FINANCIAL ASSISTANCE
FUNDING OPPORTUNITY ANNOUNCEMENT

U.S. Department of Energy

Office of Science

Office of Advanced Scientific Computing Research (ASCR)

Resilient Extreme-Scale Solvers ("RX-Solvers")

Funding Opportunity Number: DE-FOA-0000742

Announcement Type: Initial

CFDA Number: 81.049

ISSUE DATE: **June 8, 2012**

Pre-Application Due Date: **N/A**

Application Due Date: **August 13, 2012, 11:59 p.m. Eastern Time**

NOTE: REQUIREMENTS FOR GRANTS.GOV

Where to Submit: Applications must be submitted through Grants.gov to be considered for award. You cannot submit an application through Grants.gov unless you are registered. Please read the registration requirements carefully and start the process immediately. Remember you have to update your Central Contract Registry (CCR) registration annually. If you have any questions about your registration, you should contact the Grants.gov Helpdesk at 1-800-518-4726 to verify that you are still registered in Grants.gov.

Registration Requirements: There are several one-time actions you must complete in order to submit an application through Grants.gov (i.e., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the CCR, register with the credential provider, and register with Grants.gov). To register with Grants.gov go to "Get Registered" at http://grants.gov/applicants/get_registered.jsp. Use the Grants.gov Organization Registration Checklist at http://www.grants.gov/assets/OrganizationRegCheck.pdf to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at least 21 days to complete these requirements. It is suggested that the process be started as soon as possible.

IMPORTANT NOTICE TO POTENTIAL APPLICANTS: When you have completed the process, you should call the Grants.gov Helpdesk at 1-800-518-4726 to verify that you have completed the final step (i.e. Grants.gov registration).

Questions: Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. Part VII of this Funding Opportunity Announcement (FOA) explains how to submit other questions to the Department of Energy (DOE).

Application Receipt Notices

After an application is submitted, the Authorized Organization Representative (AOR) will receive a series of four e-mails. It is extremely important that the AOR watch for and save each of the emails. It may take up to two (2) business days from application submission to receipt of email Number 2. The titles of the four e-mails are:

Number 1 - Grants.gov Submission Receipt Number
Number 2 - Grants.gov Submission Validation Receipt for Application Number
Number 3 - Grants.gov Grantor Agency Retrieval Receipt for Application Number
Number 4 - Grants.gov Agency Tracking Number Assignment for Application Number

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PART I – FUNDING OPPORTUNITY DESCRIPTION

GENERAL INQUIRIES ABOUT THIS FOA SHOULD BE DIRECTED TO:

Technical/Scientific Program Contacts:

Program Manager: Dr. Karen Pao, (301) 903- 5384
Office of Advanced Scientific Computing Research, SC-21.1
E-mail: karen.pao@science.doe.gov
Office of Advanced Scientific Computing Research Webpage:
http://science.energy.gov/ascr/funding-opportunities/

STATUTORY AUTHORITY

Public Law 95-91, US Department of Energy Organization Act
Public Law 109-58, Energy Policy Act of 2005

APPLICABLE REGULATIONS

U.S. Department of Energy Financial Assistance Rules, codified at 10 CFR Part 600
U.S. Department of Energy, Office of Science Financial Assistance Program Rule, codified at 10 CFR Part 605

SUMMARY:

Advanced Scientific Computing Research (ASCR), Office of Science (SC), US Department of Energy (DOE), invites applications for basic research in Resilient Extreme-Scale Solvers ("RX-Solvers") that demonstrably advances the state of science and practice for scalable, resilient, extreme-scale numerical algorithms, to enable scientific discovery on the supercomputers expected to come online in the next 5-10 years and lay the foundation for research in numerical algorithms for extreme-scale scientific computing.

The advancement of computer architectures is undergoing fundamental changes. Microprocessor clock speed has now reached an upper bound dictated by prevailing technology, thus improvement in performance of computers is now achieved by adding more processors to a chip. At the same time, power considerations are reducing the amount of memory available to each processor, and I/O bandwidth is not expected to keep up with performance growth. For the exascale machine, the power consumption needs to be an order of magnitude less than that extrapolated from today's energy consumption levels; the system memory is expected to be a fraction of the traditional ratio of 1 byte per floating-point operation per second (FLOPS); and the level of total concurrency is expected to be billions, if not tens of billions.

Today, at 1-10 peta-FLOPS (PF), evolutionary approaches, or "patches," to current programming and execution models (such as "MPI+X") are often employed to keep existing science application codes running, while leaving the underpinning numerical algorithms largely intact. This is akin to adjusting the exterior of an automobile to gain some fuel efficiency through aerodynamics without reexamining the internal combustion engine. For the extreme-scale

computers – specifically, systems over 100 PF, that are expected to come online in the next 5-10 years -- the patch approach is not expected to be sustainable: even today, high-performance computational scientists have to manage data movement and communication explicitly for many existing architectures to achieve performance gains, and an increased number of soft errors and other faults have been observed or encountered. Independent of exact architectural detail of the next-generation supercomputer systems, serious refactoring or rethinking of today's numerical algorithms will be required.

