

**PROGRAM ANNOUNCEMENT
TO DOE NATIONAL LABORATORIES**



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

2017 Mathematical Multifaceted Integrated Capability Centers (MMICCs)

**DOE National Laboratory Announcement Number: LAB 17-1766
Announcement Type: Initial**

Issue Date:	05/05/2017
Pre-Proposal Due Date:	06/05/2017 at 5 PM Eastern Time (A preproposal is required.)
Encourage/Discourage Date:	06/09/2017 at 5 PM Eastern Time
Proposal Due Date:	07/11/2017 at 5 PM Eastern Time

Table of Contents

REGISTRATIONS	I
UPDATES AND REMINDERS.....	III
SECTION I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION	1
SECTION II – AWARD INFORMATION	7
A. TYPE OF AWARD INSTRUMENT.....	7
B. ESTIMATED FUNDING	7
C. MAXIMUM AND MINIMUM AWARD SIZE.....	7
D. EXPECTED NUMBER OF AWARDS.....	7
E. ANTICIPATED AWARD SIZE	7
F. PERIOD OF PERFORMANCE	8
G. TYPE OF PROPOSAL	8
SECTION III – ELIGIBILITY INFORMATION	9
A. ELIGIBLE APPLICANTS AND TOPICS	9
B. COST SHARING.....	9
C. ELIGIBLE INDIVIDUALS	9
SECTION IV – PROPOSAL AND SUBMISSION INFORMATION	10
A. ADDRESS TO REQUEST PROPOSAL PACKAGE.....	10
B. LETTER OF INTENT AND PRE-PROPOSAL.....	10
C. CONTENT AND PROPOSAL FORMS	13
D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS.....	27
E. SUBMISSION DATES AND TIMES	27
F. FUNDING RESTRICTIONS	27
G. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS	27
SECTION V - PROPOSAL REVIEW INFORMATION	29
A. CRITERIA	29
B. REVIEW AND SELECTION PROCESS	31
C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES	31
SECTION VI - AWARD ADMINISTRATION INFORMATION	32
A. AWARD NOTICES.....	32
B. REPORTING	32
SECTION VII - QUESTIONS/AGENCY CONTACTS.....	33
A. QUESTIONS	33

B. AGENCY CONTACTS	33
SECTION VIII - OTHER INFORMATION	34
A. MODIFICATIONS	34
B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE.....	34
C. COMMITMENT OF PUBLIC FUNDS.....	34
D. PROPRIETARY PROPOSAL INFORMATION.....	34
E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL.....	34
F. AVAILABILITY OF FUNDS.....	35

REGISTRATIONS

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

The DOE Office of Science performs many functions for DOE national laboratory proposals in the Portfolio Analysis and Management System (PAMS), which is available at <https://pamspublic.science.energy.gov>.

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

You must register in PAMS to submit a pre-proposal, letter of intent, or DOE national laboratory proposal.

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

Notifications sent from the PAMS system will come from the PAMS email address <PAMS.Autoreply@science.doe.gov>. Please make sure your email server/software allows delivery of emails from the PAMS email address to yours.

Registering to PAMS is a two-step process; once you create an individual account, you must associate yourself with (“register to”) your institution. Detailed steps are listed below.

1. CREATE PAMS ACCOUNT:

To register, click the “Create New PAMS Account” link on the website <https://pamspublic.science.energy.gov/>.

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

2. REGISTER TO YOUR INSTITUTION:

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this DOE National Laboratory Announcement should reference **LAB 17-1766**.

UPDATES AND REMINDERS

RECOMMENDATION

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

DATA MANAGEMENT PLAN

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

ACKNOWLEDGMENT OF FEDERAL SUPPORT

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

Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

Technical/Scientific Program Contacts:

Program Manager: Dr. Abani Patra, (301) 903-9938
Office of Advanced Scientific Computing Research, SC-21.1
E-mail: abani.patra@science.doe.gov

Program Manager: Dr. Steven L. Lee, (301) 903-5710
Office of Advanced Scientific Computing Research, SC-21.1
E-mail: Steven.Lee@science.doe.gov

SUMMARY

The Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby invites applications for basic mathematical research that addresses fundamental mathematical challenges within DOE's mission areas of energy, environment and security, from a mathematical perspective that require new integrated efforts across multiple mathematical, statistical and computational disciplines. This solicitation seeks to address mathematics for enabling successful development of increasingly complex DOE-relevant systems for scientific discovery, design, optimization and risk assessment – targeted through Mathematical Multifaceted Integrated Capability Centers (MMICCs), three of which were established following solicitation LAB 12-698 and have operated successfully from 2012-present.

This solicitation is seeking new proposals for Mathematical Multifaceted Integrated Capability Centers addressing an interrelated set of mathematical research challenges arising from DOE mission needs that require integrated approaches across multiple mathematical disciplines. Proposals tightly focused on solution of application problems will be considered outside the scope of this solicitation.

These MMICCs will enable applied mathematics researchers to work together in large, collaborative teams to develop the mathematics needed to address multiple DOE mission needs. The MMICCs allow researchers to take a broader view of the problem as a whole, and devise solution strategies that attack the problem in its entirety by building fundamental, multidisciplinary mathematical capabilities and tools cognizant of both extant and emerging computing paradigms. The MMICCs teams will have the flexibility and technical expertise to simultaneously consider all aspects of the problem-solving process ranging from the mathematical formulation to the development, analysis, and integration of appropriate models and methods to the demonstration of results and capabilities. These Centers will also serve as interfaces for engaging applied mathematicians and other mathematical researchers in the broader community to contribute to the solution of the mathematical challenges of DOE-relevant problems in the focus area.

More specific information is included under SUPPLEMENTARY INFORMATION below.

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

SUPPLEMENTARY INFORMATION

Mathematical Multifaceted Integrated Capability Centers

Building on the success of the first set of Mathematical Multifaceted Integrated Capability Centers running from 2012-2017, this solicitation is seeking new proposals for Mathematical Multifaceted Integrated Capability Centers addressing an interrelated set of mathematical research challenges arising from DOE mission needs. This solicitation is seeking to support research collectives that address challenges of increasing complexity within DOE's mission areas of energy, environment and security that require new integrated processes across multiple mathematical and statistical disciplines. This new paradigm will address mathematics for increasingly complex DOE-relevant systems for scientific discovery, design, optimization and risk assessment – this will be achieved through Mathematical Multifaceted Integrated Capability Centers (MMICCs). These MMICCs will enable applied mathematics researchers to work together in large, collaborative teams to more effectively address grand challenge problems from a mathematical perspective much earlier in the problem-solving process. The MMICCs allow researchers to take a broader view of the problem as a whole, and devise solution strategies that attack the problem in its entirety by building fundamental, multidisciplinary mathematical capabilities and tools. The MMICCs will have the scale and technical expertise to simultaneously consider all aspects of the problem-solving process ranging from the mathematical formulation to the development, analysis, and integration of appropriate data, models and mathematical methods to the demonstration of results and capabilities. These Centers will help serve as entry points for applied mathematicians and other mathematical researchers to more readily understand the mathematical challenges of DOE-relevant problems. It is expected that the operations of the MMICCs will create a cadre of well-trained mathematical scientists, in sync with the needs of the DOE mission, in the National Laboratories and in academic institutions.

The DOE Applied Math Summit [1], the DOE ASCR 2012 Workshop for Mathematics for the Analysis, Simulation, and Optimization of Complex Systems [2], and workshop report, A Multifaceted Mathematical Approach for Complex Systems [3] all concluded that future DOE challenges will require the ability to model systems of unprecedented complexity. The rapid convergence of compute and data intensive modes of research [17] and DOE leadership role therein guides new strategic directions as do Federal Governments Big Data initiatives. The proximal availability of exascale and beyond computing systems [12,13,14,17], big data and artificial intelligence driven discovery and innovation processes [15] raise many new and interesting demands on the mathematical infrastructure. Some of these were articulated in a series of reports on workshops [12,13,14] set up to establish requirements for the exascale age. Dealing with these increasingly complex systems will require new types of analysis and modeling that couple a broad array of diverse processes spanning a wide range of spatial and temporal scales and integrate the power of extreme scale computing with analysis of large and diverse data [17]. The models will likely combine both deterministic and stochastic elements; they are likely to have

multiple representations; and they are likely to have dynamic properties. The goal is not to simply produce high fidelity simulations, or couple existing models and methods, but rather to answer difficult questions regarding design, risk analysis, or optimization, while quantifying errors and uncertainties. These types of highly complex systems cannot be analyzed at the required fidelity with monolithic mathematical models. Effective models will be hierarchical and include multiple sub-models that represent different phenomena with vastly differing scales. These models can range from the representation of detailed physical processes to the description of complex engineered systems that must be optimized to obtain desired performance. This will require new approaches for understanding the impact on system behavior based on the interplay between sub-models at different physical resolutions or between decision points in an engineered system. Answering key questions about these systems may also require a much tighter coupling between data and simulation, and require new approaches to aggregate information from multiple sources.

