

**PROGRAM ANNOUNCEMENT
TO DOE NATIONAL LABORATORIES**



**U. S. Department of Energy
Office of Science
Advanced Scientific Computing Research (ASCR)**

**Scientific Discovery Through Advanced Computing (SciDAC)
Institutes**

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REGISTRATIONS

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

The DOE Office of Science 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>.

There are many activities that you can perform in PAMS, and more functionality will be added throughout the near future. DOE national laboratories will submit pre-proposals, letters of intent, and proposals directly into PAMS.

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 the Office of Science 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, 9AM – 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 Announcement should reference **LAB 17-1787**.

UPDATES AND REMINDERS

RECOMMENDATION

The Office of Science encourages you to register in all systems as soon as possible. You are also encouraged to submit letters of intent, pre-proposals, and proposals before the deadline.

DATA MANAGEMENT PLAN

The Office of Science has published a new Statement on Digital Data Management, published at <http://science.energy.gov/funding-opportunities/digital-data-management/>, which governs applications submitted under this FOA, and is detailed in Part IV of this FOA.

ACKNOWLEDGMENT OF FEDERAL SUPPORT

The Office of Science published guidance about how its support should be acknowledged at <http://science.energy.gov/funding-opportunities/acknowledgements/>.

Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

Technical/Scientific Program Contacts:

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SUMMARY

The Advanced Scientific Computing Research (ASCR) Program in the Office of Science (SC), U.S. Department of Energy (DOE), hereby announces its interest in receiving proposals to the Scientific Discovery through Advanced Computing (SciDAC) program for SciDAC Institutes.

The SciDAC program (<http://www.scidac.gov> or <http://science.energy.gov/ascr/research/scidac>) is a recognized leader for the employment of high-performance computing (HPC) for scientific discovery. Initiated in 2001, re-competed in 2006, and most recently re-competed in 2011-2012, SciDAC involves SC programs and other Partners with a goal to dramatically accelerate progress in scientific computing through deep collaborations between discipline scientists, applied mathematicians, and computer scientists. This LAB announcement announces the third re-competition of the SciDAC (hereafter, SciDAC-4) Institutes. The mission of the SciDAC-4 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 through modeling and simulation in areas of strategic importance to the SC and DOE.

This Announcement is open to Laboratory-led consortium proposals submitted through a DOE national laboratory. Laboratories are strongly encouraged to engage university and industry partners that will be funded through subcontracts.

Pre-proposals or letters of intent are not required for this Announcement.

SCOPE AND STRUCTURE OF THE PROPOSED INSTITUTES

Specific goals and objectives for the SciDAC-4 Institutes are to support, complement or develop:

- Mechanisms for taking on computational grand challenges across application areas of strategic importance to DOE and SC missions. Funding opportunities for SciDAC-4 Partnerships have been announced through several Program Announcements and Funding Opportunity Announcements (FOAs). These Announcements, issued by ASCR's SciDAC-4 Partners, include opportunities for linking applied mathematics and computer science research to science-domain specific challenges through SciDAC-4 partnerships (see Supplementary Information).
- 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, the National Energy Research Scientific Computing Center, and similar world-class computing facilities over the next 3 years.

- Mechanisms for incorporating and demonstrating the value of basic research results from Applied Mathematics and Computer Science. It is expected that the proposed Institutes will be structured around these two main topics.
- Plans for building up and engaging our nation's computational science research communities.

This Announcement describes the process by which proposals for individual SciDAC-4 Institutes are to be developed, submitted, and merit reviewed. The overall portfolio 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 support of DOE and SC missions. 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 for DOE and SC missions. 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-4 Partnerships, the SciDAC-4 Institutes will be Outward-Looking and Multi-Faceted. To expand their circle of influence beyond SciDAC-4 Partnerships, the proposed Institutes will be equipped with tools, resources and capabilities that will facilitate potential interactions with notable SC research centers such as Basic Energy Sciences (BES) sponsored Energy Frontier Research Centers (EFRCs), SC programs that do not participate in SciDAC-4 Partnerships such as Biological and Environmental Research (BER) Computational Biosciences program as well as major DOE-wide initiatives such as High Performance Computing for Manufacturing HPC4Mfg. It is also important for the proposed Institutes to have the built-in flexibility to adapt and rethink their efforts according to the needs and priorities of these communities, including the SciDAC-4 Partnerships, which are likely to evolve over the duration of the projects. Institutes' connection with the Partnerships is further described in the Supplementary Information.

