PROGRAM ANNOUNCEMENT
TO DOE NATIONAL LABORATORIES

U. S. Department of Energy
Office of Science
Advanced Scientific Computing Research

Scientific Data Management, Analysis and Visualization at Extreme Scale 2

DOE National Laboratory Announcement Number: LAB 14-1043
Announcement Type: Amendment 3

Note: Page 25 edited to add underlined text shown below.

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the project director/principal investigator (PD/PI) and each senior/key person.

Amendment 3 Issue Date:	**03/18/2014 (Lab Announcement only)**
Pre-Proposal Due Date:	**02/07/2014 at 5:00 PM Eastern Time** **A Pre-Proposal is required**
Encourage/Discourage Date:	**02/21/2014 at 5:00 PM Eastern Time**
Proposal Due Date:	**04/02/2014 at 5:00 PM Eastern Time**

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REGISTRATIONS

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

The DOE Office of Science performs many functions for DOE national laboratory proposals in the Portfolio Analysis and Management System (PAMS), which is available at 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 14-1043.**

Section I – DOE NATIONAL LABORATORY OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS ANNOUNCEMENT SHOULD BE DIRECTED TO:

Technical/Scientific Program Contact:

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      Email : Lucy.Nowell@science.doe.gov
      FAQ : http://science.energy.gov/ascr/funding-opportunities/

SUMMARY

The Office of Advanced Scientific Computing Research (ASCR) in the Office of Science (SC), U.S. Department of Energy (DOE), hereby invites proposals for basic research that significantly advances management, analysis and visualization of data in scientific disciplines supported by DOE in the context of emerging architectures for extreme scale computing platforms.

Future extreme scale systems will require fundamental rethinking of the way science is enabled on our largest computing platforms. The current approach to data analysis by the high performance computational science community has been to store simulation data and analyze it at a later time, away from leadership-class supercomputers. However, because the design of new leadership-class machine architectures will be driven by energy efficiency constraints, especially with regard to the memory architecture, this approach will be infeasible. Minimizing data movement will be essential to meeting the power constraints and it will be possible to store only a very small percentage of the data generated by simulations at scale. These limitations will drive science towards increased reliance on *in situ* data reduction and analysis, with implications for data management, resilience, the process of co-design, etc.

The purpose of this announcement is to invite proposals for basic computer science research on five major themes:

1. Usability and user interface design;
2. *In situ* methods for data management, analysis and visualization;
3. Design of *in situ* workflows to support data management, processing, analysis and visualization;
4. New approaches to scalable interactive visual analytic environments; and/or
5. Proxy applications or workflows and/or simulations for data management, analysis and visualization software to support co-design of extreme scale systems

The supported research will lay the foundation for building the software infrastructure to support scientific data management, analysis and visualization in the context of extreme scale computing.

While described in the context of extreme scale supercomputing and simulations, these topics also have broad implications for data intensive science at scale and have been called out as synergistic challenges.

More specific information is included under SUPPLEMENTARY INFORMATION below.

Proposals must be submitted through a DOE National Laboratory. A companion funding opportunity announcement (DE-FOA-0001043) available on Grants.gov describes the funding opportunity for institutions that are not DOE national Laboratories. Consult DE-FOA-0001043 for information on eligibility for that announcement.

SUPPLEMENTARY INFORMATION

With this announcement DOE invites proposals for basic computer science research that will lay the foundation for building the software infrastructure to support scientific data management, analysis and visualization in the context of extreme scale computing.

Significant changes in computer architectures will occur over the next few years and will impact the full spectrum of computational devices. Providing support for unprecedented levels of parallelism in application software, the new architectures will also drive dramatic changes in the way data are managed and analyzed in all scientific disciplines. Continued research is needed across a range of topics and issues to ensure our ability to make sense of data and continue to make scientific discoveries in support of national priorities.

The next-generation of scientific discovery will be enabled by research developments that can effectively harness significant and possibly disruptive advances in computing technology. Extreme scale applications will generate results with orders of magnitude higher resolution and fidelity, achieving a time-to-solution significantly shorter than possible with today's high performance computing (HPC) platforms.

Challenges of Expected Supercomputing Hardware Architecture

In order to support scientific discovery in the context of extreme scale computing platforms and across the spectrum of computational devices, advances in scientific data management and analysis must take into account a variety of challenges:

1. Energy efficient hardware and software will be constrained to a power envelope of approximately 20 Megawatts (MW);
2. Machine architecture that may be heterogeneous or hybrid in chip components;
3. Users will be required to manage deep memory hierarchies and multi-stage storage systems within the severe energy constraints;

4. Data movement will be constrained, both internode and on/off the machine, in the interest of conserving power;
5. The bottleneck for input/output will continue to worsen as improvements in storage device capabilities do not keep pace with those for computing;
6. The presence of predicted high rates of hard and soft faults that will necessitate new approaches to ensuring the integrity of data and processing; and
7. Use of the machines will require managing unprecedented parallelism, especially at the node level of exascale systems.

Additional information about expected changes to the architecture of and system software for DOE supercomputing systems can be found in a variety of sources, including [1], [2] and [3].

