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Scientific Discovery through Advanced Computing Program: SciDAC-3 Overview

Steven L. Lee

**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 ...



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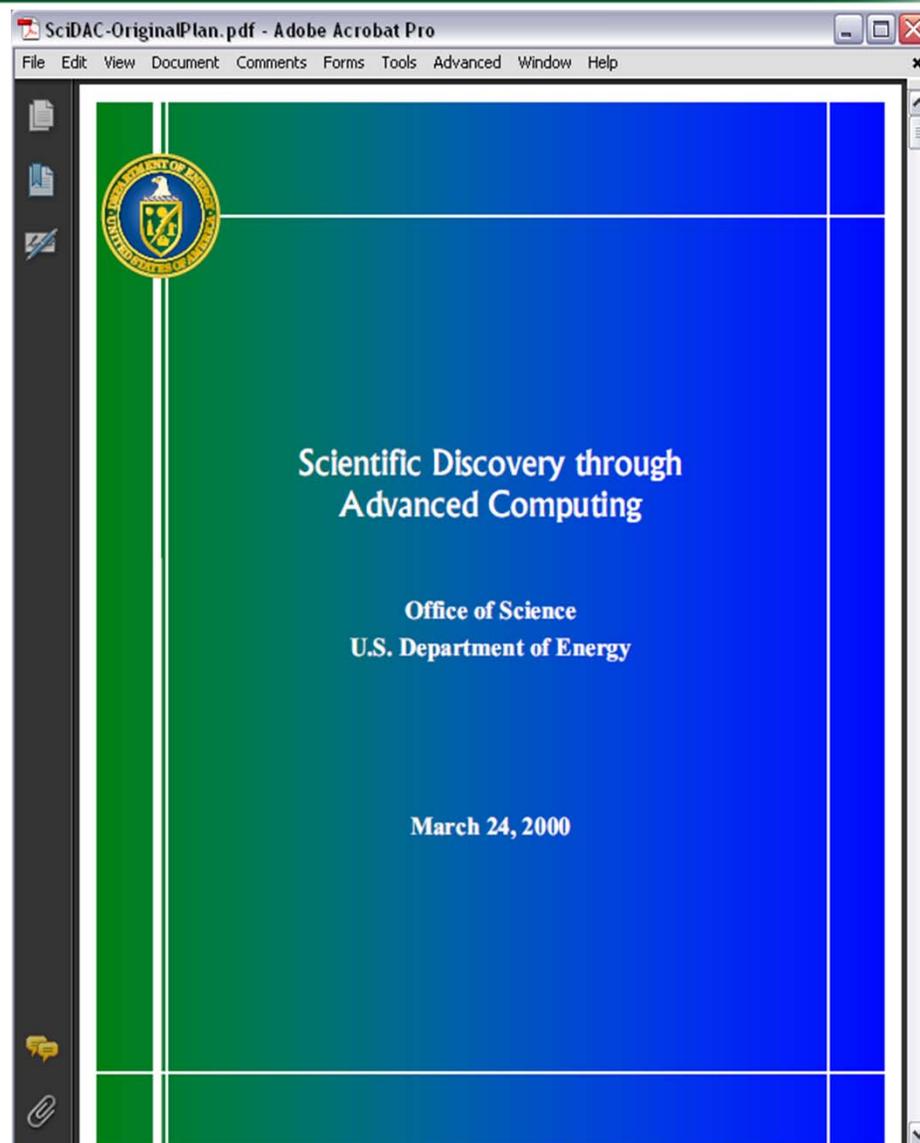
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SciDAC plan – March 24, 2000

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.”



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Scientific Discovery through Advanced Computing Program

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.”

