Program Announcement
To DOE National Laboratories
LAB 10-07

Exascale Co-Design Center

<u>SUMMARY</u>:

The Office of Advanced Scientific Computing Research (ASCR) of the Office of Science (SC), U.S. Department of Energy (DOE), hereby announces its interest in receiving peer-reviewable Field Work Proposals (FWPs) from integrated teams of scientific researchers, applied mathematicians, computer scientists and computer architects with the goal of standing up an **Exascale Co-Design Center**. Co-design refers to a computer system design process where scientific problem requirements influence architecture design and technology and constraints inform formulation and design of algorithms and software. To ensure that future architectures are well-suited for DOE target applications and that major DOE scientific problems can take advantage of the emerging computer architectures, major ongoing research and development centers of computational science need to be formally engaged in the hardware, software, numeric methods, algorithms, and applications co-design process that will be responsible for making key tradeoffs in the design of exascale systems. Multi-institutional proposals built upon co-design principles and focused on exploring new scientific problem formulations, algorithms, and execution programming models in close collaboration with the design of exascale computer systems and software are encouraged.

Exascale computer systems are expected to be comprised of as many as a billion cores. Such systems will be capable of 10 billion-way concurrency in simultaneous operations. Industry reports indicate that because of power constraints, data movement, rather than computational operations, will be the limiting factor for exascale systems. Memory per core is expected to decline sharply while the performance of storage systems will continue to lag far behind. Multi-level storage architectures that span multiple types of hardware are anticipated and will require new approaches to run-time data management and analysis.

This Program Announcement invites proposals for integrated co-design centers to address a variety of challenges in creating scientific codes for exascale computing systems, including the design and development of hardware, system software, architectural-aware numeric methods, algorithms and new formulations of the basic application problem. It is anticipated that these co-design centers will need to address: application formulation, advanced programming languages, integrated uncertainty quantification, validation and verification, new mathematics and approaches to implementing multi- physics problems that naturally express parallelism and locality, and data management analysis, including visualization; all in the context of a scientific problem area important to the DOE.

DATES:

Full proposals submitted in response to this Announcement must be received no later than Friday, 8:00 pm ET, July 9, 2010, to be accepted for merit review and to permit timely consideration for award in Fiscal Year 2010.

Please see the "Addresses" section below for further instructions on the method of submission for the proposal.

ADDRESSES and SUBMISSION INSTRUCTIONS:

Have your LAB administrator submit the entire LAB proposal and FWP via Searchable FWP (https://www.osti.gov/fwp). If you have questions about who your LAB administrator is or how to use Searchable FWP, please contact the Searchable FWP Support Center. All submissions and inquiries about this Program Announcement must reference Program Announcement Lab 10-07.

FOR FURTHER INFORMATION CONTACT:

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SUPPLEMENTARY INFORMATION:

The barriers to exascale are many and well understood. Proposed exascale computer systems designs share some of the following challenges:

1. Clock frequencies are expected to decrease to conserve power; as a result, the number of processing units on a single chip will have to increase;
2. The energy costs of moving data both on-chip and off-chip will become much more important;
3. Total concurrency in the applications must rise by a factor of ~1 million;
4. Although the memory per flop may be acceptable, memory per processor will fall dramatically which will make current weak scaling approaches problematic;
5. For both power and performance reasons, locality of data and computation is much more important so flat cache hierarchies will no longer be helpful;

6. The failure rates for components and manufacturing variability make it unreasonable to assume the computer is deterministic. This is true for performance today and will affect the results of computations by 2018 due to silent errors.
7. Synchronization will be very expensive and the work required to manage synchronization will be high.
8. The I/O system at all levels – chip to memory, memory to I/O node, I/O node to disk— will be much harder to manage due to the relative speeds of the components.

These challenges represent a change in the computing cost model, from expensive flops coupled with almost free data movement, to free flops coupled with expensive data movement.

In any architectural design, it will be more complicated to manage energy-efficiency, concurrency, and resiliency in operating system software and programming models. Numerical algorithms, mathematical models, and scientific software codes must also be reformulated, perhaps radically, to take full advantage of these emerging computational platforms. New methods of data management and analysis must be developed, since scientists will not be able to rely on exporting data for later analysis and/or visualization. Achieving these improvements will require an unprecedented cooperation, in co-design centers, between computer architects, domain scientists, application developers, applied mathematicians, and computer scientists.

