# PROGRAM ANNOUNCEMENT TO DOE NATIONAL LABORATORIES



# U. S. Department of Energy Office of Science Office of Advanced Scientific Computing Research and Office of Biological and Environmental Research

Extreme-Scale Application Software Development Productivity (Extreme-Scale Software Infrastructure)

DOE National Laboratory Announcement Number: LAB 14-0001 Announcement Type: Initial

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Letter of Intent Due Date: 06/04/2014 at 5:00 PM Eastern Time

A Letter of Intent is required

Pre-Proposal Due Date: N/A

Proposal Due Date: 06/25/2014 at 5:00 PM Eastern Time

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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>.

- 1. Click the "No, I have never had an account" link and then the "Create Account" button.
- 2. 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.
- 3. 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.
- 4. 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.
- 5. 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, <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 14-0001**.

# Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

# GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

# **Technical/Scientific Program Contacts:**

DOE Office of Advanced Scientific Computing Research

Dr. Thomas Ndousse-Fetter Phone: 301-903-5710

Email: thomas.ndousse-fetter@science.doe.gov

FAQ: http://science.energy.gov/ascr/funding-opportunities/

DOE Office of Biological and Environmental Research

Dr. David Lesmes Email: 301-903-2977

Email: <u>David.Lesmes@science.doe.gov</u>

### **SUMMARY**

The Offices of Advanced Scientific Computing Research (ASCR) and Office of Biological and Environmental Research in the Office of Science (SC) at the U.S. Department of Energy (DOE) hereby invites proposals with the potential to improve the productivity of application software development for multiscale and multi-physics modeling and simulation on heterogeneous extreme-scale computing systems. Extraordinary advances in computing hardware technologies and architectures have produced several orders of magnitude of computing performance improvements in the last decade. However, these improvements have not been directly translated into corresponding performance gains in application software development productivity in terms of exploiting advanced hardware capabilities, reduced time to application software development, and improved application software performance at execution time. Developers of multiscale and multi-physics application software increasingly find it difficult to build parallel software that adapts to rapidly changing hardware and at the same time harnesses the full capabilities of these emerging extreme-scale computing systems. This has created what is now commonly referred to as "the extreme-scale software productivity gap." The focus of this Program Announcement is on parallel-software productivity improvement tools and methodologies to address the software development productivity gap.

Information that is more specific is included under SUPPLEMENTARY INFORMATION below.

# SUPPLEMENTARY INFORMATION

With the introduction of a new generation of multicore-based computing hardware featuring specialized accelerators, high fidelity simulations of coupled multiscale and multi-physics problems that were once intractable are now becoming feasible in many domain science areas. However, using these computing systems effectively will require a significant effort in the

development of parallel application software. For domain scientists developing parallel application software, the challenges are three fold: a) developing a new-generation of application software that exploits the multi-level parallelism, b) refactoring or transforming legacy application software using advanced parallel software engineering approaches, and c) ensuring that both new and refactored application software are engineered to be reusable, interoperable, and portable across heterogeneous extreme-scale computing systems. The main objective of this Program Announcement is to develop scalable parallel software tools and methodologies to enable development of reusable and portable application software that works efficiently with emerging heterogeneous extreme-scale computing systems. Applicants interested in submitting to this Program Announcement should do so in the context of parallel application software for multiscale and multi-physics simulation on extreme-scale systems, using the case study provided in this Program Announcement as an extreme-scale application software development environment to test and validate their proposed approaches, tools, and methodologies. Specific issues of interest for this Program Announcement include, but are not limited to, the following in the context of the case study multiscale and multi-physics described below:

- a) Parallel software development tools and methodologies —The complexity of parallel application software rises sharply with the complexity of the underlying parallel hardware architectures, programming models, and multiscale/multi-physics system structure and functions. Addressing the complexities requires a suite of new automated parallel software development tools such as parallel software patterns and stencils, tools for exploiting multi-level parallelism, numerical couplers, unit and integration testing tools, model driven and/or agile methodologies, etc., that assist application software developers to build codes that are reusable, portable, interoperable, easily testable, and that exploit the underlying hardware capabilities;
- b) **Portable and reusable parallel software components and libraries** Widely used scientific software components, especially numerical libraries such as PETSc, Trilinos, Chombo, to name but few, have inherent limitations in exploring multilevel parallelism and other software productivity concepts. These libraries have to be transformed to enable interoperability, modularity, reusability, and portability across heterogeneous multicore/many core hardware systems (with or without attached accelerators) without major re-writing and without sacrificing performance portability and numerical accuracy;
- c) Scalable parallel software tools and methodologies to re-factor legacy Code Legacy software represent several decades of major software investments in major domain sciences. These include major numerical and software libraries not optimized for heterogeneous multicore/many-core systems used in the development of scientific codes. Changing the structure of legacy code to exploit the new capabilities of multicore-based systems without altering its behavior and numerical accuracy remains a software development challenge. Addressing these challenges requires new software refactoring tools and software engineering that produces minimum disruption to scientific communities.

