

DOE/NNSA Advanced Simulation and Computing

Predictive Science Academic Alliance Program II (PSAAP II)

Request for Information (RFI), Amendment 001

Reference: DE-FOA-0000528 [Pre-Proposal Conference for ASC Predictive Science Academic Alliance Program (PSAAP)]

I. Background and Pre-proposal Request:

As the result of the initial pre-proposal conference held on May 10-11, 2011, Amendment 001 to the RFI revises the original description of the three major integrated areas, clarifies the scope of this effort and provides a more detailed description of the proposed work. Please review the following description and provide a pre-proposal to Thuc Hoang, National Nuclear Security Administration ASC Alliance Program Manager, at thuc.hoang@nnsa.doe.gov by 4 PM EDT July 25, 2011, with a copy to the Grants Contracting Officer, Robert Lowther at rlowther@doeal.gov. Pre-proposals submitted after this date will not be accepted or considered. If proprietary data is included in the pre-proposal, it must be marked “Proprietary” and this information will be protected as required by 10 CFR 600 and other applicable financial assistance regulations. A more detailed description of the major areas is provided in Section II. Pre-proposal submission requirements are addressed in Section III below.

The intent of the pre-proposal request is to obtain a more detailed description of potential applicant ideas for the purpose of developing the Funding Opportunity Announcement (FOA). A competitive FOA will be released in early 2012. Section IV provides an estimated schedule for this financial assistance action.

II. The NNSA Office of Advanced Simulation and Computing (ASC), in collaboration with Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL) and Sandia National Laboratories (SNL), are initiating the next phase of the academic computational science program, called Predictive Science Academic Alliance Program II (PSAAP II). The vision for PSAAP II consists of participation by leading U.S. universities focusing on three major integrated areas:

- Predictive Science based on verification and validation and uncertainty quantification (V&V/UQ) for large-scale simulations;
- Discipline-focused research needed to further predictive science and enabled by effective Exascale computing¹; and
- Developing and demonstrating technologies and methodologies to support effective Exascale computing in the context of science/engineering applications.

¹ The phrase “Exascale computing” used herein refers to the next High Performance Computing (HPC) paradigm shift to extreme, heterogeneous, multi-core on-node parallelism – and not necessarily to any hardware or system at such scale.

NNSA is issuing this RFI as an invitation for your institution to submit a pre-proposal in accordance with the guidelines stated herein.

The PSAAP II program is anticipated to consist of the following two types of Centers:

1. ***Multi-disciplinary Simulation Center (MSC)*** - whose research will focus on scalable application simulations, targeting large-scale, integrated multidisciplinary problems to be carried out on ASC's unclassified HPC systems that will be made available to the funded PSAAP II Centers. The MSC must (1) develop and demonstrate computer science technologies and methodologies that will advance Exascale computing, and (2) demonstrate an integrated, verified, validated predictive simulation with uncertainty quantification. Both (1) and (2) must be demonstrated within the context of the proposed integrated multidisciplinary application. It is expected that an MSC will demonstrate a significant advance in predictive science, in the context of their application. The overall advance may require a combination of advances in some Exascale-enabled piece of science, integration science, or UQ science, together with wider use of state-of-the-art techniques. The advance would consist of better predictive capability, manifested as predictions of a wider range of phenomena, with improved predictive accuracy and reduced uncertainty, in comparison to existing capability at the beginning of the project. Integrated system simulation results must be produced each year during the life of the program.
2. ***Single-Discipline Center (SDC)*** - whose research will focus on scalable application simulations, targeting a broad single science/engineering discipline, to be carried out on ASC's unclassified HPC systems that will be made available to the funded PSAAP II Centers. The SDC must (1) develop and demonstrate computer science technologies and methodologies that will advance Exascale computing, and (2) demonstrate a verified, validated predictive simulation with uncertainty quantification. Both (1) and (2) must be demonstrated within the context of the proposed problem. It is anticipated that an SDC will demonstrate a compelling and significant scientific advance in the single discipline, enabled by Exascale computing. The technical advance should ideally represent a qualitative step up in the discipline, as opposed to incremental progress. While the research efforts within an SDC may follow several divergent paths under the broad umbrella of the single science/engineering discipline, it is required that *all* research paths be integrated into a *single demonstration problem*, for which simulation results must be produced each year during the life of the program. The demonstration problem is the vehicle by which progress in verified, validated, and uncertainty-quantified predictive simulation will be assessed each year.