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 Oak Ridge and Argonne Leadership Computing Facilities, the National Energy Research Scientific Computing Center, and similar world-class computing facilities over the next 3 years. We anticipate two SciDAC-4 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 3 years, the main architectural features of existing and planned computing environments include: heterogeneous nodes (CPUs, GPUs), deep memory hierarchies, and varying trade-off costs for computation versus data movement. Tools and methodologies for coping with and taking full advantage of such architectural complexities are an important practical consideration as well as coordination of the proposed capabilities with past work across disciplines. The following provides a snapshot of existing and planned computational systems at the Oak Ridge and Argonne Leadership Computing Facilities (ALCF and OLCF), the National Energy Research Scientific Computing Center (NERSC):

http://science.energy.gov/~media/ascr/pdf/facilities/ASCR_Computiing_Facility_Upgrades.pdf.

Application portability among ALCF, OLCF, and NERSC architectures is a critical concern of DOE and remaining engaged with the ASCR facilities is a central role that the SciDAC-4 Institutes are expected to play. Applicants are encouraged to refer to ASCR Facilities Joint Application Readiness Plan:

http://science.energy.gov/~media/ascr/ascac/pdf/meetings/20141121/ASCAC_Application_Readiness.pdf as they devise their 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-4 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.

The SciDAC-4 Institutes will cover a significant portion of expertise in Applied Mathematics and Computer Science and should ensure that there is no duplicative work among different parts within an Institute. The proposed 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 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 will be funded by the SciDAC-4 Partnerships that are currently under review or by other potential collaborative efforts between the Institutes and the application areas of strategic importance to 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-4 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-4 Partnerships as well as the Institute's strategy for outreach and impact to the broader computational science community including the notable SC programs and major DOE-wide initiatives (see above Application-aware). To underpin the plan, the proposed Institutes may choose to identify points of contacts assigned to work with the other Institute, the ASCR Facilities, specific SciDAC-4 Partnership areas and other targeted application areas of strategic importance to SC and DOE. 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 Laboratory. 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).

In addition to the information above, the application must include tables reflecting the institutional and primary topic area budgets as described in Section IV.

SciDAC-4 Partnerships. Beginning in early FY2017, a series of focused Announcements were released for the Partnership component of SciDAC-4 to be jointly funded and managed with the Partners. Further information on this series of Announcements and the SciDAC-4 Institutes' connection with the Partnerships can be found in the Supplementary Information section that follows.

SUPPLEMENTARY INFORMATION

Institutes' Connection with the Partnerships. The SciDAC program was initiated in 2001 as a partnership involving Office of Science (SC) program offices 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 SciDAC-4 Institutes will depend on the Institutes' ability to directly engage with the scientists in the formation and execution of these deep collaborations.

Beginning in early FY2017, a series of SciDAC-4 Partnership Announcements were released where ASCR's SciDAC Partners described areas of joint strategic importance that are positioned to be met through SciDAC-4 Partnerships. Below are summaries of these descriptions.

Applicants are strongly encouraged to identify the potential tools and capabilities needed to support these areas. More information on current and previous SciDAC portfolios can be found in this link: www.scidac.gov.

Basic Energy Sciences (BES)

https://science.energy.gov/~media/grants/pdf/lab-announcements/2017/LAB_17-1748.pdf

Basic Energy Sciences (BES) 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-4 Partnership Projects

Materials Science

Quantum Materials: Topological materials, topological interface states, superconductors, spin liquids, and strongly correlated materials. Development of novel techniques for quantum many body systems. Proposals on the quantum Hall effect or device optimization/engineering will not be accepted.

Chemical Sciences, Geosciences, and Biosciences

Low-Temperature and Low-Pressure Catalysis, Photocatalysis, and Separations: Catalysis or separations, with or without driving fields, under low-temperature and low-pressure, for processes related to water splitting, ammonia production, and/or carbon-dioxide reduction in realistic systems. Proposals that rely upon initial excitation to a highly non-equilibrium state will not be accepted.

Nanoscale Transport: Transport in porous media at nanoscale to subnanoscale; flow and diffusion in systems dominated by heterogeneously charged surfaces; breakdown of Navier-Stokes/continuum scale; coupling of tomographic imaging and molecular scales. Proposals that do not connect molecular and continuum scale problems and proposals that do not address heterogeneously charged surfaces will not be accepted.

Additional information about BES programs can be found at:

<http://science.energy.gov/bes/>

<https://science.energy.gov/bes/community-resources/reports/>

Biological and Environmental Research (BER)

https://science.energy.gov/~media/grants/pdf/lab-announcements/2017/LAB_17-1681.pdf

https://science.energy.gov/~media/grants/pdf/lab-announcements/2017/LAB_17-1682.pdf

Biological and environmental Research (BER) 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 relies upon ultra-high resolution and variable-resolution (ocean, atmosphere, land and cryosphere) coupled simulation, in which processes are increasingly resolved in high resolution regions. Cloud-resolving and land-process-resolving models inform and may eventually be embedded within high-resolution regions of the DOE global Earth system model. The global model faces particularly acute challenges for computational performance, component coupling, and predictability. Topics demanding more research involving applied mathematics, computer science and software advances for modeling and simulation therefore include: coupling methods, time-stepping, and load-balancing for multi-physics and multi-scale (in space and time) systems; methods to accelerate system spin-up and equilibration of Earth systems; algorithms for physics and biogeochemistry for high or variable resolution; mathematical methods to determine system predictability; methods to derive statistics and diagnostics during simulation; algorithm design that map to new architectures and memory structures; and coupled model performance and portability.

Additional information about the DOE global Earth system model can be found at:

<https://climatemodeling.science.energy.gov/projects/accelerated-climate-modeling-energy>

Additional information about modeling challenges in the areas of Earth system science, systems biology and BER programs in general can be found at:

<http://science.energy.gov/ber/>

Fusion Energy Sciences (FES)

https://science.energy.gov/~media/grants/pdf/lab-announcements/2017/LAB_17-1670.pdf

The Fusion Energy Sciences (FES) program mission 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 advanced 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 develop a Whole Device Modeling (WDM) capability, by enabling fusion scientists to fully exploit the potential of modern computing architectures at today's DOE HPC systems and increase their readiness for the upcoming exascale era.

Additional information about FES programs can be found at:

<http://science.energy.gov/fes/>

<http://science.energy.gov/~media/fes/pdf/workshop-reports/>

High Energy Physics (HEP)

https://science.energy.gov/~media/grants/pdf/lab-announcements/2017/LAB_17-1697.pdf

The mission of the High Energy Physics (HEP) program is to understand how the universe works at its most fundamental level, which is done by discovering the elementary constituents of matter and energy, probing the interactions between them, and exploring the basic nature of space and time. Recent successes for HEP include the discovery of dark energy and the Higgs Boson. The goal of the HEP-ASCR SciDAC-4 Partnership program is to facilitate advanced and effective use of DOE HPC by major ongoing HEP experiments along with related theory and simulation activities and current and near term accelerator projects, via appropriate partnerships between the HEP and ASCR communities. Major data-intensive HEP experiments including their related simulations, as well as computing-intensive HEP research including accelerator modeling, theoretical, and computational physics are within the scope of the HEP-ASCR

SciDAC-4 Partnership program. Partnerships that propose new research for HEP data-intensive experiments via coordinated campaigns for computational research that cross cut the HEP program are strongly encouraged. These may include innovative plans to better exploit CORI at NERSC and other DOE HPC architectures that foster data intensive computing.

