# PROGRAM ANNOUNCEMENT TO DOE NATIONAL LABORATORIES



# U. S. Department of Energy Office of Science Advanced Scientific Computing Research and Office of Nuclear Energy Office of Accelerated Innovation in Nuclear Energy

# Scientific Discovery through Advanced Computing: Partnership in Nuclear Energy Research

DOE National Laboratory Announcement Number: LAB 17-1674
Announcement Type: Initial

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Letter of Intent Due Date: 02/15/2017 at 5 PM Eastern Time

(A Letter of Intent is strongly encouraged)

Proposal Due Date: 04/05/2017 at 5 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>.

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

#### 2. REGISTER TO YOUR INSTITUTION:

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

For help with PAMS, click the "External User Guide" link on the PAMS website, <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 17-1674**.

# **UPDATES AND REMINDERS**

#### RECOMMENDATION

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

# DATA MANAGEMENT PLAN

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

# ACKNOWLEDGMENT OF FEDERAL SUPPORT

"This material is based upon work supported by the U.S. Department of Energy, Office of Nuclear Energy, Office of Accelerated Innovation in Nuclear Energy, and Office of Science, Office of Advanced Scientific Computing, SciDAC Partnership for Nuclear Energy Research, under Award Number(s) [Enter the award number(s)]."

# Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

# GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

# **Technical/Scientific Program Contacts:**

Mr. Dan Funk 301-903-3845 Dan.Funk@nuclear.energy.gov

Dr. Randall Laviolette
301-903-5195
Randall.Laviolette@science.energy.gov

#### **SUMMARY**

The Office of Nuclear Energy (NE) and the Office of Advanced Scientific Computing Research (ASCR, in the Office of Science (SC)), both of the U.S. Department of Energy (DOE), hereby announce their interest in receiving applications to the *Scientific Discovery through Advanced Computing (SciDAC)* program for SciDAC Partnerships (hereafter, Partnerships), in areas of particular relevance to the research goals of the Office of Nuclear Energy.

This solicitation is part of the 2017 re-competition of the SciDAC Partnerships for jointly funded and managed collaborations between engineers or scientists sponsored by NE and applied mathematicians or computer scientists sponsored by ASCR.

Additional details and guidance are provided under SUPPLEMENTARY INFORMATION below. A companion Funding Opportunity Announcement will be posted on the SC Grants and Contracts web site at: <a href="http://science.energy.gov/grants/lab-announcements/open/">http://science.energy.gov/grants/lab-announcements/open/</a>.

# SUPPLEMENTARY INFORMATION

The SciDAC Program - Background and Objectives: The SciDAC program (<a href="http://www.scidac.gov">http://science.energy.gov/ascr/research/scidac</a>) has been a recognized leader for the employment of high-performance computing for scientific discovery. Initiated in 2001, re-competed in 2006, and most recently re-competed in 2011-2012, SciDAC had involved all of the SC programs with a goal to dramatically accelerate progress in scientific computing. This SciDAC Partnership therefore must demonstrate deep, necessary, and productive collaborations between scientists or engineers on the one hand and applied mathematicians or computer scientists on the other, which overcome the barriers between these disciplines, fully exploit the capabilities of DOE HPC systems, and accelerate scientific discovery. In this way, partnerships enable scientists or engineers to conduct complex computations at a level of fidelity needed to simulate real-world conditions and accelerate advances in nuclear energy research.

**NE Objectives:** The NE mission encourages the development and exploration of advanced nuclear science and technology. NE promotes nuclear energy as a resource capable of meeting the Nation's energy, environmental, and national security needs by resolving scientific, technical, and regulatory challenges through research, development, and demonstration. The challenge of accelerating innovation and concept development in applied nuclear technologies requires the development and deployment of advanced modeling and simulation capabilities that are more predictive, and can be fully integrated into applied R&D in a manner that significantly improves the ability to achieve new insights and applications. A critical element in achieving such transformation in NE's applied R&D is to develop new scientific understanding by employing new methods for improving physical models and advancing the computational tools in which these models are used. Another primary goal of such collaboration are the concomitant advancements in the relevant areas of math, physics, and computational science, which will help build the foundation for future collaboration and new advancements not otherwise possible.