Co-design methodology requires the combined expertise of vendors, hardware architects, system software developers, domain scientists, computer scientists, and applied mathematicians working together to make informed decisions about features and tradeoffs in the design of the hardware, software and underlying algorithms. Co-design teams should leverage the experience in embedded systems co-design and consider disciplines such as formal methods, co-simulation modeling, hardware and software synthesis, optimization, verification, validation, integrated error analysis and uncertainty quantification.

 A co-design center should include at least the following components:

1. A principal investigator, who is accountable to the goals and objectives of the co-design research activities. The PI will plan, facilitate, and oversee research and development activities, maintain proper balance of project personnel, and coordinate interactions with other co-design centers, if necessary.
2. A well defined overarching application directly relevant to DOE mission whose solution will be optimized for exascale computer systems.
3. Strong ties to a DOE Hub, Energy Frontier Research Centers (EFRC), SciDAC Science Applications or similar organizations to facilitate buy-in from the domain science community and ensure that the innovations will reach the broad community of practitioners.
4. A well balanced interdisciplinary team that includes
   - Scientific domain experts, applied mathematicians, computational scientists, computer scientists, hardware architects and software engineers.
   - A critical mass of developers organized in a "code-team" who would be able to evaluate and implement multiple alternatives on an aggressive schedule to support the architecture development timeline

- Experience with application codes, i.e. an existing body of work with one or more codes that are under active development, targeting at the exascale design points of approximately 1-10 billion degree concurrency on hundreds of millions cores.
- Experience with scientific kernels and algorithms design, and optimization, uncertainty quantification, verification, and validation techniques.
- Knowledge and practical experience with advanced architectures in the following areas: micro-architecture hardware design, circuit design, co-simulation, hardware and software synthesis, formal specification and verification methods, simulation modeling, hardware and system software optimization.

Additional background information on ASCR efforts to enable science communities to address scientific grand challenges through extreme scale computational science can be found at

- *Scientific Grand Challenges Workshop Series* http://extremecomputing.labworks.org

This web site is a portal to 10 ASCR-sponsored workshops held between November 2008 and February 2010, covering extreme scale computing applied to different topic areas. Several workshop web sites contain completed workshop reports and all of them contain valuable additional reference material.

COMMUNITY BUILDING:

An important goal of this notice is to foster an active, integrated research community of versatile researchers who are committed to the common goal of achieving exascale computation for advancing scientific discovery. Accordingly,

- The successful proposal will provide a management plan for maintaining open communications among all team members, for example regular teleconferences, individual face-to-face meetings, team meetings, and other collaboration-inducing techniques.

The application will need to include plans for the dissemination of research results, such as:

- Publications, conferences, and educational activities for the science user community: what mechanisms will the project employ to present its work to a broader community to ensure sustained activities in the research area and promote adoption by communities of scientists?
- Lessons learned: How will the project disseminate lessons learned about application re-formulation for proposed exascale computing systems to the larger scientific community?

PROGRAM FUNDING:

It is anticipated that up to a total $8,000,000 of ASCR funds will be available for award in Fiscal Year 2010, contingent on the availability of appropriated funds. Proposals may request project support up to five year with the possibility for renewing for an additional five years. Multi-lab and/or multi-institutional proposals are expected and should request between $5,000,000 and $10,000,000 funding per year. Out-year support is contingent on the availability of funds and on

the progress of research and programmatic needs. Funding for this research will come from the program. 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.

Proposals may address one or more of the topics of interest. However, there is no limitation to the number of proposals a LAB or a Principal Investigator can submit.

SUBMISSION INFORMATION:

The instructions and format described below must be followed. All submissions and inquiries about this Program Announcement must reference Program Announcement Lab 10-07.

The research project description must be **25 pages or less,** exclusive of attachments. The proposals must include a one-page abstract of the proposed research. All collaborators should be listed at the top of the abstract. Attachments include curriculum vitae, a listing of all current and pending federal support and letters of intent when collaborations are part of the proposed research. Curriculum vitae should be limited to no more than two pages per individual. All proposals submitted in response to this Announcement must explicitly state how the proposed project will support program goals and the ASCR mission, including the project's impact on applications of interest to the Office of Science.

The following is a list of essential items that a proposal must contain. Follow this order:

1. Field Work Proposal (FWP) Format - Complete and signed by appropriate officials.

2. Proposal Cover Page – Include announcement title and number: Exascale Co-Design Center (LAB 10-07)

3. Table of Contents

4. Budget Page(s) (Form DOE F 4620.1) - Complete a separate Budget Page for the entire multi-year period for each separate participating institution, if applicable.
http://www.science.doe.gov/grants/budgetform.pdf

5. Other Project Information

   a) **A one-page abstract (on a page by itself).** The abstract should include: name of the laboratory; name of the principal investigator and the principal investigator's email address and phone number; name of the co-principal investigator(s) (if any) and their email address(es) and phone number(s); a summary of the project narrative.

   b) **Project Narrative: (limit 25 pages)** A detailed description of the proposed project (research plan), including the justification and objectives of the project, its relationship to the Office of Science program and the researcher's plan for carrying it out. The narrative should be limited to 25 pages maximum (8.5x11-inch pages of single-spaced, standard 11-point type with 1-inch margins), exclusive of attachments such as figures or references.

i)   Introduction – Should contain enough background material, including review of the relevant literature, to demonstrate sufficient knowledge of the state of the science.
ii) Research Plan - 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, should indicate which project personnel will be responsible for which activities and how this expertise maps on to the components for co-design. Include a plan that describes how the project results or resources will be disseminated in a timely manner and in an accessible and usable form to the broader scientific community.
iii) Management Plan for multi-lab proposals – Should outline how the work will be coordinated among the participating institutions, the overall chain of command, the communication plan, the leads for each area, the overall allocation of resources among the various partners, etc. The lead PI must include a budget summery of all participants, in a table format.

c) **Curriculum Vitae**: Detailed information about the background and experience of the principal investigator and co-principal investigator (if any). Biographical sketches are limited to two pages for the principal investigator, and two pages for the co-principal investigator (if any).

d) **Long Term Measure:** The proposal must explain how the proposed research will advance the goals of the program and the ASCR mission, as well as its overall impact on applications of interest to the Office of Science.

e) **Facilities and Resources**: Include information on the experience of the proposer's organization, its facilities, and resources that would be relevant to successful operation of the project.

f) **Statement of all current and pending support** for the principal investigator and co-principal investigator (if any), including the time devoted to each project by the principal investigator and co-principal investigator (if any).

The instructions and format described should be followed. You must reference Program Announcement LAB 10-07 on all submissions and inquiries about this program.

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OFFICE OF SCIENCE
GUIDE FOR PREPARATION OF SCIENTIFIC/TECHNICAL PROPOSALS
TO BE SUBMITTED BY NATIONAL LABORATORIES

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Proposals from National Laboratories submitted to the Office of Science (SC) as a result of this Program Announcement will follow the Department of Energy Field Work Proposal process with additional information requested to allow for scientific/technical merit review. The following guidelines for content and format are intended to facilitate an understanding of the requirements necessary for SC to conduct a merit review of a proposal. Please follow the guidelines carefully, as deviations could be cause for declination of a proposal without merit review.

1. Evaluation Criteria

After an initial screening for eligibility and responsiveness to this Announcement, proposals will be subjected to a formal scientific merit review (peer review). The proposals will be evaluated against the following criteria, which are 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 Researcher's Personnel and Adequacy of Proposed Resources; and
> 4) Reasonableness and Appropriateness of the Proposed Budget.

The evaluation process will include program policy factors such as the relevance of the proposed research to the terms of the 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.

2. Summary of Proposal Contents

- Field Work Proposal (FWP) Format (Reference DOE Order 412.1A) (DOE ONLY)
- Proposal Cover Page - **Include announcement title and number: Exascale Co-Design Center (LAB 10-07)**
- Table of Contents
- Budget (DOE Form 4620.1) and Budget Explanation
- Abstract (one page)
- Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel - 20-page limit)
- Literature Cited
- Biographical Sketch(es)
- Description of Facilities and Resources
- Other Support of Investigator(s)
- Appendix (optional)

2.1 Submission Instructions

Have your LAB administrator submit the entire LAB proposal and FWP via Searchable FWP (https://www.osti.gov/fwp). All submissions and inquiries about this Program Announcement must reference Program Announcement Lab 10-07. If you have questions about who your LAB administrator is or how to use Searchable FWP, please contact the Searchable FWP Support Center.

3. Detailed Contents of the Proposal

Adherence to type size and line spacing requirements is necessary for several reasons. No researcher should have the advantage, or by using small type, of providing more text in his or her proposal. Small type may also make it difficult for reviewers to read the proposal. Proposals must have 1-inch margins at the top, bottom, and on each side. Type sizes must be at least 11 point. Line spacing is at the discretion of the researcher but there must be no more than 6 lines per vertical inch of text. Pages should be standard 8 1/2" x 11" (or metric A4, i.e., 210 mm x 297 mm).