We seek basic research in the design, synthesis, analysis, implementation, and demonstration of resilient numerical algorithms that are at the heart of DOE high-performance computing science and engineering applications, so that these applications will fully realize the promises of the next-generation extreme-scale supercomputers. These algorithms must address resilience or fault tolerance at an algorithmic level. The research team is expected to demonstrate the level of performance of the proposed algorithms through a combination of numerical analysis and numerical experiments, based on a suite of relevant, nontrivial performance metrics identified and specified by the research team itself.

More specific information is included under SUPPLEMENTARY INFORMATION below.

A companion Program Announcement to DOE National Laboratories, LAB 12-742, will be posted on the SC Grants and Contracts web site at: http://www.science.doe.gov/grants

SUPPLEMENTARY INFORMATION:

The advancement of computer architectures is undergoing fundamental changes. These changes are expected to be disruptive, especially with regard to conventional wisdoms accumulated in the last 20-30 years of high-performance scientific computing.

Today, top supercomputers are capable of performing at around 1-3 PF. They consume 2-7 MW/year (at a cost of roughly $1M per MW per year). These systems may have around 20,000 processors, with a total concurrency of up to around 250,000. These systems may have a few hundred tera-bytes (TB) of total memory, 10's of peta-bytes (PB) of storage, and I/O bandwidth around a few hundred giga-bytes per second (GB/s).

An exascale system would be capable of performing 10^18 operations per second, one thousand times of the peta-scale machines. A 2008 DARPA study has determined that it is impossible to "scale" today's machine up to 1 EF; the power required to operate such a computer is the biggest obstacle. If one limits the power to about 20 MW, the exascale machine would still have O(100,000) – O(1,000,000) processors, with 10's – 100's of billions of total concurrency. The system memory is expected to be about 60 PB, with 500-1000 PB of storage. The I/O bandwidth may be around 60 TB/s.

In the next few years, before the exascale system would be designed, one may expect a few intermediate systems capable of performing at few hundred petaflops coming online. These intermediate systems will also not be scaled from today's 1-10 PF systems. Power consumption is expected to be an issue; by employing heterogeneous architectures, however, it may be

feasible to build 100-300 PF systems that consume ~15 MW/year. In addition to heterogeneity, these systems also have a formidable level of concurrency: they may have 50,000 – 500,000 processors, with 10's – 100's of millions of total concurrency – at least 2-3 orders of magnitude of today's level of concurrency. The system memory may be around 5 PB -- continuing the trend of decreasing byte-per-flops, with a complex memory hierarchy. The storage may be around 150 PB, and the I/O bandwidth around 10 TB/s. Thus, even though not at exaflops, these intermediate machines embody the significant hurdles for the deployment of application codes – and for scientific discovery through simulation -- as we march towards exascale.

For a transition of DOE applications from today's 1-10 PF Leadership-class machines to the machines of the next 5-10 years, expected to be 100 PF or more, the main algorithmic challenges are

- Extreme concurrency: estimates of two to three orders-of-magnitude of parallelism over today's levels will require solvers to pay particular attention to Amdahl's Law;
- Complex memory hierarchies: algorithms that assume rapid access to large memory may end up having to access data from far away via (generally slower) interconnects; algorithms that wish to utilize local memory (such as cache or scratchpad) may face added complexities;
- Costly data movement: the energy required for communication is far greater than that required for floating point operations; optimizing the movement of data in algorithms may potentially reduce the power requirement;
- Nondeterministic behavior in hardware: due to manufacturing challenges and the high level of concurrency, the numbers of failures, soft-errors, and other faults are expected to increase to levels that cannot be ignored.

These challenges are not completely independent. As microprocessor clock speed reaches a plateau, increased concurrency becomes the predominant mechanism to increase performance. Technologies for memory systems have unfortunately not progressed as quickly as microprocessor; increasing the complexity of memory hierarchy can be viewed a compromise between the need to pack in more memory and the need to control the cost of the overall high-performance computing system. The current implementations of many applications, however, assume the availability of memory somewhere, thus further increasing communication and data movement – and increasing the energy consumption in the process. The unrealistic level of projected energy consumption is in turn driving hardware vendors to reduce or manage power consumption at a low level. With increased density and complexity of components operating near the limit of current technology, we expect to observe in future hardware "nondeterministic" behavior that may be attributed to increased stress and damage to system components and that are realized as faults, failures, and other errors.

Arguably, extreme concurrency, complex memory hierarchies, and costly data movement are challenges that may be overcome with technology (that is, with sufficient investment, sophistication, and advancement in hardware technology). Nondeterministic behavior in hardware, however, has its root cause in the laws of physics and will be far more difficult, even infeasible, to mitigate by technological advances alone. All these challenges are expected to persist for exascale systems and beyond.

Application performance on supercomputers has traditionally been measured by maximizing the number of FLOPS, often at the expense of data placement, storage, and movement. Numerical algorithms that are at the heart of high-performance scientific applications have counted on having sufficient – or sufficiently rapid access to -- memory, where necessary data, frequently multiple copies of data, would be stored. The impending architectural changes, brought on by increased level of concurrency and reduced memory, have significantly lowered the relative cost of floating point operations to data movement: once high-performing algorithms will become communication-bound and memory-bound, or slow and expensive.

