Program Statement for the Advanced Simulation and Computing (ASC) Predictive Science Academic Alliance Program (PSAAP)

Executive Summary

This document lays out the goals for a multi-year program as a follow-on to the present ASC Alliance program. The new program, to be called Predictive Science Academic Alliance Program (PSAAP), will focus on "Predictive Science" based on verified and validated, large-scale simulation. "Predictive Science" is the application of verified and validated computational simulations to predict properties of complex systems, particularly in cases where routine experimental tests are not feasible. This process is potentially applicable to a variety of applications, including simulations of such diverse domains as biological systems, global economics, nuclear weapons effects, climate modeling, to efficient manufacturing. Each of these simulations requires the integration of a diverse set of disciplines; each discipline in its own right is an important component of many applications. Success requires both software and algorithmic frameworks for integrating models and code from multiple disciplines into a single application and significant disciplinary strength and depth to make that integration effective.

The program consists of two components:

1. Multidiscipline Simulation Centers (MSCs) research will focus on large-scale, multidisciplinary, scalable and integrated simulations to be carried out on massively parallel ASC systems.

2. Collaborating Research Activities (CRAs) will be much smaller research projects and tightly integrated with one or more of the MSCs and National Nuclear Security Administration (NNSA) Laboratories.

The PSAAP program portfolio will eventually include a mix of MSCs and CRAs (both MSCs and CRAs will change over time as described below).

The Centers will be chosen after careful review of the responses to a Request for Information (RFI) and a Request for Proposal (RFP) following a process similar to the one used to select the Centers in the present Alliance Program. Because of the tight coupling required among the MSCs, the CRAs and the NNSA Laboratories, the CRAs will not begin until the second year of the program.

The PSAAP program anticipates a procurement process wherein there is a major Center competition at periodic intervals and a CRA competition every two to three years. The actual structure of the program -- number of new centers started at any given time, duration of continuing and new centers, mix of MSCs and CRAs -- will depend on the quality of proposals, balance of funded proposals and appropriated ASC budgets.

Goals of the New Program

The new PSAAP program is intended to achieve the following:

1. Establish validated, large-scale, multidisciplinary, simulation-based "Predictive Science" as a major academic and applied research program:
    a. Demonstrate its realization via both:
        i. Simulation of large, complex problems of ASC and national interest at multiple universities, and
        ii. Discipline focused research in areas critical to stockpile stewardship predictive science as listed in the Appendix below.
    b. Produce significant science/engineering results on problems of ASC and national importance;
    c. Establish new prediction, verification, validation and uncertainty quantification methodologies;
    d. Improve the quantity & quality of tools, algorithms and models; and
    e. Integrate science/engineering, computational mathematics and computer science into a coordinated research effort.

2. Improve the relevance of this program to stockpile stewardship and the NNSA Laboratories via:
    a. Experimentation and its interaction with simulation both for experimental design and for validation and verification (V&V) and prediction. Examples might include:
        - Low cost, well-designed and instrumented small-scale science experiments of direct interest to the NNSA Laboratories;
        - Participation with the Laboratories in studying physical systems where the Laboratories provide the experiment and the Centers the simulation;
        - Using Center models to help the Laboratories design and analyze experiments;
        - Collaborative experiments where the Centers and the Laboratories provide data on different aspects of a phenomenon for model validation.

    b. Focus on discipline areas of critical interest to the stockpile stewardship program and NNSA Laboratories. Examples of potential contributions are:
        - The academic community can provide key research and development expertise in many of the disciplines critical to the Predictive Science;
        - Partnerships with the Laboratories in these areas will enable progress in precisely those directions essential to predictive

applications, both for stockpile stewardship and science more broadly;
- Discipline specific modules, tools and frameworks can contribute important technologies to the program;
- Collaboration with Laboratories can provide specific requirements for discipline specific center activities.

c. Increases in the number of students, post docs, and research staff to establish a human resources pool with more individuals capable of contributing to a "Predictive Science" and to national competitiveness.

3. Increase the visibility of the Program in the academic community generally and across government and industry.
   a. Create new Centers to demonstrate and further "Predictive Science" via verified and validated simulations.
   b. Establish smaller targeted CRAs of direct interest to one or more of the MSCs and the NNSA Laboratories to create larger webs of collaboration.
   c. Conduct an annual conference on a topic of direct interest to the NNSA Laboratories where the work of the participating universities can be highlighted.
   d. Build on the experience base of the existing Centers to rapidly expand the community of experts in validated, multi-physics, multi-scale simulation on massively parallel systems.

Structure of New Program

Multidiscipline Simulation Centers (MSCs)
MSCs are centers whose research will focus on large-scale, multidisciplinary, scalable and integrated simulations to be carried out on massively parallel ASC systems. Each Center has the primary goal to develop a verified and validated predictive capability for their specific application. They are broad in discipline and focused in application and must develop a technical and sociological framework that allows each component (discipline) to be effectively integrated into the whole. Further, significant depth in each scientific component must exist in the resulting simulations to provide for meaningful verified, validated, predictive simulation experiments to be performed to demonstrate large-scale predictive science. This type of Center is motivated by the need to demonstrate predictive science in highly visible unclassified ASC class problems, to develop the multi-discipline predictive science methodology, and establish training and education programs in this new science area. As guidelines, the selected MSCs' funding will ramp up to approximately $4M per year for up to five years.

