View from Washington

ASCR Update
March 22, 2011
Daniel Hitchcock
Acting Associate Director
Advanced Scientific Computing Research
Advanced Scientific Computing Research

Delivering world leading computational and networking capabilities to extend the frontiers of science and technology

The Scientific Challenges:
- Deliver next-generation scientific applications using today’s petascale computers.
- Discover, develop and deploy tomorrow’s exascale computing and networking capabilities.
- Develop, in partnership with U.S. industry, next generation computing hardware and tools for science.
- Discover new applied mathematics and computer science for the ultra-low power, multicore-computing future.
- Provide technological innovations for U.S. leadership in Information Technology to advance competitiveness.

FY 2012 Highlights:
- Research in **uncertainty quantification** for drawing predictive results from simulation
- **Co-design centers** to deliver next generation scientific applications by coupling application development with formulation of computer hardware architectures and system software.
- Investments in U.S. industry to address critical challenges in hardware and technologies on the path to exascale
- Installation of a **10 petaflop low-power IBM Blue Gene/Q** at the Argonne Leadership Computing Facility and a **hybrid, multi-core prototype computer** at the Oak Ridge Leadership Computing Facility.
## ASCR Budget Overview

*(dollars in thousands)*

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</thead>
<tbody>
<tr>
<td>Applied Mathematics</td>
<td>43,698</td>
<td>45,450</td>
<td>48,973</td>
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<td>Computational Partnerships (includes SciDAC)</td>
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<td>Next Generation Networking for Science</td>
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<td>SBIR/STTR</td>
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<td>4,623</td>
<td>4,873</td>
<td>+4,873</td>
</tr>
</tbody>
</table>

*Total, Mathematical, Computational, and Computer Sciences Research* 153,545 165,091 174,033  +20,488

| High Performance Production Computing (NERSC) | 54,900 | 56,000 | 57,800 | +2,900 |
| Leadership Computing Facilities             | 128,788 | 158,000 | 156,000 | +27,212 |
| Research and Evaluation Prototypes          | 15,984  | 10,052  | 35,803  | +19,819 |
| High Performance Network Facilities and Testbeds (ESnet) | 29,982  | 30,000  | 34,500  | +4,518 |
| SBIR/STTR                                  | 0       | 6,857   | 7,464   | +7,464 |

*Total, High Performance Computing and Network Facilities* 229,654 260,909 291,567  +61,913

*Total, Advanced Scientific Computing Research* 383,199* a 426,000 465,600  +82,401

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* a/ Total is reduced by $10,801, $9,643 of which was transferred to the Small Business Innovation Research (SBIR) program, and $1,158 of which was transferred to the Small Business Technology Transfer (STTR) program.
The House subcommittee recommends $163,891,000 for Mathematical, Computational, and Computer Sciences Research, $1,200,000 below the request of $165,091,000.

ASCR is also subject to a share of the government-wide $1.35 billion rescission to be allocated pro-rata to object class 20/30 funding.
New ASCR Research Division Director

William Harrod

Bill received his PhD in Mathematics from the University of Tennessee at Knoxville. Following that he was a Principal Engineer at the National Reconnaissance Office and an Engineering Manager of Computational and Applied Mathematics at SGI and the Section leader of the Mathematical Software Group at Cray. While at SGI, Dr. Harrod was the developer of the SHMEM (shared memory) architecture which provided the foundation for one-way communication libraries used on today’s high performance computers.

Most recently Bill was a Program Manager in the Information Processing Technology Office (IPTO) in the Defense Advanced Research Projects Agency (DARPA). While at DARPA he was responsible for a wide range of research activities related to the development and exploitation of advanced computing technologies and applications in support of the DoD and the Military Services. In this role, Bill led two internationally recognized hallmark studies that set the computer performance goals and strategy for achieving extreme scale computing. He also initiated a significant new research effort in Ubiquitous High Performance Computing (UHPS).
Mathematician/Physical Scientist – Steven Lee

Steve has a Ph.D. in Computer Science from the University of Illinois at Urbana-Champaign. He has spent the last 3 years at ASCR as an Applied Mathematics Program Manager on detaillee assignment from Lawrence Livermore National Laboratory. His research work at LLNL focused on the design and analysis of multiscale algorithms, the development of scalable solvers for systems of nonlinear and partial differential equations, and the use of sensitivity analysis and uncertainty quantification for large-scale science applications. Prior to that, he worked at Oak Ridge National Laboratory in the Computer Science and Mathematics Division.