3.1 Field Work Proposal Format (Reference DOE Order 412.1A) (DOE ONLY)

The Field Work Proposal (FWP) is to be prepared and submitted consistent with policies of the investigator's laboratory and the local DOE Operations Office. Additional information is also requested to allow for scientific/technical merit review.

3.2 Proposal Cover Page

The following proposal cover page information may be placed on plain paper. No form is required.

   Title of proposed project
   SC Program announcement title and number: **Exascale Co-Design Center (LAB 10-07)**
   Name of laboratory
   Name of principal investigator (PI)
   Position title of PI
   Mailing address of PI
   Telephone of PI
   Fax number of PI
   Electronic mail address of PI
   Name of official signing for laboratory*
   Title of official

Fax number of official
Telephone of official
Electronic mail address of official
Requested funding for each year; total request
Use of human subjects in proposed project:
> If activities involving human subjects are not planned at any time during the proposed project period, state "No"; otherwise state "Yes", provide the IRB Approval date and Assurance of Compliance Number and include all necessary information with the proposal should human subjects be involved.

Use of vertebrate animals in proposed project:
> If activities involving vertebrate animals are not planned at any time during this project, state "No"; otherwise state "Yes" and provide the IACUC Approval date and Animal Welfare Assurance number from NIH and include all necessary information with the proposal.

Signature of PI, date of signature
Signature of official, date of signature*

*The signature certifies that personnel and facilities are available as stated in the proposal, if the project is funded.

3.3 Table of Contents

Provide the initial page number for each of the sections of the proposal. Number pages consecutively at the bottom of each page throughout the proposal. Start each major section at the top of a new page. Do not use unnumbered pages, and do not use suffices, such as 5a, 5b.

3.4 Budget and Budget Explanation

A detailed budget is required for the entire project period and for each fiscal year. It is preferred that DOE's budget page, Form 4620.1 be used for providing budget information*. Modifications of categories are permissible to comply with institutional practices, for example with regard to overhead costs.

A written justification of each budget item is to follow the budget pages. For personnel this should take the form of a one-sentence statement of the role of the person in the project. Provide a detailed justification of the need for each item of permanent equipment. Explain each of the other direct costs in sufficient detail for reviewers to be able to judge the appropriateness of the amount requested.

Further instructions regarding the budget are given in section 4 of this guide.

* Form 4620.1 is available at web site: http://www.science.doe.gov/grants/budgetform.pdf

3.5 Abstract

Summarize the proposal in one page. Give the project objectives (in broad scientific terms), the approach to be used, and what the research is intended to accomplish. State the hypotheses to be tested (if any). At the top of the abstract give the lead DOE national Laboratory, project title,

names of all the investigators and their institutions, and contact information for the principal investigator, including e-mail address.

3.6 Narrative (main technical portion of the proposal, including background/introduction, proposed research and methods, timetable of activities, and responsibilities of key project personnel).

The narrative comprises the research plan for the project and is limited to **25 pages (maximum)**. 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 methods 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. It is important that the 25-page technical information section provide a complete description of the proposed work, because reviewers are not obliged to read the Appendices. Proposals exceeding these page limits may be rejected without review or the first 25 pages may be reviewed without regard to the remainder.

All proposals submitted in response to this LAB Announcement must explicitly state how the proposed project will support the accomplishment of the program goals and the ASCR mission, including the project's impact on applications of interest to the Office of Science.

If any portion of the project is to be done in **collaboration** with another institution (or institutions), provide information on the institution(s) and what part of the project it will carry out. Further information on any such arrangements is to be given in the sections "Budget and Budget Explanation," "Biographical Sketches," and "Description of Facilities and Resources."

3.7 Literature Cited

Give full bibliographic entries for each publication cited in the 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. Principal investigators should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the proposal.

3.8 Biographical Sketches

This information is required for senior personnel at the institution submitting the proposal and at all subcontracting institutions (if any). The biographical sketch is limited to a maximum of two pages for each investigator 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 five professional and scholarly activities related to the effort proposed.

To assist in the identification of potential conflicts of interest or bias in the selection of reviewers, the following information must also be provided in each biographical sketch.

