Scientific Discovery through Advanced Computing Program: SciDAC-3 Overview

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DOE Program Manager, Office of Science
Advanced Scientific Computing Research
Outline

SciDAC Program (Past & Present)

SciDAC-3 Institutes & Application Partnerships

Operating Plan & Program Management Team

SciDAC-3 and Beyond ...
SciDAC Executive Summary

• “Advances in computing technologies ... set the stage for major steps forward in modeling and simulation.”

• “To deliver on this promise, increased ‘peak’ computing power must be translated into increases in capabilities of scientific codes.”

• “This will only be solved by increased investments in computer software – scientific codes for simulating physical phenomena, mathematical algorithms that underlie these codes, and system software that enables the use of high-end computer systems.”
New SciDAC-3 Program is comprised of Institutes & Application Partnerships
“The overall portfolio and management of Institute awards is expected to cover a significant portion of DOE computational science needs on current and emerging computational systems.”

<table>
<thead>
<tr>
<th>SciDAC Institutes</th>
<th>SC Application Partnerships</th>
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<tbody>
<tr>
<td>✓ Institutes-aware</td>
<td>• Basic Energy Sciences</td>
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<tr>
<td>✓ Architecture-aware</td>
<td>• Biological &amp; Environmental Research</td>
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<td>✓ Application-aware</td>
<td>• Fusion Energy Sciences</td>
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<td>• Management structure</td>
<td>• High Energy Physics</td>
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<td>❏ Operating Plan</td>
<td>• Nuclear Physics</td>
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A successful Partnership will:
• “Exploit leadership class computing resources to advance scientific frontiers ... of strategic importance to the Office of Science”
• “Effectively link to the intellectual resources ... expertise in algorithms and methods ... scientific software tools ... at one or more SciDAC Institutes”
SciDAC Institutes Funding Opportunities

Specific goals and objectives for the SciDAC Institutes:
• Tools and resources for lowering the barriers to effectively use state-of-the-art computational systems;
• Procedures for taking on computational grand challenges across different science application areas;
• Procedures for incorporating and demonstrating the value of basic research results from Applied Mathematics and Computer Science; and
• Plans for building up and engaging our nation’s computational science research communities.

FY11 Program Funding – Office of Advanced Scientific Computing Research (ASCR)
• Up to $13M/year for 5 years may be available to support between 1 and 5 SciDAC Institutes
• DOE National Laboratories, Universities, Industry and other organizations may apply

Timeline
• Issued - February 23, 2011
• Letters of Intent (LOI), though not required, are strongly encouraged - March 30, 2011
• Proposal due date – May 2, 2011
• FY11 Awards for 3 SciDAC Institutes completed – July 2011
  o New SciDAC Institutes solicitation for Scientific Data Management, Analysis and Visualization
  ❑ Posted Sep 16; LOIs due Oct 12; Proposals due Nov 9; Awards expected by Dec 31, 2011
## FY11 Awards for SciDAC Institutes

**FASTMath** – Frameworks, Algorithms, and Scalable Technologies for Mathematics  
Collaborations: 4 DOE national laboratories; 1 University

**QUEST** – Quantification of Uncertainty in Extreme Scale Computations  
Collaborations: 2 DOE national laboratories; 4 Universities

**SUPER** – Institute for Sustained Performance, Energy and Resilience  
Collaborations: 4 DOE national laboratories; 7 Universities

<table>
<thead>
<tr>
<th>FASTMath Director – Lori Diachin, LLNL</th>
<th>QUEST Director – Habib N. Najm, SNL</th>
<th>SUPER Director – Robert F. Lucas, USC</th>
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<tbody>
<tr>
<td>Argonne National Laboratory</td>
<td>Los Alamos National Laboratory</td>
<td>Argonne National Laboratory</td>
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<td>Lawrence Berkeley National Lab</td>
<td>Sandia National Laboratories*</td>
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<td>Lawrence Livermore National Lab*</td>
<td>Johns Hopkins University</td>
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<td>Sandia National Laboratories</td>
<td>Massachusetts Institute of Technology</td>
<td>Oak Ridge National Laboratory</td>
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<td>Rensselaer Polytechnic Institute</td>
<td>University of Southern California</td>
<td>University of California at San Diego</td>
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<td>University of Texas at Austin</td>
<td>University of Maryland</td>
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**Budget summary:**

