DEPARTMENT OF ENERGY
OFFICE OF SCIENCE
ADVANCED SCIENTIFIC COMPUTING RESEARCH

SCIENTIFIC DISCOVERY THROUGH ADVANCED COMPUTING (SciDAC) INSTITUTES

DOE NATIONAL LABORATORY PROGRAM ANNOUNCEMENT NUMBER: LAB 20-2223

ANNOUNCEMENT TYPE: INITIAL

Announcement Issue Date:	**03/17/2020**
Submission Deadline for Letter of Intent:	**04/14/2020 at 5 PM Eastern Time** **A Letter of Intent is required**
Submission Deadline for Pre-Proposal:	**Not Applicable**
Pre-Proposal Response Date:	**Not Applicable**
Submission Deadline for Proposals:	**05/12/2020 at 5 PM Eastern Time**

Table of Contents

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 PAMS system 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 20-2223.**

UPDATES AND REMINDERS

RECOMMENDATION

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

DATA MANAGEMENT PLAN

The SC Statement on Digital Data Management, published at https://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 published at https://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.

Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

Technical/Scientific Program Contacts:
>   Dr. Ceren Susut
>   301-903-0366
>   Ceren.Susut-Bennett@science.doe.gov

SUMMARY

The DOE SC program in Advanced Scientific Computing Research (ASCR) hereby announces its interest in receiving applications from large multi-disciplinary and multi-institutional teams (requesting support of more than $3 million per year) for the Scientific Discovery through Advanced Computing (SciDAC) Institutes.

The ASCR program's mission (https://science.osti.gov/ascr and https://science.osti.gov/ascr/Community-Resources/Program-Documents) is to advance applied mathematics and computer science; deliver the most sophisticated computational scientific applications in partnership with disciplinary science; advance computing and networking capabilities; and develop future generations of computing hardware and software tools for science and engineering, in partnership with the research community. A major objective of the ASCR basic research portfolio is to enable DOE-supported science communities to take full advantage of the current and emerging high-performance computing (HPC) systems. ASCR achieves this goal through the SciDAC program (https://www.scidac.gov).

The end product of SciDAC is groundbreaking science through the use of HPC. Since its inception in 2001, the SciDAC program has been recognized as a leader in enabling scientific discoveries that would not have been possible without the deep collaborations between discipline scientists, applied mathematicians, and computer scientists. This Announcement pertains to the fourth re-competition of the SciDAC (SciDAC-5) Institutes. The mission of the SciDAC-5 Institutes is to provide intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools to advance scientific discovery in areas of strategic importance to SC and DOE.

Submitted applications must follow the guidelines and criteria provided in the supplementary information below and the following sections. Letters of Intent (LOIs) are required and must be submitted according to the guidelines in the following sections. No responses will be sent to the LOIs. Applications submitted on behalf of investigators that did not submit an LOI and applications that do not follow the guidelines and criteria established in this Announcement (see Responsiveness below) may be declined without merit review.

SUPPLEMENTARY INFORMATION

SCOPE AND STRUCTURE OF THE PROPOSED INSTITUTES

Specific goals and objectives for the SciDAC-5 Institutes are to support, complement or develop:

- Mechanisms for engaging computational grand challenges across application areas within DOE's and SC's Congressionally-authorized mission-space. Currently, 30 SciDAC-4 Partnership projects are co-funded by ASCR and its partners (https://www.scidac.gov/partnerships.html). Funding opportunities for the SciDAC-5 Partnerships will be announced through several Funding Opportunity Announcements (FOAs) and Program Announcements starting in fiscal year 2021. These Announcements, issued by ASCR's SciDAC Partners, will include opportunities for linking applied mathematics and computer science research to science-domain specific challenges (see below Institutes' Connection with the Partnerships).
- Tools and resources for lowering the barriers to effectively use state-of-the-art computational systems such as those existing and planned for at the Oak Ridge and Argonne Leadership Computing Facilities (OLCF and ALCF), the National Energy Research Scientific Computing Center (NERSC), and similar world-class computing facilities over the next 5 years.
- Mechanisms for incorporating and demonstrating the value of basic research results from ASCR investments. It is expected that the proposed Institutes will be structured around two main topics: Applied Mathematics and Computer Science, respectively.
- Plans for building up and engaging our Nation's computational science research communities.