The proposed tools and approaches must further include techniques or mechanisms to address additional parallel software requirements for extreme-scale computing, such as resilience, energy-awareness, uncertainty quantifications (UQ), and validation and verification (V&V). The proposed approaches and tools must also include strategies addressing multi-physics software strategies for coupled applications with interacting physics

at multiple scales. This will require the investigation of software coupling techniques to support interaction and interoperability of software components at different scale. This requirement is described in detail in the multiscale and multi-physics software engineering case study described in this Program Announcement.

# **Parallel Software Development Infrastructure**

The parallel software development issues outlined above are interdependent and may not be addressed effectively in isolation. The ultimate objective of the propose effort should be to build a parallel software infrastructure that consists of a suite of seamlessly integrated parallel tools, methodologies, architectures, and software engineering best-practice archives. Each proposal should therefore be structured as a multidisciplinary team effort aimed at developing software tools and methodologies that can be seamlessly integrated into a scalable parallel software development infrastructure, easily reusable and adaptable by a wide range of multiscale and multi-physics communities.

# **Validation of Proposed Research Outcome**

A specific multiscale and multi-physics application from the Office of Biological and Environmental Research (BER) in DOE's Office of Science has been selected as a use-case for this Program Announcement to enable the testing and validation of the proposed parallel software tools and methodologies. It is anticipated that the resulting parallel software developed for the representative application described in the case study below will be executed on DOE/ASCR's computing systems at the National Energy Research Scientific computing Center, Oak Ridge Leadership Computing Facility, and Argonne Leadership Computing Facility. These systems together constitute a rich extreme-scale computing environment featuring diverse hardware and architectures of the types described in this Program Announcement. Applicants are therefore encouraged to include in their research plans co-PIs from the case-study physics application described below to ensure the relevance of the application software development tools and related efforts.

# Case Study: Earth System Modeling and Simulation: A Multiscale/Multi-physics Software Challenge on Extreme-scale Computing Systems

# **Point of Contact:**

DOE Office of Biological and Environmental Research

Dr. David Lesmes Email 301-903-2977

Email: David.Lesmes@science.doe.gov

A major goal of BER is to advance a predictive understanding of terrestrial environments extending from bedrock to the atmosphere and from cellular to global scales in order to support DOE's energy and environmental missions. Capturing the multiscale and multi-physics structure and function of complex earth systems in mechanistic models is a computational grand challenge. Development of multiscale-multi-physics models demands sophisticated tools at different scales and levels of description, which, until the advent of extreme-scale computing,

have been computationally intractable. The availability of efficient software development tools remains a major productivity bottleneck in exploiting the capabilities of the advanced computational hardware for high-fidelity simulation of multiscale and multi-physics problems.

The following use-case for this Program Announcement has been selected to: a) motivate the development of a new generation of earth systems modeling software that exploits the capabilities of emerging extreme-scale computing systems; b) explore new parallel software tools and software engineering approaches to re-factor legacy codes; and c) provide a real-world multiscale and multi-physics environment to validate, test, and establish new approaches and methodologies for developing parallel-software in the climate and earth system modeling communities. The ultimate goal of the case study is to prepare climate and earth systems modeling and simulation codes for exascale computing systems in the next decade.

# Specific Case Study: Multiscale-Multi-physics Modeling of Terrestrial Environments

Improved earth system models are required to more accurately project the impacts of climate change on terrestrial systems and to inform strategies for adaptation. Improved code fidelity requires increased skill to capture the responses of complex multiscale, multi-physics interactive systems as driven by relatively subtle changes in driving conditions. The imperative to improve Earth System Model performance and climate projections requires advances in model resolution, in order to increasingly resolve rather than parameterize physics, and advances in model complexity. Earth system models, including those supported by BER, must therefore be redesigned and refactored toward efficiency in advanced architectures, but also engineered in a manner that facilitates modularity, flexibility of process resolution, and hierarchical testing.

The land components of coupled Earth System Models are highly parameterized with limited mechanistic detail especially in terms of terrestrial hydrological processes. The land component of DOE's new earth system model (ACME) uses a reactive transport code (PFLOTRAN) to model the terrestrial subsurface. As reactive transport codes are inherently three-dimensional and processes resolving the same framework can be used to model the structure and function of subsurface systems across a wide range of spatial and temporal scales with varying degrees of mechanistic detail. The next generation of reactive transport models (RTMs) should be designed to be hierarchical, modular, and scalable to advanced architectures, and to be extensible so that they can be used as the terrestrial substrate on which to build "Virtual Ecosystems". The next generation multiscale-multi-physics RTMs should support the development of virtual ecosystems that extend from a coupled plant-soil-microbiome system to crops in a field including bioenergy feedstocks, to watersheds with natural vegetation of varying complexity, to the physical hydrology of river basins. They should also be seamlessly integrated with the next generation of Earth System Models.

# Specific Multiscale and Multi-Physics Parallel Software Challenges

Particular elements in software design that will enable next-generation multiscale-multi-physics Earth System Modeling code improvements may include:

- Improvement and synthesis of libraries as needed by the chosen applications (e.g., Trilinos, PETSc, Chombo, MOAB, Dakota), with architecture-aware codes and ability to extract single modules;
- Frameworks that enable hierarchical and interoperable code building and experimental designs and that include embedded diagnostics and automated hierarchical testing;
- Coupling and building tools that enable and improve coupling within and between model components;
- Development of adaptable libraries and approaches for exposing more thread parallelism in 0D or 1D solvers-- useful, for example, for solving biogeochemical ODE's and physics routines;
- Development of libraries and approaches to working with overlapping communication of guard cells with 2D nearest-neighbor stencil operations for block-structured and unstructured meshes;
- Tools and expertise to identify and address load-imbalances and trouble-shoot communication and IO at scale;
- Software and expert support for UQ and data assimilation, needed in order to test model
  parameterizations and sensitivities, to identify coupling effects and errors, to analyze
  code skill and performance, and ultimately to link climate projection uncertainty to
  uncertainties in model components versus drivers.

The resulting software should be designed to be scalable to diverse computer architectures including at least two different DOE leadership class-computing facilities in addition to NERCS.

# **Project Management plan**

Potential applicants must provide a comprehensive management plan to effectively manage a large multi-disciplinary team. This should include effective metrics and concrete milestones to assess the progress of the overall team effort.

# **Software Engineering/Productivity References**

- ASCR Workshop on Software Productivity for Extreme-Scale Science, October 2013. workshop report
  - http://www.orau.gov/swproductivity2014/SoftwareProductivityWorkshopReport2014.pdf
- 2. H. Johansen et al, <u>Extreme-Scale Scientific Application Software Productivity: Harnessing the Full Capability of Extreme-Scale Computing</u>, whitepaper, September 9, 2013.
- 3. R. Bartlett, M. Heroux, J. Willenbring, TriBITS Lifecycle Model Version 1.0: A Lean/Agile Software Lifecycle Model for Research-based Computational Science and Engineering and Applied Mathematical Software, SANDIA REPORT SAND2012-0561, February 2012.

- 4. V. R. Basili et al., Understanding the HPC Community: A Software Engineer's Perspective, **IEEE Software**, July 2008, 25(4):29–36, http://dx.doi.org/10.1109/MS.2008.103
- J. C. Carver, Report: The Second International Workshop on Software Engineering for CSE, Computing in Science and Engineering, 11(6), 2009, http://dx.doi.org/10.1109/MCSE.2009.203
- 6. S. Falk et al., Measuring HPC Productivity, **IJHPCA**, Winter 2004, 18(4):459–473, http://dx.doi.org/10.1177/1094342004048539
- 7. W. W. Gibbs, Software's Chronic Crisis, Scientific American, Sept 1994.
- 8. C. Greenough, D. J. Worth, and L. S. Chin, Thoughts on Software Engineering for Exascale Software Development, 2011, SEG- N-018, http://www.stfc.ac.uk/CSE/resources/PDF/EESI.pdf
- 9. J. Kepner, Guest Editor, High Productivity Computing Systems and the Path Towards Usable Petascale Computing, Part B: System Productivity Technologies, **Cyberinfrastructure Technology Watch (CTWatch) Quarterly**, <a href="http://www.ctwatch.org">http://www.ctwatch.org</a>, 2 (4B), Nov 2006.
- 10. D. E. Keyes et al, Multiphysics simulations: Challenges and opportunities, **IJHPCA**, 27(1):4–83, Feb 2013, special issue, <a href="http://dx.doi.org/10.1177/1094342012468181">http://dx.doi.org/10.1177/1094342012468181</a>.
- 11. G. Miller, A Scientist's Nightmare: Software Problem Leads to Five Retractions, **Science**, Dec 22, 2006, vol. 314, no. 5807, pp. 1856-1857, <a href="http://dx.doi.org/10.1126/science.314.5807.1856">http://dx.doi.org/10.1126/science.314.5807.1856</a>
- 12. Extreme-Scale Solvers: Transition to Future Architectures Workshop Report, March 2012. Report

# **Terrestrial Environments Modeling References**

- **1.** BER Virtual Laboratory: Innovative Framework for Biological and Environmental Grand Challenges; A Report from the Biological and Environmental Research Advisory Committee, DOE/SC-0156 [pdf], February 2013
- Community Modeling and Long-Term Predictions of the Integrated Water Cycle BER
  Workshop Report, September 2012.
  <a href="http://science.energy.gov/~/media/ber/pdf/workshop%20reports/Water\_Cycle\_Report\_LR.pd">http://science.energy.gov/~/media/ber/pdf/workshop%20reports/Water\_Cycle\_Report\_LR.pd</a>
  f
- 3. Research for Sustainable Bioenergy: Linking Genomic and Ecosystem Sciences BER Workshop Report, May 2014. http://genomicscience.energy.gov/sustainability/SustainableBiofuels.pdf
- 4. Complex Systems Science for Subsurface Fate and Transport BER Workshop Report, August 2009.
  - http://science.energy.gov/~/media/ber/pdf/SubsurfaceComplexity\_03\_05\_10.pdf
- 5. R.M., Maxwell, et al., Surface-subsurface model intercomparison: A first set of benchmark results to diagnose integrated hydrology and feedbacks, **Water Resources Research**, 50(2) 1531-1549, doi:10.1002/2013WR013725, 2014

- **6.** T. D. Scheibe, et al., <u>An analysis platform for multiscale hydrogeologic modeling with emphasis on hybrid multiscale methods</u>, **Groundwater**, doi10.1111/gwat.12179, 2014.
- 7. C. I. Steefel, et al., Reactive transport modeling: An essential tool and a new research approach for the Earth science, **Earth and Planetary Science Letters**, 240: 539-558, 2005.
- 8. Developing a Hierarchical Scaling Framework for Modeling a Dynamic Arctic Landscape in a Changing Climate, A white paper by the <u>NGEE Arctic</u> science team, November 23, 2011.

  Report
- 9. Using Process Studies and Observations to Guide, Parameterize, and Evaluate a Hierarchical Scaling Framework for NGEE Arctic, A white paper by the NGEE Arctic science team, January 18, 2012.
- 10. D. Wang, et al., 2014. <u>A Functional Testing Platform for the Community Land Model</u>, <u>Environmental Modeling and Software</u>, Vol. 55, pp25-31, 10.1016/j.envsoft.2014.01.015.

### **Collaboration**

Collaborative research projects with other institutions such as universities, industry, non-profit organizations, and Federally Funded Research and Development Centers (FFRDCs), including the DOE National Laboratories are strongly encouraged but not required. Collaborative proposals submitted from different institutions should clearly indicate they are part of a proposed collaboration. All collaborative proposals must use the same title, abstract and technical narrative. In addition, such proposals must describe the work and the associated budget for the research effort to be performed under the leadership of the principal investigator in each participating institution. The first page of collaborative proposals should contain the project title followed by a tabular list of the researcher names, institutions, annual budget, and role as lead PI or co-PI of each participant. These collaborative proposals should all have the same title as the lead institution. Each collaborating institution submitting a proposal must use the same title.

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

# **Section II – AWARD INFORMATION**

# A. TYPE OF AWARD INSTRUMENT

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

# **B. ESTIMATED FUNDING**

It is anticipated that up to \$4,000,000 per year will be available under this Program Announcement and funding is contingent on satisfactory peer review and the availability of appropriate funds. Applicants should request project support for three years, with out-year support contingent on the availability of appropriated funds, progress of the research, and programmatic needs. Awards are expected to begin in Fiscal Year 2014, which ends on September 30, 2014.

