U.S. Department of Energy
Office of Science

Allocation Procedure for Leadership Computing Systems

Summary

The primary objective of the allocation procedure for the DOE Office of Science's capability or Leadership Class computing facilities is to provide substantial allocations for a small number of high-impact scientific applications through an open peer-reviewed process.

Computational science is increasingly central to progress at the frontiers of almost every scientific discipline and to our most challenging feats of engineering. The ability to model and simulate complex systems at scale under realistic conditions has become an effective tool for the research and development that the DOE, other Federal agencies, research institutions and industry conduct to meet their missions. It is widely recognized that more efficient and powerful computers are an essential underpinning of scientific inquiry and discovery in many fields and may provide the solutions to many of our most pressing scientific challenges.

To help meet this challenge, the U.S. created the multi-agency "*High End Computing Revitalization Task Force (HECRTF).*" In the HECRTF report,[1] the Task Force recommended building and operating world-class high-end capability computers, termed Leadership Systems, for leading-edge science. Further, the Task Force proposed that only a limited set of computationally intensive, high-impact scientific applications would receive substantial access to the Leadership systems and these systems

would be managed as national resources open and available to all researchers.

In May, 2004, after peer review, the DOE Office of Science selected the partnership of Oak Ridge National Laboratory (ORNL), Argonne National Laboratory (ANL) and Pacific Northwest National Laboratory (PNNL) to establish the first Leadership Computing Facility at Oak Ridge (LCF at ORNL).

Additionally, in 2004, the Office initiated the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program, which reserved 10% of the Office of Science HEC resources to allocate to the broad scientific community, including private industry, with no requirement of DOE funding. Final determination of allocations, after peer review, is made by the Director of the Office of Science.

The INCITE program is consistent with HECRTF recommendations. Therefore, to promote the open allocation of LCF resources, the INCITE program will be expanded to include at least 80% of the total hours available for allocation on the Leadership Computing Facilities at ORNL and ANL (when operational).

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[1] "Federal Plan for High-End Computing, A Report of the High-End Computing Revitalization Task Force," May, 2004, http://www.nitrd.gov/pubs/2004_hecrtf/20040702_hecrtf.pdf

Allocation Process

For the purposes of the developing the LCF allocation procedure, the following guidelines have been identified:
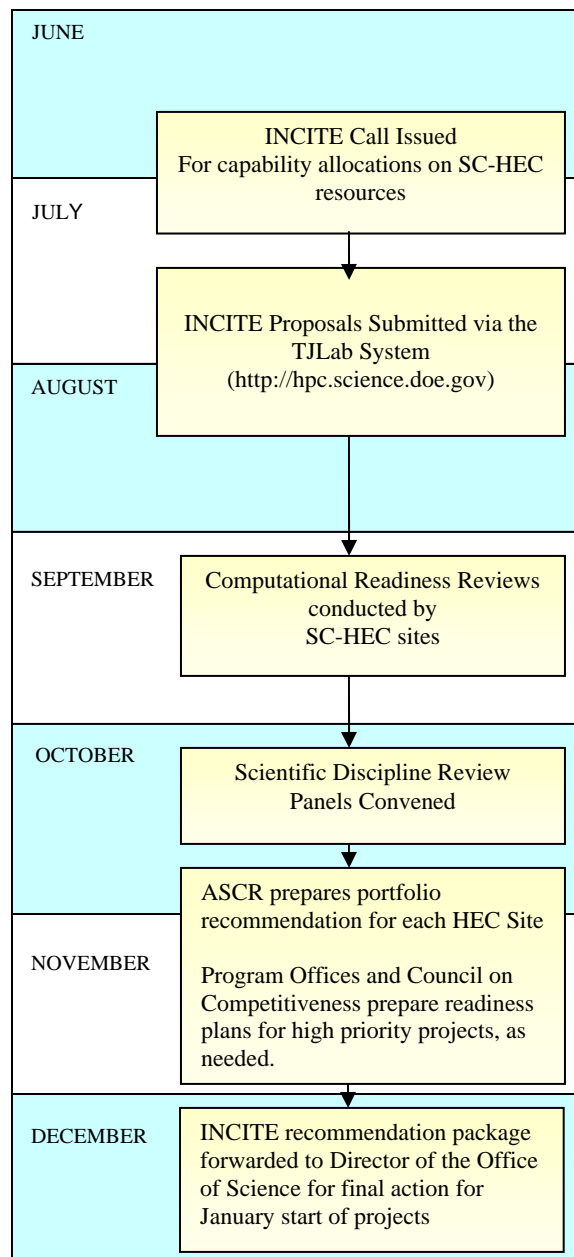
- Proposals for the capability HEC resources may request multiple year allocations. Multiple year allocations will be subject to annual review.

- A portion (up to 10%) of each resource will be reserved for allocation by the Director of the Office of Science or his designee to meet unanticipated needs.

- A portion (up to 10%) of each resource will be reserved for allocation by the site's HEC director. This portion will be negotiated yearly with the Office of Science Director or his designee. Part of the HEC director's allocation will be used to support pilot projects, including high priority projects that have been identified as "not computationally ready" and for petascale computer science and performance metrics research.

As shown in Figure 1, the LCF/INCITE allocation procedure will entail the following steps:

Computational readiness review: Each site will evaluate the readiness and the scalability of the code and its algorithms described in the proposals. Each proposal will be rated as either being ready or not ready.

Community and Federal Program Input: Prior to the Scientific review, the SC Associate Directors or their designees, Program Directors from other Federal agencies such as NSF, DOD/DARPA and NIH, and the Council on Competitiveness will provide a listing of the near-term and long-term high priority projects in their area. This listing will be included in the review panel packets and represent one scoring category on the ranking sheet.

Figure 1. Allocation process timeline

The flowchart shows a timeline from June to December with the following steps:

- JUNE / JULY: INCITE Call Issued For capability allocations on SC-HEC resources
- JULY / AUGUST: INCITE Proposals Submitted via the TJLab System (http://hpc.science.doe.gov)
- SEPTEMBER: Computational Readiness Reviews conducted by SC-HEC sites
- OCTOBER: Scientific Discipline Review Panels Convened
- NOVEMBER: ASCR prepares portfolio recommendation for each HEC Site; Program Offices and Council on Competitiveness prepare readiness plans for high priority projects, as needed.
- DECEMBER: INCITE recommendation package forwarded to Director of the Office of Science for final action for January start of projects

Scientific peer review panel: ASCR will convene scientific peer review panels to evaluate the proposal's potential for scientific impact.

- The proposals will be evaluated on scientific quality, proposed impact of the science, the ability of the principal investigator and the proposed research team, the computational plan, relation to the Office of Science mission-related research including the Scientific Discovery through Advanced Computing (SciDAC) program.
- The review panel will be composed of application domain experts from national laboratories, universities and industry, National Academy members and senior computational science researchers who have a working knowledge of the current computational challenges and opportunities in their fields.
- The review panel will also review renewal applications from multi-year requests.
- Review members will be asked to rate the proposals and renewal applications and individually propose initial allocations for each project.

Portfolio Preparation: ASCR will prepare the proposed INCITE portfolio for each site based on the input from the scientific review panel.

For any project that a Federal Program office or the Council on Competitiveness rates as "high priority", but which is judged as "not ready", before being submitted to the Director of the Office of Science, the relevant entity will

- Identify a team to develop a readiness plan

- Identify additional funding to support the implementation of the readiness plan, if needed.

Director of the Office of Science: The Director of the Office of Science or designee will review the proposed portfolio and make final recommendations on the portfolio of projects for each INCITE site.

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