# PROGRAM ANNOUNCEMENT TO DOE NATIONAL LABORATORIES



# U. S. Department of Energy Office of Science

# Resilience for Extreme Scale Supercomputing Systems

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Announcement Type: Amendment

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(A Pre-Proposal is required)

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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 <a href="https://pamspublic.science.energy.gov">https://pamspublic.science.energy.gov</a>.

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 < <u>PAMS.Autoreply@science.doe.gov</u>>. 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 <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>.

- 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 to 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, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. 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: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submission and inquiries about this DOE National Laboratory Announcement should reference **LAB 14-1059**.

## 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 Office of Advanced Scientific Computing Research (ASCR) in the Office of Science (SC), U.S. Department of Energy (DOE), hereby invites proposals for basic research that significantly improves the resiliency of scientific applications in the context of emerging architectures for extreme scale computing platforms.

The next-generation of scientific discovery will be enabled by research developments that can effectively harness significant or disruptive advances in computing technology. Applications running on extreme scale computing systems will generate results with orders of magnitude higher resolution and fidelity, achieving a time-to-solution significantly shorter than possible with today's high performance computing platforms. However, indications are that these new systems will experience hard and soft errors with increasing frequency, necessitating research to develop new approaches to resilience that enable applications to run efficiently to completion in a timely manner and achieve correct results.

Of interest are proposals that address challenges in the following topics:

- 1. Fault Detection and Categorization
- 2. Fault Mitigation
- 3. Anomaly Detection and Fault Avoidance

More specific information is included under SUPPLEMENTARY INFORMATION below.

Proposals must be submitted through a DOE National Laboratory. A companion funding opportunity announcement (DE-FOA-0001059) available on Grants.gov describes the funding opportunity for institutions that are not DOE national Laboratories. Consult DE-FOA-1059 for information on eligibility for that announcement.

#### SUPPLEMENTARY INFORMATION

## **Background:**

Research developments that effectively harness significant or disruptive advances in computing technology will enable next-generation extreme scale science. Extreme scale is defined as approximately 1,000 times the capability available today. Applications running on extreme scale computing systems will generate results with orders of magnitude higher resolution and fidelity, achieving a time-to-solution significantly shorter than possible with today's high performance computing platforms. However, indications are that these new systems will experience a variety of faults and/or errors with increasing frequency, necessitating research to develop new approaches that enable applications to run efficiently to completion and achieve correct results in a timely manner.

Twenty percent (20%) or more of the computing capacity in a large high performance computing facility is wasted due to failures and recoveries. [1] The situation is expected to worsen sharply as systems increase in size and complexity, wasting even more capacity. Research is thus required to improve the resilience of the systems and the applications that run on them.

For the purposes of this Announcement, faults are defined as the underlying causes of errors, such as bugs, stuck gates, alpha particles, etc. Errors are the part of system state that *may* lead to failure, such as an incorrect value. A failure is the transition to incorrect service, such as the start of an unplanned service outage. [2]

Three types of faults are of interest. The first is permanent (a.k.a. hard) faults in which a hardware or software component has failed and must be replaced or rebooted to continue. Transient (a.k.a. soft) faults are those in which a component may perform incorrectly for a short time and then return to normal operation. The third and more problematic type are undetected faults (a.k.a. silent errors), which can be either permanent or transient. Today's HPC systems experience all three types of errors, but their frequency, root causes and interdependencies are not well understood. [4]

A variety of factors will contribute to increased rates of faults and/or errors on extreme scale systems [1, 2, 3, 4], a few of which are

- 1. The number of components with both memory and processors will increase by an order of magnitude, and the number of system components is increasing faster than component reliability, resulting in an increase in hard and soft errors;
- 2. Constraining hardware and software to a power envelope of 20 Megawatts (MW) will necessitate operating components at near-threshold power levels and power levels may vary over time, making errors more likely; and
- 3. Use of the machines will require managing unprecedented parallelism and complexity, especially at the node level of extreme scale systems, increasing the likelihood of programmer errors.