Research Themes

The purpose of this announcement is to invite proposals for basic computer science research on five major themes:

1. Usability and user interface design;
2. *In situ* methods for data management, analysis and visualization;
3. Design of *in situ* workflows to support data management, processing, analysis and visualization;
4. New approaches to scalable interactive visual analytic environments; and/or
5. Proxy applications or workflows and/or simulations for data management, analysis and visualization software to support co-design of extreme scale systems

While described in the context of extreme scale supercomputing and simulations, these topics also have broad implications for data intensive science at scale and have been called out as synergistic challenges.

Proposals may address one or more of the announcement themes. Preference will be given to larger collaborative projects that offer more comprehensive and coherent research and solutions, provided that such proposals are appropriately integrated into a whole and not a collection of disjointed efforts.

Proposals addressing themes 2-5 must explicitly address the challenges of operating within the expected exascale environment, including severe constraints on data movement, worsening I/O bottleneck, frequent hard and soft faults, and the necessity for extremely high levels of concurrency.

The supported research will lay the foundation for building the software infrastructure to support scientific data management, analysis and visualization in the context of extreme scale computing.

Research Theme 1: Usability and User Interface Design

Computational science rests on the shoulders of scientists who push the boundaries of their disciplines and test the capabilities of the nation's fastest supercomputers, developing software to express computational models of complex phenomena for purposes of discovery and sometimes prediction. *Usability* is a concept too seldom applied to software for data management, analysis and visualization in this context. Providing a software environment for managing and analyzing data that is truly usable requires deep understanding of the culture, expectations, and processes of science in the fields to be supported. True usability is not tacked on at the end by providing a web interface to an application. Rather, usability must be designed and built in from the beginning, helping to drive functional choices at every level.

Research on this theme may involve experts from disciplines outside of computer science, such as cognitive and perceptual psychologists, cultural anthropologists, decision scientists, visual artists, etc., as well as scientists who are potential users of ASCR-supported technology for data management, analysis and visualization.

Research is required on a variety of topics related to usability, including but not limited to the following:

- If subjected to empirical usability evaluation procedures, what improvements to the user interfaces of existing applications for data management, analysis and visualization would increase ease of use and encourage broader adoption?
- Processes of data preparation and curation, analysis and visualization can be complicated to the point that it takes a team of specialists working with scientists to manage and analyze data. Can improvements to user interfaces help to alleviate confusion and give scientists more freedom and power to conduct their investigations without undue distraction by software and hardware complexities? Are the underlying software systems capable of supporting the desired user scientists' interactions with data? If not, what changes are needed from the standpoint of usability?
- Do available data abstractions adequately support scientists' thinking about their data and their science? Do the data abstractions support the types of processing and analysis that are needed? Do they help scientists reason effectively and easily about their data? If not, where are the points of failure? What characteristics are needed in new data abstractions?
- Scientists report difficulty in replicating their own analyses of data after the passage of a few weeks, let alone supporting validation by a third party. What is needed to better support management of scientific workflows and make orchestrating the processes easier and more understandable, as well as improving documentation of what has been done in order to support future validation? What are the barriers to use of existing scientific workflow systems? If we develop new workflow management software, can workflow management systems help to make it easier to explain the process of discovery? How might new workflow management approaches help to ease the burden of data management for scientists and also promote the integrity of science? From the standpoint of usability, what are the requirements for such systems?

Proposals that address this theme must show clear relevance to challenges in scientific data management, analysis and visualization in the context of science(s) that are supported by the DOE Office of Science and the ASCR supercomputing environment, which consists of the leadership class supercomputing facilities at Argonne National Lab (ANL) and Oak Ridge National Lab (ORNL), as well as the NERSC facility at Lawrence Berkeley National Lab (LBNL).

Applicants are reminded that software usability evaluation and other types of user studies are considered to be human subjects research and plans for such research must be cleared by an Institutional Review Board.

Research Theme 2: *In Situ* Data Management, Analysis and Visualization

Future extreme scale systems will require fundamental rethinking of the way science is enabled on our largest computing platforms. The current approach to data analysis by the high performance computational science community has been to store simulation data and analyze it at a later time, away from leadership-class supercomputers. However, because the new leadership-class machine architectures will be driven by energy efficiency constraints, especially with regard to the memory architecture, this approach will be infeasible. Minimizing data movement will be essential to meeting the power constraints and it will be possible to store only a very small percentage of the data generated by simulations at scale. These limitations are expected to drive science towards increased reliance on *in situ* data management, reduction, analysis and visualization, occurring in parallel with the simulation, either on the same nodes or on specially designated nodes.

A key aspect of in situ processing is that data are intelligently reduced, analyzed, transformed and indexed while they are still in memory and before being written disk or transferred over networks. In situ analysis and visualization can extract and preserve salient features of the raw data that would be lost as a result of aggressive data reduction and can characterize the extent of the data to enable runtime monitoring and even steering of the simulation. In situ data triage can effectively facilitate interactive post-processing visualization.

At the same time, changing government policies mandate that data associated with publications must be shared in order to support validation of research results. It is thus required that sufficient data must be preserved after the conclusion of a simulation, along with provenance about the data, to enable subsequent re-analysis. Furthermore, scientists observe that replicating their own analyses of data can be impossible as soon as a few weeks after completion, making it very difficult to support validation of results by a third party.