This Announcement describes the process by which proposals for individual SciDAC-5 Institutes are to be developed, submitted, and merit reviewed. The overall portfolio of the Institute awards is expected to cover a significant portion of DOE's computational science needs on current and emerging computational systems. Although the work of each proposed Institute is not application specific, we expect they will be Application-, Architecture- and Institutes-Aware, as follows:

Application-Aware

The primary metric of success for the SciDAC Institutes is the extent to which its deliverables are employed by scientists in DOE and SC communities. Nevertheless, it is difficult to anticipate the near-term and changing computational science needs of the application domains. This observation motivates the need to develop a wide array of intellectual resources and tools to meet cross-cutting or core computational science needs. Although application-aware, the overarching research strategies developed by the SciDAC-5 Institutes will not be constrained by a specific application. Applicants may propose proof-of-principle demonstrations of potential benefits – which may motivate the development of meaningful and credible suites of test applications or benchmark problems – in order to engage scientists. The latter considerations are no substitute for realistic, full-scale applications or data sets, but may be useful for development purposes and for gaining experience with the most significant issues confronting scientists.

Although their main focus will be centered upon the computational science needs of the SciDAC Partnerships, the SciDAC-5 Institutes will be Outward-Looking and Multi-Faceted. To expand their circle of influence beyond the SciDAC Partnerships, the proposed Institutes will be equipped with tools, resources and capabilities that will facilitate potential interactions with initiatives of special priority for the DOE SC (https://www.energy.gov/science/initiatives) as appropriate. For instance, the awarded Institutes will be encouraged to explore collaboration opportunities with the Basic Energy Sciences (BES) sponsored Energy Frontier Research Centers (EFRCs) (https://science.osti.gov/bes/efrc) and ASCR and National Nuclear Security Administration sponsored Exascale Computing Project (ECP) (https://exascaleproject.org/). Furthermore the awarded Institutes will be expected to develop and to support scientific machine learning based capabilities with broad impact on DOE and SC grand challenges.

It is crucial for the proposed Institutes to have the built-in flexibility to adapt and to rethink their efforts according to the needs and priorities of the DOE and SC science communities, including the SciDAC Partnerships, which will transition from SciDAC-4 to SciDAC-5 over the duration of the SciDAC-5 Institutes. Institutes' connection with the Partnerships is further described in the sections that follow.

Architecture-Aware

Another important metric of success is the extent to which the proposed Institutes lower the barriers, for the scientists, to effectively use the existing and emerging DOE HPC systems such as those existing and planned for at the OLCF and ALCF, NERSC, and similar world-class computing facilities over the next 5 years. We anticipate two SciDAC-5 Institutes that effectively leverage and incorporate the basic research results, mature technologies and areas of expertise from Applied Mathematics and Computer Science, respectively, will be needed in order to make a meaningful impact. For description of the current Institutes, go to:
www.scidac.gov/institutes.html

Over the next 5 years, the Nation will enter the exascale era with a first exascale system (Aurora) to be deployed at ALCF in 2021 and a second exascale system (FRONTIER) to be deployed at OLCF in the 2021-2022 timeframe.

Aurora (https://aurora.alcf.anl.gov) was designed in collaboration with Intel and Cray, and it will fully support machine learning and data science workloads alongside traditional modeling and simulation workloads. Aurora will have a sustained performance of over 1 exaflop and over 10 petabytes of system memory. Each node will have two Intel Xeon scalable processors coupled with six Intel Xe architecture based GP-GPUs supporting a unified memory architecture, with nodes interconnected by Cray's high-speed Slingshot interconnect. The Aurora programming environment will include fully optimized data and learning science software stacks, including numerous frameworks such as TensorFlow, PyTorch, Scikit-learn, Spark Mllib, GraphX, Intel DAAL, Intel MKL-DNN, as well as a full range of languages, libraries, and tools familiar to HPC users today.

Based on Cray's new Shasta architecture, FRONTIER (https://www.olcf.ornl.gov/frontier) will have a peak performance exceeding 1.5 exaflops. Each node on FRONTIER will contain one

AMD EPYC CPU and four Radeon Instinct GPUs fully connected by a high-speed AMD Infinity Fabric supporting fully coherent memory. Internode communication will be facilitated by Cray's high-speed Slingshot interconnect. The FRONTIER programming environment will provide full-stack support for artificial intelligence, data analytics, and simulation. This software environment will include a fully optimized scalable data science suite and the Cray Deep-learning plugin, as well as a full range of languages, libraries, and tools familiar to users of OLCF's current systems.

Additionally, NERSC will deploy a pre-exascale system (Perlmutter) in 2021. This will be a heterogeneous system comprising both CPU-only and GPU-accelerated nodes, with an expected performance of more than three times Cori, NERSC's current platform (https://www.nersc.gov/systems/perlmutter).

