Advanced Scientific Computing Research

http://www.science.doe.gov/ascr/

Academic Workshops for Under-represented Junior Faculty and Senior Graduate Students

February 25, 2011

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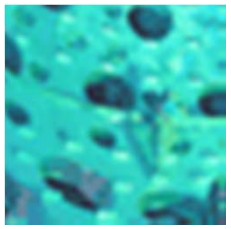
Advanced Scientific Computing Research
Office of Science, U.S. Department of Energy

Department of Energy (DOE)

- DOE is the single largest Federal government supporter of basic research in the physical sciences in the United States.
  - Fundamental research programs in basic energy sciences, biological and environmental sciences, computational science, and materials and chemical sciences.
  - Radio Isotopes program: the availability of an adequate supply of medical and research isotopes, which have become key agents in the diagnosis and effective treatment of various cancers, heart disease and other medical problems



- DOE sponsors research of thousands of PIs, post-doctoral and graduate students.
- DOE manages 24 research laboratories
- Programs:
  - Office of Science
  - ARPA-E
  - Energy Efficiency and Renewable Energy
  - Fossil Energy
  - More: http://www.energy.gov/organization/program_offices.htm

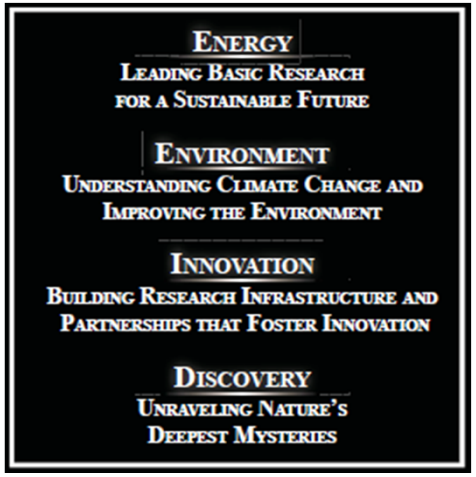
http://www.energy.gov/sciencetech/index.htm

DOE Office of Science

- The DOE Office of Science has delivered, for over sixty years, discoveries that transform our understanding of nature and advance our country's national, energy, and economic security.

- Program Offices:
- Advanced Scientific Computing Research (ASCR)
- Basic Energy Sciences (BES)
- Biological and Environmental Research (BER)
- Fusion Energy Sciences (FES)
- High Energy Physics (HEP)
- Nuclear Physics (NP)

- Today DOE Office of Science is pursuing the fundamental breakthroughs needed to create a sustainable energy economy for the 21st century.



Office of Science Workforce Development Program for Teachers and Scientists: Train the Next Generation of Scientists and Engineers

Source: http://www.sc.doe.gov/about/Trifold_2010_Final.pdf

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ASCR Mission

The mission of the Advanced Scientific Computing Research (ASCR) program is to

discover, develop, and deploy the computational and networking capabilities

that enable researchers to analyze, model, simulate, and predict complex phenomena important to the Department of Energy.

A particular challenge of the ASCR program is *fulfilling the science potential of emerging multi-core computing systems and other novel "extreme-scale" computing architectures,* which will require significant modifications to today's tools and techniques.

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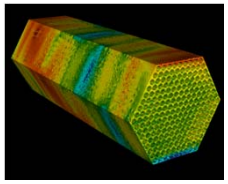
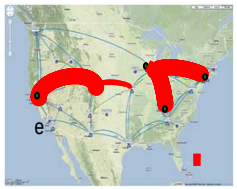
ASCR Programs

