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Advanced Scientific Computing Research Program

ASCR
Facilities Update

Vince Dattoria
October 29, 2008

Outline

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- National Energy Research Scientific Computing Center (NERSC)
- Rationale for Leadership Computing
- Argonne Leadership Computing Facility (ALCF)
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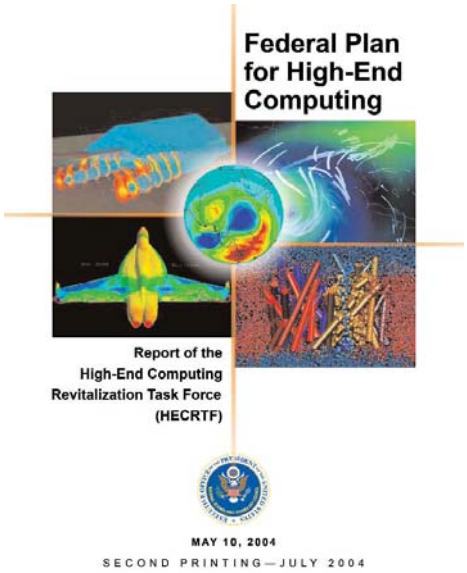
ASCR Facilities Strategy

Advanced Scientific Computing Research Program

- Providing the Tools – High-End Computing
  - High-Performance Production Computing - National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory
    - Delivers high-end capacity computing to entire DOE SC research community
  - Leadership-Class Computing – Leadership Computing Centers at Argonne National Laboratory and Oak Ridge National Laboratory
    - Delivers highest computational capability to national and international researchers through peer-reviewed **Innovative and Novel Computational Impact on Theory and Computation (INCITE)** program (80% of resources)
- Investing in the Future - Research and Evaluation Prototypes
- Linking it all together – Energy Sciences Network (ESnet)



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National Energy Research Scientific Computing Center (NERSC)

Advanced Scientific Computing Research Program

- Located at Lawrence Berkeley National Lab
- Cray XT-4 Franklin: 102 Tflop/s, 9,660 nodes, 19,320 cores
- IBM Power 5 Bassi: 6.7 Tflop/s, 888 cores
- Linux Opteron Cluster Jacquard: 3.1 Tflop/s, 712 cores
- PDSF Linux Cluster (HEP/NP): ~1K cores
- PART metric: 40% of computing time used by computations that require at least 1/8 (4,830) of the total resource
- Franklin quad-core upgrade: 350 Tflop/s, 38,640 cores in November
- NERSC-6 Project
  - RFP issued in September 2008
  - Proposals are being reviewed

Franklin

Bassi and Jacquard

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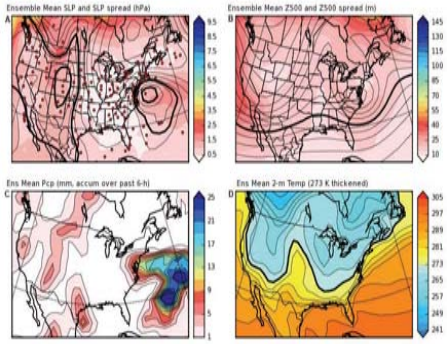
NERSC Scientific Discovery

Advanced Scientific Computing Research Program

Validating Climate Models



INCITE Award for "20th Century Reanalysis" using an Ensemble Kalman filter to fill in missing climate data since 1892

PI: Compo, U. Boulder

Reproduced 1922 Knickerbocker storm. Data can be used to validate climate and weather models

Simulation of a Low Swirl Burner Fueled with Hydrogen

Numerical simulation of flame surface of an ultra-lean premixed hydrogen flame in a laboratory-scale low-swirl burner. Burner is being developed for fuel-flexible, near-zero-emission gas turbines.

PI: Bell, LBNL

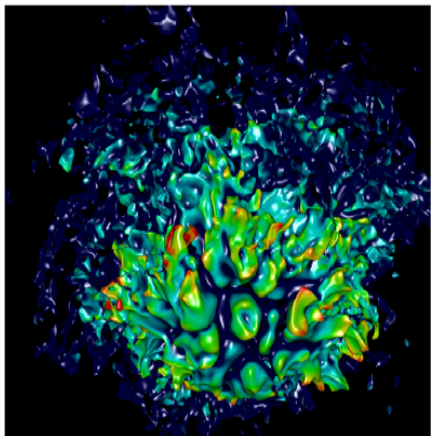
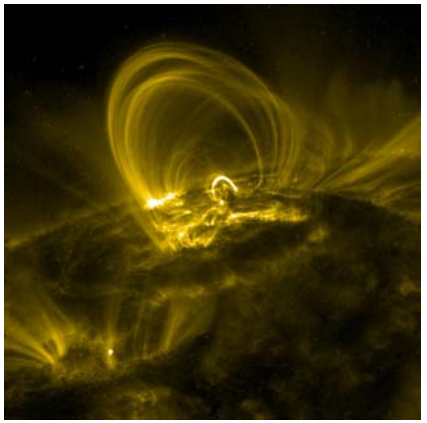


Image illustrates the cellular burning structures in hydrogen flames

AstroGK - Gyrokinetic Code for Astrophysical Plasmas

Calculation, running on 16K cores, shows how magnetic turbulence leads to particle heating.