Mathematician/Physical Scientist – Ceren Susut-Bennett

Ceren has a Ph. D. in Chemistry from Georgetown University. She has extensive research experience in diverse fields including chemical engineering, materials science and applied physics. Prior coming to ASCR, she worked as a National Research Council Postdoctoral Researcher at the Center for Nanoscale Science and Technology (CNST) at NIST where she was involved in the development of electrochromic nanodevices as well as fuel cell and battery materials. She has several published articles and three pending patent applications.
Phase Change in Computing

Performance

Top500

Concurrency Dominated

SciDAC-2

Hubs

By 2020
Typical server node chip ~ 400 cores
1k node cluster ➞ 400,000 cores
Laptop ~ 100 cores (low power)

Co-Design
X-Stack
Advanced Architectures
Data Management and Analysis at Extreme Scale

Today
Typical server node chip ~ 8 cores
1k node cluster ➞ 8,000 cores
Laptop ~ 2 cores (low power)

Laptops

2015

Time
1) **System power** is the primary constraint
2) **Memory** bandwidth and capacity are not keeping pace
3) **Concurrency** (1000x today)
4) **Processor** architecture is an open question
5) **Programming model** heroic compilers will not hide this
6) **Algorithms** need to minimize data movement, not flops
7) **I/O bandwidth** unlikely to keep pace with machine speed
8) **Reliability and resiliency** will be critical at this scale
9) **Bisection bandwidth** limited by cost and energy

Unlike the last 20 years most of these (1-7) are equally important across scales, e.g., 100 10-PF machines
- Report makes same points
  - Past performance increases have driven innovation
  - Processor speeds stalled
  - Energy is limitation
- Impacts everything
  - Data
  - Simulations
  - Control

See Kathy Yelick’s ASCAC presentation Tuesday March 22 at 4:15 pm
DOE Funding Opportunity for Scientific Discovery through Advanced Computing (SciDAC) Institutes

Program Funding – DOE, 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
- “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.”

Specific goals and objectives for the SciDAC Institutes are:
- Tools and resources for lowering the barriers to effectively use state-of-the-art computational systems;
- Mechanisms for taking on computational grand challenges across different science application areas;
- Mechanisms 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.

Timeline
- Issued - February 23, 2011
- Letters of Intent, though not required, are strongly encouraged - March 30, 2011
- Application due date – May 2, 2011
- Expect to make awards in Fiscal Year 2011

SciDAC information may be found at http://science.doe.gov/ascr/Research/SciDAC.html
For Answers to Inquiries about this Announcement – see http://science.doe.gov/ascr/research/scidac/SciDAC3InstitutesFAQ.html
Workshop Objective

- To identify the major research challenges in developing, deploying, and operating federated terabit networks to support extreme-scale science activities
- Participants from industry, academia, and nation laboratories (50 attendees)
- Major technical areas of discussions included
  - Scaling network architectures and protocols by several orders of magnitude over today’s network performance.
  - Terabit LANs, host systems, and storage
  - Advanced traffic engineering tools and services
- Workshop report pending (to be posted in two weeks)

See Rich Carlson’s ASCAC presentation Wednesday March 23 at 10:15 am
- **PI meeting for**
  - Advanced Architectures; X-Stack Software Research; Scientific Data Management, Analysis & Visualization at Extreme Scales awardees
  - Co-Design planning grant recipients
  - Exascale Software Center Planning award recipients

- **March 7-11, 2011, in San Diego, CA**

- **Expected Outcomes:**
  - Awareness **within** each solicitation communities and ASCR what members are doing and areas where they can leverage and supplement their work
  - Awareness **across** solicitation communities of what is going on and where each project fits in relation to the broad spectrum
  - Identification of gaps in ASCR exascale research portfolio
  - Lay groundwork for collaboration/cooperation with NNSA Exascale Roadmapping activities

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**See Karen Pao’s ASCAC presentation Wednesday March 23 at 8:30 am**