The architectural changes also introduce significant uncertainty in the faults application codes running on these architectures will need to deal with. Historically, errors and faults are infrequent and would be handled at a low level (for example, by the microprocessors, by error-correction codes); the only higher-level option for dealing with unexpected failures is check-pointing, or writing large "restart" files frequently so that, if failure is encountered, one may return to a nearby "checkpoint" and use the information stored in the restart file to restart a run. With the exponentially increasing number of processors and with the I/O and memory bandwidths not improving at the same rate, applications are expected to be subject to a large number of hard (failure of a device) interrupts and soft (change of a data value) errors, and it may no longer be possible to write, store, and subsequently read restart files to counter the frequency with which faults are expected to occur. Numerical algorithms may no longer be able to rely on hardware or system software alone for resilience.

For the purpose of this FOA, a "solver" is a numerical algorithm that provides a numerical solution to a mathematical model of a physical system of interest and of relevance to the Department of Energy missions. Examples of solvers include linear algebra algorithms such as direct and iterative linear solvers, nonlinear solvers, and eigensolvers, for large systems; numerical methods for solving composite systems of partial differential equations; algorithms in optimization or mathematical programming; etc. Low-level, fundamental routines such as basic arithmetic operations or Fast Fourier Transform (FFT) will not be considered as a suitable "solver" for the purpose of this FOA.

To be considered for recommendation for awards, applications to this FOA must include three elements:

1. Advances in solvers: For solvers to meet the architectural challenges of the extreme-scale machine 100 PF and beyond, they need to achieve optimal data movement and maximize available memory and I/O bandwidths. For example, strategies for achieving optimal data movement may include utilizing variable-precision arithmetic, reordering algorithms to "trade computation for communication", explicitly exploiting the machine's memory hierarchies, etc.; strategies for maximizing available bandwidths may include reducing global synchronization, "bringing computation to the data" by including more auxiliary calculations such as in situ data analysis and uncertainty quantification, designing and employing latency-tolerant algorithms such as parallel time integration, etc. Advances in solvers may be achieved by, for example, revisiting past algorithms, refactoring current, existing algorithms, or rethinking the mathematics for new classes of algorithms.

2. Fault tolerance and resilience at the algorithmic level: Future architectural challenges bring the issue of resilience to front and center. The number of faults, whether detected or corrected or not, is expected to increase with increasing system size and complexity. Traditional approaches to resilience and fault tolerance, such as assuming low-level error correction, redundancy, and checkpoint-restart, are not expected to be adequate, affordable, or possible. Algorithmic research for high-performance computers should include resilience and fault tolerance as a value-added feature of the numerical algorithm, a feature that can be "turned on" when deploying the algorithm on a new, experimental, or developmental architecture or "turned off" as the reliability of a computing system becomes predictable. . Resilience presents a rare opportunity for revolutionary innovations in algorithmic research. For resilience at the algorithmic level, solvers may consider embracing non-determinism, by, for example, employing stochastic or probabilistic methods to minimize the overall effects of faults. Solvers will need to detect, run through, or otherwise recover from various sources of faults – indeed, even defining what we mean by "correct" or "reproducible" may require research.

3. Performance of proposed algorithms: A particular difficulty in solvers research is the demonstration of the performance predictions of any new algorithm. Architecture simulators are usually not available to or easily accessible by designers of numerical algorithms, who are typically applied mathematicians and numerical analysts, as are appropriate abstract machine models, performance simulation tools, and (preferably – architecture-independent) programming models. Performance measurement tools are needed in order to guide the implementation of algorithms; these tools should measure all aspects of performance, including execution time, memory performance, data movement, faults, and energy consumption. For the extreme-scale systems, many of these models and tools are current research topics in computer science. Without the means of measuring, characterizing, validating, or otherwise quantifying the performance predictions of the new algorithms on upcoming architectures, solvers designers alone may find it difficult to gauge progress. Researchers in numerical algorithms are encouraged to perform traditional numerical analysis and, in collaboration with other experts, leverage and explore tools and models that will help them characterize new algorithms beyond using the traditional flop count, propose performance metrics that more closely represent the realities of scientific computing in the extreme-scale era. Researchers are expected to devise a suitable suite of performance metrics and demonstrate, beyond "toy problems", "linearized analysis", or "back-of-the-envelope estimates", measurable progress towards conquering the extreme-scale challenges.

Preference will be given to integrated algorithmic research projects ("large teams") that consider a broad spectrum of the challenges to solvers holistically; however, a small number of smaller projects ("small teams") that propose technically sound and imaginative research for specific challenges in solvers may be considered. Please see Award Information (Part II) below for detail. All projects will be subject to the same Merit Review criteria. Please see Application Review Information (Part V) below for the Merit Review criteria.

No architectural or hardware research will be considered for funding, either as a part of a collaboration or as a stand-alone project. Requests may not include funds for hardware lease or purchase.

Applications whose research plans do not include numerical algorithms research in a substantive manner will be deemed nonresponsive. Applications whose research plans do not include work in resilience or fault tolerance in a substantive manner will be deemed nonresponsive. Applications whose research plans do not include characterization and demonstration of the performance of proposed algorithms in a substantive manner will be deemed nonresponsive.