Research is needed to improve our understanding of and ability to utilize in situ methods for data management, analysis and visualization. [4] [5] Issues to be investigated include the following:

- How do simulations, data analysis and visualization calculations and data manipulations best share the same processors, memory space and domain decomposition to exploit data locality? If sharing is not feasible, how can data be reduced and shipped to processors dedicated to data analysis and visualization?
- Which data processing, analysis and visualization operations are best performed in situ? To what extent is a monitoring scenario relevant and how is monitoring effectively coupled with domain knowledge-driven data reduction? What types of reduction or transformation are appropriate to support both exploratory analysis and validation of results? As we store less raw data to disk, what metadata (e.g., data provenance) and supplemental information (e.g., uncertainty) should be generated and captured in situ?
- To date, in situ processing has been used primarily for operations that are known to be necessary a priori. Will this continue to be the case? If the scientist has little a priori knowledge about what is interesting or important in the data, how should data reduction be done? Will it be possible to do sufficient in situ data reduction that scientists will be able to do subsequent exploratory analysis offline? Will scientists be able to engage in exploration-oriented activities that have a scientist user "in the loop"? If so, will these activities occur concurrently with the simulation? Will the user be able to interact with the simulation and perhaps change its course, based on discoveries or observations of system behavior?
- What are the unique requirements of in situ data analysis and visualization algorithms? Some are fundamentally memory-heavy and some are compute-heavy, so that some algorithms may not be usable for in situ processing. Are reformulations for those algorithms possible and/or necessary? Can we create data abstractions or data structures and related traversal algorithms that minimize data movement while supporting both *in situ* and *post hoc* data management, analysis and visualization? Some analysis requires looking at large windows of time. Are incremental analysis methods needed to meet this requirement?
- What fraction of the supercomputer time should be devoted to in situ data processing/ analysis/visualization? As in situ data analysis and visualization become a necessity rather than an option, scientists must accept "embedded analysis" as an integral part of the simulation. What can be done to make this an attractive approach rather than an unwelcome disruption?
- What similarities can be exploited over multiple simulation projects? Can the Data Management, Analysis and Visualization communities develop a code base that can be re-used across a variety of simulations? Can existing commercial and/or open-source visualization software tools be directly extended to support in situ visualization at extreme scale?

Research Theme 3: In Situ Data Management and Workflow Management Systems

As datasets increase in size and complexity, assumptions and educated guesses will be made to reduce dataset size and manage the output. These assumptions and educated guesses need to be captured to provide context and increase reproducibility. A provenance infrastructure is needed

that makes the capture and curation of datasets automatic. On the simulation side, it needs to capture metadata information about the environment and settings of the simulation. On the analysis side, the captured information needs to accessible as feedback to the user. [4]

Furthermore, the shift to in situ data reduction and analysis that are more tightly coupled with simulations represents a new kind of workflow for scientists, creating both challenges and opportunities. Existing workflow engines coordinate tasks within the HPC environment through the scheduler and remote connections to the HPC machine. They do little to help orchestrate tasks that must run concurrently and share memory-based data objects.

A new kind of workflow management system for science is needed. Like the score for an orchestra, a scientific workflow should be both sharable and portable. This means that a workflow must be readily understandable by scientists other than those who created it and that it must be capable of operation on diverse hardware systems. It should also include the capability to capture and reuse data provenance during both in situ and post hoc processing, providing support for replicating an analysis and/or validation of results. Such workflows should be useful in the education of those entering a discipline or beginning research in a new area.

Research is needed to design in situ workflow management methods and/or systems to support data management, processing, analysis and visualization in residence with simulations at scale, as well as providing for capture of sufficient data provenance to support subsequent re-analysis and/or validation of results. [4] [5] [6]

Challenges to be addressed include but are not limited to:

- How and to what degree must codes for data management, analysis and visualization be tightly coupled to application codes to address power constraints on data movement on extreme-scale platforms? How will in situ data processing, analysis and visualization activities be controlled by and/or coordinated with simulations?
- What data transformations or adaptations are required to allow data analysis and visualization to share memory and data access with applications, preferably in a zero-copy manner?
- Given the need to support replication of results and possible post-hoc analysis, how can the capture of data provenance metadata be automated for in situ workflows in the face of a dynamic software stack and frequent hard and soft faults? What knowledge representation schemes and machine reasoning capability are required to support the use and re-use of data provenance metadata for subsequent in situ and/or post hoc use?

Research Theme 4: Visualization and Interactive Visual Analytics

Research is required to design and develop more powerful visual analytic environments for representation of and interaction with scientific data. New scientific visual analytic systems must be sufficiently scalable to address the challenges of extreme scale simulations and data intensive science and provide better understanding for multi-physics ensemble data, comparative analysis of data, and/or integrated analysis of simulation and experimental data. New methods must be developed that leverage the knowledge of domain scientists to improve the efficiency and

efficacy of the resulting analysis, including research in related areas of knowledge representation and machine reasoning methods to support scientific data analysis and visual analytics. [4] [5] [6][7]

Real time or near real time analysis of data, coupled with the shift to asynchronous models of computation, offers the possibility for a more interactive kind of computational science, allowing scientists an option to intervene in simulations in ways that have not been possible in the past. Exploratory research is needed to develop visual analytic methods and interfaces that enable scientists to assess the state of a simulation and the system running it, along with mechanisms that support interaction with the simulation environment and parameters.