III. Pre-proposal Requirements. A university may submit more than one pre-proposal, provided that it meets all of the following conditions:

- Each submission must have a different lead Principal Investigator (PI).
- Each submission must target a significantly different application and/or Exascale issue.
- Each submission should follow the page restrictions as described herein and in Appendix A.
- The Vice President for Research, or someone in a comparable position, must include a letter acknowledging the pre-proposal submission. Please note that there will be a

requirement in the full FOA proposal submission for the lead institution to comply with the Minimum Requirements identified in Appendix B in order to be considered.

The preliminary proposals should include the following information, with the font size NOT any smaller than Times New Roman 11 and in a Portable Document Format (pdf):

(1) Executive Summary: A *one-page* executive summary of the approach, goals, and tasks proposed for the Center. Indicate whether the response is for a MSC or a SDC.

(2) Technical and Scientific Approach: No more than *seven pages* describing the technical and scientific approaches and objectives for the work, with an outline plan that presents the simulation of a large, complex problem (MSC) or a significant single-discipline advance (SDC) that is of ASC programmatic and national interest, a well-defined simulation and modeling roadmap, an integrated plan for advancing and demonstrating Exascale technologies, and a timetable showing key milestones for each research area during the proposed life of the Center. The research and simulation plan should provide for and outline significant simulations at the end of each year of the program. The plan should include how to leverage existing computer science frameworks and science/engineering codes to more quickly bring up an integrated simulation capability for the selected problem so more effort can be focused on the Exascale science/engineering, V&V/UQ, and computer science components. The approach should include a verification and validation plan and associated plan for how the required data is to be obtained. The Exascale technology plan should show a convincing path to initial demonstration by end of the third year.

(3) Budget Estimate: A *one-page* budget estimate and outline for the five years of the Center, including estimated costs for manpower and other resources, with supporting cost and burden rate data, and requirements for no-cost ASC Laboratory computational resources (e.g. time, processing elements, memory, archival storage, etc.). The funding amount for an MSC is estimated to be \$4.0M/year and for an SDC is \$2.0M/year for 5 project years. Some discussion of the source of matching funds in the form of cash or direct cash equivalents of minimally 10% should be included.

(4) Ideas to Attract Students: A brief discussion of ideas for attracting US citizen graduate students and post docs, and associating them or involving them with the NNSA Laboratories (*one page maximum*).

(5) Ideas to Interact with NNSA Laboratories: A brief list of ideas for interacting with the NNSA Laboratories (*one page maximum*).

(6) List of Potential Participants and Collaborators: A list of all supported participants from the proposing institution and from other participating universities and laboratories, including a BRIEF paragraph describing the nature of the contribution by the external collaborator(s) (*two pages maximum*).

(7) Optional Partnership Management Plan: If there are multiple institutions on the team, the pre-proposal should contain a clear plan for how the “prime” institution will manage the overall program with particular attention given to the partner university(ies). This should include a plan, not to exceed one page, for how the “prime” institution will manage adding or deleting partner

universities and associated faculty and staff, as refocusing is needed or for non-performance. Clearly established roles and responsibilities of the “prime” and partner universities must be part of this plan (*one page maximum*).

(8) Outline of Center Management Structure: A *one-page* outline of the coordinated multi-department/discipline structure of the Center with a corresponding organizational chart. Include a list of senior endorsing officials (vice-chancellor, provost, etc.), heads of participating departments and key research personnel. Do not provide resumes or vitae, but a listing of sponsor names and contacts (and/or publication references) for 3-6 key related projects which are already completed or in process.

(9) Contact Information: Names, addresses, e-mail references, phone and facsimile numbers for a point of contact, the Principal Investigator, and a person authorized to execute any resulting contract (*one page maximum*).

(10) Comments on Current Scope of PSAAP II: A *one-page* discussion of your feedback to the PSAAP II program’s scope as described herein and suggestions to strengthen the program. Please note that this page will only be viewed by the ASC Alliance Strategy Team. It can be submitted as a separate pdf file if desired.

For purposes of the competitive FOA, final applications will be evaluated by a panel of experts, including, but not limited to, NNSA ASC program and Laboratory personnel. Draft evaluation criteria are provided in Appendix B. The following will be considered criteria:

(1) Relevance and practicality of the proposed research plan, simulation and modeling methodology, V&V/UQ methodology, Exascale technology, and Center organization and management structure to the advancement of Exascale computing and PSAAP II goals;

(2) The likelihood that the proposed computer science research can be shown to lead to more effective Exascale computing;

(3) Clarity of the goals and objectives of the proposed research and the technical feasibility of the simulation sequences being coupled to accomplish them;

(4) Degree to which the proposed advances in predictive science, whether multidisciplinary or single-discipline, are compelling, significant, and clearly demonstrate the power of Exascale computing to enable scientific progress;

(5) Degree to which the various disciplines, particularly the computer science efforts focused on Exascale computing, are integrated within the proposed Center:

(5a) For a Multi-discipline Simulation Center (MSC): degree to which the proposed research will demonstrate a significant advance in predictive capability (i.e., predictions of a wider range of phenomena, with improved predictive accuracy and reduced uncertainty), via a combination of advances in Exascale-enabled physical science/engineering, integration science, or UQ science, together with wider use of state-of-the-art techniques;

(5b) For a Single-Discipline Center (SDC): degree to which the various directions of research are integrated into a single demonstration problem that clearly advances the science of the discipline, and the degree to which simulation results produced each year during the life of the program will be used to demonstrate progress in verified, validated, uncertainty-quantified predictions.