SciDAC Institutes

- ✓ Institutes-aware
- ✓ Architecture-aware
- ✓ Application-aware
- Management structure
- Operating Plan

SC Application Partnerships

- Basic Energy Sciences
- Biological & Environmental Research
- Fusion Energy Sciences
- High Energy Physics
- Nuclear Physics

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”



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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**
- 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

FASTMath Director – Lori Diachin, LLNL	QUEST Director – Habib N. Najm, SNL	SUPER Director – Robert F. Lucas, USC
Argonne National Laboratory	Los Alamos National Laboratory	Argonne National Laboratory
Lawrence Berkeley National Lab	Sandia National Laboratories*	Lawrence Berkeley National Lab
Lawrence Livermore National Lab*	Johns Hopkins University	Lawrence Livermore National Lab
Sandia National Laboratories	Massachusetts Institute of Technology	Oak Ridge National Laboratory
Rensselaer Polytechnic Institute	University of Southern California	University of California at San Diego
	University of Texas at Austin	University of Maryland
		University of North Carolina
		University of Oregon
		University of Southern California*
		University of Tennessee at Knoxville
		University of Utah

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



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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)**

The screenshot shows a PDF document titled "FASTMath-overview.pdf" in Adobe Acrobat Pro. The document content includes:

- FASTMath** logo and title: "Frameworks, Algorithms, and Scalable Technologies for Mathematics SciDAC Institute".
- The FASTMath Team** section, listing:
 - Institute Director:** Lori Diachin, LLNL
 - Executive Council:** Phil Colella, LBNL; Esmond Ng, LBNL; Andy Salinger, SNL; Mark Shephard, RPI; Barry Smith, ANL
 - Key Personnel:** Mark Adams, Columbia; Ann Almgren, LBNL; Mihai Anitescu, ANL; John Bell, LBNL; Jim Demmel, Berkeley; Karen Devine, SNL; Milo Dorr, LLNL; Rob Falgout, LLNL; Dan Graves, LBNL; Jeff Hittinger, LLNL; Jonathan Hu, SNL; Ken Jansen, Colorado; Vitus Leung, SNL; Sherry Li, LBNL; Peter McCorquodale, LBNL; Lois McInnes, ANL; Esmond Ng, LBNL; Todd Munson, ANL; Carl Ollivier-Gooch, UBC; Dan Reynolds, SMU; Onkar Sahni, RPI; Tim Tautges, ANL; Brian Van Straalen, LBNL; Carol Woodward, LLNL; Chao Yang, LBNL; Ulrike Yang, LLNL
- A paragraph describing the FASTMath SciDAC Institute's mission: "The FASTMath SciDAC Institute will develop and deploy scalable mathematical algorithms and software tools for reliable simulation of complex physical phenomena and will collaborate with DOE domain scientists to ensure the usefulness and applicability of FASTMath technologies." It also discusses the challenges of next-generation computing.
- FASTMath Topical Areas:** FASTMath work is organized around the following broad topical area themes:
 - **Structured mesh capabilities:** block structured adaptive mesh refinement, embedded boundary methods, particle techniques, high-order discretization
 - **Unstructured mesh capabilities:** complex geometry representations, adaptive mesh refinement, dynamic partitioning, mesh quality improvement, high-order discretization
 - **Linear solvers:** geometric and algebraic multigrid, domain decomposition, Krylov iterative techniques, ILU and LU factorizations
 - **Nonlinear solvers:** Newton based with various globalization schemes including line search and trust region
 - **Time integrators:** implicit/explicit methods, symplectic, multiscale, backward differentiation, generalized linear, differential algebraic equations, error control
 - **Variational inequality solvers:** Newton-based active set methods and semi-smooth methods
 - **Eigensolvers:** Krylov & non-Krylov subspace methods, optimization-based techniques
- A paragraph titled "Addressing the Challenges of Next Generation Computing" discussing the shift to multi-/many-core nodes and million-way parallelism.
- Logos for Argonne, Berkeley, Columbia University, Rensselaer, SMU, and the University of British Columbia.