A key challenge will be to develop and validate visual analysis systems that support scientific discovery, in addition to confirmatory analysis and communication, while maintaining user scientists' ability to control the course of analysis and ensuring their faith (and that of policy makers and the public) in the integrity of the process of scientific analysis. It is not enough to produce an answer; scientists must be able to understand, trust and explain the results of analytic processes, communicating them effectively to other scientists and sometimes to policy makers. Providing deep integration of visualization processes with data analytic engines and the data will be especially challenging on the I/O-constrained platforms of the future. Such integration is essential to support scientists' interaction with their data, and such interaction is essential to supporting human insight, intuition, and learning. Visualization alone is not enough.

Challenges to be addressed in scientific visual analysis include but are not limited to the following:

- Can real time or near real time visual analytics provide for new kinds of interactivity with simulations? What are the implications of such interactivity in terms of capturing data provenance and/or support for validation of results? Would increased interactivity enhance scientific understanding, increase the pace of scientific discovery, and/or improve the utilization or usability of supercomputing platforms? Can we increase the ability of scientists to interact with their simulations without adverse effects on the resiliency of the applications and the supercomputing system itself?
- How can we increase the level of interaction with scientific data so as to better support the perceptual and cognitive abilities of the user scientists, increasing their ability to understand the phenomena represented in their data, detect patterns and anomalies, and increase the pace of scientific discovery?
- How can systems for visual analysis represent and leverage the knowledge of user scientists to improve the accuracy and speed of analysis? Can such knowledge representations be preserved and made reusable or possibly sharable?
- How can a visual analytics system represent data sets for which there is not even one pixel per data point without falsely conveying a sense of uniformity in data? How can small anomalies in petascale to exascale data be made perceptible? How can data from multi-scale, multi-physics simulations and experiments be represented so that the

complexity of the science is accessible while also maintaining comprehensibility of the displays?

- How can we validate the efficacy of scientific visualizations and visual analytic environments in supporting scientific understanding and discovery and also improve their usability?

Proposals that address this theme must provide for formative usability evaluation of user interface designs that will result from the research. Applicants are reminded that software usability evaluation and other types of user studies are considered to be human subjects research and plans for such research must be cleared by an Institutional Review Board.

Research Theme 5: Proxy Applications and/or Simulation Support for Co-Design

To support co-design of supercomputing systems that will support in situ management, processing, analysis, and visualization of data, research is also needed to design and develop proxy applications for data management, processing, analysis and visualization software and/or simulations of the behavior of these tools. In the past supercomputers have been designed to support scientific simulation, with the assumption that data analysis and visualization would occur post hoc on machines with a different architecture. Tighter integration of simulation and analytics in the scientific workflow on the same system that runs the simulation will impact the system architecture and operating and runtime systems in ways that are not well understood and will impact co-design of the systems for future workloads. Use of proxy applications and modeling and simulation to support system design is becoming the norm in the extreme scale research community [8] and it is important that data management, analysis and visualization software should be represented. [4] [5][7]

- What aspects of scientific data management, analysis and visualization software and/or workflows should be captured in proxy applications or mini-apps? Are additional representations of these technologies needed to support co-design of the hardware, operating and runtime systems, and applications?
- Because data management, analysis and visualization will occur in situ, perhaps using the same memory as simulations that generate the data, execution may be interleaved with that of the simulation or they may occur in parallel. Can we build proxy applications that are composable so as to represent the entire in situ data life cycle? Do we need to do so?
- What models and simulations of the behavior of data management, analysis and visualization software and/or workflows are needed to support design of extreme scale systems?

Proposed projects that address this theme should develop and deliver proxy applications and/or modeling and simulation software that will be useful in the co-design of extreme scale system hardware and the software stack. To be successful in this research theme, proposals must reveal

sufficient awareness of ongoing activities in the areas of co-design, development of the software stack, and modeling and simulation for design of DOE extreme scale HPC systems [1] [5] to make the case for potential impact.

Support for Partnerships

Data management, analysis and visualization are inherently involved in the process of scientific discovery at scale. Especially in the context of in situ processing, changes in data management, analysis and visualization technology could have potentially dramatic impact on scientific applications and discovery processes. Close collaboration with domain scientists is thus essential to successful design and deployment in these areas.

The ASCR Computer Science program does not ordinarily provide support for research that is applicable to only one domain science. Therefore, proposals must clearly make the case that the proposed research is relevant to multiple scientific disciplines that are supported by the Office of Science and/or propose discipline-specific research with the potential for a co-funding partnership with the relevant Office of Science program office.

Applications that propose funding partnerships with other Office of Science program offices are welcome, but such partnerships are not required. If a partnership proposal is considered, applicants should contact the ASCR program manager and the relevant program manager in the other Office of Science program office(s) to discuss potential partnership applications in order to ensure that the application will benefit both ASCR and the other Office of Science program office(s) and that funds are available in the other office(s).

Additional Information

Proposals may address one or more of the announcement themes. Preference will be given to larger collaborative projects that offer more comprehensive and coherent research and solutions, provided that such proposals are appropriately integrated into a whole and not a collection of disjointed efforts.

Proposals that address Theme 1 must show clear relevance to challenges in scientific data management, analysis and visualization in the context of science disciplines supported by the DOE Office of Science and the ASCR supercomputing environment at ANL, ORNL and LBNL.

Proposals addressing Themes 2-5 must explicitly address the challenges of operating within the expected exascale environment, including severe constraints on data movement, worsening I/O bottleneck, frequent hard and soft faults, and the necessity for extremely high levels of concurrency.

