areas of research.

FAIR Frameworks for Data and AI Models:
Tools for training AI models on data are readily available and widely used. What is lacking, however, is a theoretical framework for understanding relationships between data and models. For example, given a specific data set and problem, we lack rigorous methods for identifying the

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1 Wilkinson, M. D. et al. The FAIR Guiding Principles for Scientific Data Management and Stewardship. Sci. Data 3:160018 doi: 10.1038/sdata.2016.18 (2016)

best model, hyper-parameters, and training method to use. Given a specific data set and problem, which additional data would be helpful to include in the training set? What information about a dataset can be deduced from a model trained on the data? What attributes of the data can be reverse engineered from a model? What can we learn about model robustness and transfer learning by looking at relationships between data and models?

The primary focus of this announcement topic is to advance our understanding of the relationship between data and models by exploring relationships among them through the development of FAIR frameworks for relating data and models. Such frameworks should provide capabilities that advance our understanding of AI, provide new insights to help researchers with applications of AI techniques, and provide an environment where novel approaches to AI can be explored. Proposed frameworks may focus on specific disciplines or sub-disciplines within the SC congressionally mandated mission space; or may focus on particular aspects or sub-areas within AI.

SUPPLEMENTARY INFORMATION

SC's mission is the delivery of scientific discoveries and major scientific tools to transform our understanding of nature and to advance the energy, economic, and national security of the United States. The ASCR program provides national leadership in high-performance computing and in a broad set of computationally based technologies, tools, and approaches. This includes research and development that significantly advances the fields of artificial intelligence and big data analytics (BD) of interest to DOE-supported researchers.

Data are essential and strategic assets for addressing SC priorities in AI. In particular, data can be used to train AI algorithms in areas where AI can have a large impact on the SC mission; data can be used by researchers to develop new types of algorithms, particularly in areas where industry is unlikely to invest; and finally, data can be used to improve our understanding of AI, and ultimately control and design AI methods that are more robust, transparent, and sensitive to biases and ethical concerns. SC-supported research programs, laboratories, and large-scale scientific facilities create and collect enormous amounts of data. Leveraging these data for AI, however, can require significant investments in data management, curation, and sharing.

Proposals must follow the guidelines and criteria provided in this supplementary information and the following sections.

FAIR Benchmark Data:
Much of the recent progress in AI has been fueled by the availability of unprecedented amounts of data. Publicly available benchmark datasets are important tools to compare, enhance, train, and analyze AI models. For example, it has been argued that the ImageNet competition and benchmark dataset sparked the deep learning revolution, specifically by demonstrating the capabilities of convolutional neural networks in object recognition tasks in natural images. Similarly, the advancement of AI research for scientific applications can be greatly enhanced by facilitating access to science data.

A focus of this announcement is the publication of benchmark datasets that exemplify the distinguishing attributes of scientific data and/or tasks performed on the data with appropriate storage, access rights, and integration with computational capabilities and analysis tools to focus the development of AI tools and techniques on science needs. Benchmark datasets will have greater reusability if domain experts collaborate with data management experts to define the data and metadata, and provide explanations about what phenomena they describe and the nature of tasks that can be performed on them. Benchmark datasets will have greater impact with active cooperation or engagement with AI R&D and application development communities. To achieve this, applicants may choose to propose teaming arrangements, outreach activities, and/or competitions or challenges around FAIR science data.

FAIR Frameworks for Data and AI Models:
An AI model is an inference method that can be used to perform a "task" such as prediction, diagnosis, classification, etc. Conceptually, AI models fall somewhere between data and theory—neither entirely empirical, nor entirely derived from first principles. When used for control or autonomous decision making in a scientific workflow, the trained model may be an important digital artifact for reproducibility of the results. It may also be an important element of provenance for the resulting scientific data set. In other cases, the model may be better viewed as an approximation of data—either the data used to train it, or the data it generates, as in the case of Generative Adversarial Networks. As digital research objects, however, AI models are in their infancy with very few schemas for syntax, ontologies or even controlled vocabulary, or metadata standards.

Educated trial and error continues to guide advances in science applications of AI. Currently, there is no holistic, theoretical approach unifying data, AI models, and the tasks performed by models that would help us answer critical, foundational questions such as: What information about a dataset can be deduced from a model trained on the data? Do models inherit the access limitations or classifications of the training data? For a given data set and task, what are the best model, hyper-parameters, and training method? When are more data needed, and how much incremental information will they have? Which data would make the biggest improvement? In what circumstances can a model be transferred to new data?

Presently, many science applications of AI begin with the desire to perform a particular task on a given data set or data stream. Training data are chosen and prepared, and then a model is identified and trained. The choice of model often involves some educated guess work. Furthermore, to improve the accuracy of the model, it is not clear whether more training data, a different model or hyper-parameters, or the addition of domain knowledge would be beneficial. Research is needed to relate the models to previously collected data, or find out what other tasks are relevant. The missing theoretical framework for data, AI models, and tasks has important implications for performance and optimization of AI in science as well as overall productivity of AI applications, the reusability of models, and our understanding of reproducibility of AI workflows.

The lack of a unifying theory also influences decisions in regards to the sharing of AI models and techniques. Since it is not known what attributes of a dataset can be derived from a model trained on that data, AI models trained on restricted data are not shared more broadly than the

data themselves. Having a better understanding of the relationships between data and models would have an enormous impact in connecting research on restricted data with advances in open science.

Frameworks for tracking relationships among data, AI models, and tasks can address strategically important open questions in AI research that significantly advance the field of AI for public benefit within SC's Congressionally-authorized mission-space. Envisioned here is a framework that would link all salient aspects of an AI workflow including, for example, the data, AI model, task, training methodology, and accuracy metrics and measures. An important feature of this framework is the holistic view of this workflow.

Data Management Plan:

Proposed Data Management Plans (DMPs) should clearly describe how the data will be managed for the duration of the award. The DMP should also describe how the management of data align with best practices and FAIR principles.

DMPs should clearly address how data will be shared and accessed. Data should be open and free to the user whenever possible. Any exceptions to this should be justified in the DMP.

In the final year of funding, DOE and the lead PI will jointly determine a plan regarding long-term preservation and curation. Proposals should, therefore, include a plan for preparing and possibly transferring data for long-term preservation, noting that it may not be necessary to preserve all data long-term. Proposals should include metrics or other plans for assessing the impact of data made available under this award on AI application development and or AI research and development.

