TO:	Distribution
FROM:	ASC Capability Planning Advisory Committee (CPAC)
RE:	RFP for Capability Computing Campaign allocations – Cielo Campaign 5

Since early 2011, ASC Cielo has been operated as a National User Facility with access and allocations granted through a proposal review process. Proposed major programmatic computing efforts shall be organized as computing work packages and will be reviewed and prioritized for relevance, importance and technical rationale to the Stockpile Stewardship Program (SSP). To be considered, proposals must address a significant and compelling SSP mission-related problem or milestone. Cielo follows the Capability Compute System Scheduling Governance Model http://www.lanl.gov/orgs/hpc/cielo/docs/CCC_policy.pdf for allocation of resources and scheduling the stockpile stewardship workload.

Any questions should be directed to your Laboratory ASC Capability Planning Advisory Committee (CPAC) Point of Contact (listed below) or to either Jean Harris, jeharris@lanl.gov, 505-667-5778, or Cheryl Wampler, clw@lanl.gov, 505-667-0147.

Cielo CCC 5 proposals must be submitted by **July 8, 2013** to each lab's Point of Contact (POC) to be considered for the next round of Cielo allocations. Laboratory POCs may require earlier submissions so make sure you check with them. The CPAC plans to allocate Cielo for approximately six months. It is important to submit your CCC proposals on time to be considered for an allocation. Cielo CCC 5 is scheduled to start on or about **August 5, 2013.** Cielo CCC 4 will conclude on or about Sunday, August 4, 2013.

PIs who submitted proposals for earlier campaigns must resubmit for Cielo CCC 5 for evaluation against all proposals, and must clarify the new scope included in the proposal. Continuing projects are also asked to provide data on the resources consumed by the project in the previous cycle. Cielo CCC 5 ranking will be made independent of any previous ranking.

PIs of chosen CCCs are expected to prepare a presentation on their results due within two weeks of the completion of the CCC period.

Each proposed work package, called a *Capability Computing Campaign* (CCC), consists of at least one capability job together with related supporting jobs of smaller sizes. Cielo CCC 5 will allocate up to 8518 nodes (Each Cielo node = 16 cores) for this activity. Proposals are encouraged to demonstrate the need for Cielo resources by running problems that require the full resources of each node. A capability job is defined as a job that uses 30% or more of the available nodes, on Cielo this is 2550 nodes or bigger. While smaller jobs can be accommodated, Cielo is designed to run a limited number of simultaneous large jobs. CCCs that propose running capability jobs

for most of their allocation are the most desired. Usage will be tracked to ensure time is used as allocated and job sizes meet proposal requirements.

Approved projects will be assigned a campaign allocation of some number of Cielo days. A “fair share” resource management system will be used to prioritize and schedule jobs. The scheduler tries to deliver to you your “fair share” (allocation) over a window in time, approximately a couple of weeks. If you are inactive during this period, those cycles will be lost to you. In all cases, projects are advised and encouraged to keep jobs in the queue to ensure that they maximize their opportunity to fully use their allocation. If you have questions about job scheduling, please let us know. We require jobs requesting 4096 or more nodes to schedule DAT time to improve utilization and throughput. The system will be over allocated to ensure high utilization.

PROPOSAL SUBMISSION:

To submit a classified or unclassified proposal, please send e-mail to your laboratory POC containing the information specified below. Be sure to include proper classification markings on classified proposals. It is important to note that your particular Lab may have earlier deadlines or different procedures for you to follow. Please contact your Lab POC (see below) for details. Laboratory POCs should forward proposals by July 12, 2013, to Jean Harris, jeharris@lanl.gov, 505-667-5778, and Cheryl Wampler, clw@lanl.gov, 505-667-0147 for CPAC review.

Your proposal must contain

1. Principal Investigator information: Name, Username, Work Phone, Unclassified e-mail Address, and your Lab/Dept./Div/Group
2. One-line unclassified title
3. Programmatic justification that includes your overall goal or objective and any specific milestones supported.
4. Readiness justification concerning your ability to effectively utilize this capability resource and the ability of your codes to scale to the level you propose to run.
5. Requested Resources. There are three categories of scale on Cielo; C1 (job size >= 6385 nodes, >= 75% of available nodes), C2 (2550 nodes < job size < 6384 nodes) and C3 (850 nodes < job size < 2549 nodes). Job sizes greater than 4096 nodes will be asked to request DAT time to improve utilization and throughput.
    a. Total number of jobs in each category that you propose to run during this campaign.
    b. Average run time for your jobs in each category.
    c. Aggregated request in Cielo Days. One Cielo Day equals dedicated access to 8518 compute nodes for 24 hours.
6. Names of your project members may be included now or upon award notification.