Tools and methodologies for coping with and taking full advantage of the existing and emerging DOE HPC systems including the exascale systems are of critical importance to SciDAC and this will require close interactions with the ASCR facilities. SciDAC-5 Institutes are expected to play a central role in coordinating and facilitating these interactions through a robust engagement strategy with the ASCR facilities.

Software engineering best practices can greatly help in the productivity of software developers and the long-term maintainability of the software as the computational systems and science evolve over time. An important contributor to software productivity is code portability across the ASCR computational facilities. SciDAC-5 Institutes will be responsible for promoting the adoption of software engineering best practices by the SciDAC community in the end-to-end computational science pipeline and for providing basic tools supporting these practices.

Together the SciDAC-5 Institutes will cover a significant portion of expertise in Applied Mathematics and Computer Science through an integrative approach between topics traditionally supported by ASCR base research programs such as solvers, uncertainty quantification, software tools, data and others, and emerging topics such as scientific machine learning. While adopting this integrative approach, the proposers should ensure that there is no duplicative work among different parts within an Institute. The Institutes will also bring together communities who may not be accustomed to work jointly therefore should demonstrate the proposed synergistic activities and merged capabilities among these communities by examples.

Institutes-Aware

Active collaboration among the SciDAC-5 Institutes researchers is essential to fulfill the purpose of SciDAC. Consequently, a proposed Institute must not only make a compelling case for its own intrinsic capabilities, but also describe processes for effectively leveraging expertise and results from the other potential Institute. The development of capabilities tailored for specific science applications are funded by the SciDAC Partnerships or by other potential collaborative efforts between the Institutes and the application areas stewarded by SC and DOE. A key point of the Institutes is that innovative science projects can be accommodated by the Institutes' pooling of a broad range of complementary but non-duplicative computational skills that is otherwise not readily available to DOE scientists.

Management Structure

Each Institute must identify a management structure in the form of an organization chart and a plan that enable it to function efficiently and to collaborate effectively and quantifiably with the SciDAC Partnerships as well as with each other. Institute structure must have sufficient flexibility to adapt quickly to changing technical challenges and scientific needs and the plan should specify the procedure for adjusting the expertise within the Institute when needed. Institute management plan must use appropriate metrics to measure technical progress and contributions and outline a risk mitigation strategy. The plan must also describe the communication and coordination processes among different parts of the Institute, with the other Institute, the ASCR Facilities and the SciDAC Partnerships as well as the Institute's strategy for outreach and impact to the broader computational science community including initiatives of special priority for the DOE SC (see above Application-aware). The proposed Institutes may choose to identify points of contacts assigned to work with the other Institute, the ASCR Facilities, specific SciDAC Partnership areas and other targeted areas such as ECP. Additionally, each Institute must identify a Director, a Deputy Director, Leads for Primary Topic Areas, Principal Investigator(s), and Senior/Key Personnel. Typical duties, responsibilities and authorities for each category are provided below:

- **Institute Director:** The SciDAC Institute Director is the Lead Principal Investigator and must be employed by the Lead Institution. The SciDAC Institute Director will serve as the primary contact responsible for communications with the DOE Program Manager on behalf of all of the Principal Investigators in the Institute. The Director will be responsible for adjusting the areas of expertise within the Institute. This could involve personnel actions.
- **Institute Deputy Director:** The Deputy Director will assist the Institute Director in leading the project and will serve as the secondary contact for the DOE program management.
- **Lead(s) for Primary Topic Areas:** The lead(s) for Primary Topic Areas will be responsible of leading and coordinating the members and technologies under their topic areas. The Lead(s) will also work together to build synergies and merged capabilities (as applicable) among the topic areas, and to avoid duplicative work.
- **Principal Investigator:** A Principal Investigator is the individual designated by the research organization and empowered with the appropriate level of authority and responsibility for the proper conduct of the research within that organization. These authorities and responsibilities include the appropriate use of funds and administrative requirements such as the submission of scientific progress reports to DOE. When an organization designates more than one Principal Investigator, it identifies them as individuals who share the authority and responsibility for leading and directing the research, intellectually and logistically.
- **Senior/Key Personnel:** A senior/key person is an individual who contributes in a substantive, measurable way to the scientific/technical development or execution of the project. This definition includes, but is not limited to, the SciDAC Institute Director, the Deputy Director, the Leads for Primary Topic Areas and the Principal Investigator(s).

The Application must include in addition tables of the institutional and primary topic area budgets as described in Section IV.

PI Meetings

The selected awardees will be asked to attend the annual SciDAC PI meetings and participate in coordination activities with other SciDAC-funded projects. Applicants should anticipate a need for travel to effectively communicate with other SciDAC researchers and request appropriate funding in their budgets.