Proposals that address a combination of Theme 1 with one or more of Themes 2-5 are welcome.

Proposals must clearly establish that the proposed research supports the missions of the Advanced Scientific Computing Research office and the Computer Science program, as well as

showing relevance to other Office of Science disciplines. Proposed research must also be relevant to future extreme scale computing platforms operated by ASCR and must advance pertinent aspects of computer science.

All recipients of awards resulting from this FOA must comply with the terms of the ASCR policyupolicy on open source software: http://science.energy.gov/~/media/ascr/pdf/research/docs/Doe_lab_developed_software_policy.pdf.

Limitations of Scope

Proposals previously submitted to DE-FOA-0000918 [or Lab13-918] Mathematical and Statistical Methodologies for DOE Data-Centric Science at Scale or substantially the same will be deemed out of scope and declined without review.

Also out of scope for this announcement are research aimed at quantum computing; networking; computer supported collaboration; social network analysis; analysis of Internet or network traffic data; natural language understanding and/or generation; digital data preservation and/or archiving; data discovery, creation and/or use of data registries; generalized research in human computer interaction that is not responsive to Research Theme 1; and/or research which is only or primarily applicable to hand-held, portable, desktop, cluster or cloud computing.

Proposals for discipline-specific approaches to data management and/or analysis and visualization are within scope only if there is potential support from the relevant Office of Science program component.

REFERENCES

1. *The Opportunities and Challenges of Exascale Computing, ASCAC Subcommittee Report,* http://science.energy.gov/~/media/ascr/ascac/pdf/reports/Exascale_subcommittee_report.pdf
2. *Final Report of the U.S. Department of Energy Fault Management Workshop,* June 6, 2012, http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/FaultManagement-wrkshpRpt-v4-final.pdf
3. Exascale Research Conference meeting materials: http://exascaleresearch.labworks.org/oct2012/
4. *Scientific Discovery at the Exascale: Report from the DOE ASCR 2011 Workshop on Exascale Data Management, Analysis and Visualization*, Houston, TX, http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Exascale-ASCR-Analysis.pdf
5. *Synergistic Challenges in Data-Intensive Science and Exascale Computing, DOE ASCAC Data Subcommittee Report*, March 2013, http://science.energy.gov/~/media/ascr/ascac/pdf/reports/2013/ASCAC_Data_Intensive_Computing_report_final.pdf

6. *Data Crosscutting Requirements Review, April 4-5, 2013*, http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/ASCR_DataCrosscutting2_8_28_13.pdf
7. Report out from the *Exascale Research Planning Workshop Working Session on Data Management, Visualization, IO and Storage,* http://exascaleresearch.labworks.org/apr2012planningworkshop/application/layouts/exascale-planning-workshop//public/docs/PRES_WorkingSession-DataIO_120420.pdf
8. *Report on the ASCR Workshop on Modeling and Simulation of Exascale Systems and Applications, August 2012,* http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/ModSim_Report-2012_AH_5.pdf

Collaboration

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

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

Collaborative applications from institutions other than DOE National Laboratories should be submitted following the above rules in response to the companion announcement, DE-FOA-0001043.

<center>**Section II – AWARD INFORMATION**</center>

A. TYPE OF AWARD INSTRUMENT

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

B. ESTIMATED FUNDING

It is anticipated that up to $4,000,000 per year will be available under this Program Announcement and the funding opportunity announcement DE-FOA-0001043, contingent on satisfactory peer review and the availability of appropriate funds. Applicants should request project support for three years, commensurate with the scope of proposed research, with out-year support contingent on the availability of appropriated funds, progress of the research, and programmatic needs. Awards are expected to begin in Fiscal Year 2014, which ends on September 30, 2014. Some awards may be made in Fiscal Year 2015, depending on the availability of funds.

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

C. MAXIMUM AND MINIMUM AWARD SIZE

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

The minimum award size is anticipated to be $150,000 per year for a small project at a single institution.

The maximum award size is expected to be $1.5 million for a large project spanning multiple institutions.

D. EXPECTED NUMBER OF AWARDS

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

E. ANTICIPATED AWARD SIZE

Under this Program Announcement, it is anticipated that each funded project will have a total annual budget of $150,000 for a small project at a single institution up to $1.5 million for a project spanning a larger portion of the scope of research and multiple institutions. Separate awards to individual institutions are preferred but sub-awards to DOE National Laboratory awards are permitted with appropriate justification.

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

F. PERIOD OF PERFORMANCE

DOE anticipates making awards with a project period of three years, commensurate with the scope of research proposed.

G. TYPE OF PROPOSAL

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

Section III – ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS AND TOPICS

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

A given DOE National Laboratory may submit at most three proposals to this Announcement as a project lead. There is no limit on the number of proposals that may be submitted as a sub-awardee or collaborator.

For official postings see the Office of Science Grants and Contracts web site, http://www.science.doe.gov/grants.

B. COST SHARING

Cost sharing is not required.

C. ELIGIBLE INDIVIDUALS

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

A given individual may participate in at most three proposals to this announcement, including participation as a sub-awardee or collaborator.

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
Not required.

2. Pre-proposal (required)

PRE-PROPOSAL DUE DATE
February 7, 2014, by 5:00 PM Eastern Time

ENCOURAGE/DISCOURAGE DATE
February 21, 2014, by 5:00 PM Eastern Time

A pre-proposal is required and must be submitted by February 7, 2014, at 5 PM Eastern Time. Only the Lead Institution must submit the pre-proposal. 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/. **Failure to submit a pre-proposal will preclude the full proposal from consideration.**

Pre-proposals will be reviewed and DOE will send a reply by e-mail to each applicant encouraging or discouraging the submission of a full proposal. A discouragement decision does not necessarily reflect judgment on the scientific or technical merits of the proposed project and it seeks to avoid the preparation of a proposal that is not likely to be selected for award negotiations. Applicants who have not received a response regarding the status of their pre-proposals by February 21, 2014, are responsible for contacting the program to confirm this status. **Only those applicants that receive notification from DOE encouraging a full proposal may do so.** No other full proposals will be considered.

Pre-proposals will be evaluated with respect to the scope and research areas as outlined in the SUMMARY and SUPPLEMENTARY INFORMATION sections. The pre-proposal should contain (1) a one-page cover sheet, (2) a two-page technical narrative, and (3) conflict of interest information.

The one-page cover sheet identifies the name, institutional affiliation, e-mail address and telephone number of the Lead Principal Investigator and Senior/Key personnel expected to be involved in the project, and an estimated amount of funding requested for each year and for each funded institution. No biographical data need be included.

The technical narrative may not exceed two pages, with a minimum text font size of 11 point and margins no smaller than one inch on all sides. Figures and reference, if included, must fit within the two-page limit. The technical narrative must provide a clear and concise description of the objectives and technical approach of the proposed research.

To help the Office of Science avoid conflicts of interest (COI) in identifying potential reviewers, a list of collaborators, co-editors, and graduate/postdoctoral advisors and advisees must be submitted with the pre-proposal. **This list should be the final set of pages in the pdf for the pre-proposal. A single, consolidated COI list for the Lead Principal Investigator and each project collaborator (supported or unsupported) is required that includes, for all project participants collectively, an alphabetized list** of collaborative co-investigators including co-authors of the past 48 months, co-editors of the past 24 months, graduate and postdoctoral advisors/advisees.

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.

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

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

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

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

Submit Your Pre-Proposal:
- Create your pre-proposal (called a 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 / 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 pre-proposal. Save the pre-proposal for later work by clicking the "Save" button at the bottom of the screen. It will be stored in "My Pre-proposals" for later editing.
- Enter a title for your pre-proposal.
- Select the appropriate technical contact from the Program Manager dropdown.
- To upload the pre-proposal file into PAMS, click the "Attach File" button at the far right side of the screen. Click the "Browse" (or "Choose File" depending on your browser) button to search for your file. You may enter an optional description of the file you are attaching. Click the "Upload" button to upload the file.
- At the bottom of the screen, click the "Submit to DOE" button to save and submit the pre-proposal to DOE.
- Upon submission, the PI will receive an email from the PAMS system <PAMS.Autoreply@science.doe.gov> acknowledging receipt of the pre-proposal.

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

For help with PAMS, click the "External User Guide" link on the PAMS website, 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 DOE National Laboratory Program Announcement should reference **LAB 14-1043.**

Pre-proposals submitted outside PAMS will not be considered.

C. CONTENT AND PROPOSAL FORMS

April 2, 2014 by 5:00 PM Eastern Time

LETTERS

Letters of collaboration may be included in an appendix, especially for unfunded collaborators.

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

1. Summary of Proposal Contents and Information about PAMS

Each DOE National Laboratory proposal will contain the following sections:

- Budget, entered into PAMS as structured data using the PAMS budget form
- Abstract (one page), entered into PAMS as a separate pdf, containing the following information:
    - Proposal title
    - List of all participants by institutional affiliation
    - Summary of project narrative
- 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 – 15 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: 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 14-1043.** Full proposals submitted in response to this Program Announcement must be submitted to PAMS no later than April 2, 2014 at 5:00 PM Eastern Time.

All PIs and those submitting on behalf of PIs are encouraged to establish PAMS accounts as soon as possible to ensure timely submissions. To register, click "Create New PAMS Account" on the website 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 14-1043.**

2. Detailed Contents of the Proposal

BUDGET AND BUDGET EXPLANATION

The budget must be submitted into PAMS using the PAMS budget form. Research proposed under this Announcement should have four budget periods, commensurate with the scope of research proposed. Please enter the following budget period start and end dates into PAMS for proposals submitted to this Announcement:
- Budget Period 1: 8/1/2014 – 4/30/2015
- Budget Period 2: 5/1/2015 – 4/30/2016
- Budget Period 3: 5/1/2016 – 4/30/2017
- Budget Period 4: 5/1/2017 – 7/31/2017

PAMS will calculate the cumulative budget totals for you.

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

PROJECT SUMMARY/ABSTRACT (NO MORE THAN ONE PAGE)

The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to the public. It should be a self-contained document that identifies the name of the applicant, the Principal Investigator (PI) and all collaborators by institution, 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 narrativepage limitation.

- The project title:
- Applicant/Institution:
- Street Address/City/State/Zip:
- Postal Address:
- Administrative Point of Contact name, telephone number, email:
- Lead PI name, telephone number, email:
- DOE National Laboratory Announcement Number: **LAB 14-1043**
- DOE/Office of Science Program Office: **Office of Advanced Scientific Computing Research**
- DOE/Office of Science Program Office Technical Contact: **Dr. Lucy Nowell**
- PAMS Pre-proposal Number:
- A list of research themes from the Announcement that are addressed in the proposal
- A copy of the budget summary table described in the budget section below

COVER PAGE SUPPLEMENT FOR COLLABORATIONS

Collaborative proposals submitted from different institutions must clearly indicate they are part of a collaborative project/group. Every partner institution must submit a proposal through its own sponsored research office. Each proposal within the collaborative group, including the narrative

and all required appendices and attachments, must be identical with one exception: The exception is that each proposal must contain unique budget and budget justification documents corresponding to the expenditures for that proposal's submitting institution only. Each collaborative group can have only one lead institution. The common narrative must identify the lead institution and must contain a summary table describing the budget breakdown by institution for all participants.

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

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

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

Example budget table ($ in thousands)

* Note that collaborating proposals must be submitted separately.

The project narrative **must not exceed 15 pages** of technical information, including charts, graphs, maps, photographs, and other pictorial presentations, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right). The font must not be smaller than 11 point. Merit reviewers will only consider the number of pages specified in the first sentence of this paragraph.

The Project Narrative comprises the research plan for the project. It should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The narrative should provide a clear, concise statement of the specific objectives/aims of the proposed project. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project.

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

APPENDIX 1: BIOGRAPHICAL SKETCH

Provide a biographical sketch for the project director/principal investigator (PD/PI) and each senior/key person. As part of the sketch, provide information that can be used by reviewers to evaluate the PI's potential for leadership within the scientific community. Examples of information of interest are invited and/or public lectures, awards received, scientific program committees, conference or workshop organization, professional society activities, special international or industrial partnerships, reviewing or editorship activities, or other scientific leadership experiences. The biographical information (curriculum vitae) must not exceed 2 pages when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include the following:

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

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

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

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

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

Graduate and Postdoctoral Advisors and Advisees: List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s). Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates.

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

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

APPENDIX 2: CURRENT AND PENDING SUPPORT

Provide a list of all current and pending support (both Federal and non-Federal) for the Principal Investigator(s) (PI) for ongoing projects and pending proposals. For each organization providing support, show the total award amount for the entire award period (including indirect costs) and the number of person-months per year to be devoted to the project by the PI. Do not list start-up funds provided to the PI by the employing academic institution. Provide the Current and Pending Support as an appendix to your project narrative. Concurrent submission of a proposal to other organizations for simultaneous consideration will not prejudice its review.

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

APPENDIX 3: BIBLIOGRAPHY & REFERENCES CITED

Provide a bibliography of any references cited in the Project Narrative. Each reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication.

For research areas where there are routinely more than ten coauthors of archival publications, you may use an abbreviated style such as the Physical Review Letters (PRL) convention for citations (listing only the first author). Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal. Provide the Bibliography and References Cited information as an appendix to your project narrative.

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

APPENDIX 4: FACILITIES & OTHER RESOURCES

This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. Please provide the Facility and Other Resource information as an appendix to your project narrative.

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

APPENDIX 5: EQUIPMENT

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

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

APPENDIX 6: OTHER ATTACHMENTS

Information not easily accessible to a reviewer may be included in this appendix, but do not use this appendix to circumvent the page limitations of the proposal. Reviewers are not required to consider information in this appendix, and reviewers may not have time to read extensive appendix materials with the same care they would use with the proposal proper.

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

3. Detailed Instructions for the Budget

Budgets are required for the entire project period. A budget form should be completed for each budget period of the award, and a cumulative budget form for the entire project period will be populated by PAMS. A detailed budget justification narrative should be included after the budget pages. The justification should cover labor, domestic travel, equipment, materials and supplies, and anything else that will be covered with project funds. Justification must be provided for any proposed sub-awards, explaining the need for the sub-award and why these collaborators have not submitted a separate collaborative proposal.

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.

The travel budget should allow for the cost of attending an initial kickoff meeting and an annual PI meeting, as well as costs for coordination among collaborating institutions and participation in professional meetings as appropriate.

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

Section F. Other Direct Costs:
Enter Other Direct Costs information for each item listed.
- **Materials and Supplies:** Enter total funds requested for materials and supplies in the appropriate fields. In the budget justification, indicate general categories such as glassware, and chemicals, including an amount for each category (items not identified under "Equipment"). Categories less than $1,000 are not required to be itemized. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; quotes/catalog prices of similar or like items; or something else (describe).
- **Publication Costs:** Enter the total publication funds requested. The proposal budget may request funds for the costs of documenting, preparing, publishing or otherwise making available to others the findings and products of the work conducted under the award. In the budget justification, include supporting information. In the budget justification, indicate whether cost estimates are based upon past experience of purchase of similar or like items; vendor quotes of similar publication services; or something else (describe).
- **Consultant Services:** Enter total funds requested for all consultant services. In the budget justification, identify each consultant, the services he/she will perform, total number of days, travel costs, and total estimated costs. In the budget justification, indicate whether consultant cost estimate is based upon previous experience/quotes for similar or like services; or something else (describe).
- **ADP/Computer Services:** Enter total funds requested for ADP/Computer Services. The cost of computer services, including computer-based retrieval of scientific, technical and education information may be requested. In the budget justification, include the established computer service rates at the proposing organization if applicable. In the budget justification, indicate whether cost estimates are based upon quotes/past experience of purchase of similar computer services; established computer service rates at the proposing institution; or something else (describe).