Budget requests associated with Justification for any budget requests associated with data management including, for example, storage or computational resources, should be included in the budget justification and elaborated on and justified in the DMP. Existing resources should be leveraged whenever possible.

Open Science

SC is dedicated to promoting the values of openness in Federally-supported scientific research, including, but not limited to, ensuring that research may be reproduced and that the results of Federally-supported research are made available to other researchers. These objectives may be met through any number of mechanisms including, but not limited to, data access plans, data sharing agreements, the use of archives and repositories, and the use of various licensing schemes.

The use of the phrases "open" and "open-source" do not refer to any particular licensing arrangement, but are to be understood as encompassing any arrangement that furthers the objective of openness.

Collaboration

Collaborative proposals submitted from different institutions must clearly indicate they are part of a collaborative project/group. Every partner institution must submit a proposal through its own sponsored research office. Each collaborative group can have only one lead institution. Each proposal within the collaborative group, including the narrative and all required appendices and attachments, must be identical with the following exceptions:

- Each proposal must contain a correct cover page for the submitting institution only.
- Each proposal must contain a unique budget corresponding to the expenditures for that proposal's submitting institution only.
- Each proposal must contain a unique budget justification corresponding to the expenditures for that proposal's submitting institution only.

SC's intent is to create from the various proposals associated with a collaborative group one document for merit review that consists of the common, identical proposal materials combined with a set of detailed budgets from the partner institutions. Thus, it is very important that every proposal in the collaborative group be identical (including the title) with the exception of the budget and budget justification pages.

Collaborative proposals from institutions other than DOE National Laboratories should be submitted following the above rules in response to the companion announcement, DE-FOA-0002306. Each proposal within the collaborative group submitted in response to a Laboratory Announcement and its companion Funding Opportunity Announcement (FOA), including the narrative and all required appendices and attachments, must be identical with the following exceptions:

- Each proposal must contain a correct SF-424 (R&R) cover page for the submitting institution only.
- Each proposal must contain a unique budget corresponding to the expenditures for that proposal's submitting institution only.
- Each proposal must contain a unique budget justification corresponding to the expenditures for that proposal's submitting institution only.

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REFERENCES:

[1] Baker, Nathan, Alexander, Frank, Bremer, Timo, Hagberg, Aric, Kevrekidis, Yannis, Najm, Habib, Parashar, Manish, Patra, Abani, Sethian, James, Wild, Stefan, Willcox, Karen, and Lee, Steven. Workshop Report on Basic Research Needs for Scientific Machine Learning: Core Technologies for Artificial Intelligence. United States: N. p., 2019. Web. doi:10.2172/1478744. http://www.osti.gov/biblio/1478744

[2] Fagnan, Kjiersten, Nashed, Youssef, Perdue, Gabriel, Ratner, Daniel, Shankar, Arjun, and Yoo, Shinjae. Data and Models: A Framework for Advancing AI in Science. United States: N. p., 2019. Web. doi:10.2172/1579323. http://www.osti.gov/biblio/1579323

[3] Berry, Michael, Potok, Thomas E., Balaprakash, Prasanna, Hoffmann, Hank, Vatsavai, Raju, and Prabhat, . Machine Learning and Understanding for Intelligent Extreme Scale Scientific Computing and Discovery. DOE Workshop Report, January 7–9, 2015, Rockville, MD. United States: N. p., 2015. Web. doi:10.2172/1471083. http://www.osti.gov/biblio/1471083

Section II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding laboratory work authorizations under this DOE National Laboratory Program Announcement.

Any awards made under this Announcement will be subject to the provisions of the contract between DOE and the awardee National Laboratory.

DOE will consider funding multi-institution collaborations under this Announcement.

B. ESTIMATED FUNDING

A total of $8,500,000 is expected to be available to support this DOE National Laboratory Announcement and the companion FOA DE-FOA-0002306, subject to the appropriation of funds by Congress. A precise distribution of funds between this Program Announcement and the companion FOA will depend on the number of meritorious applications and the availability of appropriate funds.

DOE is under no obligation to pay for any costs associated with preparation or submission of a proposal. DOE reserves the right to fund, in whole or in part, any, all, or none of the proposal submitted in response to this DOE National Laboratory Announcement.

C. MAXIMUM AND MINIMUM AWARD SIZE

The award size will depend on the availability of appropriated funds.

Ceiling

$750,000 per year

Floor

$300,000 per year

D. EXPECTED NUMBER OF AWARDS

Approximately 3 to 7 awards are expected.

The exact number of awards will depend on the number of meritorious proposals and the availability of appropriated funds.

E. ANTICIPATED AWARD SIZE

The award size will depend on the number of meritorious proposals and the availability of

appropriated funds.

F. PERIOD OF PERFORMANCE

DOE anticipates making awards with a project period of two or three years as befitting the project.

Continuation funding (funding for the second and subsequent budget periods) is contingent on: (1) availability of funds appropriated by Congress and future year budget authority; (2) progress towards meeting the objectives of the approved application; (3) submission of required reports; and (4) compliance with the terms and conditions of the award.

G. TYPE OF PROPOSAL

DOE will only accept new DOE National Laboratory Proposals under this DOE National Laboratory Announcement. Please only submit a PAMS lab technical proposal in response to this Announcement; do not submit a DOE Field Work Proposal (FWP) at this time. SC will request FWPs later from those selected for funding consideration under this Announcement.

Section III – ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS AND TOPICS

This is a DOE National Laboratory-only Announcement. FFRDCs[2] from other Federal agencies are not eligible to submit in response to this Program Announcement.

B. COST SHARING

Cost sharing is not required.

C. ELIGIBLE INDIVIDUALS

Eligible individuals with the skills, knowledge, and resources necessary to carry out the proposed research as a Principal Investigator (PI) are invited to work with their organizations to develop a proposal. Individuals from underrepresented groups as well as individuals with disabilities are always encouraged to apply.

D. LIMITATIONS ON SUBMISSIONS

Applicant institutions are limited to no more than *3* letters of intent or proposals for each PI at the applicant institution. DOE will consider the latest received submissions to be the institution's intended submissions.
- Applications in excess of the limited number of submissions will be declined without review.