Coming soon: www.fastmath-scidac.org



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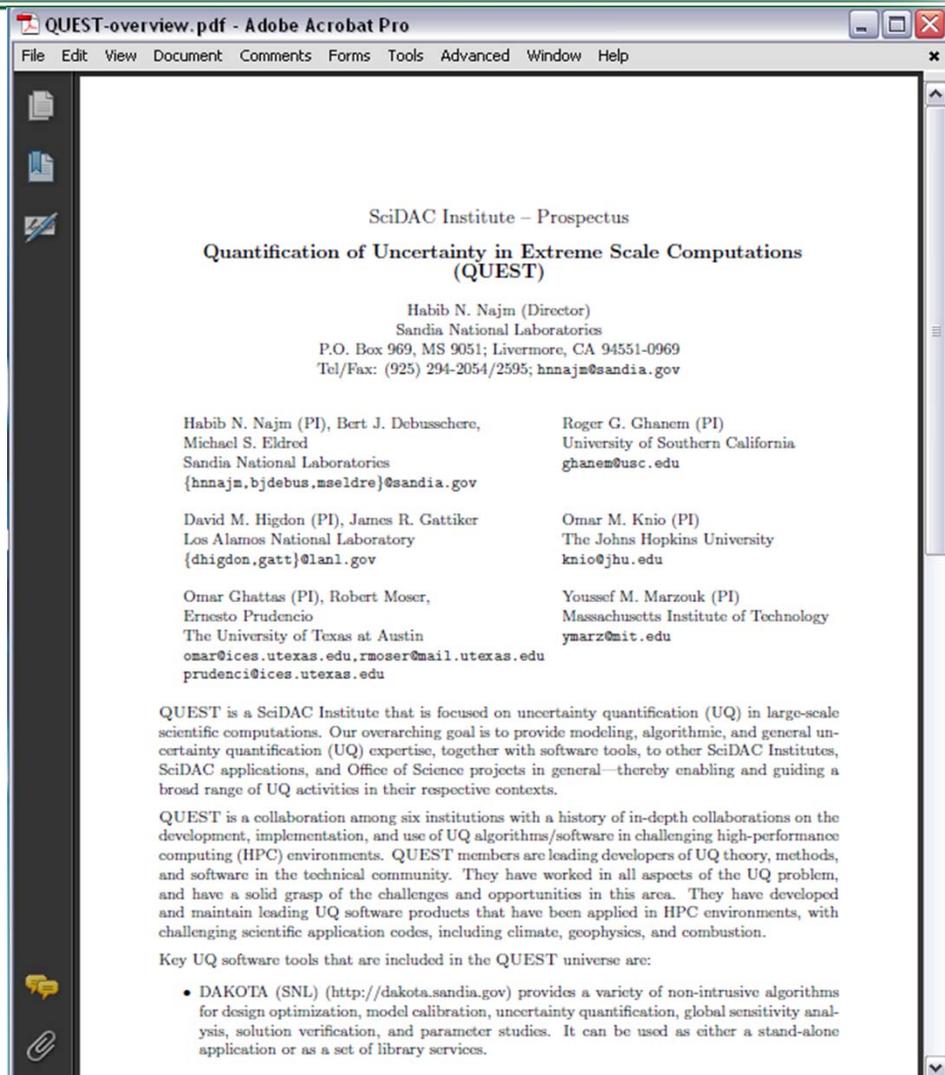
QUEST – Quantification of Uncertainty in Extreme Scale Computations

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/>



QUEST-overview.pdf - Adobe Acrobat Pro

File Edit View Document Comments Forms Tools Advanced Window Help

SciDAC Institute – Prospectus

Quantification of Uncertainty in Extreme Scale Computations (QUEST)

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QUEST is a SciDAC Institute that is focused on uncertainty quantification (UQ) in large-scale scientific computations. Our overarching goal is to provide modeling, algorithmic, and general uncertainty quantification (UQ) expertise, together with software tools, to other SciDAC Institutes, SciDAC applications, and Office of Science projects in general—thereby enabling and guiding a broad range of UQ activities in their respective contexts.

QUEST is a collaboration among six institutions with a history of in-depth collaborations on the development, implementation, and use of UQ algorithms/software in challenging high-performance computing (HPC) environments. QUEST members are leading developers of UQ theory, methods, and software in the technical community. They have worked in all aspects of the UQ problem, and have a solid grasp of the challenges and opportunities in this area. They have developed and maintain leading UQ software products that have been applied in HPC environments, with challenging scientific application codes, including climate, geophysics, and combustion.

Key UQ software tools that are included in the QUEST universe are:

- DAKOTA (SNL) (<http://dakota.sandia.gov>) provides a variety of non-intrusive algorithms for design optimization, model calibration, uncertainty quantification, global sensitivity analysis, solution verification, and parameter studies. It can be used as either a stand-alone application or as a set of library services.