For existing systems, the most common approach to achieving fault tolerance is global checkpoint-restart (C/R) that captures the full state of the machine by writing it to stable storage (checkpoint) and reinstates (restarts) it at (or rolls it back to) the last point of known correctness, which is the last checkpoint. However, extreme scale systems are expected to have characteristics that make traditional methods of global C/R infeasible:

- 1. Data movement will be constrained, both internode and on/off the machine, in the interest of conserving power, so that the power cost of global C/R may be unacceptable;
- 2. The bottleneck for input/output (I/O) will continue to worsen as improvements in storage device capabilities do not keep pace with those for computing, making traditional C/R impractical because of the time required for disk access in relation to the frequency of faults; and
- 3. It is expected that the power cost of data movement and the worsening I/O bottleneck will make it necessary for data analysis and data reduction to occur *in situ*, or on the supercomputer in parallel or interleaved with the simulation, necessitating new approaches to ensuring the integrity of data and analytic processes.

DOE mission drivers with respect to fault tolerance and correctness are described in [4].

Additional information about expected changes to the architecture of and system software for DOE extreme-scale systems can be found in a variety of sources: [5, 6, 7 and 8].

Information about the changing paradigm for data management, analysis and visualization may be found in [9 and 10].

Additional information about challenges in resilience and resiliency in extreme scale systems and applications may be found in [1, 2, 3, 4, and 11].

Information about research already in progress that is related to planned extreme scale systems may be found in [12].

Proposals may address any or all of the research issues described below. Preference will be given to well-focused proposals that offer promise of significant advances in the ability of applications to run to completion in a timely manner and achieve correct results despite the occurrence of faults and/or errors.

## **Research Topic 1: Fault Detection and Categorization**

We need a deeper understanding of the depth and magnitude of the resilience problem and how current and future systems will be impacted. We also need to understand how faults and errors propagate in a system, as a critical step toward whole system evaluations and realistic fault prediction and analysis techniques. The first phase in achieving such understanding begins with better understanding of the problems for current supercomputing systems, with the expectation that similar fault mechanisms and system behavior will occur on future systems.

Research is needed on methods to detect faults in hardware and/or software, including soft faults that currently go undetected, and categorize faults so that the system can determine the best approach to handling them. Challenges of interest include but are not limited to:

- What are the underlying causes of faults and/or errors?
- What types of errors should be detected?
- What instrumentation of hardware is required to support fault detection at the system level?
- How do faults and errors propagate in a system?
- How might runtime systems and/or applications need to be instrumented to detect faults and/or errors?
- What taxonomy of faults will best support fault mitigation?
- Can fault categorization be automated cost effectively?
- At what level in the software stack should detected faults be addressed?
- Which faults, if any, are best handled by applications? By the operating or runtime system?
- What types of software error detection are both feasible and cost effective?

## **Research Topic 2: Fault Mitigation**

Fault mitigation requires solutions that allow an application to run to completion and achieve a result that is correct or within an acceptable tolerance for error. Two research topics of interest include (1) the need for more efficient and effective checkpoint/restart (C/R) and (2) the need for effective alternatives to C/R including understanding correctness and errors in applications, transmitting that information to software stack, developing fault-tolerant algorithms in the software stack, and reducing code impacted by fault mitigation strategies.

Research is needed to increase the efficiency and efficacy of checkpoint/restart (C/R). Traditional C/R is problematic because of the power costs of data movement and the worsening I/O bottleneck, as well as the time consumed. To be effective, the time required for C/R must be significantly less than the mean time between failures. Furthermore, the presence of soft errors requires increased attention to data integrity in checkpoints, since the previous one should not be erased before the integrity of the most recent one is assured. Topics for research include but are not limited to:

- How can we reduce the amount of data movement and I/O required for C/R?
- How can we reduce the frequency of C/R?
- How can we ensure integrity of the data in a checkpoint?

Research is needed to develop cost-effective alternatives to traditional C/R that allow an application to continue running in the face of faults and/or that lessen the amount of code that must be restarted, while still allowing the application to reach a correct result or one that is within acceptable tolerance for error. Research topics that need to be addressed include but are not limited to the following:

- In the context of soft errors, what is required to ensure the correctness of simulations and processing?
- How can an application establish its tolerance for error and communicate that information to the system components handling errors?