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2 2 An authoritative list of all Federally Funded Research and Development Centers (FFRDCs) may be found at
https://www.nsf.gov/statistics/ffrdclist/

Section IV – PROPOSAL AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST PROPOSAL PACKAGE

Proposal submission instructions are available in this Announcement on the DOE SC Portfolio Analysis and Management System (PAMS). Screenshots showing the steps in DOE National Laboratory proposal submission are available in the PAMS External User Guide, accessible by navigating to https://pamspublic.science.energy.gov and clicking on the "PAMS External User Guide" link.

Proposals submitted outside of PAMS will not be accepted.

B. LETTER OF INTENT AND PRE-PROPOSAL

1. Letter of Intent

LETTER OF INTENT DUE DATE

See Section IV, Part E.

A Letter of Intent is required and must be submitted by the deadline in Section IV, Part E.

The LOI is to help in planning the review and the selection of potential reviewers for the proposal. For this purpose, the LOI must include the following:
- At the top of the first page, the following information:
  Title of Preapplication
  Principal Investigator Name, Job Title
  Institution
  PI Phone Number, PI Email Address
  Lab Announcement Number: **LAB-20-2306**

- This information must be followed by a clear and concise description of the objectives and technical approach of the proposed research. The LOI may not exceed two pages, with a minimum text font size of 11 point and margins no smaller than one inch on all sides. Figures and references, if included, must fit within the two-page limit.

- The LOI must also include a list of the names and institutional affiliations of all participating investigators, including collaborators and consultants on the proposed project. For each funded investigator, provide a list of collaborative co-investigators including co-authors of the past 48 months, co-editors of the past 24 months, graduate and postdoctoral advisors/advisees, and close associations. This list of participants and collaborators will not count toward the page limit for the LOI.

The LOI must be submitted electronically through the DOE SC Portfolio Analysis and Management System (PAMS) website https://pamspublic.science.energy.gov/. It is important that the LOI be a single file with extension .pdf, .docx, or .doc. The Principal Investigator (PI)

and anyone submitting on behalf of the PI must register for an account in PAMS before it will be possible to submit a letter of intent. **All PIs and those submitting LOIs on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.**

You may use the Internet Explorer, Firefox, Google Chrome, or Safari browsers to access PAMS.

Please see [Registrations, DOE Office of Science Portfolio Analysis and Management System (PAMS)](#), above, for instructions about how to register in PAMS.

Submit Your Letter of Intent:
- Create your letter of intent outside the system and save it as a file with extension .docx, .doc, or .pdf. Make a note of the location of the file on your computer so you can browse for it later from within PAMS.
- Log into PAMS and click the Proposals tab. Click the "View / View / Respond to DOE National Laboratory Announcements" link and find the current announcement in the list. Click the "Actions/Views" link in the Options column next to this announcement to obtain a dropdown menu. Select "Submit Letter of Intent" from the dropdown.
- On the Submit Letter of Intent page, select the institution from which you are submitting this LOI from the Institution dropdown. If you are associated with only one institution in the system, there will only be one institution in the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per LOI; to do so, click the "Select PI" button on the far-right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the "Actions" link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose "Select PI."
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the "Invite PI" link at the top left of the "Select PI" screen. You can enter an optional personal message to the PI in the "Comments" box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the LOI. Save the LOI for later work by clicking the "Save" button at the bottom of the screen. It will be stored in "My Letters of Intent" for later editing.
- Enter a title for your letter of intent.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the LOI file into PAMS, click the "Attach File" button at the far-right side of the screen. Click the "Browse" (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the "Upload" button to upload the file.
- At the bottom of the screen, click the "Submit to DOE" button to save and submit the LOI to DOE.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the LOI.

You are encouraged to register for an account in PAMS at least a week in advance of the LOI submission deadline so that there will be no delays with your submission.

> **WARNING**: The PAMS website at https://pampspublic.science.energy.gov/ will permit you to edit a previously submitted LOI in the time between your submission and the deadline. If you choose to edit, doing so will remove your previously submitted version from consideration. If you are still editing at the time of the deadline, you will not have a valid submission. Please pay attention to the deadline.

For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this Laboratory Announcement should reference **LAB 20-2306.**

1. Pre-proposal

N/A

C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

See Section IV, Part E.

Files that are attached to the forms must be PDF files unless otherwise specified in this announcement. Attached PDF files must be plain files consisting of text, numbers, and images without editable fields, signatures, passwords, redactions, or other advanced features available in some PDF-compatible software. Do not attach PDF portfolios.

> **WARNING**: The PAMS website at https://pampspublic.science.energy.gov/ will permit you to edit a previously submitted proposal in the time between your submission and the deadline. If you choose to edit, doing so will remove your previously submitted version from consideration. If you are still editing at the time of the deadline, you will not have a valid submission. Please pay attention to the deadline.

RESUBMISSION OF PROPOSALS

Proposals submitted under this Announcement may be withdrawn from consideration by using SC's PAMS website at https://pamspublic.science.energy.gov. Proposals may be withdrawn at any time between when the Laboratory submits the application and when DOE makes the application available to merit reviewers. Such withdrawals take effect immediately and cannot be reversed.

After a proposal is withdrawn, it may be resubmitted, if this Announcement is still open for the submission of applications. Such resubmissions will only count as one submission if this

Announcement restricts the number of proposals from an applicant.

SC will usually consider the last submission, according to its timestamp, to be the intended version. Please consult with your program manager to resolve any confusion about which version of a proposal should be considered.

IMPROPER CONTENTS OF PROPOSALS

Proposals submitted under this Announcement will be stored in controlled-access systems, but they may be made publicly available if an award is made, and they will be made available to merit reviewers. As such, it is critical that Laboratories follow these guidelines:
- Do not include information subject to any legal restriction on its open distribution, whether classified, export control, or unclassified controlled nuclear information.
- Do not include sensitive and protected personally identifiable information, including social security numbers, birthdates, citizenship, marital status, or home addresses. Pay particular attention to the content of biographical sketches and curriculum vitae.
- Do not include letters of support from Federal officials.
- Do not include letters of support on Federal letterhead. Letters that are not letters of support (such as letters confirming access to sites, facilities, equipment, or data; or letters from cognizant contracting officers) may be on Federal letterhead.
- Clearly mark all proprietary or trade-secret information.

LETTERS

Letters of recommendation are not allowed. A department chair letter is not required and should not be included. Applications that include recommendation letters or department chair letters will be subject to elimination from consideration during DOE's initial review.

Optional letters of collaboration for unfunded or funded collaborations may be placed in Appendix 7 (Other Attachments). Letters of collaboration should state the intention to participate, but they must not be written as recommendation or endorsement letters, which are not allowed. Each optional letter of collaboration may contain two and only two sentences and must use the following format:

Dear <Principal Investigator Name>:

If your application entitled, "<Application Name>," is selected for funding under the DOE SC Advanced Scientific Computing Research Program, it is my intent to collaborate in this research by <Complete Sentence With a Very Short Description of What the Collaborator Offers to Do or Provide>. Thank you for the opportunity to participate.

Sincerely,
<Collaborator's Name and Signature Block>

1. Summary of Proposal Contents and Information about PAMS

Each DOE National Laboratory proposal will contain the following sections:

- Budget, entered into PAMS as structured data using the PAMS budget form
- Abstract (one page), entered into PAMS as a separate pdf
- Budget justification, entered into PAMS as a separate pdf
- Proposal, combined into a single pdf containing the following information:
  - Proposal Cover Page
  - Table of Contents
  - Project Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel)
  - Appendix 1: Biographical Sketch(es)
  - Appendix 2: Current and Pending Support
  - Appendix 3: Bibliography and References Cited
  - Appendix 4: Facilities and Other Resources
  - Appendix 5: Equipment
  - Appendix 6: Data Management Plan
  - Appendix 7: Other Attachments (optional)

SUBMISSION INSTRUCTIONS

Completed proposals must be submitted into the DOE SC Portfolio Analysis and Management System (PAMS). For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 20-2306.** Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than May 15, 2020 at 5:00 PM Eastern Time.

All PIs and those submitting on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to ensure timely submissions**.** To register, click "Create New PAMS Account" on the website https://pamspublic.science.energy.gov/ and follow the instructions for creating an account.

The following information is provided to help with proposal submission. Detailed instructions and screen shots can be found in the user guide. To find the user guide, click the "External User Guide" link on the PAMS home page. Onscreen instructions are available within PAMS.

- Log into PAMS. From the proposals tab, click the "View DOE National Laboratory Announcements" link and find the current announcement in the list. Click the "Actions/Views" link in the Options column next to this Announcement to obtain a dropdown menu. Select "Submit Proposal" from the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per proposal; to do so, click the "Select PI" button on the far-right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have

- to sort, filter, or search through the list if it has multiple pages.) Click the "Actions" link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose "Select PI."
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the "Invite PI" link at the top left of the "Select PI" screen. You can enter an optional personal message to the PI in the "Comments" box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the proposal. Save the proposal for later work by selecting "Save" from the dropdown at the bottom of the screen and then clicking the "Go" button. It will be stored in "My Proposals" for later editing. As a minimum, you must complete all the required fields on the PAMS cover page before you can save the proposal for the first time.
- The cover page, budget, and attachments sections of the lab proposal are required by PAMS before it can be submitted to DOE.
- Complete the sections in PAMS one at a time, starting with the cover page and following the instructions for each section.
- Click the "+View More" link at the top of each section to expand the onscreen instructions. On the budget section, click the "Budget Tab Instructions" link to obtain detailed guidance on completing the budget form.
- Save each section by selecting either "Save" (to stay in the same section) or "Save… and Continue to the Next Section" (to move to the next section) from the dropdown menu at the bottom of the screen, followed by clicking the "Go" button.
- If you save the proposal and navigate away from it, you may return later to edit the proposal by clicking the "View My Existing Proposals" or "My Proposals" links within PAMS.
- You must enter a budget for each annual budget period.
- You must also enter a budget for each proposed sub-award. The sub-award section can be completed using the same steps used for the budget section.
- In the attachments section of the lab proposal, the abstract, the budget justification, and the proposal narrative are required and must be submitted as separate files.
- You must bundle everything other than the budget, abstract, and budget justification into one single PDF file to be attached under "Proposal Attachment."
- Do not attach anything under "Other Attachments."
- To upload a file into PAMS, click the "Attach File" button at the far-right side of the screen. Click the "Browse" (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the "Upload" button to upload the file.
- Once you have saved all of the sections, the "Submit to DOE" option will appear in the dropdown menu at the bottom of the screen.
- To submit the proposal, select "Submit to DOE" from the dropdown menu and then click the "Go" button.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the proposal.
- The proposal will also appear under My Proposals with a Proposal Status of "Submitted to DOE."

Please only submit a PAMS lab technical proposal in response to this Announcement; do not submit a DOE Field Work Proposal (FWP) at this time. SC will request FWPs later from those selected for funding consideration under this Announcement.

For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 20-2306.**

2. Detailed Contents of the Proposal

BUDGET AND BUDGET EXPLANATION

The budget must be submitted into PAMS using the PAMS budget form. Research proposed under this Announcement may only have one annual budget period.

PAMS will calculate the cumulative budget totals for you.

A written justification of each budget item is to follow the budget pages. The budget justification should be placed in a separate, single pdf document and attached on the appropriate screen in PAMS. Further instructions regarding the budget and justification are given below and in the PAMS software.

PROJECT SUMMARY/ABSTRACT (NO MORE THAN ONE PAGE)

The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to the public. It should be a self-contained document that identifies the name of the applicant, the Principal Investigator (PI), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes). This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed 1 page when printed using standard letter-size (8.5 x 11 inch) paper with 1 inch margins (top, bottom, left and right) with font not smaller than 11 point. The one-page project summary/abstract should be placed in a separate, single pdf document and attached on the appropriate screen in PAMS.

The abstract may be used to prepare publicly accessible reports about DOE-supported research.

DOE COVER PAGE
(PART OF PROJECT NARRATIVE)

The following proposal cover page information may be placed on a plain page. No form is required. This cover page will not count in the project narrative page limitation.

- The project title:
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Administrative Point of Contact name, telephone number, email:
- Lead PI name, telephone number, email:
- DOE National Laboratory Announcement Number: **LAB 20-2306**
- DOE/SC Program Office: Advanced Scientific Computing Research
- DOE/SC Program Office Technical Contact: Dr. Laura Biven
- PAMS Letter of Intent Tracking Number**:**
- Research area (site) identified in Section I of this Announcement

COVER PAGE SUPPLEMENT FOR COLLABORATIONS
(PART OF PROJECT NARRATIVE)

Collaborative proposals submitted from different institutions must clearly indicate they are part of a collaborative project/group. Every partner institution must submit a proposal through its own sponsored research office. Each collaborative group can have only one lead institution. Each proposal within the collaborative group, including the narrative and all required appendices and attachments, must be identical with one exception:
- Each proposal must contain the correct "cover-page" information for the submitting institution only.
- Each proposal must contain a unique budget corresponding to the expenditures for that proposal's submitting institution only.
- Each proposal must contain a unique budget justification corresponding to the expenditures for that proposal's submitting institution only.

SC will use the multiple proposals associated with a collaborative group to create one consolidated document for merit review that consists of the common, identical proposal materials combined with a set of detailed budgets from the partner institutions. It is very important that every proposal in the collaborative group be identical (including the title) with the exception of the budget and budget justification pages.

If the project is a collaboration, provide the following information on a separate page as a supplement to the cover page.
- List all collaborating institutions by name with each institution's principal investigator on the same line.
- Indicate the lead PI who will be the point of contact and coordinator for the combined research activity.
- Provide a statement explaining the leadership structure of the collaboration.
- Include a description of each collaborating institution's facilities, equipment, and resources that will be made available to the collaborative group.
- Include a table modeled on the following chart providing summary budget information from all collaborating institutions. Provide the total costs of the budget request in each year for each institution and totals for all rows and columns.

Collaborative Proposal Information					
	Names	**Institution**	**Year 1 Budget**	**Year 2 Budget**	**Year 3 Budget**
Lead PI					
Co-PI					
Co-PI					
Co-PI					

Example budget table ($ in thousands)

* Note that collaborating proposals must be submitted separately.

PROJECT NARRATIVE (NO MORE THAN 10 PAGES LONG)

The project narrative **must not exceed 10 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard letter-size (8.5 x 11 inch) paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph. This page limit does not apply to the Cover Page, Budget Page(s), Budget Justification, biographical material, publications and references, and appendices, each of which may have its own page limit.

Do not include any Internet addresses (URLs) that provide supplementary or additional information that constitutes a part of the proposal. Merit reviewers are not required to access Internet sites; however, Internet publications in a list of references will be treated identically to print publications. See Part VIII.D for instructions on how to mark proprietary proposal information. To attach a Project Narrative, click "Add Attachment."

Background/Introduction: Explanation of the importance and relevance of the proposed work as well as a review of the relevant literature.

Proposed Research and Methods: Identify the hypotheses to be tested (if any) and details of the methods to be used including the integration of experiments with theoretical and computational research efforts.

Timetable of Activities: Timeline for all major activities including milestones and deliverables.

Project Management Plan: Multi-institutional proposals must include a project management plan that clearly indicates the roles and responsibilities of each organization and indicates how activities will be coordinated and communicated among team members.

Project Objectives: This section should provide a clear, concise statement of the specific objectives/aims of the proposed project.

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative

should be devoted to a description and justification of the proposed project, including details of the method to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities. There should be no ambiguity about which personnel will perform particular parts of the project, and the time at which these activities will take place.

Do not include any Internet addresses (URLs) that provide supplementary or additional information that constitutes a part of the proposal. Using Internet sites in an attempt to avoid page limits will fail: The content of those sites will not be reviewed. See Part VIII.D for instructions on how to mark proprietary proposal information.

For Collaborative Proposals Only: Each collaborating institution must submit an identical common narrative. Collaborative proposals will necessarily be longer than single-institution proposals. The common narrative may exceed the page limit described for the research narrative by 50%; i.e., if the page limit is 12 pages, a collaboration is subject to a limit of 18 pages. The common narrative must identify which tasks and activities will be performed by which of the collaborating institutions in every budget period of the proposed project. The budget and the budget justification—which are unique to each collaborating institution—may refer to parts of the common narrative to further identify each collaborating institution's activities in the joint project. There should be no ambiguity about each institution's role and participation in the collaborative group.

SC will use the multiple proposals associated with a collaborative group to create one consolidated document for merit review that consists of the common, identical proposal materials combined with a set of detailed budgets from the partner institutions. It is very important that every proposal in the collaborative group be identical (including the title) with the exception of the budget and budget justification pages.

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the PI and each senior/key person as an appendix to your technical narrative.

As part of the sketch, provide information that can be used by reviewers to evaluate the PI's potential for leadership within the scientific community. Examples of information of interest are invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences.

- Provide the biographical sketch information as an appendix to your project narrative.
- Do not attach a separate file.
- The biographical sketch appendix will not count in the project narrative page limitation.
- The biographical information (curriculum vitae) for each person must not exceed 2 pages

when printed on standard letter-size (8.5 x 11 inch) paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include:

SC does not require a particular format for a biosketch. Applicants may use a format developed for other agencies or generated by any software package, including SciENcv, a cooperative venture maintained at https://www.ncbi.nlm.nih.gov/sciencv/. The biographical information (curriculum vitae) must include the following items within its page limit:

- **Education and Training**: Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.
- **Research and Professional Experience**: Beginning with the current position list, in chronological order, professional/academic positions with a brief description.
- **Publications**: Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications.
- **Synergistic Activities**: List no more than 5 professional and scholarly activities related to the effort proposed.

In addition, the biographical sketch must include information to permit DOE to identify individuals who are conflicted with or potentially biased (favorably or unfavorably) against the investigator. Include a section entitled "**Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers**" that will not count in a page limit: Provide the following information in this section:

- **Collaborators and Co-editors**: List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this application. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the Principal Investigator interacted on a regular basis while the research was being done. Also, list any individuals who are currently, or have been, co-editors with you on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this application. If there are no collaborators or co-editors to report, state "None."
- **Graduate and Postdoctoral Advisors and Advisees**: List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s). Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates.

Personally Identifiable Information: Do not include sensitive and protected personally identifiable information including social security numbers, birthdates, citizenship, marital status, or home addresses. Do not include information that a merit reviewer should not make use of.

This appendix will not count in the project narrative page limitation.

APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the PI and senior/key persons, including subawardees, for ongoing projects and pending applications. List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid. SC does not require a particular format for current and pending support. Applicants may use a format developed for other agencies or generated by any software package, including SciENcv, a cooperative venture maintained at https://www.ncbi.nlm.nih.gov/sciencv/.
For every activity, list the following items:
- The sponsor of the activity or the source of funding
- The award or other identifying number
- The title of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The award period (start date – end date).
- The person-months of effort per year being dedicated to the award or activity
- Briefly describe the research being performed and explicitly identify any overlaps or synergies with the proposed research.

Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. For research areas where there are routinely more than ten coauthors of archival publications, you may use an abbreviated style such as the Physical Review Letters (PRL) convention for citations (listing only the first author). For example, your paper may be listed as, "A Really Important New Result," A. Aardvark et. al. (MONGO Collaboration), PRL 999. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal. Provide the Bibliography and References Cited information as an appendix to your project narrative.
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 4: FACILITIES & OTHER RESOURCES

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their

capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. For proposed investigations requiring access to experimental user facilities maintained by institutions other than the applicant, please provide a document from the facility manager confirming that the researchers will have access to the facility. Please provide the Facility and Other Resource information as an appendix to your project narrative.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 5: EQUIPMENT

List major items of equipment already available for this project and, if appropriate identify location and pertinent capabilities. Provide the Equipment information as an appendix to your project narrative.

- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 6: DATA MANAGEMENT PLAN

Provide a (DMP) that addresses the following requirements:
1. DMPs should describe whether and how data generated in the course of the proposed research will be shared and preserved. If the plan is not to share and/or preserve certain data, then the plan must explain the basis of the decision (for example, cost/benefit considerations, other parameters of feasibility, scientific appropriateness, or limitations discussed in #4). At a minimum, DMPs must describe how data sharing and preservation will enable validation of results, or how results could be validated if data are not shared or preserved.
2. DMPs should provide a plan for making all research data displayed in publications resulting from the proposed research digitally accessible to the public at the time of publication. This includes data that are displayed in charts, figures, images, etc. In addition, the underlying digital research data used to generate the displayed data should be made as accessible as possible to the public in accordance with the principles stated in the SC Statement on Digital Data Management (http://science.osti.gov/funding-opportunities/digital-data-management/). This requirement could be met by including the data as supplementary information to the published article, or through other means. The published article should indicate how these data can be accessed.
3. DMPs should consult and reference available information about data management resources to be used in the course of the proposed research. In particular, DMPs that explicitly or implicitly commit data management resources at a facility beyond what is conventionally made available to approved users should be accompanied by written approval from that facility. In determining the resources available for data management at SC User Facilities, researchers should consult the published description of data management resources and practices at that facility and reference it in the DMP. Information about other SC facilities can be found in the additional guidance from the sponsoring program.

4. DMPs must protect confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, regulations, and DOE orders and policies. There is no requirement to share proprietary data.

DMPs will be reviewed as part of the overall SC research proposal merit review process. Applicants are encouraged to consult the SC website for further information and suggestions for how to structure a DMP: http://science.osti.gov/funding-opportunities/digital-data-management/

- This appendix should not exceed four (4) pages including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard letter-size (8.5 x 11 inch) paper with 1 inch margins (top, bottom, left, and right)
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

APPENDIX 7: OTHER ATTACHMENT

If you need to elaborate on your responses to questions 1-6 on the "Other Project Information" document, please provide the Other Attachment information as an appendix to your project narrative. Information not easily accessible to a reviewer may be included in this appendix, but do not use this appendix to circumvent the page limitations of the proposal. Reviewers are not required to consider information in this appendix.
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

2. Detailed Instructions for the Budget

Budgets are required for the entire project period. A budget form should be completed for each budget period of the award, and a cumulative budget form for the entire project period will be populated by PAMS. A detailed budget justification narrative should be included after the budget pages. The justification should cover labor, domestic travel, equipment, materials and supplies, and anything else that will be covered with project funds.

To edit a section on the budget, click the edit icon ( ) for each section on the page. Remember to save all budget periods before moving on to the next section. You can save the budget periods by selecting "Save All Budget Periods" from the dropdown on the lower right corner of the PAMS budget entry screen and then clicking the "Go" button. You can also save any data entry page in PAMS using the blue diskette icon ( ) in the floating toolbar on the bottom of the screen.

Section A. Senior/Key Person (Required)
For each Senior/Key Person, enter the appropriate information. List personnel, salary funds, and the number of months that person will be allocated to the project. Also include a written narrative in the budget justification that fully justifies the need for requested personnel.

Section B. Other Personnel
List personnel, salary funds, and the number of months that person will be allocated to the project. Also include a written narrative in the budget justification that fully justifies the need for requested personnel.

Section C. Equipment Description
For the purpose of this budget, equipment is designated as an item of property that has an acquisition cost of $5,000 or more and an expected service life of more than one year. (Note that this designation applies for proposal budgeting only and differs from the DOE definition of capital equipment.) List each item of equipment separately and justify each in the budget justification section. Allowable items ordinarily will be limited to research equipment and apparatus not already available for the conduct of the work. General-purpose office equipment, such as a personal computer, is not eligible for support unless primarily or exclusively used in the actual conduct of scientific research.

Section D. Travel
In the budget justification, list each trip's destination, dates, estimated costs including transportation and subsistence, number of staff traveling, the purpose of the travel, and how it relates to the project. Indicate whether travel cost estimates are based upon quotes from travel agencies; upon past experience of similar number of trips to similar travel destinations; or something else (describe). To qualify for support, attendance at meetings or conferences must enhance the investigator's capability to perform the research, plan extensions of it, or disseminate its results.

Section E. Participant/Trainee Support Costs:
If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and postgraduate) must list each trainee cost that includes stipend levels and amounts, cost of tuition for each trainee, cost of any travel (provide the same information as needed under the regular travel category), and costs for any related training expenses. Participant costs are those costs associated with conferences, workshops, symposia or institutes and breakout items should indicate the number of participants, cost for each participant, purpose of the conference, dates and places of meetings and any related administrative expenses. In the budget justification, indicate whether trainee cost estimates are based upon past experience of support of similar number of trainees on similar projects; past experience of support of similar number of participants attending similar conferences/workshops/symposia; or something else (describe).

Section F. Other Direct Costs:
Enter Other Direct Costs information for each item listed.
- **Materials and Supplies:** Enter total funds requested for materials and supplies in the appropriate fields. In the budget justification, indicate general categories such as glassware, and chemicals, including an amount for each category (items not identified under "Equipment"). Categories less than $1,000 are not required to be itemized. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; quotes/catalog prices of similar or like items; or

something else (describe).

- **Publication Costs:** Enter the total publication funds requested. The proposal budget may request funds for the costs of documenting, preparing, publishing or otherwise making available to others the findings and products of the work conducted under the award. In the budget justification, include supporting information. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; vendor quotes of similar publication services; or something else (describe).
- **Consultant Services:** Enter total funds requested for all consultant services. In the budget justification, identify each consultant, the services he/she will perform, total number of days, travel costs, and total estimated costs. In the budget justification, indicate whether consultant cost estimate is based upon previous experience/quotes for similar or like services; or something else (describe).
- **ADP/Computer Services:** Enter total funds requested for ADP/Computer Services. The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested. In the budget justification, include the established computer service rates at the proposing organization if applicable. In the budget justification, indicate whether cost estimates are based upon quotes/past experience of purchase of similar computer services; established computer service rates at the proposing institution; or something else (describe).
- **Subawards/Consortium/Contractual Costs:** Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details.
- **Equipment or Facility Rental/User Fees:** Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. In the budget justification, indicate whether cost estimates are based upon past experience with similar or like items; vendor quotes of similar items; or something else (describe).
- **Alterations and Renovations:** Enter total funds requested for Alterations and Renovations.
- **In the budget justification**, itemize by category and justify the costs of alterations and renovations, including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs.
- **Other:** Add text to describe any other Direct Costs not requested above. Enter costs associated with "Other" item(s). Use the budget justification to further itemize and justify.

Section G. Direct Costs
This represents Total Direct Costs (Sections A thru F) and will be calculated by PAMS.

Section H. Other Indirect Costs
Enter the Indirect Cost information for each field. Only four general categories of indirect costs are allowed/requested on this form, so please consolidate if needed.

Section I. Total Direct and Indirect Costs
This amount will be calculated by PAMS (Sections G + H)

D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

If selected for award, DOE reserves the right to request additional or clarifying information.

E. SUBMISSION DATES AND TIMES

1. Letter of Intent Due Date

April 17, 2020 at 5:00 PM Eastern Time

You are encouraged to submit your LOI well before the deadline. LOIs may be submitted at any time between the publication of this Announcement and the stated deadline.

2. Pre-proposal Due Date

N/A

3. Proposal Due Date

May 15, 2020 at 5:00 PM Eastern Time

You are encouraged to transmit your proposal well before the deadline. Proposals may be submitted at any time between the publication of this Announcement and the stated deadline.

4. Late Submissions

Delays in submitting letters of intent and proposals may be unavoidable. DOE has accepted late submissions when applicants have been unable to make timely submissions because of widespread technological disruptions or significant natural disasters. DOE has made accommodations for incapacitating or life-threatening illnesses and for deaths of immediate family members. Other circumstances may or may not justify late submissions. Unacceptable justifications include the following:
- Failure to begin submission process early enough.
- Failure to provide sufficient time to complete the process.
- Failure to understand the submission process.
- Failure to understand the deadlines for submissions.
- Failure to satisfy prerequisite registrations.
- Unavailability of administrative personnel.
- A non-incapacitating illness the week of the deadline.

You are responsible for beginning the submission process in sufficient time to accommodate reasonably foreseeable incidents, contingencies, and disruptions.

Applicants must contact the Program Office/Manager listed in this Funding Opportunity Announcement to discuss the option of a late submission. Contacting the Program Office/Manager after the deadline may reduce the likelihood that a request will be granted.

DOE notes that not all requests for late submission will be approved.

F. FUNDING RESTRICTIONS

Funding for all awards and future budget periods are contingent upon the availability of funds appropriated by Congress and the availability of future-year budget authority.

G. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

1. Where to Submit

Proposals must be submitted through PAMS to be considered for award.

Please only submit a PAMS lab technical proposal in response to this Announcement; do not submit a DOE Field Work Proposal (FWP) at this time. SC will request FWPs via the Searchable FWP system later from those selected for funding consideration under this Announcement.

2. Registration Process

ONE-TIME REGISTRATION PROCESS

You must complete the one-time registration process (all steps) before you can submit your first proposal through PAMS. Registration instructions appear in the front matter of this Announcement.

For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this DOE National Laboratory Program Announcement should reference **LAB 20-2306.**

3. Proposal Receipt Notices

Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the proposal.

4. Viewing Submitted Proposals

Upon submission, the proposal will appear under My Proposals for the PI and the Submitter with a Proposal Status of "Submitted to DOE."

Section V - PROPOSAL REVIEW INFORMATION

A. CRITERIA

1. Initial Review Criteria

Prior to a comprehensive merit evaluation, DOE will perform an initial review to determine that (1) the applicant is eligible for the award; (2) the information required by the Program Announcement has been submitted; (3) all mandatory requirements are satisfied; (4) the proposed project is responsive to the objectives of the Program Announcement, and (5) the proposed project is not duplicative of programmatic work. Proposals that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

2. Merit Review Criteria

Proposals will be subjected to scientific merit review (peer review) and will be evaluated against the following criteria, listed in descending order of importance.

- 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; and
- Reasonableness and Appropriateness of the Proposed Budget.

The evaluation process will also include program policy factors such as the relevance of the proposed research to the terms of the DOE National Laboratory Announcement and the agency's programmatic needs, the balance of activities within the program, and the utility of the proposed activities to the broader scientific community. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of an proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

The questions below are provided to the merit reviewers to elaborate the criteria:

SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH

- What is the scientific innovation of proposed research?
- What is the likelihood that the proposed work will enable important new applications of AI and/or advances in AI R&D?
- How might the results of the proposed work impact the direction, progress, and thinking in relevant scientific fields of research?
- How does the proposed work compare with other efforts in its field, both in terms of scientific and/or technical merit and originality?

APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

- How logical and feasible are the proposed approaches?
- Does the proposed research employ innovative concepts or methods?
- Are the conceptual framework, methods, and analyses well justified, adequately developed, and likely to lead to scientifically valid conclusions?
- Does the applicant recognize significant potential problems and consider alternative strategies?
- Is the Data Management Plan appropriate to achieve the desired impact? Does the DMP recognize best practices in data management and open science principles to enable data reuse?

COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

- What is the past performance and potential of the Principal Investigator (PI)?
- How well qualified is the research team to carry out the proposed research?
- Are the research environment and facilities adequate for performing the research?
- Does the proposed work take advantage of unique facilities and capabilities?
- Does the proposal include appropriate expertise to achieve the desired impact?

REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

- Are the proposed budget and staffing levels adequate to carry out the proposed work?
- Is the budget reasonable and appropriate for the scope?

B. REVIEW AND SELECTION PROCESS

1. Merit Review

Proposals that pass the initial review will be subjected to a formal merit review and will be evaluated based on the criteria above.

2. Program Policy Factors

The Selection Official may consider any of the following program policy factors in making the selection, listed in no order of significance:

- Availability of funds
- Relevance of the proposed activity to SC priorities
- Ensuring an appropriate balance of activities within SC programs
- Performance under current awards
- Maximizing the use of DOE user facilities
- Quality of international collaboration
- Commitment to sharing the results of research

3. Selection

The Selection Official will consider the findings of the merit review and may consider any of the Program Policy Factors described above.

4. Discussions and Award

The Government may enter into discussions with a selected applicant for any reason deemed necessary. Failure to resolve satisfactorily the issues identified by the Government will preclude award to the applicant.

C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES

DOE is interested in seeing projects supported under this Announcement begin work by September 1, 2020.

Section VI - AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES

1. Notice of Selection

Selected Applicants Notification: DOE will notify applicants selected for award. This notice of selection is not an authorization to begin performance.

Non-selected Notification: Organizations whose proposals have not been selected will be advised as promptly as possible. This notice will explain why the proposal was not selected.

2. Notice of Award

A work authorization/contract modification issued by the Contracting Officer is the authorizing award document.

B. REPORTING

Annual progress reports from the award investigator will be required and will be due 90 days before the end of each budget year.

C. OTHER CONDITIONS

1. Publications

Researchers are expected to publish or otherwise make publicly available the results of the work conducted under any authorization resulting from this Announcement. Publications and other methods of public communication describing any work based on or developed under an authorization resulting from this Announcement must contain an acknowledgment of SC support. The format for such acknowledgments is provided at https://science.osti.gov/funding-opportunities/acknowledgements/. The author's copy of any peer-reviewed manuscript accepted for funding must be announced to DOE's Office of Scientific and Technical Information (OSTI) and made publicly available in accordance with the instructions contained in the Reporting Requirements Checklist incorporated in all Assistance Agreements.

2. Environmental, Safety and Health (ES&H) Performance of Work at DOE Facilities

With respect to the performance of any portion of the work under this award which is performed at a DOE-owned or controlled site, the recipient agrees to comply with all state and Federal ES&H regulations, and with all other ES&H requirements of the operator of such site.

Prior to the performance on any work at a DOE-Owned or controlled site, the recipient shall contact the site facility manager for information on DOE and site specific ES&H requirements.

The recipient shall apply this provision to all subawardees at any tier.

3. Federal, State, and Local Requirements

With respect to the performance of any portion of the work under this award, the recipient agrees to comply with all applicable local, state, and Federal ES&H regulations. The recipient shall apply this provision to all sub awardees at any tier.

Section VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

For help with PAMS, click the "External User Guide" link on the PAMS website, https://pamspublic.science.energy.gov/. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this DOE National Laboratory Program Announcement should reference **LAB 20-2306.**
        Please contact the PAMS help desk for technological issues with the PAMS system.

Questions regarding the specific program areas and technical requirements may be directed to the technical contacts listed for each program within the DOE National Laboratory Program Announcement or below.
        Please contact the program staff with all questions not directly related to the PAMS system.

B. AGENCY CONTACTS

PAMS Customer Support	855-818-1846 (toll-free) 301-903-9610 sc.pams-helpdesk@science.doe.gov
Program Manager Scientific Contact	Dr. Laura Biven 301-903-5000 Laura.Biven@science.doe.gov

C. DEPARTMENT OF ENERGY, OFFICE OF INSPECTOR GENERAL HOTLINE:

The Office of Inspector General (OIG) maintains a Hotline to facilitate the reporting of allegations of fraud, waste, abuse, or mismanagement in DOE programs or operations. If you wish to report such allegations, you may call, send a letter, or email the OIG Hotline ighotline@hq.doe.gov. Allegations may be reported by DOE employees, DOE contractors, or the general public. OIG contact information is available at http://energy.gov/ig/services.

Section VIII - OTHER INFORMATION

A. MODIFICATIONS

Notices of any modifications to this DOE National Laboratory Announcement will be posted on the Grants and Contracts website (http://science.osti.gov/grants/).

B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE

DOE reserves the right, without qualification, to reject any or all proposals received in response to this DOE National Laboratory Announcement and to select any proposal, in whole or in part, as a basis for negotiation and/or award.

C. COMMITMENT OF PUBLIC FUNDS

The Contracting Officer is the only individual who can make awards or commit the Government to the expenditure of public funds. A commitment by other than the Contracting Officer, either explicit or implied, is invalid.

D. PROPRIETARY PROPOSAL INFORMATION

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in a proposal only when such information is necessary to convey an understanding of the proposed project. The use and disclosure of such data may be restricted, provided the applicant includes the following legend on the first page of the project narrative and specifies the pages of the proposal which are to be restricted:

"The data contained in pages _____ of this proposal have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes."

To protect such data, each line or paragraph on the pages containing such data must be specifically identified and marked with a legend similar to the following:

"The following contains proprietary information that (name of applicant) requests not be released to persons outside the Government, except for purposes of review and evaluation."

E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL

In conducting the merit review evaluation, the Government may seek the advice of qualified non-Federal personnel as reviewers. The Government may also use non-Federal personnel to conduct routine, nondiscretionary administrative activities. The applicant, by submitting its proposal, consents to the use of non-Federal reviewers/administrators. Non-Federal reviewers must sign a conflict of interest and a certificate of confidentiality prior to reviewing a proposal. Non-Federal personnel conducting administrative activities must sign a non-disclosure

agreement.

F. AVAILABILITY OF FUNDS

Funds are not presently available for this award. The Government's obligation under this award is contingent upon the availability of appropriated funds from which payment for award purposes can be made. No legal liability on the part of the Government for any payment may arise until funds are made available to the Contracting Officer for this award and until the awardee receives notice of such availability, to be confirmed in writing by the Contracting Officer.