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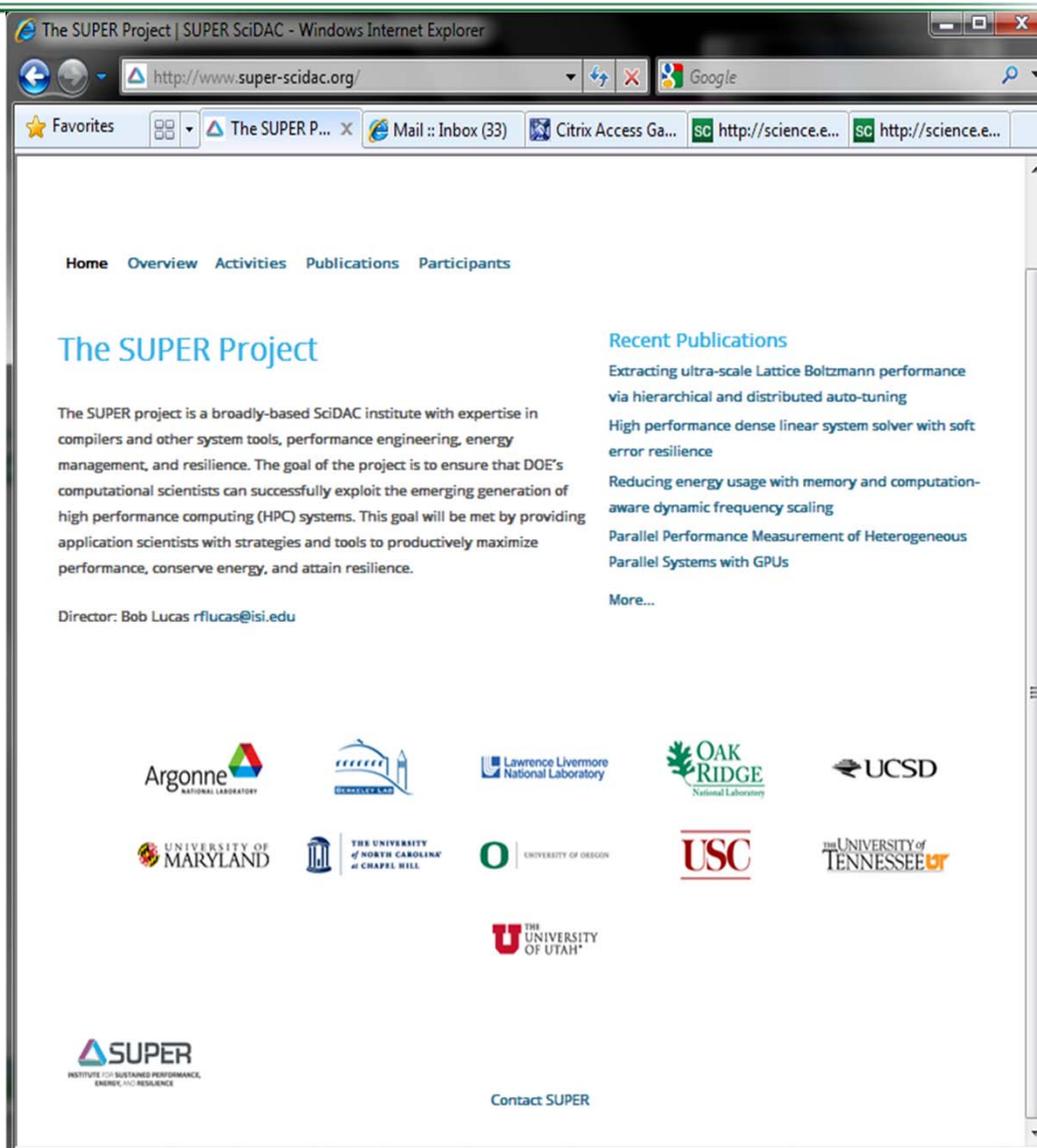
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SUPER – Institute for Sustained Performance, Energy and Resilience

Topic areas:

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



The screenshot shows a web browser window titled "The SUPER Project | SUPER SciDAC - Windows Internet Explorer". The address bar displays "http://www.super-scidac.org/". The page content includes a navigation menu with "Home", "Overview", "Activities", "Publications", and "Participants". The main heading is "The SUPER Project", followed by a paragraph describing the project's goals: "The SUPER project is a broadly-based SciDAC institute with expertise in compilers and other system tools, performance engineering, energy management, and resilience. The goal of the project is to ensure that DOE's computational scientists can successfully exploit the emerging generation of high performance computing (HPC) systems. This goal will be met by providing application scientists with strategies and tools to productively maximize performance, conserve energy, and attain resilience." Below this is the director's name and email: "Director: Bob Lucas rflucas@isi.edu". To the right, there is a "Recent Publications" section with links to articles such as "Extracting ultra-scale Lattice Boltzmann performance via hierarchical and distributed auto-tuning" and "High performance dense linear system solver with soft error resilience". At the bottom, there is a grid of logos for partner institutions: Argonne National Laboratory, Lawrence Livermore National Laboratory, Oak Ridge National Laboratory, UCSD, University of Maryland, The University of North Carolina at Chapel Hill, University of Oregon, USC, and The University of Tennessee. The SUPER logo is also present at the bottom left, and a "Contact SUPER" link is at the bottom right.

See www.super-scidac.org



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Timeline for New SciDAC Announcements

Solicitation issued – green Proposal due – blue
 Pre-proposal due – orange Review & award - gray

	2011					2012			Max Total Budget Over Duration
	Aug	Sep	Oct	Nov	Dec	Jan	Feb	Mar-Jun	
FES	8/3	9/9	10/26						\$33M / 5 years
DATA		9/16	10/12	11/9	*				\$25M / 5 years
BER		9/16	10/17		12/5				\$32.5M / 5 years
NP		9/16	10/30			1/5			\$20M / 5 years
HEP		9/16				1/9			\$12M / 3 years
BES		9/21			12/9			3/12	\$30M / 5 years

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 for Grants and Contracts information on each Announcement



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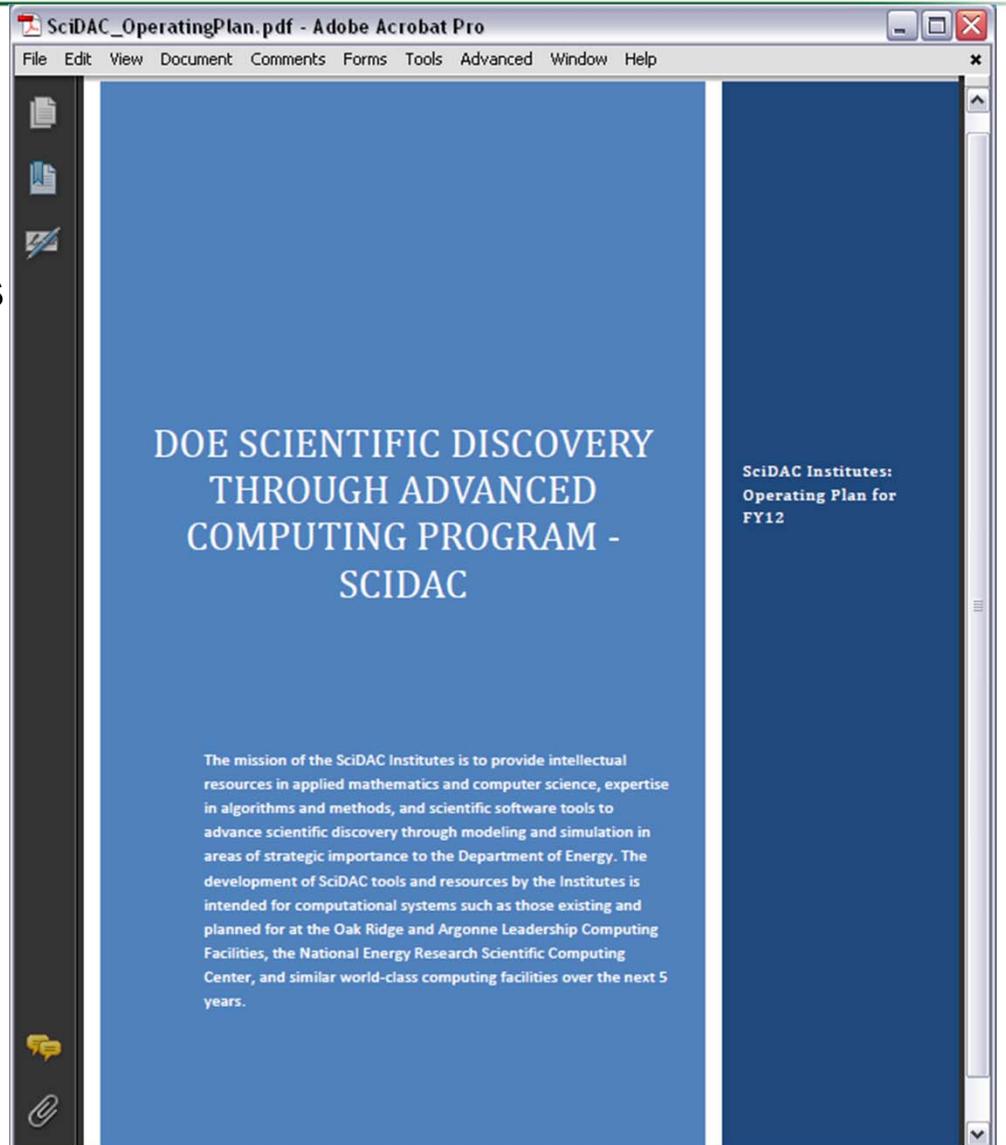
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SciDAC-3 Institutes Operating Plan