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

Research through a SciDAC collaboration would include development of high-performance computing tools capable of predicting microstructural evolution in both current (UO2) and advanced (*e.g.*, metallic, uranium-silicide, TRISO) nuclear fuel and associated cladding materials, by leveraging DOE-HPC capabilities, along with mathematical and physics expertise. These tools would be based on new insights in the physics that affect microstructure, and on application of codes and methods capable of spanning the multiple length and time scales needed to address the complex physical changes that affect fuel and cladding performance. Physical changes of interest include (but are not limited to): grain growth, fission gas release, and fracture for UO2; species transport, phase change, and swelling in U-Zr; fission gas transport and swelling in U-Si; hydride formation and behavior in Zircaloy cladding; and microstructural changes in FeCr alloys. Proposed outcomes should include improved insights into relevant atomistic processes and how they should be implemented into microscale simulations. Outcomes should also help set the stage for future research activities, including comprehensive uncertainty quantification analysis for coupled-physics simulations.

**ASCR Objectives**: The challenge of the effective employment of DOE HPC for scientific computing is one that confronts applied mathematicians, computer scientists, and discipline scientists. Therefore, we expect that the kind of collaborations required by this solicitation should result in advances that would not have been accomplished by those same researchers working separately. We expect that these applied mathematicians or computer scientists, whose proposed contributions will be reviewed by their peers, would be those who have accomplished significant research in scientific computing on the most advanced high performance supercomputing systems. A record of funding from ASCR for such research, while not a

prerequisite, may be regarded as evidence of relevant experience. Some of the research conducted and expertise contributed by applied mathematicians would likely include, for example: Discretization methods for structured and unstructured grids; particle methods; multiphysics coupling techniques; direct, iterative, and multi-level solvers for linear & nonlinear systems; time integrators; resilient algorithms, adaptive error estimation and UQ (or UQ-aware) methods; scalability to million-way parallelism; algorithm and code interoperability. Computer scientists might be expected to conduct research and contribute to: Application performance modeling and benchmarking, tuning and analysis, code profiling and optimization; fault tolerance and resilience; management, analytics and visualization of massive and heterogeneous scientific data sets; usability and user experience; runtime systems, portable programming, advanced debugging capabilities and computational methods for hybrid, many and multi-core architectures; efficient use of new and emerging memory systems; workflow management, rapid prototyping, parallel I/O tools, and storage systems.

We would further expect that the research and contributions to the collaboration by applied mathematicians and computers scientists would be "architecture aware", i.e., the main architectural features of existing and planned computing environments, include: heterogeneous nodes (e.g., CPUs + GPUs), deep memory hierarchies, and varying trade-off costs for computation versus data movement. Therefore, tools and methodologies for coping with and taking full advantage of such architectural complexities are an important practical consideration as well as coordination of the proposed capabilities with past work across disciplines. Furthermore, the applied mathematicians and computer scientists should be aware of and have plans to incorporate the software engineering best practices that can contribute to the productivity of software developers and the long-term maintainability of the software as the computational systems and science evolve over time. An important contributor to software productivity is code portability across the DOE HPC systems. It is important that best practices are tailored to fit within the constraints of the scientific problem of the proposal and that close interactions are formed between software engineering experts, scientific software developers and scientists. Some examples of exclusively ASCR funded past research via the SciDAC Institutes can be viewed at http://www.scidac.gov/institutes.html. Finally, we would expect that both the applied mathematicians and computer scientists would contribute to a strong verification and validation (V&V) plan that employs advanced UQ methods integrated with sophisticated computational strategies.