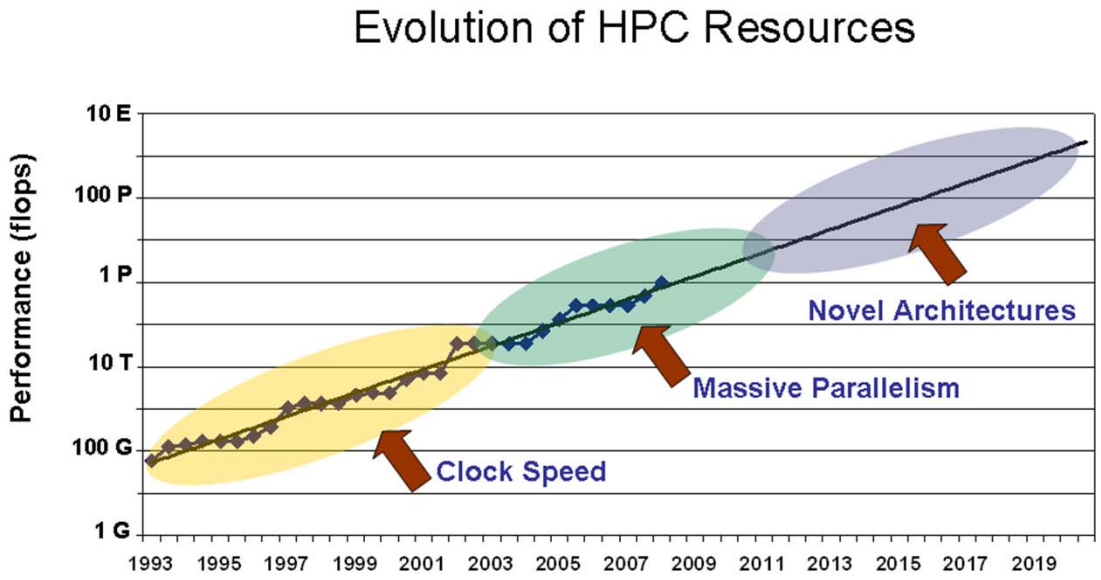
- Applied Math: development of mathematical descriptions, models, methods and algorithms to enable scientists to accurately describe and understand the behavior of complex systems involving processes that span vastly different time and/or length scales
- Computer Science: research that enables computing at extreme scales and the understanding of extreme scale data from both simulations and experiments, making scientific computers as easy and effective to use as possible.
  - Extreme scale: the use of Exascale (10^18 FLOPS) computing platforms that will operational in the 2018–2020 timeframe.
- SciDAC – Scientific Discovery Through Advanced Computing: advancing key areas of computational science and discovery that advance the mission of the Office of Science through mutually beneficial partnerships.
- Next Generation Networking: To develop networking and collaboration tools and facilities that enable scientists worldwide to work together.
- Facilities: delivering the forefront computational and networking capabilities, enabling world-class researchers to extend the frontiers of science.





Technology Challenges

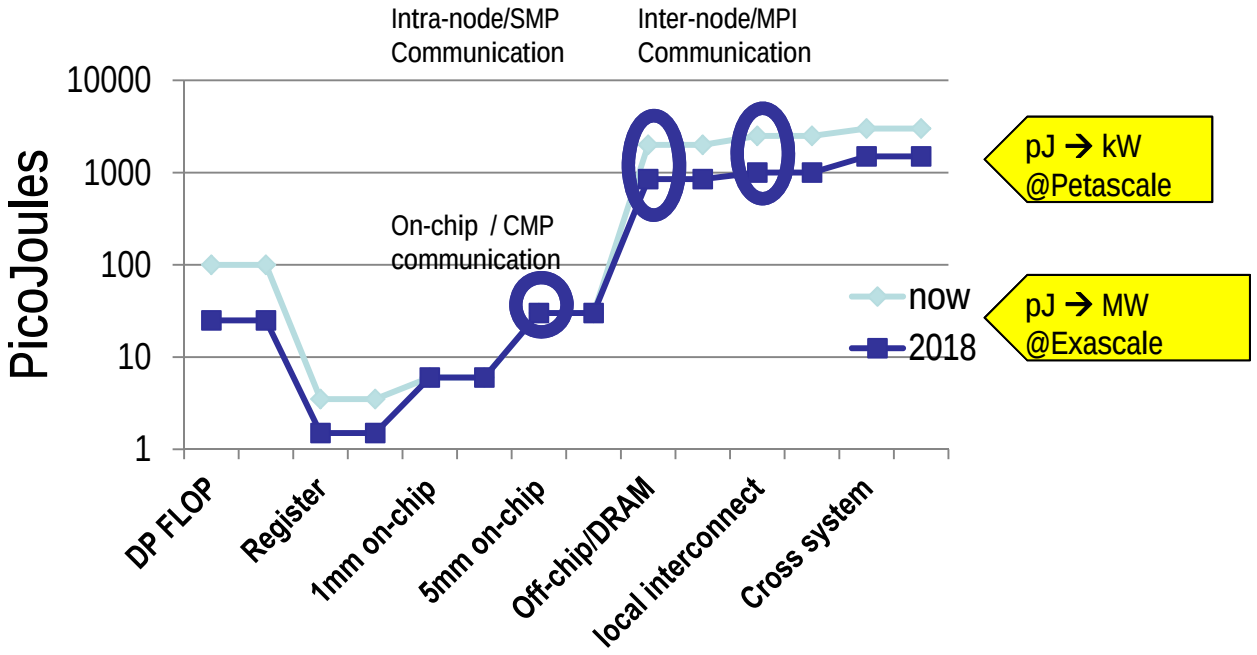
- Evolution of Computing Systems
  - Until early in this decade: increase clock speed
  - Most of this decade: massive parallelism ➔ Petaflops capability
  - For the 2012–2020 timeframe: novel architectures ➔ Exaflops capability



Computer Science at the Exascale

Exascale ≠ Petascale X 1000

- Traditionally, applications have expected 10x increase in resolution with each 1000x increase in compute capability, *but not this time:*
  - We won't have 1000x the memory available
  - The processors won't be 10x faster
  - Proportionally, we won't be able to move as much data on or off each processor
  - Introduction of massive parallelism at the node level is a significant new challenge
- However, Exascale computing is an opportunity for…
  - *More Fidelity:* Incorporate more physics instead of increased resolution
  - *Greater Understanding:* Develop uncertainty quantification (UQ) to establish confidence levels in computed results and deliver predictive science



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Technology Challenges

- What are the technology challenges:
  - Clock frequencies are expected to decrease to conserve power; as a result, the number of processing units on a single chip will have to increase;
  - The energy costs of moving data both on-chip and off-chip will become much more important;
  - Total concurrency in the applications will be on the order of ~1 billion;
  - Although the memory per flop may be acceptable, memory per processor will fall dramatically which will make current weak scaling approaches problematic;
  - For both power and performance reasons, locality of data and computation is much more important so flat cache hierarchies will no longer be helpful;
  - The failure rates for components and manufacturing variability make it unreasonable to assume the computer is deterministic. This is true for performance today and will affect the results of computations by 2018 due to silent errors.
  - Synchronization will be very expensive and the work required to manage synchronization will be high.
  - The I/O system at all levels – chip to memory, memory to I/O node, I/O node to disk—will be much harder to manage due to the relative speeds of the components.

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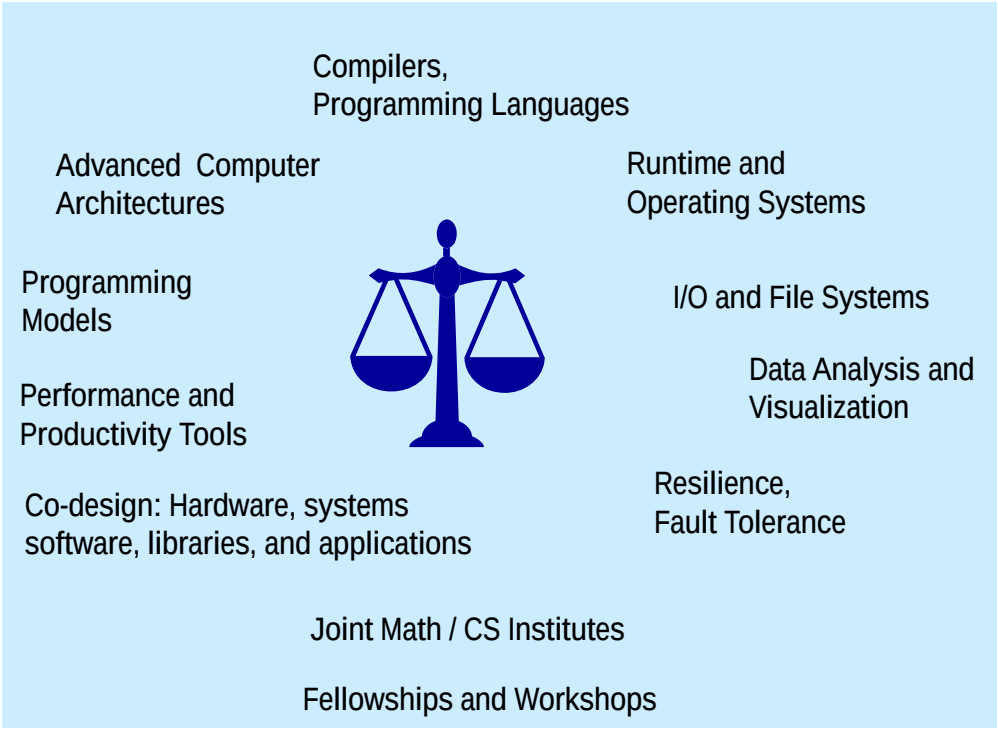
ASCR Priorities: CS

- Current CS research project areas:
  - advanced hardware and software architectures for Exascale computing systems;
  - hardware and software approaches to power/energy management for HPC systems;
  - scalable and fault tolerant operating and runtime systems, including file systems and input/output bottlenecks;
  - compilers, programming models, languages, and environments;
  - auto-tuning and performance modeling, monitoring, analysis, and optimization tools;
  - software development tools and methods;
  - scientific data management;
  - integration, analysis and visualization for petabyte to Exabyte data sets, both static and streaming, including in-situ methods.