“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**



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SciDAC-3 Program Management Team

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>



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SciDAC-3 and Beyond

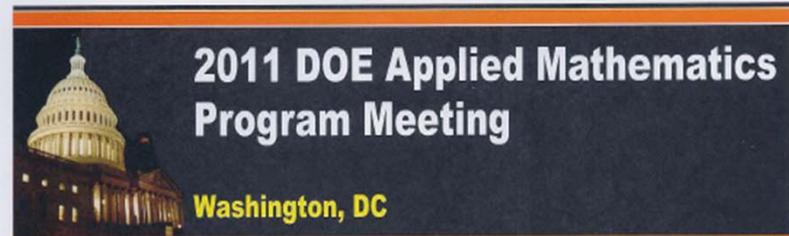
SciDAC-3 for 2011-2016

- 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

OCTOBER 17 - 19, 2011



Organizing Committee

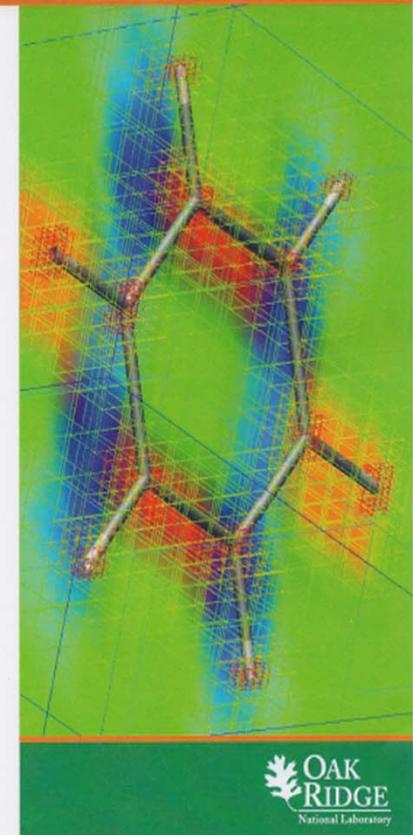
- Eduardo D'Azevedo - Oak Ridge National Laboratory
- Leslie Greengard - Courant Institute of Mathematical Sciences, New York University
- Chandrika Kamath - Lawrence Livermore National Laboratory
- Sven Leyffer - Argonne National Laboratory
- Barney Maccabe - Oak Ridge National Laboratory
- Youssef Marzouk - Massachusetts Institute of Technology
- Esmond Ng - Lawrence Berkeley National Laboratory
- Ali Pinar - Sandia National Laboratories
- Petr Plechac - University of Delaware
- Ivan Yotov - University of Pittsburgh

PROGRAM MANAGERS:

Sandy Landsberg and Karen Pao
Office of Advanced Scientific Computing Research
Office of Science U.S. Department of Energy



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