The following links contain further information on HEP programs:

<http://science.energy.gov/hep/hepap/>

<http://science.energy.gov/hep/research/>

Nuclear Energy (NE)

https://science.energy.gov/~media/grants/pdf/lab-announcements/2017/LAB_17-1674.pdf

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. An important focus for NE is advancement of nuclear fuels modeling and simulation, and incorporation of their results in applied nuclear fuels R&D. NE-ASCR SciDAC-4 Partnership program seeks to achieve a greater understanding of the physics associated with microstructural changes in various fuel materials under irradiation at high temperatures, and how these changes would affect key traits such as thermal conductivity and structural integrity. The results should help enable not only the development of more predictive, higher fidelity models, but also the accelerated development of advanced engineering-scale simulation tools.

Research areas of interest include development of HPC tools capable of predicting microstructural evolution in both current (UO₂) and advanced (e.g., metallic, uranium-silicide, TRISO) nuclear fuel and associated cladding materials, by leveraging DOE-HPC capabilities, along with mathematical and physics expertise. These tools would be based on new insights in the physics that affect microstructure, and on application of codes and methods capable of spanning the multiple length and time scales needed to address the complex physical changes that affect fuel and cladding performance.

Additional information about NE programs can be found at:

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

Nuclear Physics (NP)

https://science.energy.gov/~media/grants/pdf/lab-announcements/2017/LAB_17-1698.pdf

The mission of the Office of Nuclear Physics (NP) 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

numerical 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-4 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.

The principal NP research areas and examples of associated computational research topics are: Heavy Ion NP (QCD thermodynamics and phase diagram; nuclear collisions); Medium Energy NP (hadron structure and spectroscopy); and Low Energy NP. Computational research topics of relevance to the NP-ASCR SciDAC-4 Partnership program therefore include but are not limited to the following:

- a. Heavy Ion Collider Physics (HICP): 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; and algorithmic developments for the numerical simulations of systems with nonzero chemical potential.
- b. Medium Energy Nuclear Physics (MENP): QCD spectroscopy, including exotic mesons; hadron structure, decays, and photocouplings; hadron-hadron interactions.
- c. Low Energy Nuclear Physics (LENP): Nuclear structure calculations (ab initio and models); nuclear forces from LQCD; nuclear reactions; microscopic models of nuclear fission; the nuclear matter EOS; nuclear astrophysics; nuclear matrix elements for “fundamental symmetries” and “beyond the Standard Model” (BSM) studies.

In addition to specific results-oriented computational research, Partnerships that address longer-range topics such as novel algorithms, processing of large datasets in the field of nuclear physics, and code developments of importance for future numerical studies in these and related areas will also be considered.

Additional information regarding current NP research topics may be found at:

<http://science.energy.gov/np/about/>
<http://science.energy.gov/np/research/>.

Data Management Plan

A Data Management Plan as described in Section IV C. “Application Contents and Forms” - Appendix 6, is required. Applications that do not have a Data Management Plan will be deemed nonresponsive and will be declined without review.

Computing Resources

Proposals will not request computing resources. The allocation of HPC resources available to individual projects is contingent on review and award through the processes as described at https://science.energy.gov/~media/ascr/pdf/incite/docs/Allocation_process.pdf. Within the

available computational resources, every effort will be made to ensure that successful applications will have the resources needed to support their efforts.

REFERENCES

- [1] BES Energy Frontier Research Centers (EFRCs).
<https://science.energy.gov/bes/efrc/> and <http://www.energyfrontier.us/>
- [2] “SciDAC-EFRC Collaboration: WastePD”, April 2017.
<https://science.energy.gov/~media/ascr/ascac/pdf/meetings/201704/Windl-Riegner-WastePD.pdf>
- [3] “Exploration of Collaborative Opportunities Across SciDAC Institutes and Genomic Sciences Program”, February 2017.
<http://www.scidac.gov/documents/BSSD-SciDACreport.pdf>
- [4] High Performance Computing for Manufacturing HPC4Mfg.
<https://hpc4mfg.llnl.gov/>
- [5] SciDAC-3 PI Meetings.
<http://www.ornl.gov/scidac3pi2012/>
<http://www.ornl.gov/scidac3pi2013/>
<http://www.ornl.gov/scidac3pi2014/>
<http://www.ornl.gov/scidac3pi2015/>

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.