Computer Science Research Portfolio



FY10 Funding Opportunity Announcements (FOAs)

- URL for all FOAs: http://www.science.doe.gov/ascr/Funding/Funding.html
- Computer Science
  - X-Stack Software Research -- $10M / year for 3 years to fund 11 awards, Closed April 2, 2010
    - Development of a scientific software stack that supports extreme scale scientific computing, from operating systems to development environments.
  - Advanced Architectures and Critical Technologies for Exascale Computing -- $5M / year for 3 years to fund 5 awards, Closed March 26, 2010
    - Design of energy-efficient, resilient hardware and software architectures and technology for high performance computing systems at exascale.
  - Scientific Data Management and Analysis at the Extreme Scale -- $5M / year for 3 years for 10 awards, Closed March 18, 2010
    - Management and analysis of extreme-scale scientific data in the context of petascale computers and/or exascale computers with heterogeneous multi-core architectures.

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Funding Announcements (Continued)

- Computational Partnerships FOA
  - Exascale Co-design Center -- $10M, Closed July 9, 2010
    - Engaging major ongoing R&D centers of computational science in the hardware, systems software, numeric methods, algorithms, and applications co-design process that will be responsible for making key tradeoffs in the design of exascale systems.
- Unsolicited Proposals
  - Annual Notice, FY10 closes September 30, 2011
    - Covers ASCR priority areas. See: http://www.science.doe.gov/grants/pdf/DE-FOA-0000178.pdf
- SciDAC – Scientific Discovery through Advanced Computing Institutes
  - Published 02/23/2011, closes May 2, 2011
  - http://science.doe.gov/grants/announcements.asp?stat=1

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Funding Announcements (Continued)

- Early career Research Program Funding Opportunity
  - FOA in 2010 issued July 1 and pre-application due August 13
  - PI must be an **untenured** Assistant Professor or an **untenured** Associate Professor on the tenure track at a U.S. academic institution.
  - No more than ten (10) years can have passed between the year the PI's Ph.D. was awarded and the year of the application.
  - Highly competitive
  - More details: http://www.science.doe.gov/SC-2/early_career.htm
- DOE's Computational Science Graduate Fellowship (CSGF)
  - U. S. citizens or permanent resident aliens pursuing a PhD in scientific or engineering disciplines with an emphasis in high-performance computing
  - Up to four years of support: tuition, fees and yearly stipend of $36,000
  - Academic allowance of $5,000 the first year and $1,000 in the remaining years for the professional development of the fellow
  - 12 week research experience at a DOE Lab.
  - This year deadline for submission was January 11, 2011
  - Also very competitive
  - Check http://www.krellinst.org/csgf/ (for announcements, workshops, annual conferences).