INSTITUTES' CONNECTION WITH THE PARTNERSHIPS

The SciDAC program (https://www.scidac.gov) was initiated in 2001 as an SC-wide program to dramatically accelerate progress in scientific computing. SciDAC consists of the Institutes, as described above, and the Partnerships, as outlined below. Today the Partnerships consist of jointly funded (and managed) collaborations between scientists (sponsored by Partners) and applied mathematicians or computer scientists (sponsored by ASCR). In SciDAC-4, DOE's Office of Nuclear Energy (NE) joined ASCR's SciDAC Partners extending the Partnerships, for the first time, beyond SC programs to engage Applied Energy offices and their communities. ASCR relies upon the SciDAC Institutes to connect basic research in applied mathematics and computer science to scientific challenges by forming the foundation to address commonalities in multiple (and different) SciDAC Partnerships. As in previous cycles of SciDAC, the success of the SciDAC-5 Institutes will depend on their ability to directly engage with the scientists in the formation and execution of deep collaborations.

Currently, there are 30 SciDAC-4 Partnership projects (https://www.scidac.gov/partnerships.html). The SciDAC-5 Institutes will be expected to work with the SciDAC-4 Partnership projects as well as the upcoming SciDAC-5 Partnership projects. Funding opportunities for the SciDAC-5 Partnerships will be announced through several FOAs and Program Announcements starting in fiscal year 2021. Below ASCR's SciDAC Partners describe areas of strategic importance that are positioned to be met through the SciDAC-5 Partnerships. Applicants are strongly encouraged to identify the potential tools and capabilities needed to support these areas.

Basic Energy Sciences (BES)

https://www.energy.gov/science/bes/basic-energy-sciences
The BES program supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.

Targeted Topics for BES-ASCR SciDAC-5 Partnership Projects may include:

Quantum Phenomena
Theory and computation to understand quantum phenomena for materials and chemical sciences, emphasizing development of novel computational techniques for quantum many-electron systems that include far from equilibrium dynamics.

Data Science, Machine Learning and Artificial Intelligence

New data science, machine learning and artificial intelligence techniques to predict and to control key materials and chemical systems, including materials discovery for rare-earth materials, soft matter, including polymer up-cycling, separation science, geosciences, and bio-inspired science.

Quantum Computing or Quantum Devices will be out of scope.

Additional information about BES programs can be found at:
https://science.osti.gov/bes/Community-Resources/Reports

Biological and Environmental Research (BER)

https://www.energy.gov/science/ber/biological-and-environmental-research
The BER program supports fundamental, interdisciplinary research to achieve a predictive systems-level understanding of coupled Earth system changes and systems biology, which requires the organization and integration of diverse interdisciplinary data and models in innovative ways. In particular, BER seeks to develop advanced mathematical methods and computational models for systems ranging from molecular to global scales and an ability to connect large and diverse datasets with models, which enables more holistic and robust predictions of complex system behavior.
BER-supported Earth system modeling increasingly demands ultra-high resolution and variable-resolution coupled (ocean, atmosphere, land and cryosphere) simulation, in which processes are increasingly resolved in high resolution regions using unstructured grids. The global high-resolution coupled model faces particularly acute challenges for computational performance, communication across model components, model initialization, and managing increasingly high-volume output. Topics demanding more research involving applied mathematics, computer science and software advances therefore include: time-stepping and load-balancing for multi-scale simulations; code portability; new algorithms that reduce inter-node communications and memory needs for solving PDEs on unstructured grids; linear algebra kernels that work efficiently across upcoming exascale platforms; methods for coupled earth system model initialization and spin-up that reduce the time and computational cost to reach model equilibrium; software tools for performance analysis and automation of regression testing; and computationally efficient methods, including machine learning approaches, for analysis of high-volume simulation output.
Additional information about BER's Earth and Environmental System Modeling can be found at:
https://science.osti.gov/ber/Research/cesd/Earth-and-Environmental-System-Modeling

Fusion Energy Sciences (FES)

https://science.osti.gov/fes
The mission of the FES program is to expand the fundamental understanding of matter at very high temperatures and densities and to build the scientific foundations needed to develop a fusion energy source. As fusion research enters the era of burning plasmas, large-scale integrated simulations based on high fidelity physics models will be necessary to develop the experimentally validated predictive capability needed for addressing the FES mission. Advanced fusion simulation codes are based on first-principles or theory-based reduced descriptions of the

fundamental Maxwell-Boltzmann system of equations describing the properties and behavior of magnetically confined plasmas and on comparable materials science descriptions of the interaction of the confined plasma with the material walls. The intrinsic nonlinearities (expected to be stronger in self-heated burning plasmas), complicated three-dimensional geometries and magnetic topologies, extreme anisotropies, wide ranges of overlapping temporal and spatial scales, and multi-physics effects associated with a realistic description of the magnetically confined plasma state pose significant challenges to the solution of these equations, especially in an integrated simulation approach. Contributions from the applied mathematics and computer science communities are essential for overcoming these challenges and developing a Whole-Device Modeling (WDM) capability, by enabling fusion scientists to fully exploit the potential of SC HPC resources at today's multi-petascale level and increase their readiness for the upcoming exascale era.

High-priority computational capabilities needed to advance the FES mission include fast I/O for handling large sets of data; in-situ on-memory data analysis; tools and algorithms for GPU performance optimization on upcoming exascale architectures; porting of parallel scalable solver libraries to exascale; performance profiling and optimization; support for unstructured meshes, adaptive mesh refinement, and grid generation for complex 3D geometries; adaptive time stepping and time parallelization methods; fault tolerant algorithms; real-to-complex FFTs; artificial intelligence and machine learning tools including pattern discovery from extreme-scale simulation and experimental data, data-driven discovery of governing equations, machine learning in high-dimensional dataspaces, and federated data science management frameworks for remote connections between exascale computers and big experiments; implicit / explicit (IMEX) methodologies; and visualization, uncertainty quantification, and feature extraction tools.

Additional information about FES programs can be found at:
https://science.osti.gov/fes/Community-Resources/Workshop-Reports

High Energy Physics (HEP)

https://science.osti.gov/hep
The mission of the HEP program is to understand how our universe works at its most fundamental level. We do this by discovering the most elementary constituents of matter and energy, exploring the basic nature of space and time itself, and probing the interactions between them. To enable these discoveries, HEP supports theoretical and experimental research in both elementary particle physics and fundamental accelerator science and technology.

Computational physics incorporating advanced computing techniques is a critical requirement for multiple parts of the HEP program including complex simulations and analysis of the increasing amounts of data streaming from experiments and generated by simulations. An important role of the sophisticated scientific simulations using cutting edge scientific codes is to enable discovery along the HEP science goals that may not be accessible by other means.

HEP has participated in the SciDAC program since its inception and partnerships with the SciDAC Institutes continues to be a key part of the successful outcomes. Valuable collaborations include incorporation of portable software tools, data structure frameworks, data transfer and

analysis tools, understanding the role of uncertainty quantification and more recently optimizing use of artificial intelligence and machine learning techniques across the computational HEP program.

The following links contain further information on HEP programs:
https://science.osti.gov/hep/hepap

Nuclear Physics (NP)

https://www.energy.gov/science/np/nuclear-physics
The mission of the NP program is to discover, explore, and understand all forms of nuclear matter. Nuclear physics may be unique in the extent to which it is amenable to accurate investigation using HPC methods. This is because the fundamental particles that compose nuclear matter - quarks and gluons - and their interactions are described mathematically by the theory of Quantum Chromodynamics (QCD), and numerical predictions for observable quantities in nuclear physics can be obtained directly by solving the equations of QCD on a computer, using the methods of "lattice QCD." In addition, many more traditional many-body methods are applied to a wide range of models in computational studies of nuclei, their properties and interactions, and the properties of bulk nuclear matter.
These computational studies are of great interest to the NP experimental program, since their predictions can be used to optimize the sensitivity and effectiveness of planned experiments, and guide detector design towards the most efficient and economical choices. Accordingly, the primary goal of the NP-ASCR SciDAC Partnership program is to enable and support research on current high-profile computationally intensive topics that are of direct relevance to the experimental research programs at existing or approved NP facilities. More generally, these Partnership projects are intended to facilitate studies of the wide range of problems in nuclear physics that are amenable to solution using HPC.
Topics for NP-ASCR SciDAC-5 Partnership program may include but are not limited to the following:

- Heavy Ion Collider Physics: Lattice Quantum Chromodynamics (LQCD) studies of the properties of the quark-gluon plasma (QGP); the QCD equation of state (EOS); phase diagram and critical point; algorithmic developments for the numerical simulations of systems with nonzero chemical potential.
- Medium Energy Nuclear Physics: QCD spectroscopy including exotic mesons; hadron structure, decays, and photocouplings; hadron-hadron interactions.
- Nuclear Structure and Astrophysics: Nuclear structure calculations (ab initio and models); nuclear forces from LQCD; nuclear reactions; microscopic models of nuclear fission; the nuclear matter EOS; nuclear astrophysics.
- Fundamental Symmetries: Nuclear matrix elements for fundamental symmetries and beyond the Standard Model (BSM) studies; LQCD applications for fundamental symmetries.
- Nuclear Data: Novel algorithms and artificial intelligence and machine learning methods for processing large data sets.
- Isotope Development and Production for Research and Applications: Facilitating isotope production by unifying nuclear physics and thermal hydraulics codes to model target irradiations to generate isotope yields and target data such as temperature distributions.