- 37 Institutes - Letters of Intent requesting $217M/year
- 27 Institutes - Full proposals requesting $141M/year
- 20 Institutes reviewed at total of $106M/year
- 3 Institutes awarded at total of $10.5M/year
FASTMath – Frameworks, Algorithms, and Scalable Technologies for Mathematics

Topic areas:

- Structured & unstructured mesh tools
- Linear & nonlinear solvers
- Eigensolvers
- Particle methods
- Time integration
- Differential Variational Inequalities (DVIs)

Coming soon: www.fastmath-scidac.org
**Topic areas:**

- Forward uncertainty propagation
- Reduced stochastic representation
- Inverse problems
- Experimental design & model validation
- Fault tolerance

For QUEST and other flyers, see [http://science.energy.gov/ascr/research/scidac/scidac-institutes/](http://science.energy.gov/ascr/research/scidac/scidac-institutes/)
SUPER – Institute for Sustained Performance, Energy and Resilience

Topic areas:

• Performance engineering (includes modeling & auto-tuning)
• Energy efficiency
• Resilience
• Optimization

See www.super-scidac.org
### Timeline for New SciDAC Announcements

<table>
<thead>
<tr>
<th>Solicitation issued – green</th>
<th>Proposal due – blue</th>
<th>Pre-proposal due – orange</th>
<th>Review &amp; award - gray</th>
<th>Max Total Budget Over Duration</th>
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<tr>
<td><strong>2011</strong></td>
<td><strong>2012</strong></td>
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<td>Aug</td>
<td>Sep</td>
<td>Oct</td>
<td>Nov</td>
<td>Dec</td>
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<tr>
<td>FES</td>
<td>8/3</td>
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<td>DATA</td>
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<td>BER</td>
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<td>NP</td>
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<td>HEP</td>
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<td>BES</td>
<td>9/21</td>
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FES – Partnerships in Fusion Energy Science, 11-571
DATA – SciDAC Institute: Scientific Data Management, Analysis and Visualization, 11-589
BER – Partnerships in Earth System Science, 11-588
NP – Partnerships in Nuclear Physics, 11-581
HEP – Partnerships in High Energy Physics, 11-580
BES – Partnerships in Materials and Chemical Sciences, 11-593

See [www.science.doe.gov/grants](http://www.science.doe.gov/grants) for Grants and Contracts information on each Announcement.

SciDAC-3 Overview - Applied Mathematics PI meeting: 10/18/2011
“The mission of SciDAC Institutes is to provide intellectual resources in applied mathematics and computer science, expertise in algorithms & methods, and scientific software tools to advance scientific discovery …”

Operating Plan will describe:

- Coordination & communication processes among the Institutes
- Processes used by each Institute to review its activities & re-prioritize as appropriate
- Communicate changes throughout SciDAC-3 and to ASCR
- Document Institutes approach for working with Application Partnerships
SciDAC-3 Team is comprised of several ASCR program managers

SciDAC Institutes
- Steven Lee
- Ceren Susut-Bennett
- Sandy Landsberg
- Lucy Nowell

Application Partnerships
- Randall Laviolette
- Ceren Susut-Bennett

Work in Progress: [http://www.scidac.gov](http://www.scidac.gov)
SciDAC-3 and Beyond

SciDAC-3 for 2011-2016

- Petascale – Roadrunner, 5/26/2008
- Era of hybrid, multi-core processors

SciDAC-3 and beyond

- See original SciDAC plan & vision
- “Mainstream” petascale computing technology
- Scientific discoveries & breakthroughs for the DOE mission
- DOE Applied Mathematics is an essential part of continued SciDAC success