The goal is to have researchers simultaneously examine, in an integrated form, all of the mathematical elements needed to make significant advances in the analysis and simulation needed for scientific discovery or optimization of a complex system. This holistic approach to problem empowers researchers to arrive at the combination of formulation, discretization, and solution methodologies that will enable the most effective combination of mathematical elements to construct the tools needed to answer important questions about systems of increasing complexity while making efficient use of emerging computer architectures.

Applications for a Mathematical Multifaceted Integrated Capability Center must:

1. Advance multifaceted, integrated mathematics that spans, as appropriate, novel formulations, discretizations, algorithm development, data analysis techniques, uncertainty quantification methodologies, optimization techniques, and other mathematical and statistical approaches; and,
2. Address mathematical problems with clear relevance and significant impact to the DOE;
3. Actively engage in community building events to rapidly disseminate scientific advances and maintain clear channels of communication to the DOE user community to assure rapid uptake of mathematical advances and, provide appropriate training opportunities in topical areas for the current and next generation DOE workforce.

In addition, it is expected that each MMICC will facilitate the formation of partnerships such that applied and basic science research groups in need of the mathematical expertise contained in each MMICC will be able to rapidly access this expertise. This solicitation includes illustrative DOE examples for MMICCs and the organizational structure and management plan of a MMICC.

Illustrative DOE Examples for MMICCS

The extant centers Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4)[18], An Integrated Multifaceted Approach to Mathematics at the Interfaces of Data, Models, and Decisions (DiAMOND) [19] and M2ACS: Multifaceted Mathematics for Complex Energy Systems Project (M2ACS) [20] provide instances of scope and potential structure. However, thoughtful evolution of scope, structure, function and topics are expected in the next round of awards [21].

Organizational Structure and Management Plan for MMICCs

Each MMICC will require expertise from a variety of different mathematical sub-disciplines. In addition, the MMICCs may require long-term engagement from problem inception to demonstration of results with domain scientists, computational scientists, and/or computer scientists. Applications may include funding for domain scientists or other expertise; the level of involvement or commitment is to be determined by the Center. Each MMICC must identify an appropriate team and organizational structure that enables it to function efficiently in a collaborative manner to address the multifaceted integrated mathematical research challenges. The MMICC Director (“Center Director”) will serve as the primary contact responsible for communications with the DOE Program Office on behalf of all of the Principal Investigators in the MMICC. It is expected that the Center Director will provide overall direction for the center ensuring internal coordination and collaboration as well as appropriate external outreach. The expectation is the Center Director will need to devote at least 33% of their time to the MMICC and will have support staff as appropriate. The MMICC structure must be sufficiently flexible to adapt to changing technical challenges and scientific needs. In particular, it is expected that there will be changes in the research plans as research progresses necessitating changes in personnel and sub-projects; equally likely are potential changes in the scientific challenges. Major changes should be effected in consultation with ASCR program staff. Applications should identify key senior personnel who will contribute in a substantive, measurable way to the scientific/technical development or execution of the project. It is acceptable to not explicitly name all junior staff; however, the application should include a discussion of how the center will be fully staffed and on what timeline. Given the diversity of the expertise required for a successful MMICC, it is expected that MMICCs will involve more than one institution. Multi-institutional collaborations should be identified in the application. The role of each institution should be discussed in terms of the contributions to the MMICC. Additional collaborations both with other MMICCs and in the broader community may form after an MMICC is established; applications should include a discussion of how this may be accomplished.

Applicants should identify key milestones of the research plan, a basic mapping of tasks, milestones including interactions among researchers, key dependencies (internal or external), and level of risk. It is expected that the MMICC will have multiple levels of risk.

The application must include a concise management plan that addresses the organization, communications, and coordination of the collaborating researchers. This plan should include mitigation strategies for foreseeable risks and explain how the project will have sufficient flexibility to adapt to changing priorities, challenges, personnel, and resources. Centers will be reviewed at the end of the 1st year and 4th years and have a major review in the 3rd year; additional informal reviews and reports will be conducted throughout the program. The application must contain a plan to support technical and programmatic review of the Center.