#### **Issues and Guidance Common to All Areas**

- The project should leverage where possible, and without duplication, previous and ongoing work in modeling nuclear materials behavior in extreme environments and in applied mathematics/computer science at the participating institutions. While duplication of other project or program efforts will not be acceptable, efforts to complement or extend such efforts are encouraged.
- Successful partnerships should be able to exploit the massive concurrency of the DOE HPC systems and not merely their high capacity. Research activities that are relevant to the topical areas described above but are not planning or are not ready to take full advantage of DOE HPC resources should seek support from other program elements.

- The lead PI, the institutional Co-PIs, and the other senior investigators are expected to
  commit significant fractions of their time, consistent with their institutional practices, to lead
  or carry out the proposed tasks. Technical contributions that are needed occasionally or
  during certain phases of the project should be supported via consultancies or sub-awards to
  increase flexibility.
- A comprehensive verification & validation plan is necessary for the success of these efforts and should therefore be described in sufficient detail.
- Collaborations are expected to employ the intellectual resources in nuclear engineering, materials science, applied mathematics, and computer science communities (including expertise in algorithms and methods, and scientific software tools) in <u>multi-institutional</u> collaborations.
- Applicants will request funds from both NE and ASCR to meet proposed objectives (see also Management Plan). Proposals will not request computing resources; instead, the allocation of computing resources available to individual projects is contingent on review and award through the processes as described in <a href="http://science.energy.gov/ascr/facilities/allocation-policy">http://science.energy.gov/ascr/facilities/allocation-policy</a>. Within the available computational resources, every effort will be made to ensure that successful applications will have the resources needed to support their efforts.

All entities submitting applications to this funding opportunity announcement must recognize the moral and legal obligations to comply with export controls and policies that relate to the transfer of knowledge that has relevance to the production of special nuclear materials (SNM) and technologies with potential dual use. Please see 10 CFR 810 for further information. Do not submit applications containing restricted data, formerly restricted data, naval nuclear propulsion information, or unclassified controlled nuclear information as defined in the Atomic Energy Act of 1954, as amended, 42 USC 2011 et seq., 10 CFR 1017, 10 CFR 1045 (also <a href="https://www.osti.gov/stip/controlled">https://www.osti.gov/stip/controlled</a>).

#### **Collaboration**

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

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

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.

Collaborative proposals from institutions other than DOE National Laboratories should be submitted following the above rules in response to the companion announcement, DE-FOA-0001674. Each proposal within the collaborative group submitted in response to an FOA, including the narrative and all required appendices and attachments, must be identical with the following exceptions:

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

# Section II – AWARD INFORMATION

# A. TYPE OF AWARD INSTRUMENT

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

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

DOE will require multi-institution collaborations under this Announcement.

#### **B. ESTIMATED FUNDING**

Total funding of up to \$7,500,000 is expected to be made available for awards under this FOA and its companion LAB announcement. The precise breakdown of funds between the FOA and the LAB announcement will depend upon the number of meritorious proposals and the availability of appropriated funds.

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

# C. MAXIMUM AND MINIMUM AWARD SIZE

The award size at each institution will depend on the number of meritorious applications and the availability of appropriated funds. Note that multi-institution collaborations are expected to receive funding through one award at each participating institution.

For individual institution awards the following funding limits are specified for each award:

#### **Ceiling**

\$800,000 per year

# **Floor**

\$250,000 per year

For an entire multi-institution (including Laboratories, see LAB-1674) collaboration the following total funding limits are specified:

# Ceiling

\$1,600,000 per year

#### Floor

\$500,000 per year

#### D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

It is expected, depending upon receipt of meritorious applications and the availability of appropriated funds, that multiple awards for one collaborative project will be recommended.

# E. ANTICIPATED AWARD SIZE

(See B. Estimated Funding Section above.)

The award size will depend on the number of institutions participating in the recommended project.

# F. PERIOD OF PERFORMANCE

(See B. Estimated Funding section above.)

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

# G. TYPE OF PROPOSAL

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

# **Section III – ELIGIBILITY INFORMATION**

# A. ELIGIBLE APPLICANTS AND TOPICS

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

# **B. COST SHARING**

Cost sharing is not required.