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

This Program Announcement anticipates to fund a single large application software development project at a total budget of \$4,000,000 per for three years. Each institution that participates in a funded project receives a separate award as described in accompanying budget pages and justifications.

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

### D. EXPECTED NUMBER OF AWARDS

This Program Announcement anticipates funding a single large software co-development project at a total budget of \$4,000,000 per year for three years.

# E. ANTICIPATED AWARD SIZE

This Program Announcement anticipates funding a single large application software development project at a total budget of \$4,000,000 per year for three years. Each institution that participates in a funded project receives a separate award as described in accompanying budget pages and justifications.

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

# F. PERIOD OF PERFORMANCE

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

# 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 is a DOE Lab-only Announcement. FFRDCs from other Federal agencies are not eligible to submit in response to this Program Announcement.

For official postings, see the Office of Science Grants and Contracts web site, <a href="http://www.science.energy.gov/grants">http://www.science.energy.gov/grants</a>.

# **B. COST SHARING**

Cost sharing is not required.

# C. ELIGIBLE INDIVIDUALS

Eligible individuals with the skills, knowledge, and resources necessary to carry out the proposed research as a Principal Investigator 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 <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-PROPOSAL

### 1. Letter of Intent

LETTER OF INTENT DUE DATE
June 4, 2014 at 5 PM Eastern Time

A Letter of Intent is required and must be submitted by 06/04/2014 at 5 PM Eastern Time.

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

- A cover sheet containing the name and mailing address of the sponsoring institution; the Lead Principal Investigator and additional principal investigators (PIs) (and their planned title of the research application; the name, e-mail address, and telephone number institutions) expected to be involved in the planned application.
- A brief abstract
- Estimated budget request (annual)

The LOI 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>. It is important that the LOI be a single file with extension .pdf, .docx, or .doc. The Lead Principal Investigator and anyone submitting on behalf of the Lead PI must register for an account in PAMS before it will be possible to submit a letter of intent. All Lead PIs and those submitting LOIs on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to avoid submission delays.

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

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

0. Click the "No, I have never had an account" link and then the "Create Account" button.

- 1. 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.
- 2. 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.
- 3. 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. (If you have been an Office of Science merit reviewer or if you have previously submitted an application, you may already be linked to an institution in PAMS. If this happens, you will be taken 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 do not need to enter the exact name of the institution, but you should enter a word or phrase contained within the institution name. (If your institution has a frequently used acronym, such as ANL for Argonne National Laboratory or UCLA for the Regents of the University of California, Los Angeles, you may find it easiest to 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.
- If, after searching, you think your institution is not currently in the database, click the "Cannot Find My Institution" button and enter the requested institution information into PAMS. Click the "Create Institution" button. PAMS will add the institution to the system, associate your profile with the new institution, and return you to the "Institutions List" page when you are finished.

# **Submit Your Letter of Intent:**

- Create your letter of intent outside the system and save it as a file with extension .docx, .doc, or .pdf. Make a note of the location of the file on your computer so you can browse for it later from within PAMS.
- Log into PAMS and click the Proposals tab. Click the "View / Respond to Funding Opportunity Announcements" link and find the current announcement in the list. Click the

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

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

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 Funding Opportunity Announcement should reference **LAB 14-0001.** 

# 2. Pre-proposal

PRE-PROPOSAL DUE DATE N/A

ENCOURAGE/DISCOURAGE DATE N/A

# C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

June 25, 2014 at 5:00 PM Eastern Time

LETTERS

<u>Do not submit letters of support or endorsement as these are not used in making funding decisions and can interfere with the selection of peer reviewers.</u>

# 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:
  - 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 20 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 14-0001. Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than June 25, 2014 at 5:00 PM Eastern Time.

All PIs and those submitting on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to ensure timely submissions. To register, click "Create New PAMS Account" on the website <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 < 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, <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 14-0001.

# 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 should have three annual budget periods. Please enter the following budget period start and end dates into PAMS for proposals submitted to this Announcement:

- Budget Period 1: 9/1/2014 8/31/2015
- Budget Period 2: 9/1/2015 8/31/2016
- Budget Period 2: 9/1/2016 8/31/2017

PAMS will calculate the cumulative budget totals for you.

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

# PROJECT SUMMARY/ABSTRACT (NO MORE THAN ONE PAGE)

The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to the public. It should be a self-contained document that identifies the name of the applicant, the Principal Investigator (PI), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes). This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed 1 page when printed using standard 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:
- Lead PI name, telephone number, email:
- DOE National Laboratory Announcement Number: LAB 14-0001
- DOE/Office of Science Program Office: **Office of Advanced Scientific Computing Research**
- DOE/Office of Science Program Office Technical Contact: **Dr. Thomas Ndousse-Fetter**
- PAMS Pre-proposal Number:

# COVER PAGE SUPPLEMENT FOR COLLABORATIONS

Collaborative proposals submitted from different institutions must clearly indicate they are part of a collaborative project/group. Every partner institution must submit a proposal through its own sponsored research office. Each proposal within the collaborative group, including the narrative and all required appendices and attachments, must be identical with one exception: The exception is that each proposal must contain unique budget and budget justification documents corresponding to the expenditures for that proposal'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.

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

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

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

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

Example budget table (\$ in thousands)

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.

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 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.

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

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 Principal Investigator (PI) 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 professional and scholarly activities related to the effort proposed. Some examples might be invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society membership and/or activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences.

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 make use of.

- Do not attach a separate file.
- 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 Principal Investigator(s) (PI) for ongoing projects and pending proposals. 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. Do not list start-up funds provided to the PI by the employing academic institution. Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of a proposal 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). 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. 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 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 ATTACHMENTS**

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, and reviewers may not have time to read extensive appendix materials with the same care they would use with the proposal proper.

- 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

June 4, 2014 at 5:00 PM Eastern Time

# 2. Pre-proposal Due Date

N/A

# 3. Proposal Due Date

June 25, 2014 at 5:00 PM Eastern Time

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

Modifications to the proposal are not allowed after the proposal due date.

### 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 14-0001.

# 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 DOE National Laboratory Announcement 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. 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.

- 1. Scientific and/or Technical Merit of the Project;
- 2. Appropriateness of the Proposed Method or Approach;
- 3. Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
- 4. 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 DOE National Laboratory 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 a proposal constitutes agreement that this is acceptable to the investigator(s) and the submitting institution.

The following questions will be posed to reviewers for each of the review criterion listed above:

# 1. Scientific and/or Technical Merit of the Proposed Research

- What is the scientific or technical innovation of the proposed research?
- To what extent is the proposed research likely to achieve valuable results?
- To what extent might the results of the proposed research impact the direction, progress, and thinking in areas relevant to extreme-scale science research?
- How does the proposed research compare with other research in its field, both in terms of scientific and/or technical merit and originality?

# 2. Appropriateness of the Proposed Method or Approach

- To what extent are the research approaches logical and feasible?
- To what extent does the proposed research employ innovative concepts or methods?
- To what extent are the conceptual framework, methods, and analysis well justified, adequately developed, and likely to lead to scientifically valid conclusions?

• To what extent does the proposed research recognize significant potential problems and consider alternative strategies?

# 3. Competency of Applicant's Personnel and Adequacy of Proposed Resources

- To what extent does the project team have the requisite background and level of expertise to accomplish the proposed research?
- To what extent are the technical responsibilities of senior or key personnel clearly and adequately described?
- How well organized is the timeline for major research goals and objectives?
- To what extent does the proposed work take advantage of unique facilities and capabilities?

# 4. Reasonableness and Appropriateness of the Proposed Budget

- To what extent are the personnel staffing levels adequate for carrying out the proposed research?
- To what extent is the budget reasonable and appropriate for the scope of research?

# **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 Official will consider the merit review recommendations, program policy factors, programmatic priorities, and the amount of funding available.

### 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 August 1, 2014. It is expected that awards will be made in Fiscal Year 2014.

DOE is interested in having projects supported under this Program Announcement begin work by September 1, 2014.

# 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 14-0001.

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
	DOE Office of Advanced Scientific Computing Research
	Dr. Thomas Ndousse-Fetter
	Phone: 301-903-9960
Program Managers	Email: <u>Thomas.ndousse-fetter@science.doe.gov</u>
Scientific Contact	
	DOE Office of Biological and Environmental Research
	Dr. David Lesmes
	Email 301-903-2977
	Email: <u>David.Lesmes@science.doe.gov</u>

# **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.doe.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.