B. ESTIMATED FUNDING

It is anticipated that approximately \$10,000,000 per year will be available under this DOE National Laboratory Announcement, contingent on satisfactory peer review and the availability of appropriated funds. Applicants should request project support for three years. Following the first year award, out-year support will be contingent on the availability of appropriated funds, progress of the research, and programmatic needs. Awards are expected to begin in fiscal year 2017.

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.

C. MAXIMUM AND MINIMUM AWARD SIZE

(See B. Estimated Funding section above.)

The following total funding limits are specified for consortium proposals. The award size will depend on the availability of appropriated funds.

Ceiling

\$6,000,000 per year

Floor

\$3,000,000 per year

D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

Approximately 2 awards are expected.

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

E. ANTICIPATED AWARD SIZE

(See B. Estimated Funding Section 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 section above.)

DOE anticipates making awards with a project period of three 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 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. The Office of Science 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 Lead Principal Investigator/Principal Investigator 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.

Section IV – PROPOSAL AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST PROPOSAL PACKAGE

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

Proposals submitted outside of PAMS will not be accepted.

B. LETTER OF INTENT AND PRE-PROPOSAL

1. Letter of Intent

A letter of intent is not required.

2. Pre-proposal

A pre-proposal is not required.

C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

July 26, 2017 at 5 PM Eastern Time

Files that are attached to the forms must be in Adobe Portable Document Format (PDF) 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.

RESUBMISSION OF PROPOSALS

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

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

The Office of Science 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 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 – 20 page limit)
 - 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

Full proposals must be submitted into the DOE Office of Science Portfolio Analysis and Management System (PAMS). For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 17-1787**. Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than **July 26, 2017**, at 5 PM Eastern Time.

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

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

- Log into PAMS. From the proposals tab, click the “View DOE National Laboratory Announcements” link and find the current announcement in the list. Click the “Actions/Views” link in the Options column next to this Announcement to obtain a dropdown menu. Select “Submit Proposal” from the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per proposal; to do so, click the “Select PI” button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the “Actions” link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose “Select PI.”
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the “Invite PI” link at the top left of the “Select PI” screen. You can enter an optional personal message to the PI in the “Comments” box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the proposal. Save the proposal for later work by selecting “Save” from the dropdown at the bottom of the screen and then clicking the “Go” button. It will be stored in “My Proposals” for later editing. As a minimum, you must complete all the required fields on the PAMS cover page before you can save the proposal for the first time.
- The cover page, budget, and attachments sections of the lab proposal are required by PAMS before it can be submitted to DOE.
- Complete the sections in PAMS one at a time, starting with the cover page and following the instructions for each section.

- Click the “+View More” link at the top of each section to expand the onscreen instructions. On the budget section, click the “Budget Tab Instructions” link to obtain detailed guidance on completing the budget form.
- Save each section by selecting either “Save” (to stay in the same section) or “Save... and Continue to the Next Section” (to move to the next section) from the dropdown menu at the bottom of the screen, followed by clicking the “Go” button.
- If you save the proposal and navigate away from it, you may return later to edit the proposal by clicking the “View My Existing Proposals” or “My Proposals” links within PAMS.
- You must enter a budget for each annual budget period.
- You must also enter a budget for each proposed sub-award. The sub-award section can be completed using the same steps used for the budget section.
- In the attachments section of the lab proposal, the abstract, the budget justification, and the proposal narrative are required and must be submitted as separate files.
- You must bundle everything other than the budget, abstract, and budget justification into one single PDF file to be attached under “Proposal Attachment.”
- Do not attach anything under “Other Attachments.”
- To upload a file into PAMS, click the “Attach File” button at the far right side of the screen. Click the “Browse” (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the “Upload” button to upload the file.
- Once you have saved all of the sections, the “Submit to DOE” option will appear in the dropdown menu at the bottom of the screen.
- To submit the proposal, select “Submit to DOE” from the dropdown menu and then click the “Go” button.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the proposal.
- The proposal will also appear under My Proposals with a Proposal Status of “Submitted to DOE.”