- Accelerator Research and Development for Current and Future Nuclear Physics Facilities: Beam dynamics studies; spin tracking simulations in storage rings; strong hadron beam cooling methods; artificial intelligence and machine learning for optimizing operational efficiencies of accelerator user facilities.

Nuclear Energy (NE)

https://www.energy.gov/ne/office-nuclear-energy

The NE mission encourages the development and exploration of advanced nuclear science and technology. NE promotes nuclear energy as a resource capable of meeting the Nation's energy, environmental, and national security needs by resolving scientific, technical, and regulatory challenges through research, development, and demonstration. The challenge of accelerating innovation and concept development in applied nuclear technologies requires the development and deployment of advanced modeling and simulation capabilities that are more predictive, and can be fully integrated into applied research and development in a manner that significantly improves the ability to achieve new insights and applications. A critical element in achieving such transformation in NE's applied research and development is to develop new scientific understanding by employing new methods for improving physical models and advancing the computational tools in which these models are used. Another primary goal of such collaboration are the concomitant advancements in the relevant areas of mathematics, physics, and computational science, with a focus on multiscale or multiphysics modeling, which will help build the foundation for new advancements not otherwise possible and for future collaboration both within DOE and industry. In particular, the following capabilities will be desired in the NE-ASCR SciDAC-5 Partnership program:
- Support for extension of numerical solvers to GPU-based computing platforms
- Method development for enhanced utilization of uncertainty quantification and data analytics for applied nuclear energy problems
- Method development to allow for scalable density functional theory (DFT) calculations
- Overlapping multi-scale methods for computational fluid dynamics, and in particular methods that seamlessly integrate information across overlapping concurrent calculations at different scales for improved accuracy of transient phenomena solutions

Additional information about NE programs can be found at:
https://neams.inl.gov/SitePages/Home.aspx

RESPONSIVENESS

All proposals received in response to this Announcement will undergo a responsiveness review in addition to other initial review criteria as described in Section V. The following proposals will be deemed unresponsive:
- Proposals from single institutional collaborations
- Proposals requesting support of less than $3 million or more than $8 million per year for the collaboration
- Proposals on research within the mission space of other SC and DOE programs
- Proposals on research or technology funded by other ASCR sub-programs or duplicative of

any active SC awards and projects
- Proposals on research geared towards a specific application
- Proposals on research and engineering for hardware and architecture development

Unresponsive proposals may be declined without merit review.

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 phrase "open-source" does not refer to any particular licensing arrangement, but is 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-0002223. Each proposal within the collaborative group submitted in response to a Laboratory Announcement and its companion 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.

11

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

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

DOE anticipates that the total value of authorizations made under this Program Announcement will be between $45 and $65 million. DOE expects that, subject to the availability of future year appropriation, between $10 and $30 million will be used to support cooperative agreements under the companion FOA.

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

The total budget of a collaboration may not be lower than $3,000,000 per year or higher than $8,000,000 per year. A proposed collaboration with a total budget outside these limits may be declined without merit review.

C. MAXIMUM AND MINIMUM AWARD SIZE

(See B. Estimated Funding section above.)

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

Ceiling

$2,500,000 per year

Floor

$250,000 per year

D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding above.)

Approximately 2 collaborations are expected to be funded, with the number of collaborating

institutions depending on the nature of the proposed collaborations.

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

E. ANTICIPATED AWARD SIZE

(See B. Estimated Funding above.)

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

F. PERIOD OF PERFORMANCE

(See B. Estimated Funding above.)

DOE anticipates making awards with a project period of five years.

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 proposal; (3) submission of required reports; and (4) compliance with the terms and conditions of the award.

G. TYPE OF PROPOSAL

DOE will accept only 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 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 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

Institute Director
Applications with more than one investigator, including applications with multiple institutions, must designate one and only one investigator as the Institute Director, who will exercise overall scientific control and direction of the proposed research. The Institute Director must be employed by or have a written agreement in place to be hired by the Lead Institution. If the proposed Institute Director will not be employed by the Lead Institution at the time of award, the application may be declined without further review.