- If applications can tolerate or handle soft errors, how can they best convey that to the appropriate layer(s) of the software stack? What mechanisms can be provided to help applications to better handle soft errors?
- What fault-tolerant or self-checking algorithms might be developed that allow the software stack to continue running correctly in the presence of frequent errors? How can we develop trusted system services that support recovery from errors?
- Since checkpointing the full system state is infeasible, how can we reduce the amount of system state that must be protected from faults?
- How can we reduce the amount of code that is impacted by fault mitigation?

## **Research Topic 3: Anomaly Detection for Fault Avoidance**

Research is needed to determine whether it is possible for machine learning methods to enable anticipation of faults and/or node failure far enough in advance for an application to avoid the fault/failure, perhaps by migrating the running application to another node. Challenges of interest include but are not limited to:

- What information might be provided by hardware to support detection of anomalous behavior?
- How could a software resilience solution learn adaptively from hardware or the overall system sensor information network in order to anticipate and deal with potential faults effectively, assuming the availability of information about heat levels, power variability, prior faults and other suspected causes of faults?
- What strategies would enable the runtime system and/or the application to avoid a fault that is anticipated near term?

## **Additional Information**

Proposals may address one or more of the announcement themes. Preference will be given to projects that offer focused and coherent research and solutions. All projects should appropriately integrated into a whole and not a collection of disjointed efforts.

Proposals must explicitly address the challenges of operating within the expected exascale environment, including severe constraints on data movement, worsening I/O bottleneck, frequent hard and soft faults, and the necessity for extremely high levels of concurrency.

Proposed research must advance pertinent aspects of computer science.

All recipients of awards resulting from this Announcement must comply with the terms of the ASCR policy on open source software:

http://science.energy.gov/~/media/ascr/pdf/research/docs/Doe\_lab\_developed\_software\_policy.pdf.

## **Out of Scope:**

Out of scope for this Announcement are proposals that

• Fail to address extreme scale high performance computing systems;

- Provide discipline-specific and/or application-specific solutions that do not generalize to multiple applications;
- Request supplements to existing projects to address resiliency challenges;
- Would develop resilient solvers or math libraries;
- Aim to incorporate resilience into programming models and/or languages; and/or
- Address fault prediction through machine learning other than by anomaly detection based on information from hardware sensors.

Proposals that are deemed to be the same as or substantially similar to proposals submitted to DE-FOA-0000742/Lab Announcement 12-742 Resilient Extreme-Scale Solvers, DE-FOA-0001003/ Lab Announcement 14-1003 Exploratory Research for Extreme-Scale Science, or DE-FOA-000958/Lab 13-958 Early Career Research Program will be declined without review.

## **Collaboration**

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

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

Collaborative proposals from institutions other than DOE National Laboratories should be submitted following the above rules in response to the companion announcement, DE-FOA-0001059.

#### **References:**

- 1. System Resilience at Extreme Scale, E.N. (Mootaz) Elnozahy et al, <a href="http://institute.lanl.gov/resilience/docs/IBM%20Mootaz%20White%20Paper%20System%20Resilience.pdf">http://institute.lanl.gov/resilience/docs/IBM%20Mootaz%20White%20Paper%20System%20Resilience.pdf</a>
- 2. Addressing Failures in Exascale Computing, Marc Snir et al., March 2013 http://www.mcs.anl.gov/papers/P5022-0913.pdf
- 3. *Interagency Workshop on HPC Resilience at Extreme Scale, Final Report*, February 2012, http://institute.lanl.gov/resilience/docs/Inter-AgencyResilienceReport.pdf
- 4. Final Report from the U.S. Department of Energy Fault Management Workshop, August 2012, <a href="http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/FaultManagement-wrkshpRpt-v4-final.pdf">http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/FaultManagement-wrkshpRpt-v4-final.pdf</a>
- 5. <u>Scientific Grand Challenges: Crosscutting Technologies for Computing at the Exascale,</u> February 2010, http://science.energy.gov/~/media/ascr/pdf/programdocuments/docs/Crosscutting\_grand\_challenges.pdf