> *Collaborators and Co-editors:* A list of all persons in alphabetical order (including their current organizational affiliations) who are currently, or who have been, collaborators or co-authors with the investigator on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of the proposal. Also, include those individuals who are currently or have been co-editors of a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of the proposal. Finally, list any individuals who are not listed in the previous categories with whom you are discussing future collaborations. If there are no collaborators or co-editors to report, this should be so indicated.

> *Graduate and Postdoctoral Advisors and Advisees:* A list of the names of the individual's own graduate advisor(s) and principal postdoctoral sponsor(s), and their current organizational affiliations. A list of the names of the individual's graduate students and postdoctoral associates during the past five years, and their current organizational affiliations.

3.9 Description of Facilities and Resources

Facilities to be used for the conduct of the proposed research should be briefly described. Indicate the pertinent capabilities of the institution, including support facilities (such as machine shops), that will be used during the project. List the most important equipment items already available for the project and their pertinent capabilities. Include this information for each subcontracting institution (if any).

3.10 Other Support of Investigators

Other support is defined as all financial resources, whether Federal, non-Federal, commercial, or institutional, available in direct support of an individual's research endeavors. Information on active and pending other support is required for all senior personnel, including investigators at collaborating institutions to be funded by a subcontract. For each item of other support, give the organization or agency, inclusive dates of the project or proposed project, annual funding, and level of effort (months per year or percentage of the year) devoted to the project.

3.11 Appendix

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

The appendix may contain the following items: up to five publications, manuscripts accepted for publication, abstracts, patents, or other printed materials directly relevant to this project, but not generally available to the scientific community; and letters from investigators at other institutions stating their agreement to participate in the project (do not include letters of endorsement of the project).

4. Detailed Instructions for the Budget
(DOE Form 4620.1 "Budget Page" may be used).

4.1 Salaries and Wages

List the names of the principal investigator and other key personnel and the estimated number of person-months for which DOE funding is requested. Proposers should list the number of postdoctoral associates and other professional positions included in the proposal and indicate the number of full-time-equivalent (FTE) person-months and rate of pay (hourly, monthly or annually). For graduate and undergraduate students and all other personnel categories such as secretarial, clerical, technical, etc., show the total number of people needed in each job title and total salaries needed. Salaries requested must be consistent with the institution's regular practices. The budget explanation should define concisely the role of each position in the overall project.

4.2 Equipment

DOE defines equipment as "an item of tangible personal property that has a useful life of more than two years and an acquisition cost of $50,000 or more." Special purpose equipment means equipment which is used only for research, scientific or other technical activities. Items of needed equipment should be individually listed by description and estimated cost, including tax, and adequately justified. Allowable items ordinarily will be limited to scientific equipment that is not already available for the conduct of the work. General purpose office equipment normally will not be considered eligible for support.

4.3 Domestic Travel

The type and extent of travel and its relation to the research should be specified. Funds may be requested for attendance at meetings and conferences, other travel associated with the work and subsistence. In order 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. Consultant's travel costs also may be requested.

4.4 Foreign Travel

Foreign travel is any travel outside Canada and the United States and its territories and possessions. Foreign travel may be approved only if it is directly related to project objectives.

4.5 Other Direct Costs

The budget should itemize other anticipated direct costs not included under the headings above, including materials and supplies, publication costs, computer services, and consultant services (which are discussed below). Other examples are: aircraft rental, space rental at research establishments away from the institution, minor building alterations, service charges, and fabrication of equipment or systems not available off- the-shelf. Reference books and periodicals may be charged to the project only if they are specifically related to the research.

a. Materials and Supplies

The budget should indicate in general terms the type of required expendable materials and supplies with their estimated costs. The breakdown should be more detailed when the cost is substantial.

b. Publication Costs/Page Charges

The budget may request funds for the costs of preparing and publishing the results of research, including costs of reports, reprints page charges, or other journal costs (except costs for prior or early publication), and necessary illustrations.

c. Consultant Services

Anticipated consultant services should be justified and information furnished on each individual's expertise, primary organizational affiliation, daily compensation rate and number of days expected service. Consultant's travel costs should be listed separately under travel in the budget.

d. Computer Services

The cost of computer services, including computer-based retrieval of scientific and technical information, may be requested. A justification based on the established computer service rates should be included.

e. Subcontracts

Subcontracts should be listed so that they can be properly evaluated. There should be an anticipated cost and an explanation of that cost for each subcontract. The total amount of each subcontract should also appear as a budget item.

4.6 Indirect Costs

Explain the basis for each overhead and indirect cost. Include the current rates.