- **Subawards/Consortium/Contractual Costs:** Enter total costs for all subawards/consortium organizations and other contractual costs proposed for the project. In the budget justification, justify the details.
- **Equipment or Facility Rental/User Fees:** Enter total funds requested for Equipment or Facility Rental/User Fees. In the budget justification, identify each rental/user fee and justify. In the budget justification, indicate whether cost estimates are based upon past experience with similar or like items; vendor quotes of similar items; or something else (describe).
- **Alterations and Renovations:** Enter total funds requested for Alterations and Renovations.
- **In the budget justification**, itemize by category and justify the costs of alterations and renovations, including repairs, painting, removal or installation of partitions, shielding, or air conditioning. Where applicable, provide the square footage and costs.
- **Other:** Add text to describe any other Direct Costs not requested above. Enter costs associated with "Other" item(s). Use the budget justification to further itemize and justify.

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

Section H. Other Indirect Costs
Enter the Indirect Cost information for each field. Only four general categories of indirect costs are allowed/requested on this form, so please consolidate if needed.

Section I. Total Direct and Indirect Costs
This amount will be calculated by PAMS (Sections G + H)

D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS

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

E. SUBMISSION DATES AND TIMES

1. Letter of Intent Due Date
Not required.

2. Pre-proposal Due Date
February 7, 2014, at 5:00 PM Eastern Time

3. Proposal Due Date
April 2, 2014, at 5:00 PM Eastern Time

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

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

4. Late Submissions

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

F. FUNDING RESTRICTIONS

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

G. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

1. Where to Submit

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

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

2. Registration Process

ONE-TIME REGISTRATION PROCESS

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

For help with PAMS, click the "External User Guide" link on the PAMS website, 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 14-1043.**

3. Proposal Receipt Notices

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

4. Viewing Submitted Proposals

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

Section V - PROPOSAL REVIEW INFORMATION

A. CRITERIA

1. Initial Review Criteria

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

2. Merit Review Criteria

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

1. Scientific and/or Technical Merit of the Project;
2. Appropriateness of the Proposed Method or Approach;
3. Competency of Applicant's Personnel and Adequacy of Proposed Resources;
4. Reasonableness and Appropriateness of the Proposed Budget; and
5. Relevance to the mission of and systems operated by the Advanced Scientific Computing Research program

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

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

1. **SCIENTIFIC AND/OR TECHNICAL MERIT OF THE PROPOSED RESEARCH**

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

   1.1 What are the strengths and weaknesses of the proposed research with respect to each of the themes in the call for proposals that are addressed in the proposal?
   1.2 Evaluate the overall responsiveness of the proposed research to the call for proposals and the potential of the proposed research to have a significant impact on scientific data management, analysis and visualization on extreme scale platforms. If

successful, to what degree is the proposed research likely to improve the ability of scientists to manage, analyze and understand their data and increase the pace of scientific discovery?

2. **APPROPRIATENESS OF THE PROPOSED METHOD OR APPROACH**

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

2.1 **Evaluate the plan for conducting the research. Is there a clear and coherent plan for the proposed research so that it is an integrated endeavor? Is there strong enough leadership, communication and coordination? Does the proposal include a clear plan for deliverables, a reasonable timeline, and sound methods for assessing the effectiveness of the research?**

2.2 **What is the proposed plan for sharing the results of the proposed research and making available under open source license any software that is developed? Is the plan appropriate and credible?**

3. **COMPETENCY OF APPLICANT'S PERSONNEL AND ADEQUACY OF PROPOSED RESOURCES**

What are the past performance and the potential of the Principal Investigator (PI)? How well qualified is the research team to carry out the proposed research? Is the number of personnel appropriate and sufficient to conduct the proposed research? Are the research environment and facilities adequate for performing the research? Does the proposed work take advantage of unique facilities and capabilities? What is the past performance of the team?

4. **REASONABLENESS AND APPROPRIATENESS OF THE PROPOSED BUDGET**

Are the proposed budget and staffing levels adequate to carry out the proposed work? Is the budget reasonable and appropriate for the scope?

4.1 **Are the levels of support and commitment requested by the PI and other senior personnel appropriate and necessary to meet the research objectives?**

4.2 **Is the proposed budget for travel reasonable and appropriate for the number of people supported and the level of coordination that is necessary for the project to succeed?**

5. **RELEVANCE TO THE MISSION OF AND SYSTEMS OPERATED BY THE ADVANCED SCIENTIFIC COMPUTING RESEARCH PROGRAM**

Does the proposal reflect awareness and understanding of Office of Science and ASCR mission drivers and constraints? How important is the proposed research to fulfilling these missions?

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 and ASCR programs
- Previous performance
- Relevance to the mission of and systems operated by the Advanced Scientific Computing Research program.

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 April 2014. It is expected that awards will be made in Fiscal Year 2014 and possibly Fiscal Year 2015, depending on the availability of funds.

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

Section VI - AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES

1. Notice of Selection

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

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

2. Notice of Award

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

B. REPORTING

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

<center>**Section VII - QUESTIONS/AGENCY CONTACTS**</center>

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 14-1043.
>   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. Lucy Nowell Office of Advanced Scientific Computing Research Phone : 301-903-3191 Email : Lucy.Nowell@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.