Please only submit a PAMS lab technical proposal in response to this Announcement; do not submit a DOE Field Work Proposal (FWP) at this time. The Office of Science 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 17-1787**.

2. Detailed Contents of the Proposal

BUDGET AND BUDGET EXPLANATION

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

PAMS will calculate the cumulative budget totals for you.

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

PROJECT SUMMARY/ABSTRACT (NO MORE THAN ONE PAGE)

The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to the public. It should be a self-contained document that identifies the name of the Institute Director and the Institute Deputy Director, 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 8.5” by 11” paper with 1” margins (top, bottom, left and right) with font not smaller than 11 point. The one-page project summary/abstract should be placed in a separate, single pdf document and attached on the appropriate screen in PAMS.

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

DOE COVER PAGE (PART OF PROJECT NARRATIVE)

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

- The project title:
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Administrative Point of Contact name, telephone number, email:
- Institute Director name, telephone number, email:
- DOE National Laboratory Announcement Number: **LAB 17-1787**
- DOE/Office of Science Program Office: **Advanced Scientific Computing Research**
- DOE/Office of Science Program Office Technical Contact: Dr. Ceren Susut
- Research area (site) identified in Section I of this Announcement

On separate pages, as a supplement to the cover page, include the following four tables providing personnel and budget information for the entire project (including all institutions).

Table 1: Team Members (Institute Director, Institute Deputy Director, Lead(s) for Primary Topic Areas, Principal Investigators and Senior/Key Personnel) on the application and institutional affiliations

Team Members			Institution
Last Name	First Name	Title	Institution Name

Table 2: Collaborators of Team Members

Collaborator			Institution
Last Name	First Name	Title	Institution Name

For all team members, Table 2 must include co-authors over the past 48 months, graduate and postdoctoral advisors, graduate students and postdoctoral associates that have been supervised during the past 60 months, and any other current close associations.

Table 2 should exclude all personnel at any of the institutions listed in Table 1.

Table 3: Budget by Institution

Institution	Team Member	Role of the Institution	Y1 Budget	Y2 Budget	Y3 Budget	Total Budget
Total						

Table 4: Budget by Primary Topic Areas

Primary Topic Area	Lead for Primary Topic Area	Y1 Budget	Y2 Budget	Y3 Budget	Total Budget
Total					

Tables 1-4 will not count in the application 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 8.5” by 11” paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph. This page limit does not apply to the Cover Page, Budget Page(s), Budget Justification, biographical material, publications and references, and appendices, each of which may have its own page limit.

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

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

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

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

Project Management Plan: Multi-institutional proposals must include a project management plan that clearly indicates the roles and responsibilities of each organization and indicates how

activities will be coordinated and communicated among team members.

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

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the method to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities. There should be no ambiguity about which personnel will perform particular parts of the project, and the time at which these activities will take place.

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

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the Institute director/principal investigator and each senior/key person, including the sub-awardees, 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. The biographical information (curriculum vitae) must not exceed 3 pages when printed on 8.5" by 11" paper with 1-inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include the following:

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. An abbreviated style such as the Physical Review Letters (PRL) convention for citations (list only the first author) may be used for publications with more than 10 authors.

Synergistic Activities: List no more than 5 professional and scholarly activities related to the effort proposed.

Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers: 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 Principal Investigator interacted on a regular basis while the research was being done. Also, list any individuals who are currently, or have been, co-editors with you on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this 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 personally identifiable information such as a Social Security Number, date of birth, or city of birth. Do not include information that a merit reviewer should not consider.

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 Institute Director/Principal Investigator(s) and senior/key persons, including sub-awardees, for ongoing projects and pending applications. List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid.

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 person-months of effort per year being dedicated to the award or activity

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 Office of Science Statement on Digital Data Management (<http://science.energy.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 Office of Science 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 Office of Science 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 Office of Science research proposal merit review process. Applicants are encouraged to consult the Office of Science website for further information and suggestions for how to structure a DMP: <http://science.energy.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 8.5” by 11” 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 should be completed for each budget period of the award, and a cumulative budget form for the entire project period will be populated by PAMS. A detailed budget justification narrative should be included after the budget pages. The justification should cover labor, domestic travel, equipment, materials and supplies, and anything else that will be covered with project funds.

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

Section A. Senior/Key Person (Required)

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

Section B. Other Personnel

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

Section C. Equipment Description

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

Section D. Travel

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

its results.

Section E. Participant/Trainee Support Costs:

If applicable, submit training support costs. Educational projects that intend to support trainees (precollege, college, graduate and 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

A letter of Intent is not required or invited.

2. Pre-proposal Due Date

A pre-proposal is not required or invited.

3. Proposal Due Date

July 26th, 2017

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.

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. The Office of Science 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, 9AM – 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 17-1787**.

3. Proposal Receipt Notices

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

4. Viewing Submitted Proposals

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

Section V - PROPOSAL REVIEW INFORMATION

A. CRITERIA

1. Initial Review Criteria

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

2. Merit Review Criteria

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

- Scientific and/or Technical Merit of the Project;
- Appropriateness of the Proposed Method or Approach;
- Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
- Reasonableness and Appropriateness of the Proposed Budget.
- Strength of 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-4 Partners and other DOE communities?
- Evaluate how the tools, resources and capabilities of the proposed Institute will facilitate potential interactions with notable SC research centers, SC programs that do not participate in SciDAC and major DOE-wide initiatives.

- Assess the plan for the development of tools and resources intended for current and emerging DOE HPC systems available to researchers within the next three years and the likelihood that these will lower the barriers to the effective employment 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

- Does the applicant have a process for leveraging 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

- Does the applicant have a proven record of success in managing diverse teams of scientific and technical experts and delivering results for advanced computational science research?
- Do the members of the proposed Institute have a proven record of research and development in the disciplines needed for success in projects of this complexity and magnitude?
- Are the roles and intellectual contributions of the Director, Deputy Director, and Leads for Primary Topic Areas, Principal Investigator(s), and each Senior/Key Personnel adequately described?
- 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 team 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 MANAGEMENT PLAN

- Is there a clear lead organization and a qualified Project Director?

- Does the applicant present a comprehensive management plan that includes mitigation strategies 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?
- Does the applicant present an organizational structure that delineates the roles and responsibilities of the members of the Institute?
- Evaluate the proposed Institute's plans to effectively communicate and coordinate its activities to the potential SciDAC-4 Institute(s) and SciDAC-4 Partnerships and ASCR program management as well as for outreach to the broader computational science community including ASCR Facilities.

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. Selection

The Selection Officials will consider the following items, listed in no order of significance:

- Scientific and technical merit of the proposed activity as determined by merit review;
- Potential impact of proposed research activities on SciDAC-4 goals;
- Relation of the proposed research activities to other research efforts supported by ASCR;
- Potential for developing synergies with the other SciDAC-4 Institute; SciDAC-4 Partnerships and other targeted application areas of strategic importance to SC and DOE;
- Previous performance.

3. 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, 2017. It is expected that awards will be made in Fiscal Year 2017.

DOE is interested in seeing projects supported under this Announcement begin work by September 30th, 2017.

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.

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, 9AM – 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 17-1787**.

Please contact the PAMS help desk for technological issues with the PAMS system.

Questions regarding the specific program areas and technical requirements may be directed to the technical contacts listed for each program within the DOE National Laboratory Program Announcement or below.

Please contact the program staff with all questions not directly related to the PAMS system.

B. AGENCY CONTACTS

PAMS Customer Support	855-818-1846 (toll-free) 301-903-9610 sc.pams-helpdesk@science.doe.gov
Program Manager Scientific Contact	Advanced Scientific Computing Research, SC-21.1 Dr. Ceren Susut 301-903-0366 Ceren.Susut-Bennett@science.doe.gov

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.energy.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.