U.S. DEPARTMENT OF ENERGY | Office of Science

Scientific Discovery through Advanced Computing: SciDAC-3 Committee of Visitors (COV) Response

Randall Laviolette, **Steven Lee**, Ceren Susut

Computational Partnerships

Advanced Scientific Computing Research

Office of Science, Department of Energy

March 24, 2015

SciDAC-3 COV Members

- **Roscoe Giles** (Chair), Professor, Department of Electrical & Computer Engineering, Boston University
- **Thomas Clune**, Senior Computational Scientist, Advanced Software Technology Group (ASTG), National Aeronautics and Space Administration (NASA)
- **Jeff Greeley**, Associate Professor, School of Chemical Engineering, Purdue University
- **David Keyes**, Professor, Applied Mathematics and Computational Science, King Abdullah University of Science and Technology (KAUST)
- **Claudio Rebbi**, Professor, Department of Physics, Boston University

SciDAC-3 COV Charge & Timeline

Assess the **efficacy and quality of the FY11-FY13 processes** used to:

- Solicit, review, recommend, and document proposal actions, and
- Monitor active award, projects and programs

Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:

- The **breadth and depth of portfolio elements**
- The degree to which the program is anticipating and **addressing emerging challenges from high performance computing and DOE missions**, and
- The **national and international standing** of the program with regard to other computational science programs that are also focused on harnessing high performance scientific computing and using massive datasets to advance science

COV Timeline:

Charge Letter – March 31, 2014

COV Review – October 6-7, 2014

COV Report/Draft – November 21, 2014

COV Response – January 5, 2015

SciDAC-3 COV Report, 8 Recommendations, Bottom Line

- Solicit, review, recommend, and document proposal actions
  - **3 Recommendations**
- Monitor active award, projects and programs
  - **No Recommendations**

- The **breadth and depth of portfolio elements**
  - **3 Recommendations**
- The degree to which the program is anticipating and **addressing emerging challenges from high performance computing and DOE missions**
  - **2 Recommendations**
- The **national and international standing** of the program with regard to other computational science programs that are also focused on harnessing high performance scientific computing and using massive datasets to advance science
  - **No Recommendations**

Bottom Line from SciDAC-3 COV Report … SciDAC remains the gold standard for fostering interaction between disciplinary scientists and HPC. The PMs are to be commended on continuing the excellence of the SciDAC "brand."

Solicit, review, recommend, and document proposal actions

COV Recommendation (1 of 8):

- Preserve decision documents, even for declined proposals, and provide summary feedback in the declination letter.

Program Response:

- ASCR agrees with this recommendation. The Portfolio Analysis and Management System (PAMS) has been developed and employed to support and document the complete research funding process for Office of Science research programs, including SciDAC. Decision documents for declined proposals are in PAMS.

Solicit, review, recommend, and document proposal actions

COV Recommendation (2 of 8):

- It is important that the Program Managers can impose the SciDAC priority filter over and above the peer reviewers, who (properly within their sphere) rank based on the traditional merits of quality and originality.

Program Response:

- ASCR agrees with this recommendation. The overall quality of the SciDAC program relies on the careful management of the solicitation, review, and selection process relative to each science discipline.

SciDAC Institutes are 4 large team projects involving National Laboratory, University and Industry collaborators

FASTMath Director – Lori Diachin Scalable solvers & discretizations	QUEST Director – Habib Najm Uncertainty Quantification	SDAV Director – Arie Shoshani Scalable data management, analysis & visualization	SUPER Director – Robert Lucas Performance tools & code optimization
Lawrence Livermore (CA)	**Sandia (CA)**	**Lawrence Berkeley (CA)**	**Univ of Southern CA**
Argonne (IL)	Los Alamos (NM)	Argonne (IL)	Argonne (IL)
Lawrence Berkeley (CA)	Duke University (NC)	Lawrence Livermore (CA)	Lawrence Berkeley (CA)
Sandia (CA & NM)	MIT (MA)	Los Alamos (NM)	Lawrence Livermore (CA)
RPI (NY)	Univ of Southern CA	Oak Ridge (TN)	Oak Ridge (TN)
	Univ of Texas, Austin (TX)	Sandia (NM)	Univ of CA, San Diego (CA)
		Univ of CA, Davis (CA)	Univ of Maryland (MD)
		Georgia Tech (GA)	Univ of North Carolina (NC)
		North Carolina St Univ (NC)	Univ of Oregon (OR)
		Northwestern (IL)	Univ of Tenn, Knoxville (TN)
		Ohio State Univ (OH)	Univ of Utah (UT)
		Rutgers Univ (NJ)	
		Univ of Utah (UT)	
		Kitware, Inc (NY)	

FASTMath - Frameworks, Algorithms & Scalable Technologies for Mathematics

QUEST - Quantification of Uncertainty in Extreme-Scale Computations

SDAV - Scalable Data Management, Analysis & Visualization

SUPER - Institute for Sustained Performance, Energy & Resilience

Lead
National Labs
Universities
Industry

Solicit, review, recommend, and document proposal actions

COV Recommendation (3 of 8):

- Coordination between science programs and ASCR priorities in timing decisions pertaining to future proposals should be maintained.