Each project is expected to have a management plan appropriate for the size and complexity of the project. The roles of senior and key personnel must be clearly articulated. A communication plan, both for communication within the project and for communication with the broader community, is expected from each project. The Principle Investigator is expected to commit sufficient time to be accountable for the successful execution of the project's plans. Other senior project personnel are expected to commit sufficient time in order to make significant technical contributions to the project. The project's management and communication plans and the levels of commitment of effort of lead project investigator, key personnel, and other senior personnel will be considered in Merit Review.

References

"Scientific Grand Challenges: Crosscutting Technologies for Computing at the Exascale", report from the workshop held February 2-4, 2010.
http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/Crosscutting_grand_challenges.pdf

"The Opportunity and Challenges of Exascale Computing", summary report of the Advanced Scientific Computing Advisory Committee (ASCAC) Subcommittee. Fall 2010.
http://science.energy.gov/~/media/ascr/ascac/pdf/reports/Exascale_subcommittee_report.pdf

Kogge, Peter, "Next-Generation Supercomputers", IEEE Spectrum, February 2011.
http://spectrum.ieee.org/computing/hardware/nextgeneration-supercomputers/0
"Exascale Programming Challenges", report from the Workshop on Exascale Programming Challenges held July 27-29, 2011.
http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/ProgrammingChallengesWorkshopReport.pdf

"Tools for Exascale Computing: Challenges and Strategies", report from the Exascale Tools Workshop held October 13-14, 2011.
http://science.energy.gov/~/media/ascr/pdf/research/cs/Exascale%20Workshop/Exascale_Tools_Workshop_Report.pdf

"Workshop on Extreme-Scale Solvers: Transition to Future Architectures", report from the Extreme-Scale Solvers Workshop held March 8-9, 2012.
http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/reportExtremeScaleSolvers2012.pdf

Collaborations

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. Collaborative applications submitted from different institutions should clearly indicate they are part of a proposed collaboration and contain the same title, abstract and narrative for that research project. In addition, such applications must describe the work and the associated budget for the research effort being performed under the leadership of the Principal Investigator at that participating institution.

These collaborative applications should all have the same title as the Lead Institution. Each collaborating institution submitting an application must use the same title in Block 11 of the SF 424 (R&R) form.

PART II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT.

DOE anticipates awarding grants under this FOA.

B. ESTIMATED FUNDING.

Awards are expected to be made for a period of three years at a funding level of up to $4,500,000 per year to support multiple awards in Fiscal Year 2012, with out-year support contingent on the availability of appropriated funds and satisfactory progress.

The awards will be made in the following two categories:

- Large team awards: awards involving multiple investigators from two or more institutions. The funding level for these awards will be roughly around $1M -- $2.5M per year for up to three years.
- Small team awards: awards involving single investigators or small teams. The funding level for these awards will be up to $250K per year for up to three years.

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

C. MAXIMUM AND MINIMUM AWARD SIZE.

The award size will depend on the number of meritorious applications and the availability of appropriated funds. It is expected that the maximum award size for universities would be up to $1.5M per year and the minimum would be $150K.

D. EXPECTED NUMBER OF AWARDS.

The exact number of awards will depend on the number of meritorious applications and the availability of appropriated funds. We expect to make up to three large team awards and no more than two single investigator awards.

E. ANTICIPATED AWARD SIZE.

The award size will depend on the number of meritorious applications and the availability of appropriated funds. The total project size is anticipated to range from $150,000 up to $4,500,000 per year.

F. PERIOD OF PERFORMANCE.

Grants are expected to be made for a period of three years at a funding level appropriate for the proposed scope, with out-year support contingent on the availability of appropriated funds and satisfactory progress.

G. TYPE OF APPLICATION.

DOE will accept new applications under this FOA.

PART III - ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS.

All types of domestic entities are eligible to apply, except other Federal agencies, Federally Funded Research and Development Center (FFRDC) Contractors, and nonprofit organizations described in section 501(c)(4) of the Internal Revenue Code of 1986 that engaged in lobbying activities after December 31, 1995.

B. COST SHARING.

Cost sharing is not required.

C. OTHER ELIGIBILITY REQUIREMENTS.

N/A

PART IV – APPLICATION AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST APPLICATION PACKAGE.

Application forms and instructions are available at Grants.gov. To access these materials, go to http://www.grants.gov, select "**Apply for Grants**", and then select "**Download a Grant Application Package**". Enter the CFDA and/or the funding opportunity number located on the cover of this FOA and then follow the prompts to download the application package.

B. LETTER OF INTENT AND PRE-APPLICATION

1. Letter of Intent.

N/A

2. Pre-Application.

N/A

C. CONTENT AND FORM OF APPLICATION – SF 424 (R&R)

You must complete the mandatory forms and any applicable optional forms (e.g., SF-LLL-Disclosure of Lobbying Activities) in accordance with the instructions on the forms and the additional instructions below. **Files that are attached to the forms must be in Adobe Portable Document Format (PDF) unless otherwise specified in this FOA.**

1. SF 424 (R&R)

Complete this form first to populate data in other forms. Complete all the required fields in accordance with the pop-up instructions on the form. The list of certifications and assurances referenced in Field 17 can be found on the DOE Financial Assistance Forms Page at http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms under Certifications and Assurances.