- 6. <u>The Opportunities and Challenges of Exascale Computing</u>, ASCAC Subcommittee Report,

  <a href="http://science.energy.gov/~/media/ascr/ascac/pdf/reports/Exascale\_subcommittee\_report.pdf">http://science.energy.gov/~/media/ascr/ascac/pdf/reports/Exascale\_subcommittee\_report.pdf</a>
- 7. Scientific Grand Challenges: Architectures and Technology for Extreme Scale Computing, December 2009, <a href="http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Arch\_tech\_grand\_challenges\_report.pdf">http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Arch\_tech\_grand\_challenges\_report.pdf</a>
- 8. Exascale Operating Systems and Runtime Software Report, December 2012, <a href="http://science.energy.gov/~/media/ascr/pdf/research/cs/Exascale%20Workshop/ExaOSR-Report-Final.pdf">http://science.energy.gov/~/media/ascr/pdf/research/cs/Exascale%20Workshop/ExaOSR-Report-Final.pdf</a>
- 9. Scientific Discovery at the Exascale: Report from the DOE ASCR 2011 Workshop on Exascale Data Management, Analysis and Visualization, Houston, TX, <a href="http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Exascale-ASCR-Analysis.pdf">http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Exascale-ASCR-Analysis.pdf</a>
- 10. Synergistic Challenges in Data-Intensive Science and Exascale Computing, DOE ASCAC Data Subcommittee Report, March 2013, <a href="http://science.energy.gov/~/media/ascr/ascac/pdf/reports/2013/ASCAC\_Data\_Intensive\_Computing\_report\_final.pdf">http://science.energy.gov/~/media/ascr/ascac/pdf/reports/2013/ASCAC\_Data\_Intensive\_Computing\_report\_final.pdf</a>
- 11. Report-back slides from the Exascale Planning Workshop, April 2012, http://exascaleresearch.labworks.org/apr2012planningworkshop/
- 12. Exascale Research Conference Meeting materials: http://exascaleresearch.labworks.org/oct2012/

## Section II – AWARD INFORMATION

## A. TYPE OF AWARD INSTRUMENT

DOE anticipates awarding laboratory work authorizations under this DOE National Laboratory Program Announcement. At most two applications as a Prime/Lead institution will be accepted from each National Laboratory. There is no ceiling on the number of applications as a collaborating institution that may be submitted by each National Laboratory. However, the same work should not be included in more than one application.

Participation by non-DOE/NNSA Federal agencies and their Federally Funded Research and Development Center (FFRDC) contractors will be funded under an interagency agreement (but see Section III. A. ELIGIBLE APPLICANTS).

## **B. ESTIMATED FUNDING**

It is anticipated that up to \$4,000,000 per year will be available under this DOE National Laboratory Program 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 may begin in either FY 2015 or FY 2016, depending on the availability of funds.

DOE is under no obligation to pay for any costs associated with preparation or submission of proposals. 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 Program Announcement.

## C. MAXIMUM AND MINIMUM AWARD SIZE

(See B. Estimated Funding section above.)

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

#### Ceiling

\$1,250,000 per year per project, including any collaborating institutions

#### Floor

Suggested minimum: \$100,000 for a university PI collaborating with a DOE national laboratory as part of a larger project. \$300,000 is the expected minimum project size.

## D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

Four to six funded projects are anticipated. 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 Section above.)

It is anticipated that project sizes may range from \$300,000 per year to \$1,250,000 per year, including awards to any and all collaborators.

Award sizes will range from \$100,000 per year to \$1,250,000 per year. The award size will depend on the number of meritorious applications and the availability of appropriated funds.

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

## F. PERIOD OF PERFORMANCE

(See B. Estimated Funding section above.)

DOE is interested in seeing projects supported under this Announcement begin work by February 1, 2015, for awards made in Fiscal Year 2015 and April 1, 2016, for awards made in Fiscal Year 2016.

Awards are expected to be made for a period of three years. Out-year funding will depend upon suitable progress and the availability of appropriated funds.