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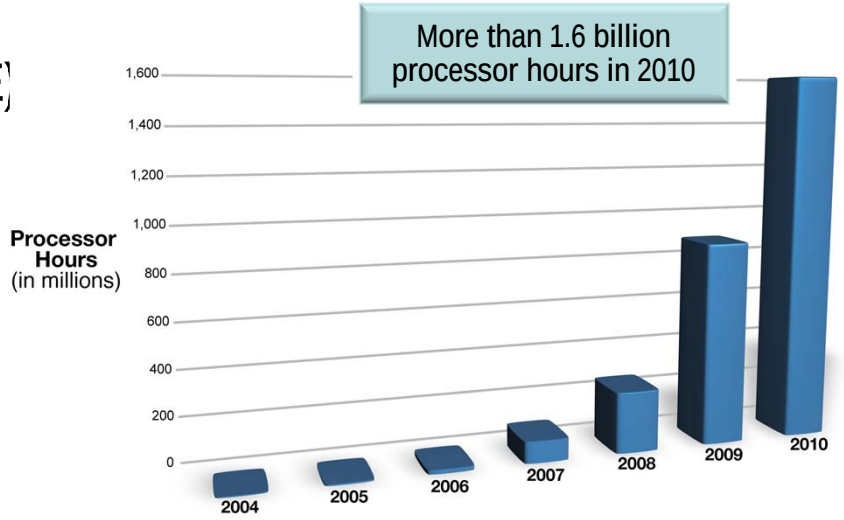
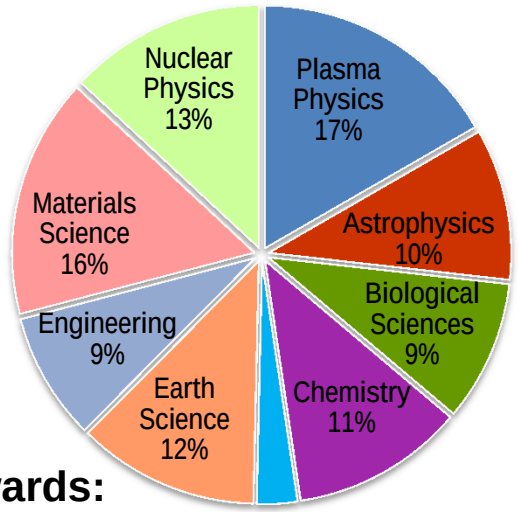
ASCR Facilities Allocation

- Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program started in 2004.
  - Provides Office of Science computing resources to a
    - computationally intensive research
    - high-impact scientific advances
  - Open to national and international researchers, including industry
  - No requirement of DOE or Office of Science funding or topic area
  - Peer and computational reviews

- http://www.sc.doe.gov/ascr/INCITE/index.html





INCITE 2010 awards: 35 new projects and 34 renewal projects

ASCR Facilities Allocation

- ERCAP (Energy Research Computing Allocations Process): Researchers working on SC relevant projects may request allocations of resources at NERSC via a NERSC call for proposals issued annually in August and closed in October for allocations that begin the following January. http://www.nersc.gov/nusers/accounts/allocations/ercap/
- ALCC (ASCR Leadership Computing Challenge) Open to academia and industry for special situations of interest to the Department with emphasis on high-risk, high-payoff simulations in areas directly related to the Department's energy mission, for national emergencies, or for broadening the community of researchers capable of using leadership computing resources. http://www.sc.doe.gov/ascr/Facilities/ALCC.html

Hopper, a Cray XE6 system at NERSC, is the fifth most powerful machine on the list of Top 500 supercomputers in the world

ALCC program allocates up to 30% of the computational resources at NERSC and the Leadership Computing Facilities at Argonne and Oak Ridge

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Getting to Know ASCR

- Serve as a peer reviewer
- Attend workshops, meetings, and conferences on the key areas of interest to ASCR
  - ➔input (e.g., reports) from the broad community is very important to the Office of Science and ASCR
- Track funding opportunities:
  - ASCR Funding Opportunities: http://science.doe.gov/ascr/Funding/Funding.html
- Track publications:
    - SciDAC Review: http://www.scidacreview.org/1002/index.html
    - ASCR Discovery Magazine: http://ascr-discovery.science.doe.gov/index.shtml
    - ASCR Workshops and Conferences: http://science.doe.gov/ascr/WorkshopsConferences/WorkshopsConferences.html
    - Other ASCR news and reports: http://science.doe.gov/ascr/Accomp/Accomplishments.html

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Increasing Awareness

- Check the reports from the quarterly Advanced Scientific Computing Advisory Committee (ASCAC) meetings: http://www.science.doe.gov/ascr/ASCAC/Reports.html
- Understand the Office of Science mission and its computational programs
  - http://www.scidac.gov/
  - Understand the needs of DOE mission-based scientific applications
  - Reach out to the ASCR-funded CS, Applied Math, and SciDAC teams at Labs and Universities, as their research currently addresses scientific applications needs
- Arrange to make presentations at DOE Laboratories and at the ASCR office
  - So that you may be able to start a fruitful collaboration with DOE researchers, and/or get feedback from program managers
- Communicate with the program managers before applying
  - Sending white papers and discussing ideas with program managers
  - (Be persistent, as Dilma said, we have too many emails, it is easy to miss yours: resend, call, resend and call again, until we respond)

Thank You!

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http://www.science.doe.gov/ascr/index.html

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Backup

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Exascale Co-design Centers

- Collaboration among DOE Labs, Universities, and Industry
- Mission-oriented funding: scientific applications matter!