By submitting an application in response to this FOA the Applicant certifies that:

- It is **not** a corporation that has been convicted (or had an officer or agent of such corporation acting on behalf of the corporation convicted) of a felony criminal violation under any Federal law within the preceding 24 months,

- It is **not** a corporation that has any unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or have lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability,

- If the Applicant's financial assistance application is chosen for award and the award is in excess of $1,000,000, the applicant will, by the end of the fiscal year, upgrade

the efficiency of their facilities by replacing any lighting that does not meet or exceed the energy efficiency standard for incandescent light bulbs set forth in Section 325 of the Energy Policy and Conservation Act (42 U.S.C. 6295).

2. RESEARCH AND RELATED Other Project Information.
Complete questions 1 through 6 and attach files. The files must comply with the following instructions:

Project Summary/Abstract (Field 7 on the Form).
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 project director/principal investigator(s) (PD/PI), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes), and major participants (for collaborative projects). 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. To attach a Project Summary/Abstract, click "Add Attachment."

Project Narrative (Field 8 on the Form).
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). EVALUATORS WILL ONLY REVIEW THE NUMBER OF PAGES SPECIFIED IN THE PRECEDING SENTENCE. The font must not be smaller than 11 point.

Please do not submit general letters of support as these are not used in making funding decisions and can interfere with the selection of peer reviewers.

Do not include any Internet addresses (URLs) that provide information necessary to review the application, because the information contained in these sites will not be reviewed. See Part VIII.D for instructions on how to mark proprietary application information. To attach a Project Narrative, click "Add Attachment."

The application narrative should begin with a cover page that includes: the project title, the Lead PI's name and complete contact information.

The cover page must also include the following information (this page will not count in the project narrative page limitation):

Applicant/Institution:
Street Address/City/State/Zip:
Principal Investigator:
Postal Address:
Telephone Number:

Email:
Funding Opportunity Announcement Number: DE-FOA-0000742

DOE/Office of Science Program Office: Office of Advanced Scientific Computing Research (ASCR)
DOE/Office of Science Program Office Technical Contact: Dr. Karen Pao

Is this a Collaboration? If yes, please list ALL Collaborating Institutions/PIs and indicate which ones will also be submitting applications. Also indicate the PI who will be the point of contact and coordinator for the combined research activity.

The Lead-PI should include the following table on the cover page.

Sample Table for the Lead Institution ($ in thousands)

	Year 1	**Year 2**	**Year 3**	**Total**
Name of PI and Institution	$	$	$	$
Name of Co-PI and Institution	$	$	$	$
Name of Co-PI and Institution	$	$	$	$
Name of Co-PI and Institution	$	$	$	$
Total	$	$	$	$

Project Objectives:

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

The Project Narrative comprises the research plan for the project; it should contain enough background material in the Introduction, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the method to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities.

Appendix 1: Biographical Sketch.

Provide a biographical sketch for the project director/principal investigator (PD/PI) and each senior/key person listed in Section A on the R&R Budget form. **Provide the Biographical Sketch information as an Appendix to your project narrative. Do not attach a separate file. The Biographical Sketch Appendix will not count in the project narrative page limitation.**

The biographical information (curriculum vitae) for each person 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:

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.

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

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

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

Graduate and Postdoctoral Advisors and Advisees: List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s) during the last 5 years. Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates during the past 5 years.

Appendix 2: Current and Pending Support.
Provide a list of all current and pending support (both Federal and non-Federal) for the Project Director/Principal Investigator(s) (PD/PI) and senior/key persons, including subawardees, for ongoing projects and pending applications. 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 senior/key person. **Provide the Current and Pending Support as an Appendix to your project narrative. Do not attach a separate file. The Current and Pending Support Appendix will not count in the project narrative page limitation.** Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.

Appendix 3: Bibliography and 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. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the application. **Provide the Bibliography and References Cited information as an Appendix to your project narrative. Do not attach a separate file. The Bibliography and References Cited Appendix will not count in the project narrative page limitation.**

Appendix 4: Facilities and 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. **Provide the Facility and Other Resource information as an Appendix to your project narrative. Do not attach a separate file. The Facility and Other Resource Appendix will not count in the project narrative page limitation.**

Appendix 5: Equipment.
List major items of equipment already available for this project and, if appropriate identify location and pertinent capabilities. **Provide the Equipment information as an Appendix to your project narrative. Do not attach a separate file. The Equipment Appendix will not count in the project narrative page limitation.**

Appendix 6: Other Attachment.
If you need to elaborate on your responses to questions 1-6 on the "Other Project Information" document, **please provide the Other Attachment information as an Appendix to your project narrative. Do not attach a separate file. The Other Attachment Appendix will not count in the project narrative page limitation.**

Do not attach any of the requested Appendices described above as files for fields 9, 10, 11, and 12. Instead follow the above instructions to include the information as Appendices to the project narrative file (these Appendices will not count in the project narrative page limitation).

3. RESEARCH AND RELATED BUDGET.

Complete the Research and Related Budget form in accordance with the instructions on the form and the following instructions. You must complete a separate budget for each year of support requested. The form will generate a cumulative budget for the total project period. You must complete all the mandatory information on the form before the NEXT PERIOD button is activated. You may request funds under any of the categories listed as long as the item and amount are necessary to perform the proposed work, meet all the criteria for allowability under the applicable Federal cost principles, and are not prohibited by the funding restrictions in this FOA (See PART IV, G).

Budget Justification (Field K on the form).

Provide the required supporting information for the following costs: equipment; domestic and foreign travel; participant/trainees; material and supplies; publication; consultant services; ADP/computer services; subaward/consortium/contractual; equipment or facility rental/user fees; alterations and renovations; and indirect cost type. Provide any other information you wish to submit to justify your budget request. **Attach a single budget justification file for the entire project period in Field K.** The file automatically carries over to each budget year.

4. R&R SUBAWARD BUDGET ATTACHMENT(S) FORM.

Budgets for Subawardees, other than DOE FFRDC Contractors. You must provide a separate cumulative R&R budget for each subawardee that is expected to perform work estimated to be more than $100,000 or 50 percent of the total work effort (whichever is less). If you are selected for award, you must submit a multi-year budget for each of these subawardees. Download the R&R Budget Attachment from the R&R SUBAWARD BUDGET ATTACHMENT(S) FORM and e-mail it to each subawardee that is required to submit a separate budget. After the Subawardee has e-mailed its completed budget back to you, attach it to one of the blocks provided on the form. Use up to 10 letters of the subawardee's name (plus .xfd) as the file name (e.g., ucla.xfd or energyres.xfd).

5. PROJECT/PERFORMANCE SITE LOCATION(s)

Indicate the primary site where the work will be performed. If a portion of the project will be performed at any other site(s), identify the site location(s) in the blocks provided.

Note that the Project/Performance Site Congressional District is entered in the format of the 2 digit state code followed by a dash and a 3 digit Congressional district code, for example VA-001. Hover over this field for additional instructions.

Use the Next Site button to expand the form to add additional Project/Performance Site Locations.

SF-LLL Disclosure of Lobbying Activities

If applicable, complete SF- LLL. Applicability: If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the grant, you must complete and submit Standard Form - LLL, "Disclosure Form to Report Lobbying."

Summary of Required Forms/Files

Your application must include the following documents:

Name of Document	Format	Attach to
SF 424 (R&R)	Form	N/A
RESEARCH AND RELATED Other Project Information	Form	N/A
Project Summary/Abstract	PDF	Field 7
Project Narrative, including required appendices	PDF	Field 8
RESEARCH & RELATED BUDGET	Form	N/A
Budget Justification	PDF	Field K
PROJECT/PERFORMANCE SITE LOCATION(S)	Form	N/A
SF-LLL Disclosure of Lobbying Activities, if applicable	Form	N/A

D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS.

If selected for award, DOE reserves the right to request additional or clarifying information for any reason deemed necessary, including, but not limited to:

- Indirect cost information
- Other budget information
- Name and phone number of the Designated Responsible Employee for complying with national policies prohibiting discrimination (See 10 CFR 1040.5)
- Representation of Limited Rights Data and Restricted Software, if applicable
- Commitment Letter from Third Parties Contributing to Cost Sharing, if applicable.

E. SUBMISSION DATES AND TIMES.

1. Letter of Intent.

N/A

2. Pre-Application.

N/A

3. Formal Applications.

APPLICATION DUE DATE: August 13, 2012, 11:59 PM Eastern Time

Formal applications submitted in response to this FOA must be received by **August 13, 2012**, 11:59 PM Eastern Time, to permit timely consideration of awards in Fiscal Year 2013. **You are encouraged to submit your application well before the deadline. APPLICATIONS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.**

F. INTERGOVERNMENTAL REVIEW.

This program is not subject to Executive Order 12372 Intergovernmental Review of Federal Programs.

G. FUNDING RESTRICTIONS.

Cost Principles**.** Costs must be allowable in accordance with the applicable Federal cost principles referenced in 10 CFR Part 600. The cost principles for commercial organization are in FAR Part 31.

Pre-award Costs**.** Recipients may charge to an award resulting from this FOA pre-award costs that were incurred within the ninety (90) calendar-day period immediately preceding the effective date of the award, if the costs are allowable in accordance with the applicable Federal cost principles referenced in 10 CFR Part 600. Recipients must obtain the prior approval of the contracting officer for any pre-award costs that are for periods greater than this 90-day calendar period.

Pre-award costs are incurred at the applicant's risk. DOE is under no obligation to reimburse such costs if for any reason the applicant does not receive an award or if the award is made for a lesser amount than the applicant expected.

H. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS.

1. Where to Submit.

APPLICATIONS MUST BE SUBMITTED THROUGH GRANTS.GOV TO BE CONSIDERED FOR AWARD.

Submit electronic applications through the "Apply for Grants" function at www.Grants.gov. If you have problems completing the registration process or submitting your application, call Grants.gov at 1-800-518-4726 or send an email to support@grants.gov.

2. Registration Process.

Registration Requirements: There are several one-time actions you must complete in order to submit an application through Grants.gov (i.e., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the CCR, register with the credential provider, and register with Grants.gov). To register with Grants.gov go to "Get Registered" at http://grants.gov/applicants/get_registered.jsp. Use the Grants.gov Organization Registration Checklist at http://www.grants.gov/assets/OrganizationRegCheck.pdf to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at least 21 days to complete these requirements. It is suggested that the process be started as soon as possible.

IMPORTANT NOTICE TO POTENTIAL APPLICANTS: When you have completed the process, you should call the Grants.gov Helpdesk at 1-800-518-4726 to verify that you have completed the final step (i.e. Grants.gov registration).

Questions: Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. Part VII of this FOA explains how to submit other questions to the Department of Energy (DOE).

Application Receipt Notices

After an application is submitted, the Authorized Organization Representative (AOR) will receive a series of four e-mails. It is extremely important that the AOR watch for and save each of the emails. It may take up to two (2) business days from application submission to receipt of email Number 2. The titles of the four e-mails are:

Number 1 - Grants.gov Submission Receipt Number
Number 2 - Grants.gov Submission Validation Receipt for Application Number
Number 3 - Grants.gov Grantor Agency Retrieval Receipt for Application Number
Number 4 - Grants.gov Agency Tracking Number Assignment for Application Number

PART V - APPLICATION REVIEW INFORMATION

A. CRITERIA

Initial Review Criteria.

Prior to a comprehensive merit evaluation, DOE will perform an initial review in accordance with 10 CFR 605.10(b) to determine that (1) the applicant is eligible for the award; (2) the information required by the FOA has been submitted; (3) all mandatory requirements are satisfied; and (4) the proposed project is responsive to the objectives of the FOA. Applications that fail to pass the initial review will not be forwarded for merit review and will be eliminated from further consideration.

Merit Review Criteria

Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria codified at 10 CFR 605.10(d). Included within each criterion are specific questions that the merit reviewers will be asked to consider.

1) Scientific and/or technical merit of the project

- Does the proposed research significantly advance the state-of-the-art in numerical algorithms for scientific discovery, and will meet the architectural challenges of extreme-scale systems?
- Does the proposed research clearly address fault tolerance and resilience at an algorithmic level?
- Does the research plan contain scientifically valid performance metrics that will allow progress to be measured?
- Does the proposed research have the potential to have significant, far-reaching impact beyond the next-generation extreme-scale computers?

2) Appropriateness of the proposed method or approach

- How feasible is the proposed research plan for the advancement of numerical algorithms for scientific discovery?
- How feasible is the proposed research plan to address fault tolerance and resilience at an algorithmic level?
- How feasible is the proposed plan for the characterization and demonstration of the performance of proposed algorithms?
- What is the likelihood that the applicant can overcome the key challenges and, as warranted, shift research directions in response to promising advances in basic research?

3) Competency of the applicant's personnel and adequacy of the proposed resources

- Has the applicant requested sufficient time and resources to execute the research plan successfully?
- Does the project have a sound communication plan?
- Does the project have an appropriate and effective management plan?
- Is the Principle Investigator capable of leading this project and being accountable for the successful execution of the project's technical, management, and communication plans?
- Are the roles of senior or key personnel clearly and adequately described, and have these senior or key personnel committed sufficient level of effort to ensure the success of this project?

4) Reasonableness and appropriateness of the proposed budget

- Is the requested manpower reasonable and appropriate?
- Is the travel budget appropriate?

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

- Relevance of proposed research to DOE missions;
- Potential impact of proposed research activities on ASCR Exascale goals and objectives;
- Potential for developing synergies and/or relation of the proposed research activities to other research efforts supported by ASCR, such as those in applied mathematics and computer science; and
- Total amount of DOE funds available.

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

C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES.

It is anticipated that selections will be completed by September 23, 2012. Awards will be made in Fiscal Year 2013.

PART 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. (See Part IV.G with respect to the allowability of pre-award costs.)

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

2. Notice of Award.

An Assistance Agreement issued by the contracting officer is the authorizing award document. It normally includes, either as an attachment or by reference: 1. Special Terms and Conditions; 2. Applicable program regulations, if any; 3. Application as approved by DOE; 4. DOE assistance regulations at 10 CFR Part 600; 5. National Policy Assurances to be Incorporated as Award Terms; 6. Budget Summary; and 7. Federal Assistance Reporting Checklist, which identifies the reporting requirements.

For grants and cooperative agreements made to universities, non-profits and other entities subject to Title 2 CFR the Award also includes the Research Terms and Conditions located at: http://www.nsf.gov/bfa/dias/policy/rtc/index.jsp.

B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS.

1. Administrative Requirements.

The administrative requirements for DOE grants and cooperative agreements are contained in 10 CFR 600 and 10 CFR Part 605 (See: http://ecfr.gpoaccess.gov). Grants and cooperative agreements made to universities, non-profits and other entities subject to Title 2 CFR are subject to the Research Terms and Conditions located on the National Science Foundation web site at: http://www.nsf.gov/bfa/dias/policy/rtc/index.jsp.

DUNS and CCR Requirements

Additional administrative requirements for DOE grants and cooperative agreements are contained in 2 CFR, Part 25 (See: http://ecfr.gpoaccess.gov). Prime awardees must keep their data at CCR current. Subawardees at all tiers must obtain DUNS numbers and provide the DUNS to the prime awardee before the subaward can be issued.

Subaward and Executive Reporting

Additional administrative requirements necessary for DOE grants and cooperative agreements to comply with the Federal Funding and Transparency Act of 2006 (FFATA) are contained in 2 CFR, Part 170. (See: http://ecfr.gpoaccess.gov). Prime awardees must

register with the new FSRS database and report the required data on their first tier subawardees. Prime awardees must report the executive compensation for their own executives as part of their registration profile in the CCR.