References

1. DOE 2012 Applied Math Summit <https://science.energy.gov/ascr/community-resources/workshops-and-conferences/doe-applied-math-summit/>
2. DOE ASCR 2012 Workshop for Mathematics for the Analysis, Simulation, and Optimization of Complex Systems, <https://science.energy.gov/~media/ascr/asccac/pdf/meetings/nov11/Bell.pdf>
3. DOE Basic Energy Sciences Report 2010: Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale, <https://www.osti.gov/scitech/servlets/purl/1273408>
4. DOE Basic Energy Sciences: Basic Research Needs Reports, New Science for a Secure and Sustainable Energy Future https://science.energy.gov/~media/bes/pdf/reports/files/New_Science_for_a_Secure_and_Sustainable_Energy_Future_rpt.pdf
5. DOE Basic Energy Sciences Report 2011: Computational Materials Sciences and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science, <https://www.osti.gov/scitech/biblio/1294275pdf>
6. National Science and Technology Council, Committee on Technology, Materials Genome Initiative, 2011, <https://www.mgi.gov/>
7. DOE Basic Energy Sciences Workshop Report 2007: Basic Research Needs: Catalysis for Energy, <https://www.osti.gov/scitech/biblio/927492-basic-research-needs-catalysis-energy>
8. DOE Office of Electricity Delivery and Energy Reliability 2011 Report: Computational Needs for the Next Generation Electric Grid Proceedings, http://energy.gov/sites/prod/files/FINAL_CompNeeds_Proceedings2011.pdf
9. DOE Basic Energy Sciences Workshop Report: Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems. <https://science.energy.gov/bes/efrc/research/bes-reports/>
10. DOE Basic Energy Sciences Data Workshop 2011, <https://www.ornl.gov/dataworkshop2011/default1.htm>
11. ASRC Report on Quantum Computing for Science <https://science.energy.gov/~media/ascr/pdf/programdocuments/docs/ASCRQuantumReport-final.pdf>
12. BES Computing and Data Requirements in The Exascale Age https://science.energy.gov/~media/ascr/pdf/programdocuments/docs/DOE-ExascaleReport_BES_final.pdf
13. HEP Computing and Data Requirements in the Exascale Age <https://science.energy.gov/~media/ascr/pdf/programdocuments/docs/DOE-ExascaleReport-HEP.pdf>
14. 2015 Turbulent Flow Simulation at the Exascale: Opportunities and Challenges Workshop https://science.energy.gov/~media/ascr/pdf/programdocuments/docs/turb_flow_exascale.pdf
15. The 2015 Machine Learning and Understanding For Scientific Discovery Workshop, https://science.energy.gov/~media/ascr/pdf/programdocuments/docs/Machine_Learning_DOE_Workshop_Report.pdf

16. Synergistic Challenges in Data-Intensive Science and Exascale Computing
<https://science.energy.gov/~media/40749FD92B58438594256267425C4AD1.ashx>
17. Executive Order – Creating a National Strategic Computing Initiative (Executive order),
The White House – Office of the Press Secretary, July 29, 2015
18. Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4)
<http://www.pnnl.gov/computing/cm4/>
19. DiaMonD: An Integrated Multifaceted Approach to Mathematics at the Interfaces of
Data, Models, and Decisions <http://dmd.mit.edu>
20. Multifaceted Mathematics for Complex Energy Systems
(M2ACS) <http://www.mcs.anl.gov/MACS/>
21. Applied Math Center Investments – Success at Scale
https://science.energy.gov/~media/ascr/ascac/pdf/meetings/201704/MMICCS_ASCAC_Patra.pdf

ADDITIONAL REQUIREMENTS:

Collaboration

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

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

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.

We are seeking strong teams that address novel research requiring multifaceted integrated mathematics. We will give priority to applications that clearly discuss one or more scientific or engineering grand challenges, abstract an interrelated set of mathematics research challenges that are optimally addressed through a multifaceted, integrated approach and have potential DOE impact in the 5-10+ year timeframe. Organizationally, the application must identify the Center Director, key personnel who will make significant technical contributions to the proposed research, and key collaborations.

Section II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT

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

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

DOE will consider funding multi-institution collaborations under this Announcement.

B. ESTIMATED FUNDING

Awards are expected to be made for a period of five years at a funding level of up to \$9,000,000 per year to support multiple awards in Fiscal Year 2017, with out-year support contingent on the availability of appropriated funds and satisfactory progress.