# C. ELIGIBLE INDIVIDUALS

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

# Section IV – PROPOSAL AND SUBMISSION INFORMATION

# A. ADDRESS TO REQUEST PROPOSAL PACKAGE

Proposal submission instructions are available in this Announcement on the DOE Office of Science Portfolio Analysis and Management System (PAMS). Screenshots showing the steps in DOE National Laboratory proposal submission are available in the PAMS External User Guide, accessible by navigating to <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

A Letter of Intent is strongly encouraged and should be submitted by the deadline in <u>Section IV</u>, Part E.

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 planned title of the research application; the name and mailing address of every collaborating institution; the name and e-mail address of every corresponding Principal Investigator, as well as any additional Senior Investigator(s), and Senior/Key personnel who are expected to be involved in the planned proposal.

The absence of a LOI will not negatively affect a thorough evaluation of a responsive full proposal submitted in a timely fashion.

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

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

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 the "Having Trouble Logging In?" page. (If you have been an Office of Science merit reviewer or if you have previously submitted an proposal, 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 / View / Respond to DOE National Laboratory Announcements" link and find the current announcement in the list.

- Click the "Actions/Views" link in the Options column next to this announcement to obtain a dropdown menu. Select "Submit Letter of Intent" from the dropdown.
- On the Submit Letter of Intent page, select the institution from which you are submitting this LOI from the Institution dropdown. If you are associated with only one institution in the system, there will only be one institution in the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per LOI; to do so, click the "Select PI" button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the "Actions" link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose "Select PI."
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the "Invite PI" link at the top left of the "Select PI" screen. You can enter an optional personal message to the PI in the "Comments" box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the LOI. Save the LOI for later work by clicking the "Save" button at the bottom of the screen. It will be stored in "My Letters of Intent" for later editing.
- Enter a title for your letter of intent.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the LOI file into PAMS, click the "Attach File" button at the far right side of the screen. Click the "Browse" (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the "Upload" button to upload the file.
- At the bottom of the screen, click the "Submit to DOE" button to save and submit the LOI to DOE.
- Upon submission, the PI will receive an email from the PAMS system <<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 Laboratory Announcement should reference LAB 17-1674.

# C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

April 5, 2017 at 5:00 PM Eastern Time or See Section IV, Part E.

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

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

#### RESUBMISSION OF PROPOSALS

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

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

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

#### IMPROPER CONTENTS OF PROPOSALS

Proposals submitted under this Announcement will be stored in controlled-access systems, but they may be made publicly available if an award is made, and they will be made available to merit reviewers. As such, it is critical that Laboratories follow these guidelines:

- Do not include information subject to any legal restriction on its open distribution, whether classified, export control, or unclassified controlled nuclear information.
- Do not include personally identifiable information, including social security numbers, birthdates, citizenship, marital status, or home addresses. Pay particular attention to the content of biographical sketches and curriculum vitae.
- Do not include letters of support from Federal officials.
- Do not include letters of support on Federal letterhead. Letters that are not letters of support (such as letters confirming access to sites, facilities, equipment, or data; or letters from cognizant contracting officers) may be on Federal letterhead.
- Clearly mark all proprietary or trade-secret information.

#### DEPARTURE OF PRINCIPAL INVESTIGATOR

The actions to take upon the end of the principal investigator's relationship with the Laboratory are controlled by the date.

- If the proposal due date has not passed, the Laboratory must withdraw any application for a principal investigator whose relationship with the Laboratory has ended.
- If the proposal due date has passed, the Laboratory must consult with the DOE program manager identified in the Announcement. Depending on many factors, the proposal may be withdrawn or a new principal investigator could be proposed.

These guidelines apply whenever the principal investigator's relationship with the Laboratory has ended, whether from leaving for industry, transferring to another institution, or passing away.

#### LETTERS

Please do not solicit and do not submit letters of support. Letters of commitment to participate from prospective unfunded collaborators or facilities are permitted.