Limitation on the Number of Applications: An individual may participate in no more than two applications and may be the Institute Director on no more than one application. An institution may be the Lead Institution on no more than one application. There is no limitation on the number of applications in which an institution may participate. If any of the following cases occur, the last received application that matches a qualified LOI (as described in Section IV B., below) will be accepted and all other applications will be declined without merit review:
- More than two applications are received with the same individual identified as an Institute Member in any role including the Institute Director,
Or
- More than one application is received with the same individual identified as an Institute Director,
Or
- More than one application is received with the same institution identified as the Lead Institution.

Section IV – PROPOSAL AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST PROPOSAL PACKAGE

Proposal submission instructions are available in this Announcement on the DOE SC 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

A Letter of Intent (LOI) is required and must be submitted by the due date. No responses will be sent to the LOI.

LETTER OF INTENT DUE DATE

04/13/2020 at 5 PM Eastern Time

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 information:

At the top of the first page:
<div align="center">

Title of LOI
Team Director Name, Job Title
Lead Institution
Phone Number, Email Address
Laboratory Announcement Number: LAB 20-2223

</div>

Only one LOI should be submitted for the entire project by the Lead Institution/Team Director.

In addition, the Lead Institution on the full proposal must be the same as on the LOI. The Team Director should not be changed unless unavoidable and only minor edits should be made, if necessary, to the title. If necessary, the applicant may make changes to other senior/key personnel and other participating institutions, although DOE discourages extensive changes.

This information should 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 LOIs must include the following two Tables, which will not count toward the two-page limit:

Table 1: Institute Members (Institute Director, Deputy Institute Director, Leads for Primary Topic Areas, PI's and Senior/Key Personnel) on the application and institutional affiliations

Team Members			Institution
Last Name	First Name	Title	Institution Name

Table 2: Collaborators of Institute Members

Collaborator			Institution
Last Name	First Name	Title	Institution Name

For all Institute members, Table 2 must include 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.

It is important that the LOI be a single file with extension .pdf, .docx, or .doc.

The LOI must be submitted electronically through the DOE SC PAMS website https://pamspublic.science.energy.gov. It is important that the LOI be a single file with extension .pdf, .docx, or .doc. The 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 20-2223.**

2. Pre-proposal

A pre-proposal is not required.

C. CONTENT AND PROPOSAL FORMS

05/12/2020 at 5:00 PM Eastern Time

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 proposal and when DOE makes the proposal 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 proposals. 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 support are discouraged and will not be reviewed by DOE.

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 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 20-2223.** Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than **03/31/2020**, 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 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 20-2223.**

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 must 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 must be a self-contained document that identifies the name of the applicant, the 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 must 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 20-2223**
- DOE/SC Program Office: **Advanced Scientific Computing Research**
- DOE/SC Program Office Technical Contact: Dr. Ceren Susut
- PAMS Letter of Intent Tracking Number**:**

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 PI on the same line.
- Indicate the Institute Director 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 below (Table 1) 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.

Table 1

	Names	**Institution**	**Year 1 Budget**	**Year 2 Budget**	**Year 3 Budget**	**Year 4 Budget**	**Year 5 Budget**	**Total Budget**
Institute Director								
PI								
PI								
PI								

Example budget table ($ in thousands)

* Note that collaborating proposals must be submitted separately.

In addition, the following three tables must be included as supplements to the cover page: Note Tables 2 & 3 are the same (possibly updated) as those submitted in the LOI.

Table 2: Institute Members (Institute Director, Deputy Institute Director, Leads for Primary Topic Areas, PI and Senior/Key Personnel) on the proposal and institutional affiliations

Institute Members			**Institution**
Last Name	First Name	Title	Institution Name

Table 3: Collaborators of Institute Members

Collaborator			**Institution**
Last Name	First Name	Title	Institution Name

For all Institute members, Table 3 must include 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.

Table 4: Budget by Primary Topic Areas

Primary Topic Area	Lead for Primary Topic Area	Year 1 Budget	Year 2 Budget	Year 3 Budget	Year 4 Budget	Year 5 Budget	Total Budget
Total							

Tables 1-4 will not count in the proposal page limitation.

PROJECT NARRATIVE (NO MORE THAN 20 PAGES LONG)

The project narrative **must not exceed 20 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 Section VIII.D for instructions on how to mark proprietary proposal information.

> **For Collaborative Proposals**: Each collaborating institution must submit an identical common narrative (No more than 20 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 be augmented by a statement of work 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 proposal. For publications or collaborations with more than 10 authors or participants, only list those individuals in the core group with whom the PI 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 proposal. 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 Data Management Plan (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 (https://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: https://science.osti.gov/funding-opportunities/digital-data-management/

- This appendix should not exceed 3 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.

