Scientific Discovery through Advanced Computing

-- Update & Review Plans --

ASCAC Meeting
October 28-29, 2008
Gaithersburg, MD

Walter M. Polansky
Acting Director
Computational Science
Research and Partnerships Division
SciDAC-2 Goals

• Create comprehensive, scientific computing software infrastructure to enable scientific discovery in the physical, biological, and environmental sciences at the petascale

• Develop new generation of data management and knowledge discovery tools for large data sets (obtained from scientific user and simulations)
Scientific Discovery through Advanced Computing

### Scientific Discovery
- Accelerator science and simulation
- Climate modeling and simulation
- Fusion science
- Petabyte high-energy/nuclear physics
- Nuclear physics
- Radiation transport
- Groundwater reactive transport modeling and simulation

### Applications
- Centers for Enabling Technology
- Outreach Center
- Scientific Applications Partnerships
- Institutes (University-lead)

### Compute & Network Resources
- Leadership Computing- ANL 553 TF
- Leadership Computing- ORNL 263 TF
- Production Computing- NERSC 104 TF
- ESnet: On path toward Dual rings 40Gbps/ 10 Gbps fault tolerant

### SciDAC
- Astrophysics
- Computational Biology
- High-energy physics
- Materials science and chemistry
- QCD
- Turbulence

### NERSC Allocation
- INCITE NERSC Allocation
- Algorithms Software Tools
- Scientific Discovery
- Applications
- Compute & Network Resources
SciDAC Management Policy
-- Established April 16, 2003 --

- Memorandum states Dr. Orbach’s intentions regarding management of SC SciDAC activities in each of the program budgets.
- Michael R. Strayer is the SciDAC Director

"Expect SciDAC Director to review and sign-off on SciDAC FWPs, grant initiations and renewals, and AFP changes and program guidance letters concerning formulation and execution of budgets."

ASCAC: October 28-29, 2008
Review of SciDAC Portfolio

• Timeline
  – Science Applications: Jan – April, 2009
  – Centers and Institutes: April - May, 2009

• Process
  – Peer Review (with Panels)
  – Reviewer Selection:
    • Science Applications: Funding office(s), in partnership with ASCR
    • CETs, Institutes and Outreach Center: ASCR, in consultation with other SC offices, NNSA and/or NSF.
SciDAC Coordination Group

Comprised of Program managers from ASCR, BER, BES, FES, HEP, NP, and NNSA

(ASCR SciDAC Team- Lali Chatterjee, Christine Chalk, Bill Spotz, Osni Marques, Susan Turnbull, Walt Polansky)

- Formulated Notice and Announcement
- Managed peer reviews
- Recommended projects for funding
- Prepared award packages
- Managed awarded projects

- Developing procedures for organizing, scheduling and conducting peer reviews of the SciDAC portfolio.
## Review Schedule

### Tentative

<table>
<thead>
<tr>
<th>Project Title</th>
<th>PI, Inst</th>
<th>Timelines</th>
<th>Partners</th>
<th>Review schedule</th>
<th>Participants</th>
</tr>
</thead>
<tbody>
<tr>
<td>Framework Application for Core-Edge Transport Simulations (FACETS)</td>
<td>J Cary, Tech X</td>
<td>Project '11, SAP 09</td>
<td>FES (Lead), ASCR</td>
<td>May, 2009 (DC)</td>
<td>4 labs, 4 universities, 3 industry</td>
</tr>
<tr>
<td>Computational Astrophysics Consortium: Supernovae,...........</td>
<td>S Woosley, UC Santa Cruz</td>
<td>Project '11, SAP 09</td>
<td>HEP (Lead), NP, NNSA, ASCR</td>
<td>Jan 21-22, 2009 (CA)</td>
<td>3 labs, 5 universities</td>
</tr>
<tr>
<td>A...... Earth System Model for Climate Change Science</td>
<td>J Drake, ORNL</td>
<td>Project '11, SAP 09</td>
<td>BER (Lead), ASCR</td>
<td>April 9-10, 2008 (DC)</td>
<td>8 labs, 2 universities (counting NCAR)</td>
</tr>
<tr>
<td>Design and Testing of a Global Cloud-Resolving Model</td>
<td>D Randall, Colo State U</td>
<td>Project '11, SAP 09</td>
<td>BER (Lead), ASCR</td>
<td>April 9-10, 2008 (DC)</td>
<td>1 lab, 2 universities</td>
</tr>
<tr>
<td>Hybrid....Simulations of Subsurface Biogeochemical Processes</td>
<td>T. Scheibe, PNNL</td>
<td>Project '10, SAP 09</td>
<td>BER (Lead), ASCR</td>
<td>TBD</td>
<td>3 labs, 1 university</td>
</tr>
<tr>
<td>Modeling ..... Subsurface Reactive Flows using Advanced Computing</td>
<td>P Lichtner, LANL</td>
<td>ends '11 - review early</td>
<td>BER (Lead), ASCR</td>
<td>TBD</td>
<td>4 labs, 1 university</td>
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<tr>
<td>National Computational Infrastructure for Lattice Gauge Theory</td>
<td>R Sugar, UC SantaBarbara</td>
<td>ends '11</td>
<td>HEP(lead), NP, ASCR</td>
<td>Jan, 2009 (DC)</td>
<td>3 labs, 10 universities</td>
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<tr>
<td>ComPASS (Accelerator Modelling)</td>
<td>P Spentzouris, FNAL</td>
<td>ends '11</td>
<td>HEP(lead), NP, BES, ASCR</td>
<td>March, 2009</td>
<td>6 labs, 3 universities, 1 industry</td>
</tr>
<tr>
<td>Quantum Simulations of Material and Nanostructures (Q-SIMAN)</td>
<td>G Galli, UC Davis</td>
<td>ends '11</td>
<td>NNSA(lead), ASCR</td>
<td>TBD</td>
<td>1 lab, 5 universities</td>
</tr>
</tbody>
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