# 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 personnel – 10 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: Data Management Plan
  - o Appendix 7: Other Attachments (optional)

#### SUBMISSION INSTRUCTIONS

Full proposals must be submitted into the DOE Office of Science Portfolio Analysis and Management System (PAMS). For help with PAMS, click the "External User Guide" link on the PAMS website, <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 17-1674. Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than 04/05/2017, 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 <<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 17-1674.** 

# 2. Detailed Contents of the Proposal

**BUDGET AND BUDGET EXPLANATION** 

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

PAMS will calculate the cumulative budget totals for you.

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

PROJECT SUMMARY/ABSTRACT (NO MORE THAN ONE PAGE)

The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to the public. It should be a self-contained document that identifies the name of the applicant, the Principal Investigator (PI), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes). This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed 1 page when printed using standard 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 17-1674
- Pick one pair:
  - o DOE/Program Office: Office of Accelerated Innovation in Nuclear Energy
  - o DOE/Program Office Technical Contact: Dan Funk

or

- o DOE/Program Office: Advanced Scientific Computing Research
- o DOE/ Program Office Technical Contact: Randall Laviolette
- PAMS Letter of Intent Tracking Number:
- Research area (site) identified in Section I of this Announcement

COVER PAGE SUPPLEMENT FOR COLLABORATIONS (PART OF PROJECT NARRATIVE ATTACHED TO FIELD 8 ON THE FORM)

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

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

The **lead proposal** <u>must</u> provide the following information on a separate page as a supplement to the cover page.

- List all collaborating institutions by name with each institution's principal investigator on the same line.
- Indicate the lead PI who will be the point of contact and coordinator for the combined research activity.
- Provide a statement explaining the leadership structure of the collaboration.

- Include a description of each collaborating institution's facilities, equipment, and resources that will be made available to the collaborative group.
- Include a table modeled on the following chart providing summary budget information from all collaborating institutions. Provide the total costs of the budget request in each year for each institution and totals for all rows and columns.

**Budget by Institution** 

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Institution	PI	Role	Y1 Budget NE/ASCR	Y2 Budget NE/ASCR	Y3 Budget NE/ASCR	Y4 Budget NE/ASCR	Y5 Budget NE/ASCR	Total NE/ASCR
		Lead PI						
Total								

**Budget by Task** 

Task	Task Leader	Y1 Budget NE/ASCR	Y2 Budget NE/ASCR	Y3 Budget NE/ASCR	Y4 Budget NE/ASCR	Y5 Budget NE/ASCR	Total NE/ASCR
Task 1							
Task n							
Total							

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

PROJECT NARRATIVE (NO MORE THAN 30 PAGES LONG)

The project narrative **must not exceed 30 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph. This page limit does not apply to the Cover Page, Budget Page(s), Budget Justification, biographical material, publications and references, and appendices, each of which may have its own page limit.

Do not include any Internet addresses (URLs) that provide supplementary or additional information that constitutes a part of the proposal. Merit reviewers are not required to access Internet sites; however, Internet publications in a list of references will be treated identically to

print publications. See Part VIII.D for instructions on how to mark proprietary proposal information. To attach a Project Narrative, click "Add Attachment."

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

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

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

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

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

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

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

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 multiple proposals associated with a collaborative group will be used to create one consolidated document for merit review that consists of the common, identical proposal materials combined with a set of detailed budgets from the partner institutions. It is very important that every proposal in the collaborative

group be identical (including the title) with the exception of the budget and budget justification pages.

#### APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the 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 3 pages when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include the following:

**Education and Training**: Undergraduate, graduate and postdoctoral training; provide institution, major/area, degree and year.

**Research and Professional Experience**: Beginning with the current position list, in chronological order, professional/academic positions with a brief description.

**Publications**: Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically. Patents, copyrights and software systems developed may be provided in addition to or substituted for publications. An abbreviated style such as the Physical Review Letters (PRL) convention for citations (list only the first author) may be used for publications with more than 10 authors.

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

**Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers**: Provide the following information in this section:

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

Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates.