3. Detailed Instructions for the Budget

Budgets are required for the entire project period. A budget form must 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 must be included after the budget pages. The justification must 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 post graduate) 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

04/14/2020 5 PM Eastern Time

You are encouraged to submit your Letter of Intent well before the deadline.

2. Pre-proposal Due Date

A pre-proposal is not required.

3. Proposal Due Date

05/13/2020 5 PM Eastern Time

You are encouraged to transmit your proposal well before the deadline.

4. Late Submissions

Proposals received after the deadline will not be reviewed or considered for award.

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.

Computing Resources: Proposals will not request computing resources. The allocation of High Performance Computing (HPC) resources available to individual projects is contingent on review and award through the processes as described at https://science.osti.gov/-/media/ascr/pdf/incite/docs/Allocation_process.pdf?la=en&hash=CBF42998D83C9B4761051F8 C468118AF71A86B72. Within the available computational resources, every effort will be made to ensure that successful proposals will have the resources needed to support their efforts.

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 20-2223.**

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 Lab Announcement (see Responsiveness in Section I); (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.

- 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

Merit reviewers will be asked to evaluate one additional criterion of lesser significance than the criteria above, established by 10 CFR 605.10 (d):
- Strength of the Management Plan.

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 a 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

- Assess how the proposed Institute will support, complement or develop mechanisms to accelerate scientific discovery in areas of strategic importance to DOE.
- Has the applicant identified commonalities in multiple (and different) application domains for addressing computational grand challenges of strategic importance to ASCR's SciDAC Partners and other DOE communities?

- Evaluate how the tools, resources and capabilities of the proposed Institute will facilitate potential interactions with initiatives of special priority for the DOE SC.
- Assess the plan for the development of tools and resources intended for current and emerging DOE HPC systems available to researchers within the next five years and the likelihood that these will lower the barriers to the effective employment of these systems.
- Is the Data Management Plan suitable for the proposed research; to what extent does it make the data available and useful to the scientific community?

APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

- Assess the processes that the proposed Institute will use to leverage basic research advances from Applied Mathematics and Computer Science.
- Evaluate the appropriateness of the performance metrics that will allow progress and contributions to be measured over the course of the research.
- Does the proposed Institute have an effective strategy to promote the adoption of software engineering best practices and provide basic tools to support these practices?

COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES

- Do the Institute Director and the other Institute Members have a proven record of research in the disciplines needed for success in projects of this complexity and magnitude?
- Is there duplicative work among the Primary Topic Areas of the Institute? Does the applicant identify the proposed synergistic activities and merged capabilities among different parts of the Institute?
- Does the proposed Institute have the necessary expertise to cope with the complexities of current and emerging DOE HPC systems?
- How does the proposed research exploit existing resources or contribute new resources (e.g., algorithms, software) or would it result in a duplication of existing resources?

REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET

- Are the requested budget and the distribution of the funds among Primary Topic Areas appropriate?
- How does the requested budget relate to the proposed specified management structure?
- Does the applicant have a process for reallocating funds to address changing priorities?

STRENGTH OF THE MANAGEMENT PLAN
- Is there a clear lead organization, a qualified Institute Director, and a qualified Deputy Director?
- Evaluate the comprehensiveness of the management plan and the organizational structure that delineates the roles and responsibilities of the Institute Members.
- Assess the mitigation strategies of the proposed Institute for foreseeable risks and explain how the Institute will have sufficient flexibility to adapt to changing priorities, challenges, and resources? What is the likelihood that the proposed Institute can overcome the key challenges and, as warranted, shift research directions in response to promising advances in

basic research?

- Evaluate the proposed Institute's plans to effectively communicate and coordinate its activities to the potential SciDAC-5 Institute(s), SciDAC-4 and SciDAC-5 Partnerships and ASCR program management as well as for outreach to the broader computational science community.

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
- Performance under current awards
- Potential impact of proposed research activities on SciDAC goals
- Relation of the proposed research activities to other research efforts and projects supported by ASCR

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

It is anticipated that the award selection will be completed by September 1st, 2020. It is expected that awards will be made in Fiscal Year 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.

4. 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 20-2223.**
  Please contact the PAMS help desk for technological issues with the PAMS system.

Questions regarding the technical requirements may be directed to the technical contact listed 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	Advanced Scientific Computing Research Dr. Ceren Susut 301-903-0366 Ceren.Susut-Bennett@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 conflict of interest and non-disclosure agreements 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.