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

#### G. TYPE OF PROPOSAL

DOE will accept new DOE National Laboratory Proposals under this DOE National Laboratory Program 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 Announcement is for proposals led by DOE laboratories, including DOE/NNSA Federally Funded Research and Development Center (FFRDC) Contractors.

At most two proposals as a Prime/Lead institution will be accepted from each National Laboratory. There is no ceiling on the number of proposals as a collaborating institution that may be submitted by each National Laboratory. Proposed work should not be the same across multiple projects.

Each Senior Person (Principal Investigator, Co-Principal Investigator, and/or other senior researchers who contribute to the intellectual content of a proposal) may participate in at most two proposals.

#### **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.

## D. OTHER ELIGIBILITY REQUIREMENTS

## **Performance of Work in the United States**

DOE requires all work performed by the prime recipient under funding agreements resulting from this Announcement to be performed in the United States – i.e., a prime recipient must expend 100% of its total project costs in the United States, except for sub-awards to foreign entities.

This requirement does not apply to travel or to equipment, materials and supply purchases. Like all proposed costs, proposed travel, equipment, and material and supply costs will be evaluated to determine whether they are necessary and appropriate for the conduct of the effort. Furthermore, it is the sense of the Congress that, to the greatest extent practicable, all equipment and products purchased with funds made available under awards resulting from this Announcement should be American-made.

## 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 <a href="https://pamspublic.science.energy.gov">https://pamspublic.science.energy.gov</a> and clicking on the "PAMS External User Guide" link.

Proposals submitted outside of PAMS will not be accepted.

## **B. LETTER OF INTENT AND PRE-APPLICATION**

#### 1. Letter of Intent

LETTER OF INTENT DUE DATE

A Letter of Intent is not required.

## 2. Pre-proposal

A pre-proposal is required. The page limit is two pages, including references. Only the lead organization should submit a pre-proposal; collaborating organizations need not do so.

Full proposals will be accepted only in response to a pre-proposal that was encouraged. Full proposals will not be accepted for pre-proposals that have been discouraged.

PRE-PROPOSAL DUE DATE

August 27, 2014, at 5:00 PM ET

ENCOURAGE/DISCOURAGE DATE

September 4, 2014, at 5:00 PM ET

The pre-proposal is to help in planning the review and the selection of potential reviewers for the application. For this purpose, the pre-proposal must include the following:

- A cover sheet containing the name and mailing address of the sponsoring institution; the planned title of the research application; the name, e-mail address, and telephone number of the Principal Investigator, additional Senior Investigator(s), and Senior/Key personnel expected to be involved in the planned application.
- A brief abstract that identifies the FOA themes that will be addressed
- Estimated budget request (annual).
- Conflict of interest information as detailed below

To help the Office of Science avoid conflicts of interest (COI) in identifying potential reviewers, a list of collaborators, co-editors, and graduate/postdoctoral advisors and advisees must be submitted with the pre-application. This list should be the final set of pages in the pdf for the pre-application. A single, consolidated COI list for the Lead Principal Investigator and each project

collaborator (supported or unsupported) is required that includes, for all project participants collectively, an alphabetized list of collaborative co-investigators including co-authors of the past 48 months, co-editors of the past 24 months, graduate and postdoctoral advisors/advisees.

Because the COI information provided in the pre-application will be used to identify proposal reviewers, additional Investigators and/or Senior/Key personnel may not be named to the project when the full application is submitted, though the intent to add someone with particular expertise may be mentioned. Project budgets may be revised between submission of the pre-proposal and the full proposal.

It is important that the pre-proposal be a single file with extension .pdf, .docx, or .doc. The pre-proposal must be submitted electronically through the DOE Office of Science Portfolio Analysis and Management System (PAMS) website <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. The Principal Investigator and anyone submitting on behalf of the Principal Investigator must register for an account in PAMS before it will be possible to submit a pre-proposal. All PIs and those submitting pre-proposals on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.

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

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.

## **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 to 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.)

## **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.

## **Submit Your Pre-Proposal:**

- Create your pre-proposal (called a pre-proposal in PAMS) 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 / 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 Pre-proposal" from the dropdown.
- On the Submit Pre-proposal page, select the institution from which you are submitting this pre-proposal 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 pre-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 pre-proposal. Save the pre-proposal for later work by clicking the "Save" button at the bottom of the screen. It will be stored in "My Pre-proposals" for later editing.