**Personally Identifiable Information**: Do not include sensitive personally identifiable information such as a Social Security Number, date of birth, or city of birth. Do not include information that a merit reviewer should not consider.

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

#### APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the Project Director/Principal Investigator(s) (PD/PI) and senior/key persons, including subawardees, for ongoing projects and pending applications. List all sponsored activities or awards requiring a measurable commitment of effort, whether paid or unpaid.

For every activity, list the following items:

- The sponsor of the activity or the source of funding
- The award or other identifying number
- The title of the award or activity
- The total cost or value of the award or activity, including direct and indirect costs. For pending proposals, provide the total amount of requested funding.
- The person-months of effort per year being dedicated to the award or activity Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.
  - Do not attach a separate file.
  - This appendix will not count in the project narrative page limitation.

#### APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. For research areas where there are routinely more than ten coauthors of archival publications, you may use an abbreviated style such as the Physical Review Letters (PRL) convention for citations (listing only the first author). For example, your paper may be listed as, "A Really Important New Result," A. Aardvark et. al. (MONGO Collaboration), PRL 999. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal. Provide the Bibliography and References Cited information as an appendix to your project narrative.

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

# APPENDIX 4: FACILITIES & OTHER RESOURCES

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. For proposed investigations requiring access to experimental user facilities maintained by institutions other than the applicant, please provide a document from the facility manager confirming that the researchers will have access to the facility. Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

# **APPENDIX 5: EQUIPMENT**

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

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

#### APPENDIX 6: DATA MANAGEMENT PLAN

Provide a Data Management Plan (DMP) that addresses the following requirements:

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

- resources and practices at that facility and reference it in the DMP. Information about other Office of Science facilities can be found in the additional guidance from the sponsoring program.
- 4. DMPs must protect confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests, business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, regulations, and DOE orders and policies. There is no requirement to share proprietary data.

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

- This appendix should not exceed 3 pages including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right)
- Do not attach a separate file.
- This appendix will not count in the project narrative page limitation.

#### **APPENDIX 7: OTHER ATTACHMENT**

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

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

# 3. Detailed Instructions for the Budget

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

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

# Section A. Senior/Key Person (Required)

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

# **Section B. Other Personnel**

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

# **Section C. Equipment Description**

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

#### Section D. Travel

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

# **Section E. Participant/Trainee Support Costs:**

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

# **Section F. Other Direct Costs:**

Enter Other Direct Costs information for each item listed.

• Materials and Supplies: Enter total funds requested for materials and supplies in the

appropriate fields. In the budget justification, indicate general categories such as glassware, and chemicals, including an amount for each category (items not identified under "Equipment"). Categories less than \$1,000 are not required to be itemized. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; quotes/catalog prices of similar or like items; or something else (describe).

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

# **Section G. Direct Costs**

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

#### **Section H. Other Indirect Costs**

Enter the Indirect Cost information for each field. Only four general categories of indirect costs

are allowed/requested on this form, so please consolidate if needed.

# **Section I. Total Direct and Indirect Costs**

This amount will be calculated by PAMS (Sections G + H)

# D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

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

# E. SUBMISSION DATES AND TIMES

#### 1. Letter of Intent Due Date

02/15/2017 5pm Eastern Time

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

# 3. Proposal Due Date

04/05/2017 5pm, Eastern Time

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

# 4. Late Submissions

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

# F. FUNDING RESTRICTIONS

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

# 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 17-1674.** 

# 3. Proposal Receipt Notices

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

# 4. Viewing Submitted Proposals

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

# **Section V - PROPOSAL REVIEW INFORMATION**

#### A. CRITERIA

#### 1. Initial Review Criteria

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

#### 2. Merit Review Criteria

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

- Scientific 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.
- Effectiveness of the Management Plan
- Alignment with Nuclear Energy Research Priorities

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

The sub-criteria below are provided to the merit reviewers to elaborate the criteria:

# • Scientific or Technical Merit of the Project

- o Is it likely that the proposed research will accelerate scientific discovery through computation with DOE HPC systems?
- How would the proposed research lead to significant improvements in simulation capability?
- o What science will become feasible with this collaboration that is not feasible now?
- o What key uncertainties are targeted by the project?
- o Is the Data Management Plan suitable for the proposed research?

C

# • Appropriateness of the Proposed Method or Approach

- O Are there significant potential problems in the proposed method or approach? If so, are the applicant's plans to address these problems—including the consideration of alternative strategies—adequate?
- O Does the project demonstrate a functional collaboration between the indicated scientists or engineers and applied mathematicians or computer scientists? If so, is the collaboration itself necessary to accomplish the proposed goals?
- Does the proposed research employ or develop state-of-the-art approaches that effectively employ DOE HPC resources? Can this project be completed on DOE HPC platforms that are currently available or are expected to be available by 2019?
- O Does the proposed research exploit existing resources, or, if it is intended to contribute new resources (e.g., algorithms, software), would that result in a duplication of existing resources? Do the proposers describe credible quality assurance principles and practices?
- O Does the proposed research include a plan to characterize model uncertainty and a plan for validation and verification?

# • Competency of Applicant's Personnel and Adequacy of Proposed Resources

- O Does the team include experts in both the science or engineering and applied mathematics or computer science research topics?
- O Does the proposal describe a well-integrated team based approach to addressing the scientific goals? Is the proposed team likely to work together in a cohesive manner?
- O Does the leadership team appear to be qualified to lead a multi-institutional and multidisciplinary collaboration? Does it have a proven record of success in managing diverse teams of scientific and technical experts and delivering results from advanced computational science research?
- o Do any deliverables depend upon the contribution of unfunded collaborators?

# • Reasonableness and Appropriateness of the Proposed Budget

- o Does the budget provide for adequate commitment by senior contributors?
- o Do critical elements rely upon efforts by unpaid contributors?
- o Does the requested budget support the proposer's specified management structure in a meaningful way?
- Are the applied mathematicians and computers scientists conducting significant research or are they merely acting as consultants?

# • Effectiveness of the Management Plan

- o Does the management plan present an organizational structure that delineates the roles and responsibilities of senior or key personnel?
- o Does it credibly enable collaboration of scientists or engineers and applied mathematicians or computer scientists?
- O Does it provide a clearly defined mechanism to evaluate success and failure and to reconfigure the project as needed?

# • Alignment with Nuclear Energy Research Priorities

o Can the results of this research substantially improve the ability of models to predict physical changes in the microstructure of uranium-oxide nuclear fuels?

• Would the results of this research be expected to be ultimately useful to NE advanced computational tools for fuel performance simulation?

# **B. REVIEW AND SELECTION PROCESS**

#### 1. Merit Review

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

#### 2. Selection

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

- Scientific and technical merit of the proposed activity as determined by merit review
- Availability of funds
- Relevance of the proposed activity to Office of Science priorities
- Ensuring an appropriate balance of activities within Office of Science programs
- Previous performance

#### 3. Discussions and Award

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

#### C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES

It is anticipated that the award selection will be completed by June 2017. It is expected that awards will be made in Fiscal Year 2017.

DOE is interested in seeing projects supported under this Announcement begin work by August 2017.

# Section VI - AWARD ADMINISTRATION INFORMATION

# A. AWARD NOTICES

# 1. Notice of Selection

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

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

# 2. Notice of Award

A work authorization/contract modification issued by the contracting officer is the authorizing award document.

#### **B. REPORTING**

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

# Section VII - QUESTIONS/AGENCY CONTACTS

# **A. QUESTIONS**

For help with PAMS, click the "External User Guide" link on the PAMS website, <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 17-1674.** 

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 for Office	Office of Accelerated Innovation in Nuclear Energy
of Nuclear Energy	Dan.Funk@nuclear.energy.gov
	301-903-3845
Program Manager for Office	Advanced Scientific Computing Research
of Science	Randall.Laviolette@science.doe.gov
	301-903-5195

# **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.