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

C. MAXIMUM AND MINIMUM AWARD SIZE

The award size will depend on the number of meritorious applications and the availability of appropriated funds. However, it is anticipated that approximately 3 to 4 centers will be awarded with total project size ranging from \$2,000,000 to \$3,500,000 per year.

D. EXPECTED NUMBER OF AWARDS

(See B. Estimated Funding Section above.)

The award size will depend on the number of meritorious applications and the availability of appropriated funds. However, it is anticipated that approximately 3 to 4 centers will be awarded with total project size ranging from \$2,000,000 to \$3,500,000 per year.

E. ANTICIPATED AWARD SIZE

(See B. Estimated Funding Section above.)

The award size will depend on the number of meritorious applications and the availability of appropriated funds. However, it is anticipated that approximately 3 to 4 centers will be awarded with total project size ranging from \$2,000,000 to \$3,500,000 per year.

F. PERIOD OF PERFORMANCE

(See B. Estimated Funding section above.)

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

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

G. TYPE OF PROPOSAL

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

Section III – ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS AND TOPICS

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

B. COST SHARING

Cost sharing is not required.

C. ELIGIBLE INDIVIDUALS

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

Section IV – PROPOSAL AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST PROPOSAL PACKAGE

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

Proposals submitted outside of PAMS will not be accepted.

B. LETTER OF INTENT AND PRE-PROPOSAL

1. Letter of Intent

N/A

2. Pre-proposal

PRE-PROPOSAL DUE DATE

June 5, 2017 or [See Section IV, Part E.](#)

ENCOURAGE/DISCOURAGE DATE

June 9, 2017 or [See Section IV, Part E.](#)

Pre-applications (**3 pages+1 page team**) are **REQUIRED** and must be submitted by June 5, 2017, 5:00 PM Eastern Time.

Pre-proposals will be reviewed for responsiveness of the proposed work to the research topics identified in this FOA. DOE will send a response by email to each applicant encouraging or discouraging the submission of a full proposal by June 9, 2017. Applicants who have not received a response regarding the status of their preproposal by this date are responsible for contacting the program to confirm this status.

Only those applicants that receive notification from DOE encouraging a full proposal may submit full proposals. No other full proposals will be considered.

The pre-proposal attachment should include, at the top of the first page, the following information:

Title of Preproposal
Principal Investigator Name, Job Title
Institution
PI Phone Number, PI Email Address
Laboratory Announcement Number: LAB 17-1766

This information should be followed by a clear and concise description of the objectives and technical approach of the proposed research. The preproposal may not exceed three pages, with a minimum text font size of 11 point and margins no smaller than one inch on all sides. Figures and references, if included, must fit within the three-page limit. An additional page may be used to enumerate the team and teaming arrangements.

The pre-proposal must also include a list of the names and institutional affiliations of all participating investigators, including collaborators and consultants on the proposed project. For each funded investigator, provide a list of collaborative co-investigators including co-authors of the past 48 months, co-editors of the past 24 months, graduate and postdoctoral advisors/advisees, and close associations.

Those pre-proposals that are encouraged will be used to help the Office of Science begin planning for the full proposal peer review process. The intent of the Office of Science in discouraging submission of certain full proposals is to save the time and effort of applicants in preparing and submitting full proposals not responsive to this Program Announcement.

The Principal Investigator will be automatically notified when the pre-proposal is encouraged or discouraged. The DOE Office of Science Portfolio Analysis and Management System (PAMS) will send an email to the Principal Investigator from PAMS.Autoreply@science.doe.gov, and the status of the pre-proposal will be updated at the PAMS website <https://pamspublic.science.energy.gov/>. Notifications are sent as soon as the decisions to encourage or discourage are finalized.

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

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 Pre-Proposal:

- Create your pre-proposal (called a preproposal in PAMS) outside the system and save it as a file with extension .docx, .doc, or .pdf. Make a note of the location of the file on your computer so you can browse for it later from within PAMS.
- Log into PAMS and click the Proposals tab. Click the “View / 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 Preproposal” from the dropdown.