Program Response:

- ASCR agrees with this recommendation. Close coordination and communication among SciDAC Program Managers has been essential in managing this complex program and will be maintained.

Timing for SciDAC-3 Partnerships

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

The breadth and depth of portfolio elements

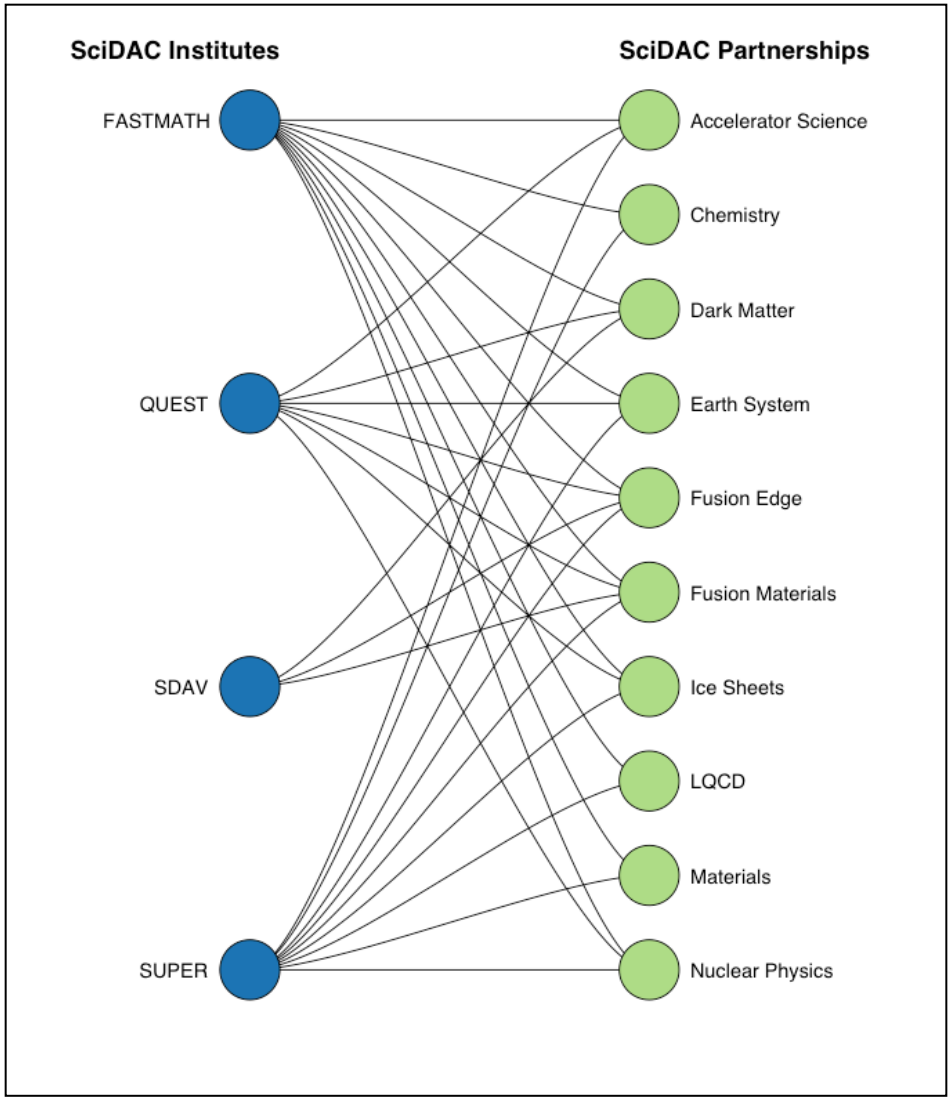
COV Recommendation (4 of 8):

- Maintain or create an appropriately balanced emphasis on science-based algorithms and insights, mathematical/computational algorithms, and high-performance computing.

Program Response:

- ASCR agrees with this recommendation. The SciDAC program will continue to balance its portfolio of high-performance algorithms and software to address the strategic research priorities of the Office of Science.

Institutes-Partnerships: Science areas leverage the capabilities of the 4 SciDAC-3 Institutes



FASTMath
Scalable solvers & discretization

QUEST
Uncertainty quantification

SDAV
Scalable data management, analysis & visualization

SUPER
Performance portability & tools

Note: Diagram aggregates 18 SciDAC Application Partnership projects into 10 main science topic areas

Each science area leverages capabilities of multiple SciDAC-3 Institutes

The breadth and depth of portfolio elements

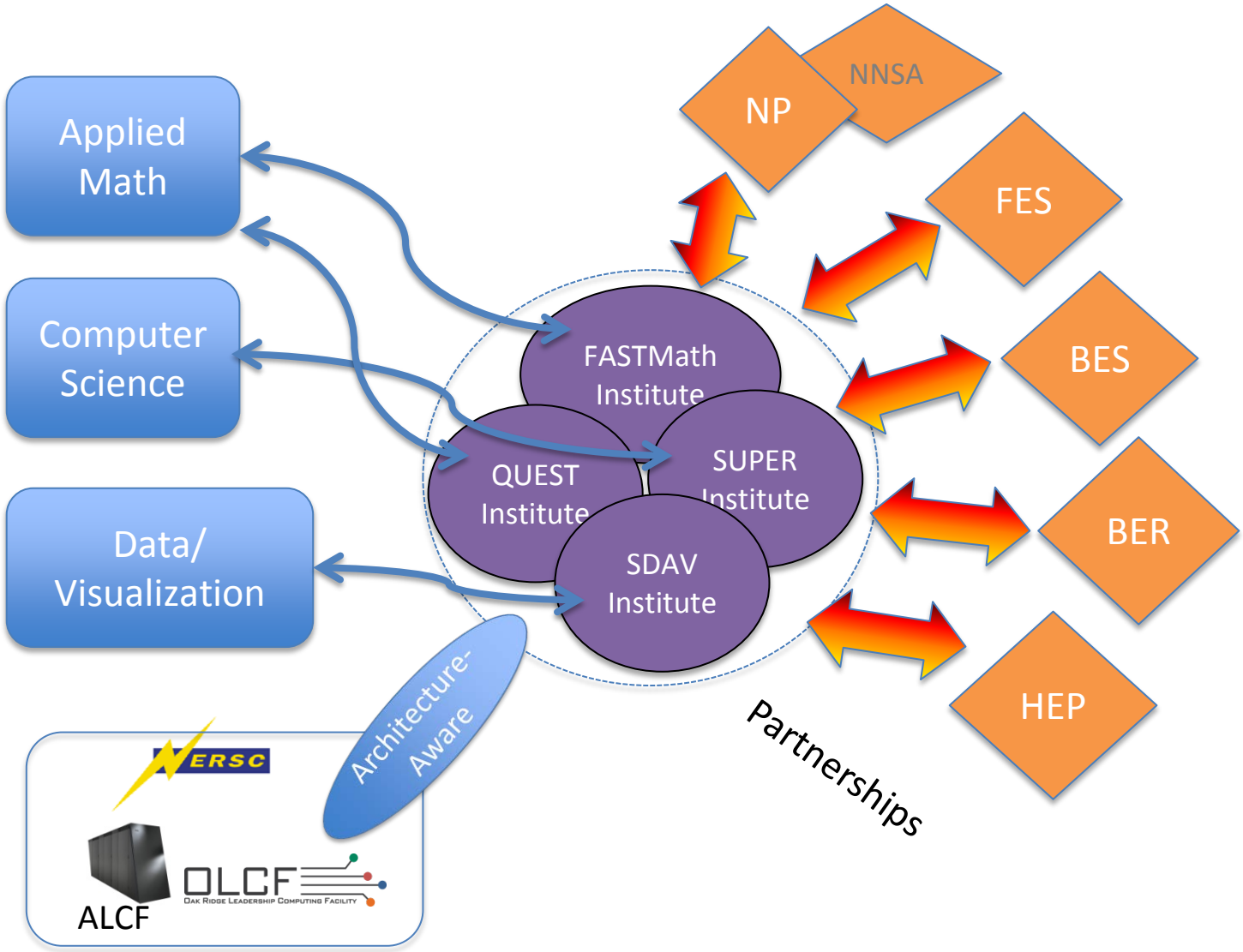
COV Recommendation (5 of 8):

- ASCR should pursue synergisms between SciDAC and Co-Design.

Program Response:

- ASCR agrees with this recommendation. Scalability and architecture-awareness are primary characteristics of SciDAC-3 software and science applications. Efforts to prepare SciDAC for future architectures will continue to benefit from leveraging results from ASCR research projects.

SciDAC-3 model: Connecting ASCR research with Science



The breadth and depth of portfolio elements

COV Recommendation (6 of 8):

- In terms of demonstrating success for SciDAC collaborations, wide adoption in the field of codes developed by the Institutes should be regarded as at least meritorious as shared post-doctoral funding (FTEs), in that it shows that the algorithmic and software technology has reached maturity.

Program Response:

- ASCR agrees with this recommendation. The wide adoption of codes produced by SciDAC projects continues to be one of our success stories.