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<table>
<thead>
<tr>
<th>Category</th>
<th>People</th>
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<tr>
<td>Advanced Architectures</td>
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<td>X-Stack Software Research</td>
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<td>Data Mgmt., Analysis &amp; Visualization</td>
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<td>Co-Design Centers</td>
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<td>Grad. Student Scribes</td>
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<td>DOE</td>
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<td>NNSA (including Tri-Lab Working Group Leads)</td>
<td>17</td>
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<tr>
<td>DOD</td>
<td>1</td>
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<tr>
<td>TOTAL Attendance</td>
<td>201</td>
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Attendees include representatives from ASCR’s Exascale Kickoff meeting to identify areas of collaboration.
The contiguous U.S. electric power transmission grid. New computational modeling and analysis tools are needed that integrate real-time information to optimize power flow and prevent outages.

- **BES/EERE Workshop- ‘Predictive Simulation for Internal Combustion Engines (PreSICE)’ - March 3, 2011**
  - The purpose of the workshop was to identify critical needs in basic and applied R&D in chemistry, physics, and engineering required for the successful realization of predictive combustion modeling for engines.

  - The purpose of the workshop is to bring together experts from various fields of computation to discuss current industry practice and provide a critical comparative review of relevant research during the next 5 to 10 years.
SciDAC 2011 Conference
“Addressing the Challenges of the Next Decade”

- Location: Brown Palace Hotel, Denver CO
- Dates: July 10-14, 2011
- 400 participants from a broad range of computational science areas expected
- Special Events:
  - Plenary Speaker: Dr. Patricia Dehmer
  - Poster Sessions
    - ARRA-funded Post-docs and SciDAC-e
    - The successes of SciDAC-2
    - Viz Night
  - Panel sessions:
    - Challenges of Starting Community Codes
    - New Challenges in the Next Decade
    - Uncertainty Quantification

Registration Open at http://events.cels.anl.gov/scidac11/

Conference Chair: Lori Diachin, LLNL
INCITE provides awards of time to researchers in academia, government, and industry to pursue transformational advances in science and technology: **1.7 billion hours** were awarded in 2011 on the DOE Leadership Computing Facilities at Oak Ridge and Argonne National Laboratories.

2011 INCITE Statistics

- **124 Proposals received**
- **57 Projects awarded**
- **5.7B Hours requested**
- **1.7B Hours awarded**

See Rich Carlson’s ASCAC presentation Wednesday March 23 at 10:15 am

Contact information
Julia C. White, INCITE Manager
whitejc@DOEleadershipcomputing.org
Juan Meza is Named One of Top 200 Most Influential Hispanics in Technology

The editors of Hispanic Engineer & Information Technology magazine (HE&IT) have selected Juan Meza, interim head of the Lawrence Berkeley National Laboratory’s Computational Research Division, as one of the “Top 200 Most Influential Hispanics in Technology.” The winners were recognized for their excellence in work, strong commitment to their communities and leadership as role models.
Recognitions: John Birge

Dr. John Birge, University of Chicago Booth School of Business, was elected to the National Academy of Engineering in February 2001 and was recognized “for contributions to the theory of optimization under uncertainty.” Dr. Birge, funded in part by the ASCR Applied Mathematics program, studies mathematical modeling of systems under uncertainty using the methodologies of stochastic programming and large-scale optimization for a variety of practical applications.
(1) Purpose of this work
- Energy/Power are the most critical challenges
- Interconnect is the dominant bottleneck
- Computation is free; communication is expensive.

(DARPA-08): Energy consumed, relative to 64b MAC

(2) Conventional State-of-the-Art
- ON-CHIP LINKS pegged to 100-200fJ/bit (per mm)
  Wire power does not scale ($CV_{DD}^2$)

(DARPA-08): $V_{DD}$ Scaling
(HO-01): Capacitance Scaling

-OFF-CHIP I/O limited to above 1mW/Gbps (1pJ/bit)
Clocking dominates energy budget (54-71%)

(DARPA-08): $V_{DD}$, (HO-01): Capacitance Scaling

(3) Goal of DOE Early CAREER Award
The research goal of this CAREER proposal is to develop energy-efficient, VLSI interconnect circuits and systems that will facilitate future massively-parallel computing:

THrust #1: ON-CHIP I/O INTERCONNECT BANDWIDTH
- Energy-Efficient, Density-Scalable Crossbars and Core-to-Core Links
- Energy-Efficient Equalization Techniques for RC-Limited Lines

THrust #2: OFF-CHIP I/O INTERCONNECT BANDWIDTH
- Sub-1mW/Gbps, High-Speed I/O for Parallel, Short-Range Interconnect
- Energy-Efficient, Multi-Gigahertz ADCs for Limited Bandwidth Channels

(4) Energy-Efficient On-Chip Wires
- Token Flow Control Network-on-a-Chip Prototype: Co-design between micro-architecture/low-swing signaling circuits

(DARPA-08): Low-swing crossbars and core-core links

[ICCD-10]: Low-swing crossbars and core-core links

(5) Energy-Efficient Off-Chip Serial Links
- Low-power clock generation/distribution using injection locking

(A) 0.6pJ/b, 6.4Gbps receiver

(B) 0.16pJ/b, 8.0Gbps receiver

(6) Future Work
- Near-threshold, parallel computing with variation resiliency
- Efficiency-scalable computing, with fine-grain control of energy-adaptive interconnects

(CAL-10) Synctium-I performance

8-Lane SIMD, near-threshold prototype

Looking for collaborations in novel interconnects (3D and optics), heterogeneous memory architectures, and resiliency software/hardware co-design.
Challenges:
As HPC platforms scale in size, physics simulations have increased:
• Raw dataset size
• Notational complexity (e.g. intrusive UQ & stochastic simulations track non-deterministic scalar quantities)
• Physical scale (e.g. increased range of feature sizes)
• Representational scale (e.g. higher-dimensional state spaces)
• Operational scale (e.g. more costly constitutive equations are evaluated)

Increased complexity poses challenges for feature analysis:
• Topological analyses become computationally intractable due to raw data size + notational complexity.
• Statistical analyses tend toward the mean and variations from the mean decrease providing little insight into the data.

Accomplishments:
Introduced several hybrid approaches to analyze the results of petascale simulations:
• By computing statistics on topologically-defined features, the averaging that can obscure insight is avoided.
• By using statistically accurate subsampling, topological features can be computed at scales otherwise impossible.
• By examining the topologically-defined features of statistical constructs such as contingency tables or random variables, information available due to increased notational complexity is communicated.

Novel “hixel” technique enables feature identification on extremely large or uncertain data. Statistically associate instances of subsets of the data, and apply topological segmentation methods per subset to recover views of large-scale features that would either be infeasible to compute or ambiguous to infer within the original data.
Objectives

- Quantify the uncertainty in numerical simulations
- Exploit knowledge of the noise level to obtain stable derivative estimates
- Provide nonintrusive stability bounds for simulations at the extreme scale

Impact

- Provide fundamental insights into how simulation tolerances affect computational noise
- Obtain optimal accuracy in estimated derivatives
- Enable sensitivity analysis and optimization of noisy simulations

Accomplishments

- New tool, ECNoise, provides reliable estimates of stochastic and deterministic noise in few simulations
- Optimal difference parameters calculated without computationally expensive parameter sweeps
- Stochastic theory provides error bounds independent of the form of underlying distributions

Optimal step was obtained with only two simulation evaluations. Classical approach (circles): result of a sweep across 100 difference parameters, each point requiring a new simulation.
MRNet – An Infrastructure for Highly Scalable and Reliable Tools and Middleware
Barton P. Miller (Univ. Wisconsin)

ASCR – Computer Science Highlight

Objectives

- Simplify the building of highly scalable tools and middleware.
- Provide reliability as a basic feature, without requiring special effort or programming.
- Proving a common infrastructure to be used across leadership class and cluster platforms.

Impact

- More rapid delivery of scalable tools on the largest of systems.
- Make fault tolerance a default feature.
- Increase the portability of tools for the leadership class platforms.

Impact Objectives

- STAT: The first debugging tool that ran easily at full scale on IBM BG/L and Cray Jaguar (> 200K processes). Collaboration with LLNL and ORNL.
- Significant number of production application bugs found with STAT (ones that could not be previously found).
- Commercial research of MRNet and STAT by Cray.
- Incorporation of MRNet into tools by Totalview, Jülich Supercomputer Center, Barcelona Supercomputer Center, TAU project, and others.