- On the Submit Preproposal page, select the institution from which you are submitting this preproposal 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 preproposal; 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 preproposal. Save the preproposal for later work by clicking the “Save” button at the bottom of the screen. It will be stored in “My Preproposals” for later editing.
- Enter a title for your preproposal.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the preproposal file into PAMS, click the “Attach File” button at the far right side of the screen. Click the “Browse” (or “Choose File” depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the “Upload” button to upload the file.
- At the bottom of the screen, click the “Submit to DOE” button to save and submit the preproposal to DOE.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the preproposal.

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this Program Announcement should reference **LAB 17-1766**.

Preproposals submitted outside PAMS will not be considered. Preproposals may not be submitted through grants.gov or www.FedConnect.net.

C. CONTENT AND PROPOSAL FORMS

PROPOSAL DUE DATE

July 11, 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 <https://pamspublic.science.energy.gov>. Proposals may be withdrawn at any time between when the Laboratory submits the application and when DOE makes the application available to merit reviewers. Such withdrawals take effect immediately and cannot be reversed.

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

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

IMPROPER CONTENTS OF PROPOSALS

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

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

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

Letters of support are discouraged and will not be reviewed by DOE.

1. Summary of Proposal Contents and Information about PAMS

Each DOE National Laboratory proposal will contain the following sections:

- Budget, entered into PAMS as structured data using the PAMS budget form
- Abstract (one page), entered into PAMS as a separate pdf
- Budget justification, entered into PAMS as a separate pdf
- Proposal, combined into a single pdf containing the following information:
 - Proposal Cover Page
 - Table of Contents
 - Project Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel – 25 page limit)
 - Appendix 1: Biographical Sketch(es)
 - Appendix 2: Current and Pending Support
 - Appendix 3: Bibliography and References Cited
 - Appendix 4: Facilities and Other Resources
 - Appendix 5: Equipment
 - Appendix 6: Data Management Plan
 - Appendix 7: Other Attachments (optional)

SUBMISSION INSTRUCTIONS

Full proposals must be submitted into the DOE Office of Science Portfolio Analysis and Management System (PAMS). For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 17-1766**. Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than **July 11, 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 <https://pamspublic.science.energy.gov/> and follow the instructions for creating an account.

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

- Log into PAMS. From the proposals tab, click the “View DOE National Laboratory Announcements” link and find the current announcement in the list. Click the “Actions/Views” link in the Options column next to this Announcement to obtain a dropdown menu. Select “Submit Proposal” from the dropdown.
- Note that you must select one and only one Principal Investigator (PI) per proposal; to do so, click the “Select PI” button on the far right side of the screen. Find the appropriate PI from the list of all registered users from your institution returned by PAMS. (Hint: You may have to sort, filter, or search through the list if it has multiple pages.) Click the “Actions” link in the Options column next to the appropriate PI to obtain a dropdown menu. From the dropdown, choose “Select PI.”
- If the PI for whom you are submitting does not appear on the list, it means he or she has not yet registered in PAMS. For your convenience, you may have PAMS send an email invitation to the PI to register in PAMS. To do so, click the “Invite PI” link at the top left of the “Select PI” screen. You can enter an optional personal message to the PI in the “Comments” box, and it will be included in the email sent by PAMS to the PI. You must wait until the PI registers before you can submit the proposal. Save the proposal for later work by selecting “Save” from the dropdown at the bottom of the screen and then clicking the “Go” button. It will be stored in “My Proposals” for later editing. As a minimum, you must complete all the required fields on the PAMS cover page before you can save the proposal for the first time.
- The cover page, budget, and attachments sections of the lab proposal are required by PAMS before it can be submitted to DOE.
- Complete the sections in PAMS one at a time, starting with the cover page and following the instructions for each section.
- Click the “+View More” link at the top of each section to expand the onscreen instructions. On the budget section, click the “Budget Tab Instructions” link to obtain detailed guidance on completing the budget form.
- Save each section by selecting either “Save” (to stay in the same section) or “Save... and Continue to the Next Section” (to move to the next section) from the dropdown menu at the bottom of the screen, followed by clicking the “Go” button.
- If you save the proposal and navigate away from it, you may return later to edit the proposal by clicking the “View My Existing Proposals” or “My Proposals” links within PAMS.
- You must enter a budget for each annual budget period.
- You must also enter a budget for each proposed sub-award. The sub-award section can be completed using the same steps used for the budget section.
- In the attachments section of the lab proposal, the abstract, the budget justification, and the proposal narrative are required and must be submitted as separate files.
- You must bundle everything other than the budget, abstract, and budget justification into one single PDF file to be attached under “Proposal Attachment.”
- Do not attach anything under “Other Attachments.”

- To upload a file into PAMS, click the “Attach File” button at the far right side of the screen. Click the “Browse” (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the “Upload” button to upload the file.
- Once you have saved all of the sections, the “Submit to DOE” option will appear in the dropdown menu at the bottom of the screen.
- To submit the proposal, select “Submit to DOE” from the dropdown menu and then click the “Go” button.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the proposal.
- The proposal will also appear under My Proposals with a Proposal Status of “Submitted to DOE.”

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

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9:00 AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free number) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submissions and inquiries about this Program Announcement should reference **LAB 17-1766**.

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 17-1766**
- DOE/Office of Science Program Office: **Advanced Scientific Computing Research**
- DOE/Office of Science Program Office Technical Contact: **Abani Patra**
- 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 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.

- 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.

Collaborative Proposal Information								
	Names	Institution	Year 1 Budget	Year 2 Budget	Year 3 Budget	Year 4 Budget	Year 5 Budget	Total Budget
Lead PI								
Co-PI								
Co-PI								
Co-PI								

Example budget table (\$ in thousands)

* Note that collaborating proposals must be submitted separately.

PROJECT NARRATIVE (NO MORE THAN 25 PAGES LONG)

The project narrative **must not exceed 25 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.

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

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

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the 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 (<http://science.energy.gov/funding-opportunities/digital-data-management/>). This requirement could be met by including the data as supplementary information to the published article, or through other means. The published article should indicate how these data can be accessed.
3. DMPs should consult and reference available information about data management resources to be used in the course of the proposed research. In particular, DMPs that explicitly or implicitly commit data management resources at a facility beyond what is conventionally made available to approved users should be accompanied by written approval from that facility. In determining the resources available for data management at Office of Science User Facilities, researchers should consult the published description of data management resources and practices at that facility and reference it in the DMP. Information about other Office of Science facilities can be found in the additional guidance from the sponsoring program.
4. DMPs must protect confidentiality, personal privacy, Personally Identifiable Information, and U.S. national, homeland, and economic security; recognize proprietary interests,

business confidential information, and intellectual property rights; avoid significant negative impact on innovation, and U.S. competitiveness; and otherwise be consistent with all applicable laws, regulations, and DOE orders and policies. There is no requirement to share proprietary data.

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

- This appendix should not exceed 4 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

N/A

2. Pre-proposal Due Date

June 5, 2017 at 5 p.m. Eastern

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

3. Proposal Due Date

July 11, 2017 at 5 p.m. Eastern

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

4. Late Submissions

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

F. FUNDING RESTRICTIONS

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

G. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

1. Where to Submit

Proposals must be submitted through PAMS to be considered for award.

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

2. Registration Process

ONE-TIME REGISTRATION PROCESS

You must complete the one-time registration process (all steps) before you can submit your first proposal through PAMS. Registration instructions appear in the front matter of this Announcement.

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this DOE National Laboratory Program Announcement should reference **LAB 17-1766**.

3. Proposal Receipt Notices

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

4. Viewing Submitted Proposals

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

Section V - PROPOSAL REVIEW INFORMATION

A. CRITERIA

1. Initial Review Criteria

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

2. Merit Review Criteria

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

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

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 questions below are provided to the merit reviewers to elaborate the criteria:

1. Scientific and/or Technical Merit of the Project

- a. What compelling, scientific grand challenge problems are identified and to what extent are they relevant to the DOE mission? What is the potential long-term impact of the MMICC?
- b. What are the main technical challenges and how well does the application articulate the difficulties that bar scientific progress?
- c. What fundamental mathematical advances are needed to achieve the desired scientific discoveries and breakthroughs?
- d. What is the likelihood and to what extent can the proposed research overcome the main technical challenges to the scientific grand challenge problems?
- e. Is the Data Management Plan suitable for the proposed research and to what extent does it make the data available to the scientific community?

2. Appropriateness of the Proposed Method or Approach

- a. How well does the application articulate a mathematical, multifaceted, integrated approach to addressing the scientific grand challenge problems?
- b. To what extent does the proposed research treat the grand challenges holistically and justify the choice of mathematical abstractions?
- c. To what extent does the proposed research identify novel mathematical models, methods and approaches of individual components as well as integrated approaches?
- d. How well does the research plan describe metrics that will allow research progress and contributions to be measured?
- e. To what extent does the application articulate a plan for effectively coordinating and managing the research activities of the Center?

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

- a. How well is the role of the Center Director articulated? What prior experience and success does the Center Director have in effectively managing collaborative teams?
- b. To what extent are the roles of key personnel adequately described? To what extent do key personnel have a proven record of success in delivering results in computational and applied mathematics?
- c. To what extent do key personnel have extensive research and development experience in the mathematical sub-disciplines needed for the success of the Center?

4. Reasonableness and Appropriateness of the Proposed Budget

- a. To what extent is the overall requested budget appropriate for the scope of the work proposed?
- b. Is the requested budget and level of effort of the Center Director and key personnel sufficient and appropriate to achieve success?
- c. How well does the requested budget support the Center's management structure? What Center procedures, if any, will be used to permit flexibility in staffing and allow for additional future collaborations?
- d. What Center procedures, if any, will be used for reallocating funds to address changing priorities?

The selection official will consider the following program policy and management factors in the selection process:

- Potential for developing synergies and/or relation of the proposed research activities to other research efforts supported by ASCR and the Office of Science;
- Total amount of DOE funds available; and
- A management plan that addresses the organization, communications, and coordination of the collaborating researchers. This plan should include mitigation strategies for foreseeable risks and explain how the project will have sufficient flexibility to adapt to changing priorities, challenges, and resources.

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

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 September 1, 2017. It is expected that awards will be made in Fiscal Year 2017/2018.

DOE is interested in seeing projects supported under this Announcement begin work by January 1, 2018.

Section VI - AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES

1. Notice of Selection

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

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

2. Notice of Award

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

B. REPORTING

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

Section VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

For help with PAMS, click the “External User Guide” link on the PAMS website, <https://pamspublic.science.energy.gov/>. You may also contact the PAMS Help Desk, which can be reached Monday through Friday, 9AM – 5:30 PM Eastern Time. Telephone: (855) 818-1846 (toll free) or (301) 903-9610, Email: sc.pams-helpdesk@science.doe.gov. All submission and inquiries about this DOE National Laboratory Program Announcement should reference **LAB 17-1766**.

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

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

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

B. AGENCY CONTACTS

PAMS Customer Support	855-818-1846 (toll-free) 301-903-9610 sc.pams-helpdesk@science.doe.gov
Program Manager Scientific Contact	Dr. Abani Patra, (301) 903-9938 E-mail: abani.patra@science.doe.gov Dr. Steven L. Lee, (301) 903-5710 E-mail: Steven.Lee@science.doe.gov

Section VIII - OTHER INFORMATION

A. MODIFICATIONS

Notices of any modifications to this DOE National Laboratory Announcement will be posted on the Grants and Contracts website (<http://science.energy.gov/grants/>).

B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE

DOE reserves the right, without qualification, to reject any or all proposals received in response to this DOE National Laboratory Announcement and to select any proposal, in whole or in part, as a basis for negotiation and/or award.

C. COMMITMENT OF PUBLIC FUNDS

The Contracting Officer is the only individual who can make awards or commit the Government to the expenditure of public funds. A commitment by other than the Contracting Officer, either explicit or implied, is invalid.

D. PROPRIETARY PROPOSAL INFORMATION

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in a proposal only when such information is necessary to convey an understanding of the proposed project. The use and disclosure of such data may be restricted, provided the applicant includes the following legend on the first page of the project narrative and specifies the pages of the proposal which are to be restricted:

“The data contained in pages _____ of this proposal have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes.”

To protect such data, each line or paragraph on the pages containing such data must be specifically identified and marked with a legend similar to the following:

“The following contains proprietary information that (name of applicant) requests not be released to persons outside the Government, except for purposes of review and evaluation.”

E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL

In conducting the merit review evaluation, the Government may seek the advice of qualified non-Federal personnel as reviewers. The Government may also use non-Federal personnel to conduct routine, nondiscretionary administrative activities. The applicant, by submitting its proposal, consents to the use of non-Federal reviewers/administrators. Non-Federal reviewers must sign conflict of interest and non-disclosure agreements prior to reviewing a proposal. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

F. AVAILABILITY OF FUNDS

Funds are not presently available for this award. The Government's obligation under this award is contingent upon the availability of appropriated funds from which payment for award purposes can be made. No legal liability on the part of the Government for any payment may arise until funds are made available to the Contracting Officer for this award and until the awardee receives notice of such availability, to be confirmed in writing by the Contracting Officer.