- Enter a title for your pre-proposal.
- Select the appropriate technical contact from the Program Manager drop-down.
- To upload the pre-proposal 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 preproposal to DOE.
- Upon submission, the PI will receive an email from the PAMS system <<u>PAMS.Autoreply@science.doe.gov</u>> acknowledging receipt of the pre-proposal.

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

For help with PAMS, click the "External User Guide" link on the PAMS website, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submission and inquiries about this DOE National Laboratory Program Announcement should reference LAB 14-1059.

Pre-proposals submitted outside PAMS will not be considered.

#### C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

## November 3, 2014, at 5:00 PM ET

Full proposals will be accepted only in response to a pre-proposal that was encouraged. Full applications will not be accepted for pre-applications that have been discouraged nor for projects that did not submit a pre-application.

#### **LETTERS**

Letters of collaboration should be included for unfunded collaborators.

Letters of support should not be included.

## 1. Summary of Application Contents and Information about PAMS

Each DOE National Laboratory application 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, containing the following information:
  - o Proposal title
  - o List of all participants by institutional affiliation
  - o Summary of project narrative
- Budget justification, entered into PAMS as a separate pdf

- Proposal, combined into a single pdf containing the following information:
  - o Proposal Cover Page
  - o 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 – 15 page limit)
  - o Appendix 1: Biographical Sketch(es)
  - o Appendix 2: Current and Pending Support
  - o Appendix 3: Bibliography and References Cited
  - o Appendix 4: Facilities and Other Resources
  - o Appendix 5: Equipment
  - o Appendix 6: 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, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. 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: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submissions and inquiries about this Program Announcement should reference LAB 14-1059. Full applications submitted in response to this Program Announcement must be submitted to PAMS no later than the application due date shown above.

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 <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a> 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 <<u>PAMS.Autoreply@science.doe.gov</u>> 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, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. 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: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submissions and inquiries about this Program Announcement should reference **LAB 14-1059**.

## 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, including proposed sub-awards, 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.

Applicants are encouraged to budget for activities and travel that support international coordination on the subjects addressed in this announcement.

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. 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 project summary/abstract is a summary of the proposed activity suitable for distribution to the public and sufficient to permit potential reviewers to identify conflicts of interest. It should be a self-contained document that identifies the name of the applicant, the Principal Investigator (PI), the names of any co-investigators and their institutional affiliations, the project title, the objectives of the project, a description of the project, including methods to be employed, and the potential impact of the project (i.e., benefits, outcomes. A sample is provided below:

## A Really Great Idea

A. Smith, Lead Institution (Principal Investigator)A. Brown, Institution 2 (Co-Investigator)A. Jones, Institution 3 (Co-Investigator)

Text of abstract

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

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. To attach a Project Summary/Abstract, click "Add Attachment."

- Do not include any proprietary or sensitive business information.
- DOE may use the abstract may to prepare public reports about 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 14-1059
- DOE/Office of Science Program Office: Advanced Scientific Computing Research
- DOE/Office of Science Program Office Technical Contact: **Dr. Lucy Nowell**
- Research Themes in the Lab Announcement to which the proposal responds
- PAMS Pre-Application Tracking Number:

## COVER PAGE SUPPLEMENT FOR COLLABORATIONS

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

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

Each collaborative group can have only one lead institution. The common narrative must identify the lead institution and must contain a summary table describing the budget breakdown by institution for all participants.

Collaborations that include non-DOE National Laboratory participants should note that proposals from organizations other than a DOE National Laboratory should be submitted in response to the companion Funding Opportunity Announcement (DE-FOA-0001059) through Grants.gov.

If the project is a collaboration, provide the following information on a separate page as a supplement to the cover page.

- List all collaborating institutions by name with each institution's principal investigator on the same line.
- Indicate the lead PI who will be the point of contact and coordinator for the combined research activity.
- Provide a statement explaining the leadership structure of the collaboration.
- Include a table modeled on the following chart providing summary budget information from all collaborating institutions. Provide the total costs of the budget request in each year for each institution and totals for all rows and columns.

			Collaborative Proposal Information				
	Names	Institution	Fiscal Year 1 Budget	Fiscal Year 2 Budget	Fiscal Year 3 Budget	Fiscal Year 4 Budget	Total Budget
Lead PI							
Co-PI							
Co-PI							
		Total Budget per Fiscal Year					

Example budget table (\$ in thousands)

Collaborations that include an institution other than DOE national laboratories should note that proposals from university, industry and/or not-for profit institutions should be submitted in response to the companion DE-FOA-0001059 through Grants.gov.

## PROJECT NARRATIVE (NO MORE THAN 15 PAGES LONG)

The project narrative **must not exceed 15 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.

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 narrative should provide a clear, concise statement of the specific objectives/aims of the proposed project. The major part of

<sup>\*</sup> Note that collaborating proposals must be submitted separately.

the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project.

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

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

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.

For Collaborative Proposals Only: Each collaborating institution must submit an identical common narrative. The common narrative must identify which tasks and activities will be performed by which of the collaborating institutions in every budget period of the proposed project. The budget and the budget justification—which are unique to each collaborating institution—may refer to parts of the common narrative to further identify each collaborating institution's activities in the joint project. There should be no ambiguity about each institution's role and participation in the collaborative group.

The Office of Science will use the multiple applications associated with a collaborative group to create one consolidated document for merit review that consists of the common, identical application materials combined with a set of detailed budgets from the partner institutions. It is very important that every application in the collaborative group have identical titles and technical narratives. Budget and budget justification pages will differ for each institution.

Management Plan and Timeline of Activities: This section should describe the management structure, how effective collaborations among the participants will be fostered, how integration of experimental and theoretical efforts will be attained, and the timeline for all major activities including performance metrics and deliverables. Include the following summary level budget tables:

Task	PI(s)	Role(s)	Year 1 Budget	Year 2 Budget	Year 3 Budget	Total Budget
Task 1						
Task 2						
Task.3.						
Total						

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 project director/principal investigator (PD/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. The biographical information (curriculum vitae) must not exceed 2 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, which does not count in the page limit for the biographical sketch:

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

**Personally Identifiable Information**: Do not include sensitive 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 lead principal investigator and each principal investigator, including sub-awardees, for ongoing projects and pending applications. For each organization providing support, show the total award amount for the entire award period (including indirect costs) and the number of person-months per year to be devoted to the project by the PI. Include the award number, title of the funded research project, and the name of the PI for the project. Briefly describe the research being performed and explicitly identify any overlaps 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 application. 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, Computer, User Facilities, 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. For access to ASCR-supported user facilities or other DOE Office of Science (SC) supported user facilities, please describe past access and experience with these facilities. 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: 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 application. 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.

Travel budgets should include support for participation in a kick-off meeting, at least one annual PI meeting, and, where appropriate, costs for project meetings that span collaborating institutions.

International travel to support participation in relevant conferences, workshops, and engagement with the broader research community is encouraged

## **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

Not applicable.

## 2. Pre-proposal Due Date

August 27, 2014, at 5:00 PM ET

(A pre-proposal is required.)

You are encouraged to submit your pre-application well before the deadline.

#### 3. Proposal Due Date

November 3, 2014, at 5:00 PM ET

You are encouraged to transmit your application 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, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. 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: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submission and inquiries about this DOE National Laboratory Program Announcement should reference **LAB** 14-1059.

## 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 - APPLICATION 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 Announcement, including the required Pre-proposal has been submitted; (3) all mandatory requirements are satisfied; (4) the proposed project is responsive to the objectives of the DOE National Laboratory Announcement, and (5) the proposed project is not duplicative of programmatic work.

Applications that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

## **B. REVIEW AND SELECTION PROCESS**

#### 2. Merit Review Criteria

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

- Scientific and/or Technical Merit of the Project;
- Appropriateness of the Proposed Method or Approach;
- Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
- Reasonableness and Appropriateness of the Proposed Budget.

The evaluation process will include program policy factors such as the relevance of the proposed research to the terms of the Announcement and the agency's programmatic needs. Note that external peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Both Federal and non-Federal reviewers may be used, and submission of an application 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 established by regulation:

SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH

What is the scientific innovation of proposed effort? How does the proposed work compare with other efforts in its field, both in terms of scientific and/or technical merit and originality? How might the results of the proposed work impact the direction, progress, and thinking in relevant scientific fields of research? What is the likelihood of achieving influential results?

- Briefly summarize the proposal technical content in your own words.
- What are the strengths and weaknesses of the proposed research with respect to each of the themes in the funding announcement that are addressed in the proposal?

- Evaluate the overall responsiveness of the proposed research to the funding announcement and the potential of the proposed research have a significant impact on the resilience of scientific applications and/or extreme scale platforms. If successful, to what degree would the proposed research be likely to improve the ability of scientific applications to run to completion and achieve results that are correct or within acceptable bounds for error on an extreme scale supercomputer?
- Does the application advance DOE's mission of supporting open-source software as
  described in the policy applicable to DOE National Laboratories at:
  <a href="http://science.energy.gov/~/media/ascr/pdf/research/docs/Doe\_lab\_developed\_software\_policy.pdf">http://science.energy.gov/~/media/ascr/pdf/research/docs/Doe\_lab\_developed\_software\_policy.pdf</a>

#### APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH

Does the proposed effort employ innovative concepts or methods? How logical and feasible are the approaches? Are the conceptual framework, methods, and analyses well justified, adequately developed, and likely to lead to scientifically valid conclusions? Does the applicant recognize significant potential problems and consider alternative strategies?

- Does the proposal reflect sufficient understanding of the challenges presented by the expected exascale architecture and software environment for the research to be successful?
- Evaluate the plan for conducting the research. Is there a clear and coherent plan for the proposed research so that it is an integrated endeavor? Especially for collaborative proposals, is there strong enough leadership, communication and coordination? Does the proposal include a clear plan for deliverables, a reasonable timeline, and sound methods for assessing the effectiveness of the research?
- What is the proposed plan for sharing the results of the proposed research and making available under open source license any software that is developed? Is the plan appropriate and credible?

COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES Does the proposed work take advantage of unique facilities and capabilities? What is the past performance of the team? How well qualified is the team to carry out the proposed work? Are the environment and facilities adequate for performing the proposed effort?

REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET Are the proposed budget and staffing levels adequate to carry out the proposed work? Is the budget reasonable and appropriate for the scope?

- Are the levels of support and commitment requested by the PI and other senior personnel appropriate and necessary to meet the research objectives? Does the budget include senior managers who will not contribute to the research?
- Is the proposed budget for travel reasonable and appropriate for the number of people supported and the level of coordination that is necessary for the project to succeed?

#### 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 expected that awards may be made in Fiscal Years 2015 and 2016.

DOE is interested in seeing projects supported under this Announcement at DOE National Laboratories begin work by January 15, 2015, for awards made in Fiscal Year 2015 and April 15, 2016, for awards made in Fiscal Year 2016. Start dates for applications chosen for award will be negotiated during the budget negotiation process.

The suggested start date for organizations other than DOE National Laboratories is February 1, 2015. For awards made in Fiscal Year 2016, the suggested start date is April 1, 2016.

## 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, <a href="https://pamspublic.science.energy.gov/">https://pamspublic.science.energy.gov/</a>. 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: <a href="mailto:sc.pams-helpdesk@science.doe.gov">sc.pams-helpdesk@science.doe.gov</a>. All submission and inquiries about this DOE National Laboratory Program Announcement should reference **LAB 14-1059**.

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	855-818-1846 (toll-free)
Customer Support	301-903-9610
	sc.pams-helpdesk@science.doe.gov
Program Manager	Technical/Scientific Program Contact:
Scientific Contact	
	Advanced Scientific Computing Research
	For topics 1 and 2:
	Dr. Lucy Nowell
	301-903-3191
	<u>Lucy.Nowell@science.doe.gov</u>
	For topic 3:
	Dr. Robinson Pino
	301-903-1263
	Robinson.Pino@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.