Progress (FY10)

http://www.youtube.com/watch?v=Lv8rR03ez04
In-situ feature tracking and visualization” J. Chen (SNL), K.L. Ma (SciDAC -Ultrascale Viz) and V. Pascucci (SciDAC-VACET)

**Objectives**

- Develop in-situ topological feature extraction & tracking and volume & particle visualization in petascale combustion simulation – take a holistic view towards end-to-end scientific discovery pipeline for large data
- Use the new in-situ analytics/visualization capability to extract combustion science relevant to power generation with alternative fuels.

**Impact**

- Reduce I/O and storage requirements for petabytes of combustion data and accelerate time to discovery
- Glean insight from petascale combustion simulation focusing on science underpinning efficient power generation coupled with carbon-capture and storage, to minimize net carbon and NO\textsubscript{x} emissions, and to provide unique benchmark validation data for engineering model development

**Progress**

- Developed algorithms for scaleable parallel merge trees for in-situ topological segmentation
- Developed highly scalable parallel algorithms for in-situ volume and particle rendering and image compositing
- Demonstrated scalability of in-situ volume and particle rendering in petascale DNS up to 15,000 Cray XT5 cores, cost is < 1% of simulation time

“I am excited to hear about Dr. Chen’s proposal to simulate a directly relevant canonical configuration, jet-in-crossflow, which has bearing on fuel injection and flame stabilization, with a variety of relevant fuels, to address the breadth of flame propagation and stabilization effects. GE will be using the conclusions of this research when they are made available to advance our development efforts.” Venkat E. Tangirala, Senior Research Scientist, General Electric Global Research Center
**APDEC’s Modeling of San Francisco Bay and Delta**
*(P. Colella, LBNL)*

**ASCR- SciDAC Math Center of Enabling Technology Highlight**

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<tr>
<th>Objectives</th>
<th>Impact</th>
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<tr>
<td>LBNL and the California Department of Water Resources are collaborating on the development of an open-source hydrodynamic, transport, and particle tracking model of the Sacramento-San Joaquin Delta (REALM) that will provide input to critical water policy decisions in CA.</td>
<td>Two-thirds of the water in California passes through the Sacramento-San Joaquin Delta, providing drinking water for 22 million Californians and supporting agriculture valued at tens of billions of dollars.</td>
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**Progress**

Provide support for computations of salinity, transport of pollutants, and the survival of young fish by supplying ASCR-funded technologies such as

- Embedded boundary methods for complex geometries.
- Adaptive mesh refinement on structured grids.
- Libraries and frameworks for implementation on parallel architectures.
The performance and lifetime of materials used in nuclear technology and in advanced power generation are severely limited by corrosive environments and extreme conditions.

Premature failure of materials can result from undetected stress corrosion cracking.

Annually, corrosion costs about 3% of the U.S. gross domestic product.

48-million-atom simulation on Argonne Leadership Computing Facility showed a link between sulfur impurities segregated at grain boundaries of nickel and embrittlement. An order-of-magnitude reduction in grain-boundary shear strength, combined with tensile-strength reduction, allows the crack tip to always find an easy propagation path in this configuration. This mechanism explains an experimentally observed crossover from microscopic fracture to macroscopic cracks due to sulfur impurities.
A team led by Southern California Earthquake Center (SCEC) director Thomas Jordan is using ORNL’s Jaguar supercomputer through INCITE to simulate a magnitude-8 quake and assess its impact on the SoCal region.

The area simulated is home to 20 million people—about one in 15 Americans. As a result, the information provided will be valuable not only to seismologists, but also to building designers and emergency planners.

The M8 simulation compare well with data averaged from many real earthquakes, in particular on rock sites.

The simulation reached 220 trillion calculations per second, or 220 teraflops, more than twice the speed of any previous seismic simulation.

“The things we learn about earthquakes here should be applicable to earthquakes around the world.”
— SCEC information technology architect Phil Maechling
ASCR at a Glance

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Relevant Websites

ASCR: science.doe.gov/ascr/
ASCR Workshops and Conferences: science.doe.gov/ascr/WorkshopsConferences/WorkshopsConferences.html
SciDAC: www.scidac.gov
INCITE: www.science.doe.gov/ascr/incite/
Exascale Software: www.exascale.org
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