Anticipating and addressing emerging challenges from high performance computing and DOE missions

COV Recommendation (7 of 8):

- The Committee strongly encourages the Institutes to expand outreach efforts in the out years of SciDAC-3 to reach a larger scientific community.

Program Response:

- ASCR agrees with this recommendation. The SciDAC Institutes are actively involved in expanding their outreach to the wider computational science community through annual summer schools, extensive tutorials, and new, research project collaborations.

Anticipating and addressing emerging challenges from high performance computing and DOE missions

COV Recommendation (8 of 8):

- Be attentive that balance between ASCR Leadership Computing Challenge (ALCC) and INCITE computing resources is tuned in light of SciDAC requirements.

Program Response:

- ASCR agrees with this recommendation. Sufficient access to advanced scientific computing resources is essential to the success of the SciDAC program and ASCR can address this risk when considering its computing resource allocation policies in FY16.

Comment: ALCC originated in 2010 and is an allocation program … for DOE projects emphasizing high-risk, high-payoff simulations in areas directly related to the DOE mission & for broadening the community of researchers capable of using leadership computing resources.

Thank You on Behalf of SciDAC-3!

Program	Time Frame	Description	Result
SciDAC-1	2001 - 2006	Created scientific software infrastructure for parallel computing; Funded collaboration in DOE science domains	Science at the Terascale
SciDAC-2	2006 - 2011	Added DOE science domains; Enhanced university involvement; Outreach to broader scientific community; Added Data Visualization	Science at the Petascale
SciDAC-3	2011 - 2016	Improved collaborations among SciDAC Institutes and ASCR-SC programs; Enhanced architecture- and applications-awareness within each Institute; Added Uncertainty Quantification	Science on multi-core & emerging hybrid architectures

SciDAC-3 Program Managers in the Office of Science (SC)

- Ted Barnes – Nuclear Physics (NP)
- Lali Chatterjee – High-Energy Physics (HEP)
- Jim Davenport – Basic Energy Sciences/Materials (BES)
- Dorothy Koch – Biological & Environmental Research (BER)
- Randall Laviolette – **ASCR**
- Steven Lee – **ASCR**
- John Mandrekas – Fusion Energy Sciences (FES)
- Mark Pederson – Basic Energy Science/Chemistry (BES)
- Ceren Susut - **ASCR**

More from COV Report: Findings (1-3 of 11)

Solicit, review, recommend, and document proposal actions:

1. The timing of the calls for Institute proposals and the interrelated Partnership proposals is a challenge. Asking the Program Managers in the science areas to define their areas of interest, followed by the Institute competition with knowledge of those areas, followed by the actual science program completion, was a good process.
2. The Program Managers are to be commended for having the courage to re-compete the Data Institute rather than accepting a sub-optimal solution among the original proposals.
3. Process documentation has much improved since the last review in 2007.

More from COV Report: Findings (4-9 of 11)

Monitor active award, projects and programs:

4. Projects are well monitored by Program Managers through frequent teleconferences.
5. Principal Investigator (PI) meetings are an excellent mechanism for oversight.
6. The Program Managers seem to be able to work together very effectively in supporting the projects. Negotiations among Program Managers were essential, and positive solutions were readily achieved.
7. The communication and interaction of Program Managers with the complex teams that are involved is essential. The level of interaction of the Program Managers with the teams is commendable.
8. The ability of Program Managers to travel to project meetings and conferences is important but is currently insufficient. Current travel support is inadequate.
9. The program was adaptive to changing circumstances. For example, when one PI became ill, there was an intervention that resulted in a two-PI arrangement that worked very well.

Managing the SciDAC-3 Program

Example for ASCR-funded SciDAC-3 Institutes

- Weekly or bi-weekly telecons with the 4 SciDAC-3 Institutes Directors
- Semi-annual Director Reports due in April & October
- Annual SciDAC-3 PI Meetings held in DC area: 2012, 2013, 2014
- Site visits, Participation in all-hands meetings
- SciDAC-3 Institutes Mid-Term Review on May 5-6, 2014
- "SciDAC: Accelerating Scientific Discovery, Transforming Computational Science" (SIAM News, April 2014)
- Each SciDAC-3 Institute and Partnership has its own project webpage
- SciDAC-3 Homepage: www.scidac.gov

More from COV Report: Findings (10-11 of 11)

National and international standing of the portfolio with regard to other computational science programs that are also focused on harnessing high performance scientific computing and utilizing massive datasets to advance science:

10. SciDAC remains the gold standard for fostering interaction between disciplinary scientists and high-performance computing. The Program Managers are to be commended on continuing the excellence of the SciDAC "brand."

11. Informal conversations of the reviewers with overseas colleagues indicate that SciDAC is seen as a model program, which they wish could be replicated in their home countries.