Collaborating Research Activities (CRAs)

In order to expand the number of universities involved, to increase the visibility of the program, and to bring unique research capabilities into the program (variable over the life of the program), a portion of the budget will be set aside for smaller efforts directly tied to one or more MSCs and the NNSA Laboratories. Such efforts will fall into the range of $200-800K per year, for up to 3 years, and cover topics such as experiments, models, tools, algorithms, etc. Each activity will likely involve only a single site. Such activities could span MSCs and NNSA Laboratories helping to form tighter relationships and sharing of common approaches. Thus the goal is not only to simply broaden the number of universities involved in the program, but also to encourage broadening the web of relationships and collaborations that might continue under other funding mechanisms later. All such efforts will have to be endorsed by each of the Centers to which the effort will be tied, and meet the criteria of NNSA Laboratory relevance and ties. Competition for these awards will occur roughly every two to three years beginning in the second year of the program. Such a schedule will allow for flexibility in targeting technical areas that need research attention and assistance from the academic community.

Mechanism for Creating the New Program

Proposal Requirements for MSCs

An RFI and RFP process will be utilized to attract proposals. Responses to the RFI must include (see RFI document for specifics):

1. Focus on the predictive science of a multi-physics, multi-scale problem in science or engineering via simulation on state of the art ASC systems using a problem of ASC and national interest.
2. A discussion of clear demonstration goals for predictive science that address fundamental questions in the chosen problem.
3. A discussion of plans to verify and validate the proposed simulation.
4. A discussion for effectively integrating science/engineering, computational mathematics and computer science into an effort focused on the chosen problem;
    a. This should include how to leverage existing computer science frameworks and science/engineering codes to more quickly bring up the integrated simulation for the selected problem so more effort can be focused on the predictive science component.
5. Some discussion of the source of matching funds in the form of cash or direct cash equivalents of approximately 10%;
6. A discussion of ideas for interacting with the NNSA Laboratories;
7. A discussion of ideas for attracting US citizen graduate students and post docs and associating them or involving them with the NNSA Laboratories.
8. A list of potential collaborators from other universities.

Following the review of the responses to the RFI, a competitive RFP for multi-year programs will be released to a subset of those responding to the RFI. In general, responses to the RFP must include (the RFP documents will provide the specifics):

1. Focus on the predictive science of a multi-physics, multi-scale problem in science or engineering via simulation on state of the art ASC systems using a problem of ASC and national interest.
2. A research plan for development and use of V&V and uncertainty quantification methodology;
3. A predictive science research plan with clear demonstration goals that address fundamental questions in the chosen problem.
4. A plan for effectively integrating science/engineering, computational mathematics and computer science into an effort focused on the chosen problem;
    a. This should include how to leverage existing computer science frameworks and science/engineering codes to more quickly bring up integrated simulation for their selected problem so more effort can be focused on the predictive science component.
5. Matching funds in the form of cash or direct cash equivalents of approximately 10%;
6. A plan for interacting with the NNSA Laboratories; for example, students supported by the program may be required to spend summers at NNSA Laboratories, and Post Docs and other staff supported by the program may be required to spend some designated period like 2 - 4 weeks.
7. A plan for attracting US citizen graduate students and post docs and associating them or involving them with the NNSA Laboratories.

While it is the intent of this program that MSCs be largely centered within a single university, a proposing Center could fill a technical need by involving other universities; however, the proposal will have to 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 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.

Proposal Requirements for CRAs

Beginning in the second year of the PSAAP program, and continuing on a regular basis, an RFP will be released for CRAs. Requirements for these activities will include:

1. A research plan focused on a particular science or engineering advancement of direct relevance to one or more of the Centers in meeting their goals of improving or demonstrating large-scale predictive science;
2. How the work affects the targeted Center(s) predictive science research plan and demonstration goal. V&V is an important component of predictive science;
3. A letter of support from the intended Center(s) advocating the value of the proposed activity to those Centers;
4. A plan for interacting with the chosen Centers;
5. A plan for interacting with the NNSA Laboratories; for example, students

supported by the program may be required to spend summers at NNSA Laboratories, and post docs and other staff supported by the program may be required to spend some designated period like 2-4 weeks;
6. A plan for attracting US citizen graduate students and post docs; and
7. A plan for how their research results will be integrated with those of the targeted Center(s).

Appendix

Research areas of importance to the NNSA Laboratories:

- Verification and Validation and Uncertainty Quantification/Uncertainty Analysis
- Equation of State (EOS)/Constitutive Properties
- Material Damage and Failure
- Plasma Physics
- Particle Transport
- Novel Materials
- Nuclear Properties
- Turbulence Mixing/Hydrodynamics
- Material Stability
- Radiation Effects
- Chemical Transformations (includes High Explosives)
- Computer Science and computational mathematics

White papers on these topics may be found at http://www.llnl.gov/asci/alliances/psaap.

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