(6) Degree to which the pre-proposal incorporates a feasible plan for demonstrating agreement of simulation predictions with physical reality, including:

- Plan for verification and validation (V&V) of simulation capability.
- Plan for acquiring validation quality data for use in the V&V effort.
- Plan for a full-system prediction demonstration with specified uncertainty using the fully V&V and UQ simulation.

(7) Degree to which the models are integrated into an overarching computational framework;

(8) The capabilities, related experience, facilities, or techniques which are available for the work and are considered to be integral factors for achieving the objective(s) of the proposed work; and

(9) The validity and practicality of the requested ASC computing resources and capability of fully utilizing such resources.

IV. Estimated Financial Assistance Procurement Schedule:

The estimated PSAAP II financial assistance schedule is as follows:

- Pre-proposal Meeting – *May 10-11, 2011*
- RFI issued – *June 16, 2011*
- Pre-proposals due – *July 25, 2011*
- Review of pre-proposals – *August 15-16, 2011*
- Estimated FOA issue date – *January 16, 2012*
- Estimated Final Applications due – *March 31, 2012*

Additional reference materials on various topics may be found at:

- ASC Program – <http://nnsa.energy.gov/asc>
- ASC Exascale Environment Workshop – <https://asc.llnl.gov/exascale/>
- ASC PSAAP II Pre-proposal conference - <http://sandia.gov/ascppc/>

If there are any questions on this RFI letter or the procurement process, please contact Robert Lowther, NNSA Grants Contracting Officer, at rlowther@doeal.gov. Once the RFI is issued and after the pre-proposals are due, all communications should be with the Grants Contracting Officer.

Appendix A – Pre-Proposal Document Template

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1. Executive Summary	NTE 1 page
2. Technical and Scientific Approach	NTE 7 pages
3. Budget Estimate	NTE 1 page
4. Ideas on attracting US grad students & post docs	NTE 1 page
5. Ideas on Interacting with NNSA Labs	NTE 1 page
6. List of all Participants and Potential Collaborators	NTE 2 pages
7. (Optional) Partnership Management Plan	NTE 1 page
8. Outline of Center Management Structure	NTE 1 page
9. Contact Information	NTE 1 page
10. Comments on current scope of PSAAP II (can be in separate file)	NTE 1 page

NOTE:

- The enumerated sections above correspond to the respective sections called out in pages 3-4 of the RFI letter.
- “NTE” = “Not To Exceed”

Appendix B

DRAFT FOA FULL APPLICATION MINIMUM QUALIFICATION REQUIREMENTS

For administrative screening of the submitted applications, the application must demonstrate the Applicant's ability to meet or exceed each of the Minimum Qualification Requirements listed below. The Applicant shall include in the application a letter of support from the Applicant's Vice President for Research, or someone in a comparable position, that affirms the PSAAP II Center will comply with the following Minimum Requirements:

- a) The Applicant shall be a United States academic institution that can grant PhD degrees.
- b) Every PhD student, who is financially supported under a resulting cooperative agreement and who is not a citizen of a sensitive country as noted on the DOE sensitive country list, shall spend at least one period of ten contiguous weeks collaborating at one of the three NNSA Defense Programs National Laboratories (associated costs shall be included in the proposed budget.) Note: this requirement means that the PSAAP II funds can only be used for students who are US citizens or who are permanent residents from non-sensitive foreign countries. Students from sensitive countries can still participate in the Center's work but would need to be supported as part of the Applicant's matching funding.
- c) Every research staff member and post doc, who is financially supported under a resulting cooperative agreement and who is not a citizen of a sensitive country, shall spend at least one week collaborating at one of the three NNSA Defense Programs National Laboratories each year. Note that this requirement means that the PSAAP II funds can only be used for students who are US citizens or who are permanent residents from non-sensitive foreign countries. Students from sensitive countries can still participate in the Center's work but would need to be supported as part of the Applicant's matching funding.
- d) The Applicant will be contributing 10% as cost matching to the NNSA award on the annual basis.