A template is attached to guide your input. You can also download the template in the open at http://www.lanl.gov/orgs/hpc/cielo/docs/CCCTemplate.doc, or at https://xweb.lanl.gov in the secure. If you have any questions about the information requested or the CCC process, please call or e-mail your laboratory POC.

You should receive an acknowledgement that your proposal was received within 24 business hours. If you do not receive this acknowledgement, please call or e-mail.

Thank you for your interest, the CPAC looks forward to reviewing your proposals.

CPAC Representatives

LLNL:	Chris Clouse (POC)	clouse1@llnl.gov	925-422-4576
	Brian Carnes (POC)	carnes1@llnl.gov	925-423-9181
LANL:	Scott Doebling (POC)	doebling@lanl.gov	505-667-6950
	Mike Haertling (POC)	haert@lanl.gov	505-667-0592
SNL:	Joel Stevenson (POC)	josteve@sandia.gov	505-845-1347
	Kenneth Alvin (POC)	kfalvin@sandia.gov	505-844-9329

Cielo CCC Proposal Template

Principal Investigator:
Name: Joseph Bishop
Username: jebisho
Work Phone: 505-845-0478
Unclassified e-mail Address: jebisho@sandia.gov
Lab/Department/Division/Group: SNL/1525

(Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.)

Please provide a one-line unclassified title for this proposal:
Understanding the Effects of Microscale Material Variability in Macroscale Structures through Direct Numerical Simulations of Embedded Microstructures

Milestones supported (if any): none

Goal/Objective:

The Predicting Performance Margins (PPM) team has developed a methodology for embedding realistic material microstructures directly into finite-element models of macroscale structures. The goal is to understand how microscale material variability is manifested at the macroscale through direct numerical simulations. Quantitative comparisons will illustrate the impact on engineering quantities of interest and provide a rationale for incorporating additional physics into the production environment. Classical homogenization techniques, used in all current finite-element software, filter out this variability except on a large scale.

This new process has been tested using a polycrystalline stainless steel structure containing approximately 0.5 million grains. Each grain is modeled using an FCC crystal plasticity material model. An ensemble of 100 simulations has been performed with resulting statistical variability among the simulations captured for analysis. Each simulation contained 35M finite elements and was run on Chama using Sierra/SM with 2400 processors. For a macroscale structure on a scale of centimeters, many more grains must be modeled (on the order of millions) and the effects of greater mesh refinement must be studied. Also, until now, only small ensembles have been run (up to 100). For more accurate uncertainty quantification, we would like to increase the ensemble size to ~1000. Also, we would like to simulate the structural response in the plastic regime which is computationally much more intensive.

Readiness Justification - Scaling: I will be using Sierra/SM.

Experience:

C1 Requirements (jobs that use 6375 or more nodes)

Number of jobs in this category that will be run:
Size (number of nodes needed):
Average run time for jobs in this category:
Code used:

C2 Requirements (jobs that use at least 2550 but less than 6374 nodes)
Number of jobs in this category that will be run:
Size (number of nodes needed):
Average run time for jobs in this category:
Code used:

C3 Requirements (jobs that use at least 850 but less than 2549 nodes)
Number of jobs in this category that will be run: 200
Size (number of nodes needed): 1000
Average run time for jobs in this category: 4 days
Code used: Sierra/SM (adagio)

Based on your C-level requirements, please provide the total number of Cielo days' allocation required to fulfill your proposal requests. Base your aggregation calculations on: 8518 compute nodes for 24 hours = 1 Cielo day. Total Cielo days required for this proposal is: 94

Data Management:

Based on your C-level requirements, please provide estimates for the following:

How much data do you expect to store in the /scratch file system? (TB) 20
How much data do you expect to store in the LANL HPSS archive? (TB) 20
How much data do you expect to transfer across the WAN? (TB)
For data to be transferred across the WAN: will it be destined for a file system, HPSS, or both?

Will your application require the use of the read-only "UDSL' file system? If so, please estimate the size of the data storage required (GB).

Application Codes and Application Development Teams

Please list the application codes that you will be running on Cielo during the campaign.

Please list the primary contact for each application development/support team for the applications you plan to run.

Visualization

What visualization software/tools will you require on Cielo? Paraview

List of users authorized to use this CCC bank. Please specify each user's name, login name, e-mail address, and work phone: