U.S. DEPARTMENT OF ENERGY | Office of Science

View from Washington

ASCR Update

November 1, 2011

Daniel Hitchcock

Acting Associate Director

Advanced Scientific Computing Research

HPC in the European Union

ASCR FY12House Budget Language

- ADVANCED SCIENTIFIC COMPUTING RESEARCH

   The Advanced Scientific Computing Research program develops world-leading computing and networking capabilities in support of science and energy research. The Committee recommends $427,093,000 for Advanced Scientific Computing Research, $5,096,000 above fiscal year 2011 and $38,507,000 below the request.

   The Office of Science and the National Nuclear Security Administration fund the development and operation of the world's fastest computing systems. These systems have consistently topped the list of the world's fastest supercomputers. More than just symbolic, American leadership in supercomputing supports domestic world leading weapons and scientific research while keeping the private sector at the leading edge of information technology. Global competition has become increasingly fierce, with the United States unseated from the top spot in late 2010. The Committee continues to support science activities in the United States that improve and develop the world's fastest supercomputing systems.

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- ADVANCED SCIENTIFIC COMPUTING RESEARCH

….While the budget request proposes funding increases to accelerate exascale research and emphasizes its importance, the Department has not yet aggregated exascale research components into a coherent effort. Several Department national laboratories have stated target years for exascale prototypes and fully-operational exascale systems, but the Department has not stated any such timeframes, nor has it provided clear funding amounts for the exascale effort in the budget request. The Department is directed to provide to the Committee, not later than February 10, 2012, a report including its current target date for developing an operational exascale platform, interim milestones towards reaching that target, estimated total ranges of Department investment likely needed to hit those targets, and a complete listing of exascale activities included in the budget request broken out by program and activity with comparisons to the current year's funding levels.

ASCR FY12 Senate Budget Language

- ADVANCED SCIENTIFC COMPUTING RESEARCH

  The Committee recommends $441,619,000 for Advanced Scientific Computing Research. The Committee recommends $90,000,000 for the exascale initiative to spur U. S. innovation and increase the country's ability to address critical national challenges. The Committee understands that exascale computing will help maintain U.S. industrial competitiveness. In particular, high-tech industries such as transportation, aerospace, nuclear energy, and petroleum will increasingly rely on high-performance computing, especially when traditional experiments would be impossible, dangerous or inordinately costly to perform.

  The Committee directs the Department's Undersecretary for Science and The National Nuclear Security Administration (NNSA) Administrator to <u>submit within 120 days of enactment of this act, a joint, integrated strategy and program plan with estimated budget needs through 2018 on how the Office of Science's Advanced Scientific Computing Research and NNSA's Advanced Simulation and Computing programs will share responsibilities and coordinate research and development activities to reach exascale computing</u> for national security, energy, environmental and other science missions and to retain the United States' global leadership and competitiveness in advanced computing.

ASCR Budget Overview
(dollars in thousands)

	FY 2011 Budget	FY 2012 Request	FY 2012 vs. FY 2011	FY 2012 House	FY 2012 Request vs. House	FY2012 Senate	FY 2012 Request vs. Senate
Total, Advanced Scientific Computing Research	421,997	465,600	+ 43,603	427,093	- 38,507	441,619	-23,981

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New DOE Funding Opportunities:
SC Application Partnerships with SciDAC Institutes

DOE Office of Science is lead federal agency in fundamental research for energy

- SC is comprised of 6 interdisciplinary scientific program offices
- Nation's largest supporter of basic research in the physical sciences
- Unique open-access scientific user facilities – including leadership-class supercomputers

Overview of funding opportunities for Application Partnerships

- Each FOA issued by an SC office & in partnership with ASCR
- DOE National Laboratories, Universities, Industry and other organizations may apply
- Partnerships will exploit leadership-class computing resources to advance scientific frontiers in areas of strategic importance to the Office of Science
- Partnerships will effectively leverage the SciDAC Institutes' intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools

Timeline for Partnerships FOAs

- SC Application Partnerships in Fusion Energy Science: DE-FOA-0000571, LAB 11-571
  - ✓ Posted August 3; Pre-proposals due September 9; Proposals due October 26
- FOAs are also being developed in partnership with other SC offices
- First awards expected in mid-FY12

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.

New Funding Opportunity: SciDAC Institutes FOA for Scientific Data Management, Analysis and Visualization

- Funded Institute will serve as a single point of contact for scientists participating in Scientific Computation Application Partnerships seeking ASCR-supported collaborators to more efficiently and effectively manage, analyze, visualize and understand their scientific.
- Up to $5M/year for 5 years;
- DOE Labs, Universities, Industry and other organizations may apply
- Posted: **September 16, 2011**
- Letters of Intents due: **October 12, 2011**
- Proposals due: **November 9, 2011**

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SciDAC SC Application Partnerships

Partner	PMs	Topics
FES	John Mandrekas, Randall Laviolette	• Edge Physics • Multiscale Integrated Modeling • Materials Science
BER	Dorothy Koch, Randall Laviolette	• Multiscale dynamics of the atmosphere, ocean or ice sheets • Tracer transport in the atmosphere or oceans
NP	Ted Barnes, Randall Laviolette	• Low-Energy Nuclear Physics • Medium-Energy Nuclear Physics • Heavy-Ion Collider Physics
HEP	Lali Chatterjee, Randall Laviolette	• Cosmic Frontier Scientific Simulations • Lattice Gauge Theory Research • Accelerator Science Modeling and Simulation
BES	Jim Davenport, Mark Pederson, Ceren Susut	• First-principles treatments of excited states • Electron correlation in finite and extended systems

SciDAC SC Application Partnerships

Partner	FES	BER	NP	HEP	BES
FOA #	571	588	581	580	593
Pre-apps	9-Sep	17-Oct	30-Oct	N/A	**9-Dec**
Proposals	26-Oct	**5-Dec**	**5-Jan**	**9-Jan**	**12-Mar**
#Projects	1-4	2-5	1-4		5-12
Duration (y)	5	5	5	3	5
max. value over lifetime (**$ in millions**)	**$33.0**	**$32.5**	**$20.0**	**$12.0**	**$30.0**

FES BER NP HEP BES
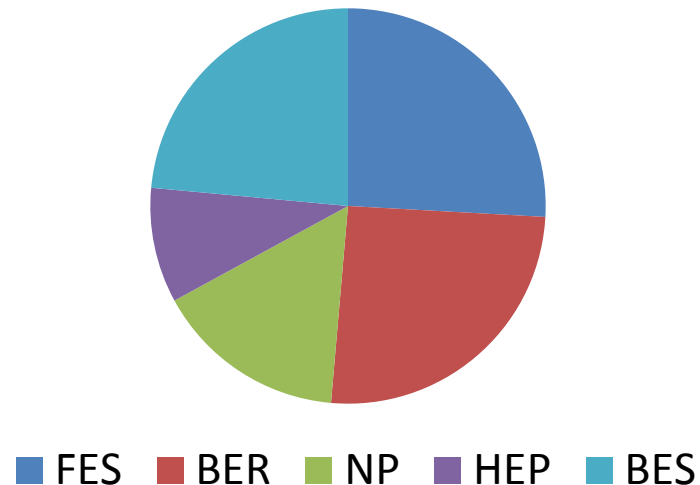
ARRA update: SciDAC-e Review

- Interim reports from SciDAC-e ERFC were reviewed by ASCR and BES PMs in early September

- Project reports for ARRA Postdocs at ASCR facilities were reviewed by ASCR and SC PMs in October

See Karen Pao's Talk for more information

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Magellan Project Status

- **No-cost extension to December 31, 2011**
  - Provides high-performance end-points for ANI 100 Gbps prototype network
  - Extends Magellan through SC'11 demo cycle
- **Disposition plans in place for continued use of Magellan hardware**
- **Final report being prepared for December release**

High level Findings

- **Magellan demonstrated potential value to DOE science communities**
  - Allowing the creation of customized environments though bare-metal and virtualized OS deployments
  - Rapid surge capability enabled by automatic deployment of customized environments
- **Magellan identified significant gaps and challenges**
  - High initial effort and skills needed to port applications to cloud computing paradigm
  - Administrative tools for managing virtual environments, workflows, data, and cyber-security are lacking
  - Scientists need to learn new computing model not based on existing HPC batch-queue usage

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Disposition Plans

- **Argonne plans**
  - Systems Biology Knowledge Base: 6 compute node racks, 8 global file servers, 200 active storage nodes, 1 GPU server rack, 12 Big Memory nodes, 16 Login/Gateway servers, and 2 Infiniband switches
  - Argonne Leadership Computing Facility: 3 GPU server racks, Tape storage equipment, and 12 Login/Gateway nodes
  - Computing Information Systems Division: 2 100 Gpbs routers
- **NERSC plans**
  - NERSC production: 3 compute node racks, 2 large memory nodes, and archival and disk storage resources
  - Kbase Project: 2 compute node racks
  - Special Projects: 2 compute node racks
  - Testbed projects: 2 compute nodes racks and flash storage system

FY12 SBIR Topics

- **Advanced Network Technologies and Services**
  - New tools, services, and devices that simplify network management and lower operational costs

- **Increasing Adoption of HPD Modeling and Simulation in the Advanced Manufacturing and Engineering Industries**
  - Outreach efforts to enable HPC by non-traditional HPC users

74 proposals received and will be reviewed

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FY12 SBIR Statistics

- **74 Proposals Received**
  - 22 for Network Technologies
  - 46 for HPC for Industry and Manufacturing
  - 6 declined without review

- **4 review panel sessions planned**
  - 3 panels to meet for half day session
  - 1 panel to meet for full day session

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Workshops

- **July 27-29, 2011 Programming Challenges Workshop**
  - USC/ISI, Marina del Rey, CA; report at http://science.energy.gov/~/media/ascr/pdf/program-documents/docs/ProgrammingChallengesWorkshopReport.pdf
- **August 2-3, 2011 2011 Workshop on Architectures I: Exascale and Beyond: Gaps in Research, Gaps in our Thinking**
  - Stanford, CA
- **August 8-10, 2011 2011 Workshop on Architectures II: Exascale and Beyond: Configuring, Reasoning, Scaling**
  - Sandia National Laboratories, Albuquerque, NM
- **September 13-14, 2011 Workshop for Mathematics for the Analysis, Simulation and Optimization of Complex Systems**
  - Sheraton Crystal City, Arlington, VA See John Bell's Talk, Nov 1, 3:30 pm
- **September 26-27, 2011 The 5th Workshop on HPC Best Practices: File Systems and Architectures**
  - San Francisco, CA
- **October 11-13, 2011 Exascale Research Principal Investigators Meeting**
  - Annapolis, MD
- **October 13-14, 2011 Exascale Tools Workshop**
  - Annapolis, MD
- **October 17-19, 2011 Applied Mathematics Principal Investigators Meeting**
  - Hyatt Regency Reston, Reston, VA
- **October Data and Communications in Basic Energy Sciences: Creating a Pathway for Scientific Discovery**
  - Bethesda, MD See Peter Nugent's talk, Nov 1, 11:00 am
- **Dec 6-7, 2011 Scientific Collaboration Workshop**
  - Gaithersburg Marriott Washingtonian
- **Dec 8-9, ESnet FES Requirements Gathering Workshop**
  - Rockville, MD

Exascale Tools Workshop

This workshop will explore the challenges for Exascale tools and identify promising approaches to meeting these challenges and measuring their progress. A goal will be to define objective criteria for assessing tool features, their usability, and their interaction with compilers, runtime systems, and hardware

- **Held:** October 13-14, 2011, Annapolis MD

- **Organizing Committee:** John Mellor-Crummey (Rice), Barton Miller (U. Wisconsin), Jeff Hollingsworth (U. Maryland), Dan Quinlan (LLNL), Martin Schulz (LLNL), Paul Hovland (ANL), Jeff Vetter (ORNL and Georgia Institute of Technology), David Skinner (LBNL)

- **Workshop Website:**
   http://science.energy.gov/ascr/research/computer-science/exascale-tools-workshop/

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Exascale Tools Workshop
Background and User's Experience

- Need for scalability, modular infrastructures, good interfaces / abstractions for interacting with apps and other layers of the software stack

- Inertia and little current use of tools

- Trends: Increasing use of I/O and threads; and decreasing performance understanding due to complex hardware.

- Wants/needs: Flexibility in choice of tools, portability, automation, usability (e.g., good interfaces), minimal invasiveness in code and workflow, analytic capability, longevity, and engagement with / feedback to tool developers so that tools are of sufficient quality.

Workshop Report due November 15, 2011

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2011 DOE Applied Mathematics Program Meeting
October 17-19, 2011 in Reston, VA

A combination of plenary talks, contributed talks, and poster sessions to highlight recent research in selected theme areas. The purpose of this meeting is to exchange technical information and foster interactions among researchers funded by the DOE Applied Mathematics Program, and to relay DOE interests to our researchers.

Statistics from Principal Investigators meetings:

	Host	Participants	Plenary talks	Contributed talks	Posters
May 2007	LLNL	136	8	38	44
Oct 2008	ANL	147	7	48	35
May 2010	LBNL	225	9	48	83
Oct 2011	**ORNL**	**207**	**8**	**48**	**96**

DOE Mission Panel: Alex Larzelere, Office of Nuclear Energy, David Lesmes, Office of Science, Biological and Environmental Research, Jim Davenport, Office of Science, Basic Energy Sciences, John Mandrekas, Office of Science, Fusion Energy Sciences, Gil Bindewald, Office of Electricity Delivery and Energy Reliability

Website: http://www.csm.ornl.gov/workshops/applmath11/index.html

2011 DOE Applied Mathematics Program Meeting

ASCR Speakers:

- Bill Harrod, *DOE Extreme Scale Computing*
- Steve Lee, *SciDAC-3 Overview*
- Barb Helland, *DOE Fellowship programs*
- Karen Pao*, Co-Design and You: Why mathematicians should care about exascale computing*
- Sandy Landsberg, *Applied Math Program Update*

Invited Speakers:

- John Bell and Mihai Anitescu, Applied Mathematics Workshop Update, *Workshop for Mathematics for the Analysis, Simulation, and Optimization of Complex Systems*
- David Keyes, *Missing Mathematics for Extreme-Scale Simulation*

Plenary Speakers:

1. Jim Demmel, UC Berkeley, *Minimizing Communication in Linear Algebra*
2. Andrew Gelman, Columbia, *Statistical computing and data analysis with complex models*
3. Jan Hesthaven, Brown, *GPU Accelerated High-Order Hybrid Methods for Shock Problems*
4. Alireza Doostan, CU-Boulder, *Stochastic PDEs, Sparse Approximations, and Compressive Sampling**
5. Luis Chacon, ORNL, *Scalable implicit algorithms for stiff hyperbolic PDE systems*
6. Alexandre Tartakovsky, PNNL*, Dimension Reduction Method for Large ODE Systems**
7. Michael Ferris, Wisconsin, *Multiple Optimization Problems with Equilibrium Constraints*
8. Mihai Anitescu, ANL, *Scalable Stochastic Programming*

*   SC/ASCR Early Career Research Program Awardees

DOE HPC Best Practices Workshops

- **In 2006, NNSA and SC identified need for large supercomputer centers to learn from each other what worked and what did not, as acquisition, installation, integration, testing, and operation of such centers became more complex and challenging under perpetual budget constraints every year.**

- **Hosting organization alternates between NERSC and LLNL**

- **Previous HPC Best Practices Workshops**
  - 2007:   System Integration
  - 2008: Risk Management
  - 2009: Software Lifecycles for HPC Centers
  - 2010: HPC Power Management

See http://outreach.scidac.gov/fsbp/ for Workshop information

2011 DOE HPC Best Practices Workshop

- **Topic:** File Systems and Archives
- **Purpose:** To address current best practices for the procurement, operation, and usability of file systems and archives. Furthermore, the workshop addressed whether system challenges can be met by evolving current practices.
- **Statistics:**
  - NERSC hosted workshop which was in San Francisco, CA, on Sep 26-27, 2011
  - 64 attendees, representing 29 different institutions and sites from around the world (DOE, DoD, NSF, NASA, Japan, France, Germany, Switzerland, and United Kingdom)
- **Workshop report:** in progress
- **Sample Best Practices:**
  - Having dedicated maintenance personnel, vendor or internal staff, is important to increasing system availability.
  - Storage systems should function independently from compute systems.
- **Participants continued discussions after workshop**

Participants identified "Data Management" as possible topic for 2012 Best Practices Workshop

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NERSC Played Key Role in Nobel Prize-Winning Discovery

Accelerating Expansion of the Universe Subject of 2011 Prize

Type Ia supernovae are used as "standard candles" to measure the distance to remote galaxies.

Simulations run at NERSC in the late 90s modeled how Type Ia supernovae should appear from Earth.

This provided the crucial calibration needed to enable the Nobel Prize-winning discovery.

When NERSC moved to Berkeley 1996, this project's work was one of the first funded in a new computational science program created to encourage collaborations between physical and computer scientists.

Berkeley Lab's Saul Perlmutter was awarded the 2011 Nobel Prize in Physics along with two others for their discovery.

It implies the existence of so-called dark energy, a mysterious force that acts to oppose gravity.

The nature of dark energy is unknown and has been termed the most important problem facing 21st century physics.

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SciDAC PI Wins Nuclear Physics Prize

American Physical Society's 2012 Tom W. Bonner Prize in Nuclear Physics Awardee:
Witold Nazarewicz, University of Tennessee

- *"For his foundational work in developing and applying nuclear Density Functional Theory, motivating experiments and interpreting their results, and implementing a comprehensive theoretical framework for the physics of exotic nuclei."*

- **Co-Director of the UNEDF SciDAC Project**

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Kathy Yelick Named to National Academies Board

- LBNL Associate Laboratory Director for Computing Sciences Kathy Yelick has been appointed to the Computer Science and Telecommunications Board (CSTB) of the National Academies

  - CSTB is composed of nationally recognized experts from across the information technology fields and complementary fields germane to the Board's interests in IT and society

  - Board members are appointed by the National Academies following a rigorous vetting process, and they serve staggered terms of three to five years.

- Yelick was previously a member of the CSTB's Committee on Sustaining Growth in Computing Performance, which published the report *The Future of Computing Performance: Game Over or Next Level?* earlier this year.

2011 PECASE Awardees

Dr. Grigory Bronevetsky, Lawrence Livermore National Laboratory
For innovative, cutting-edge research using statistical models to predict the effects of system faults leading to the development of new software tools and more reliable applications and supercomputer systems, and for his strong track record of professional service and leadership.

Dr. Christiane Jablonowski, University of Michigan
For exemplary computation science research, advancing the frontier at the interfaces of applied math, computer science, scientific computing, and atmospheric science, and for leadership in connecting diverse communities and bridging the gaps between mathematical and computational developments and the special requirements of climate modeling.

ASCR Early Career Research Program Awardees in 2010

Facility Progress

- Four ASCR facilities completed Annual Operational Assessment by September 30, 2011
    - ALCF – onsite Operational Assessment, August
    - NERSC, OLCF – mail reviews
    - ESnet – Virtual review

Oak Ridge Leadership Computing Facility

Jaguar -- > Titan Phase I
Doubles the memory
One Third more cores

Jaguar Specs	
Nodes	18,688
Memory per node	16 GB
Six-Core Opteron	2.6 GHz
Opteron performance	125 Gflops
Peak Performance	2.33 Pflops

Titan Specs (Phase 1)	
Nodes	18,688
Memory per node	32 GB + 6 GB
Sixteen Core Opteron	2.2 GHz
Opteron performance	141 Gflops
Total Opteron Flops	2.6 Pflops
NVIDIA "Fermi"	665 GFlops
# of Fermi chips	960
Peak Performance (Aggregate)	3.3 Pflops

Phase 2: Add 6,912 - 18,688 Nvidia Kepler Accelerators to reach Peak Performance of 10 - 20 Pflops (Aggregate)

See Buddy Bland's talk Nov 1, 4:15 pm

"Sustainable Silicon: Energy-Efficient VLSI Interconnect for Extreme-Scale Computing" –

Patrick Chiang, Oregon State University

ASCR- Computer Science Highlight

Objectives

- Semiconductor technology advances improve the amount of parallel computation cores possible on a single silicon die.

- Unfortunately, the energy consumed to communicate between these cores now dominates over the energy consumed to compute.

- **The research goal of this EARLY CAREER proposal is to develop energy-efficient, VLSI interconnect circuits and systems that will facilitate future massively-parallel computing.**

Impact

- Energy-efficiency is of critical importance for all classes of computing – from exascale super-computers to handheld cellphones to embedded medical devices.

- Interconnect energy between cores (on-die), processors (off-die), and different racks

Fig-1: Energy dissipated to compute 64b floating-point operation versus move that information (Shalf et. al. 2011)
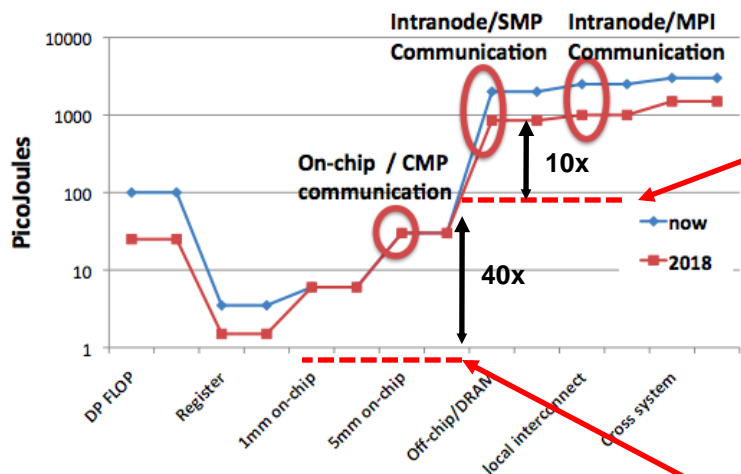
- **OFF-CHIP (Conventional): 1000 – 10,000fJ/bit**

THIS WORK: 200fJ/bit test-chip [1]
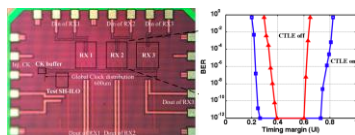
- **ON-CHIP (Conventional): 100 - 200fJ/bit/mm**

THIS WORK: 5-100fJ/bit/mm test-chip [2]

OUR GOAL: Reducing the energy required to move information around by more than 10x
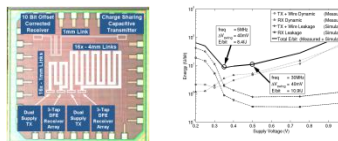
Accomplishments 2011

- Experimental validation of energy-efficient off-chip communications RX (5-10x better than conventional) [1]

- Experimental validation of energy-efficient on-chip communications (5-40x better than conventional) [2]

[1] K. Hu, T. Jiang, S. Palermo, and P. Chiang, "Low-Power 8Gb/s Near-Threshold Serial Link Receivers Using Super-Harmonic Injection Locking in 65nm CMOS", IEEE Custom Integrated Circuits Conference, 2011.

[2] J. Postman and P. Chiang, "Energy-Efficient Transceiver Circuits for Short Range On-Chip Interconnects," IEEE Custom Integrated Circuits Conference, 2011.

True Rational Materials Design

- **Organic semiconductors hold immense promise for use in flexible displays (picture an iPad you could roll up) but they aren't yet fast enough for high definition LCD screens.**

  - *Science discovery: a new organic semiconductor, amongst the speediest yet, was discovered using a predictive screening approach*

    - *Can also be used to manufacture less expensive printed solar cells leading to more widespread solar power*

- ***Would have taken <u>several years</u> to synthesize and characterize all seven candidate compounds studied.***

  - *The material discovered via this method conducts charge more than 30 times faster than what is currently used for liquid crystal displays.*

- ***A key proof of principle for supercomputer-aided materials design.***

Predicted crystal structure of the highly conductive organic semiconductor material
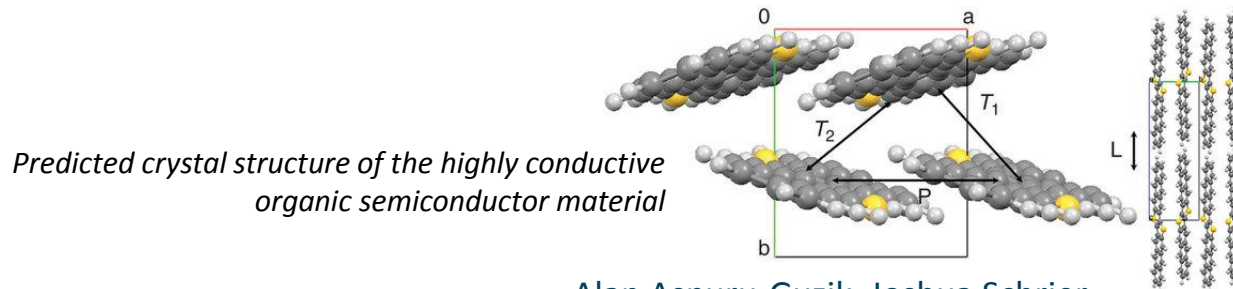
Alan Aspuru-Guzik, Joshua Schrier

September 2011

The Problem with Cellulosic Ethanol

Simulation provides a close-up look at the molecule that complicates next-generation biofuels

- A team led by ORNL's Jeremy Smith has taken a substantial step in the quest for cheaper biofuels by revealing the surface structure of lignin clumps down to 1 angstrom.

- The team's conclusion, that the surface of these clumps is rough and folded, even magnified to the scale of individual molecules, was published June 15, 2011, in the journal Physical Review E.

- Smith's team employed two of ORNL's signature strengths—simulation on Jaguar and neutron scattering—to resolve lignin's structure at scales ranging from 1 to 1,000 angstroms.

- Its results are important because lignin is a major impediment to the production of cellulosic ethanol, preventing enzymes from breaking down cellulose molecules into the sugars that will eventually be fermented.

"Nature has evolved a very sophisticated mechanism to protect plants against enzymatic attack, so it is not easy to make the fuels. What we're trying to do is understand the physical basis of biomass recalcitrance—resistance of the plants against enzymatic degradation."- team member Loukas Petridis, a computational physicist at ORNL
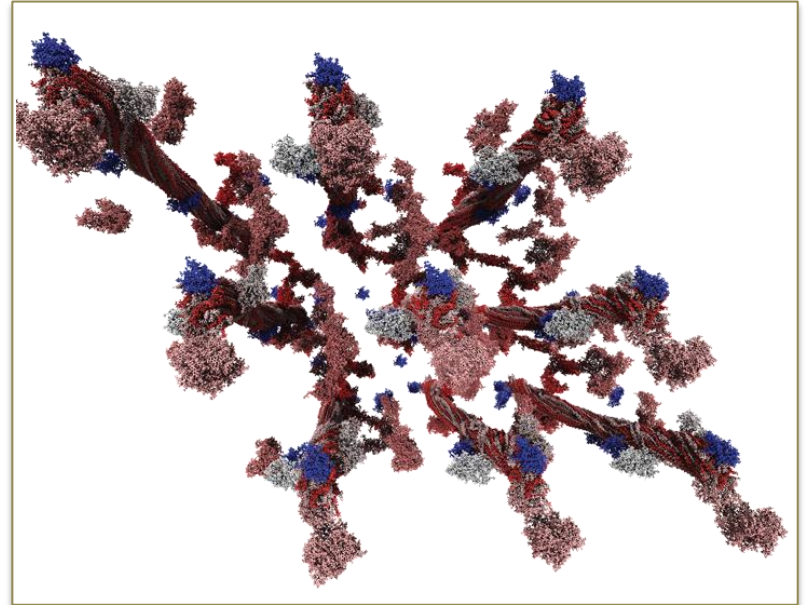
Leadership-class molecular dynamics simulation of the plant components lignin and cellulose. This 3.3 million-atom simulation was performed on 30,000 cores of the Jaguar XT5 supercomputer and investigated lignin precipitation on cellulose fibrils, a process that poses a significant obstacle to economically viable bioethanol production.

Related publications:

J. Smith, et al. 2011. "Self-Similar Multiscale Structure of Lignin Revealed by Neutron Scattering and Molecular Dynamics Simulation," *Physical Review E*, 83(6): 061911-1.

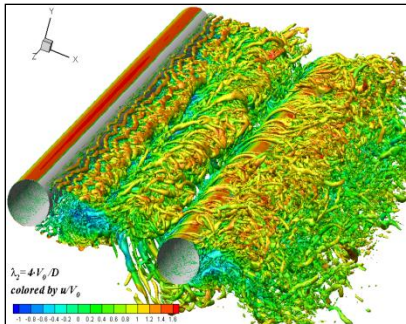U.S. DEPARTMENT OF ENERGY | Office of Science

Boeing uses ALCF BlueGene to design quieter planes


Landing gear of Boeing 777

Tandem cylinder used for V&V

- Boeing is using ALCF to simulate the turbulence created by aircraft landing gear and calculated the noise caused by two cylinders placed in tandem in an air stream.
- Boeing expects these capabilities to contribute to the design of safe and quiet technologies
- INCITE project is led by Dr. Philippe Spalart (Boeing) and Prof. Michael Stretlets (St. Petersburg State U.).
- The simulations are being carried out on eight 192 nodes (i.e. 32,768 cores) of the Blue Gene/P. The code used is the multi-purpose CFD code NTS. It allows Delayed Detached-Eddy Simulation(DDES) and Improved Delayed Detached-Eddy Simulations (IDDES) to be compared, to each other and to experimental data.
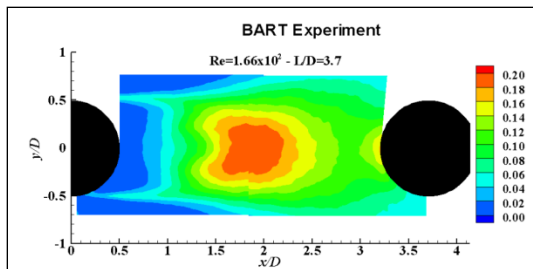
Experiment used as baseline
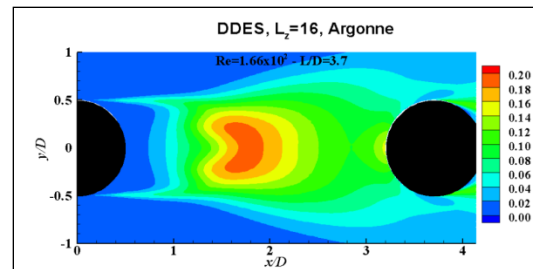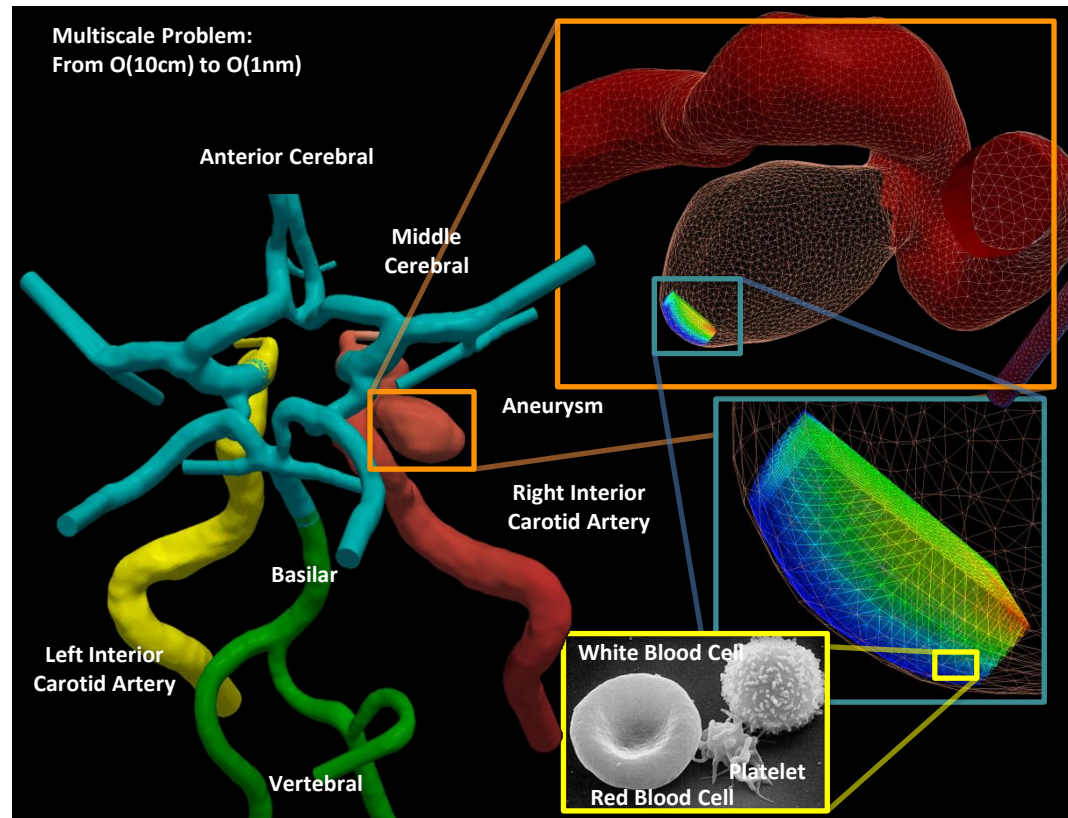

DDES method run at ALCF
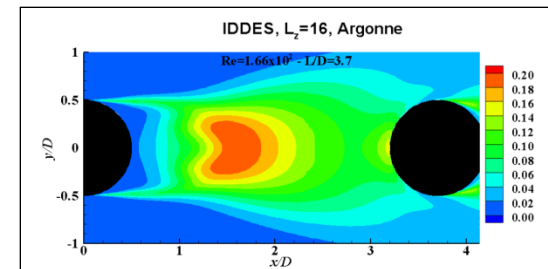
IDDES method run at ALCF

Multi-Scale Simulation

L. Grinberg, V. Morozov, D. A. Fedosov, J. A. Insley, M. E. Papka, K. Kumar, and G. E. Karniadakis. *A new computational paradigm in multi- scale simulations: Application to brain blood flow.* to appear in the Proceedings of the 2011 ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis, Seattle, WA, 2011.

Simulation run on 32 Racks of Argonne Intrepid [IBM BG/P (132K processors)]

- Macro-scale: NekTar – Spectral Element Method
  - Complex geometries from patient-specific MRI data
  - ~450K spectral elements
- Micro-scale: DPD-LAMMPS - Dissipative Particle Dynamics
- 350+ time steps
- 800 Million particles

Multiscale Problem: From O(10cm) to O(1nm)

Anterior Cerebral

Middle Cerebral

Aneurysm

Right Interior Carotid Artery

Basilar

Left Interior Carotid Artery

White Blood Cell

Platelet

Red Blood Cell

Vertebral

Simulating Materials at the Nanoscale

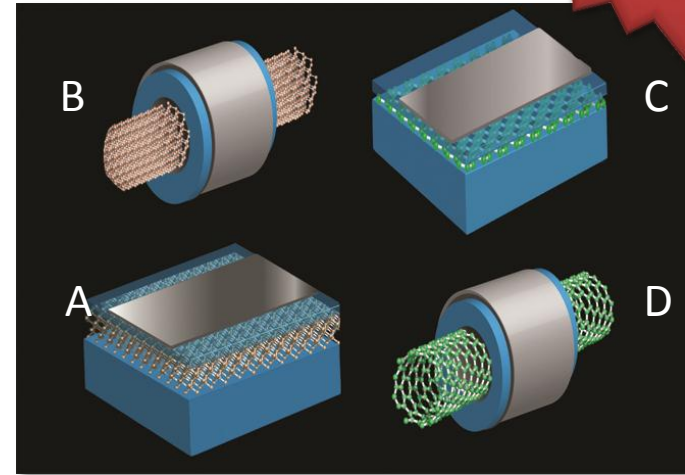## Purdue University's Gerhard Klimeck

Gordon Bell Finalist

Science Objectives and Impact

- **Model, understand, and design carrier flow in nano-scale semiconductor transistors. Identify next generation nano-transistor architectures while reducing power consumption and increasing manufacturability**

- **Demonstrate full atomistic quantum transport simulations. Coherent transport in a few minutes, scattering transport hours at the petascale**

Performance

- **Simulated two dissimilar realistic nanoelectronic devices,**
  - a high electron mobility transistor and
  - a band-to-band tunneling field-effect transistor

- **Sustained performance on Jaguar of up to 1.44 petaflops**

- **Time-to-simulation scales almost perfectly from 2,700 to 221,400 cores**

- **Team: Gerhard Klimeck and Mathieu Luisier (Purdue University), Timothy B. Boykin (University of Alabama–Huntsville), and Wolfgang Fichtner (ETH Zürich)**

(a) Single-gate and doublegate ultra-thin-body FET made of Si, Ge, or III-V semiconductors; (b) gateall-around nanowire FET; (c) graphene nanoribbon FET; and (d) coaxially gated carbon nanotube FET. Image courtesy Gerhard Klimeck, Purdue University.

2011 Gordon Bell Prize Finalist
- Performance of up to 1.44 PF using OMEN
- One of five codes with performance over one sustained petaflop on Jaguar

U.S. DEPARTMENT OF ENERGY | Office of Science

ESnet Headlines

- **October 13:** *Internet2, ESnet Complete First Transcontinental 100G Network Deployment* See Steve Cotter's talk Nov 2, 10:15 am
    - Connections are now operational between New York, Washington D.C., Cleveland, Chicago, Kansas City, Denver, Salt Lake City, and Sunnyvale spanning a distance nearly 4000 miles

- **October 25:** *ESnet, Orange Silicon Valley, and Bay Microsystems Demonstrate the World's First Long Distance 40Gbps RDMA Data Transfer*
    - RDMA, or Remote Direct Memory Access,
        - is an alternative model to TCP/IP for bulk data transfer
        - designed to significantly improve the utilization of available bandwidth resources and the processing efficiency of the end hosts
        - no need for any special network tuning
    - Experiment marks the first time that it has been demonstrated at 40 Gbps data rates over long-haul distances, in this case approximately 200 miles.
    - Demonstration showed that using RDMA moves data at up to 96 percent of the peak capacity of the network as opposed to other network technologies

ASCR At A Glance

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