2. Special Terms and Conditions and National Policy Requirements.
The DOE Special Terms and Conditions for Use in Most Grants and Cooperative Agreements are located at: http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms under Award Terms. The National Policy Assurances to be Incorporated as Award Terms are located at: http://www.nsf.gov/bfa/dias/policy/rtc/appc.pdf.

Intellectual Property Provisions.
The standard DOE financial assistance intellectual property provisions applicable to the various types of recipients are located at: http://energy.gov/gc/standard-intellectual-property-ip-provisions-financial-assistance-awards.

Statement of Substantial Involvement
Either a grant or cooperative agreement may be awarded under this FOA. If the award is a cooperative agreement, the DOE Contract Specialist and DOE Project Officer will negotiate a Statement of Substantial Involvement prior to award.

C. REPORTING.

Reporting requirements are identified on the Federal Assistance Reporting Checklist, DOE F4600.2, attached to the award agreement. For a sample Checklist, see http://energy.gov/management/office-management/operational-management/financial-assistance/financial-assistance-forms.

PART VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

Questions regarding the content of the FOA must be submitted through the FedConnect portal. You must register with FedConnect to respond as an interested party to submit questions, and to view responses to questions. It is recommended that you register as soon after release of the FOA as possible to have the benefit of all responses. More information is available at: https://www.fedconnect.net/FedConnect/PublicPages/FedConnect_Ready_Set_Go.pdf.

DOE will try to respond to a question within 3 business days, unless a similar question and answer have already been posted on the website.

Applications submitted through FedConnect will not be accepted.

Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. DOE cannot answer these questions.

B. AGENCY CONTACTS:

Technical/Scientific Program Contacts:

Program Manager: Dr. Karen Pao, (301) 903- 5384
Office of Advanced Scientific Computing Research, SC-21.1
E-mail: karen.pao@science.doe.gov
Office of Advanced Scientific Computing Research Webpage:
http://science.energy.gov/ascr/funding-opportunities/

PART VIII - OTHER INFORMATION

A. MODIFICATIONS.

Notices of any modifications to this FOA will be posted on Grants.gov and the FedConnect portal. You can receive an email when a modification or an FOA message is posted by registering with FedConnect as an interested party for this FOA. It is recommended that you register as soon after release of the FOA as possible to ensure you receive timely notice of any modifications or other FOAs. More information is available at http://www.fedconnect.net.

B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE.

DOE reserves the right, without qualification, to reject any or all applications received in response to this FOA and to select any application, 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 APPLICATION INFORMATION.

Patentable ideas, trade secrets, proprietary or confidential commercial or financial information, disclosure of which may harm the applicant, should be included in an application 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 application which are to be restricted:

"The data contained in pages _____ of this application have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes, provided that if this applicant receives an award as a result of or in connection with the submission of this application, DOE shall have the right to use or disclose the data herein to the extent provided in the award. This restriction does not limit the government's right to use or disclose data obtained without restriction from any source, including the applicant."

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 application, consents to the use of non-Federal reviewers/administrators. Non-Federal reviewers must sign conflict of interest and non-disclosure agreements prior to reviewing an application. Non-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

F. INTELLECTUAL PROPERTY DEVELOPED UNDER THIS PROGRAM.

Patent Rights. The government will have certain statutory rights in an invention that is conceived or first actually reduced to practice under a DOE award. 42 U.S.C. 5908 provides that title to such inventions vests in the United States, except where 35 U.S.C. 202 provides otherwise for nonprofit organizations or small business firms. However, the Secretary of Energy may waive all or any part of the rights of the United States subject to certain conditions. (See "Notice of Right to Request Patent Waiver" in paragraph G below.)

Rights in Technical Data. Normally, the government has unlimited rights in technical data created under a DOE agreement. Delivery or third party licensing of proprietary software or data developed solely at private expense will not normally be required except as specifically negotiated in a particular agreement to satisfy DOE's own needs or to insure the commercialization of technology developed under a DOE agreement.

G. NOTICE OF RIGHT TO REQUEST PATENT WAIVER.

Applicants may request a waiver of all or any part of the rights of the United States in inventions conceived or first actually reduced to practice in performance of an agreement as a result of this FOA, in advance of or within 30 days after the effective date of the award. Even if such advance waiver is not requested or the request is denied, the recipient will have a continuing right under the award to request a waiver of the rights of the United States in identified inventions, i.e., individual inventions conceived or first actually reduced to practice in performance of the award. Any patent waiver that may be granted is subject to certain terms and conditions in 10 CFR 784.12, http://ecfr.gpoaccess.gov/cgi/t/text/text-idx?c=ecfr&tpl=/ecfrbrowse/Title10/10cfr784_main_02.tpl.

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Domestic small businesses and domestic nonprofit organizations will receive the patent rights clause at 37 CFR 401.14, i.e., the implementation of the Bayh-Dole Act. This clause permits domestic small business and domestic nonprofit organizations to retain title to subject inventions. Therefore, small businesses and nonprofit organizations do not need to request a waiver.

H. NOTICE REGARDING ELIGIBLE/INELIGIBLE ACTIVITIES.

N/A

I. 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.