PIs: Dorland (U. of Maryland), Howes, Tatsuno

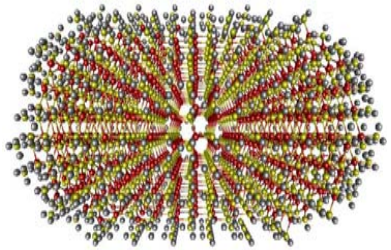


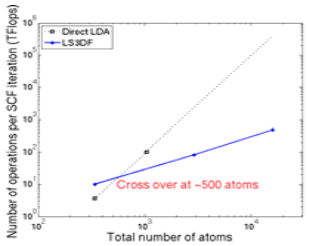
Nanoscience Calculations and Scalable Algorithms

Linear Scaling 3D Fragment (LS3DF). Density Functional Theory (DFT) calculation numerically equivalent to more common algorithm, but scales with O(n) in number of atoms rather than $O(n^3)$

PI: Wang, LBNL

Took 30 hours vs. months for $O(n^3)$ algorithm





Rationale for Leadership Computing

DOE High-End Computing Revitalization Act of 2004

The Secretary (through the Director of the Office of Science) shall

- Carry out a program of research and development (including development of software and hardware) to advance high-end computing systems
- Develop and deploy high-end computing systems for advanced scientific and engineering applications
- Establish and operate 1 or more Leadership facilities
  - Provide Leadership Systems, on a competitive, merit-reviewed basis, access to researchers in United States industry, institutions of higher education, national laboratories and other Federal agencies.
- Establish at least 1 Software Development Center (SciDAC institutes)

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Argonne Leadership Computing Facility (ALCF)

Advanced Scientific Computing Research Program

- Argonne LCF
  - 111 peak teraflop IBM Blue Gene/P with 8,192 quad-core compute nodes (32,768 processors) and 16 terabytes of memory began operations April 1, 2008
  - **IBM Blue Gene/P upgrade *accepted in March, 2008 and in transition to operations* will result in a 556 peak teraflop leadership-class computing resource with 40,960 quad-core compute nodes and 80 terabytes**

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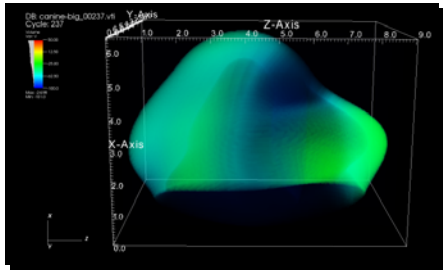
ALCF Scientific Discovery

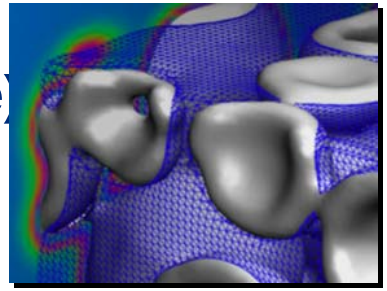
Advanced Scientific Computing Research Program

Cardiac Simulation

Study wave break and the onset of cardiac arrhythmia



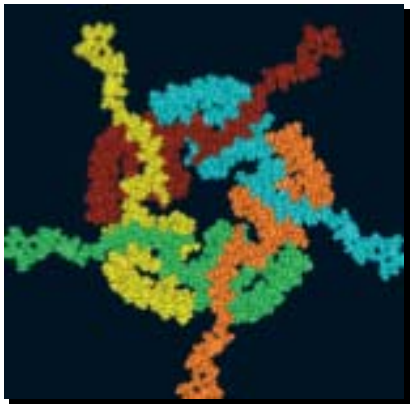
Bubble Formation (Procter & Gamble)



Improved understanding of foams and surfactants that can lead to better, safer products

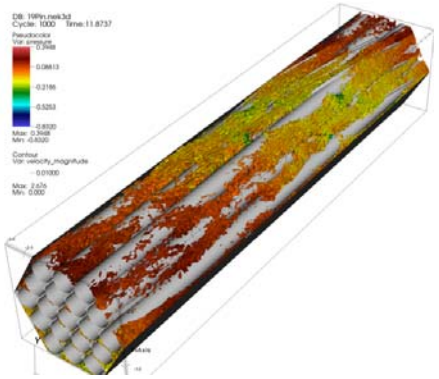
Parkinson's Disease

Provided new insights into the molecular mechanism for Parkinson's disease & its progression



Fission Reactor Design

New understanding of the effects of pin counts on reactor designs



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Oak Ridge Leadership Computing Facilities (OLCF)

Advanced Scientific Computing Research Program

- LCF at Oak Ridge
  - 263 teraflop Cray XT4 (Jaguar) with 7,832 quad core 2.1 GHz AMD Opteron compute nodes, 62 terabytes aggregate memory
  - *18.5 teraflop Cray X1E (Phoenix) with 1,024 multi-streaming vector processors (to be retired, October, 2008)*
  - **Delivery of 1 Petaflop Cray Baker (Jaguar upgrade) complete with acceptance expected by Dec, 2008**

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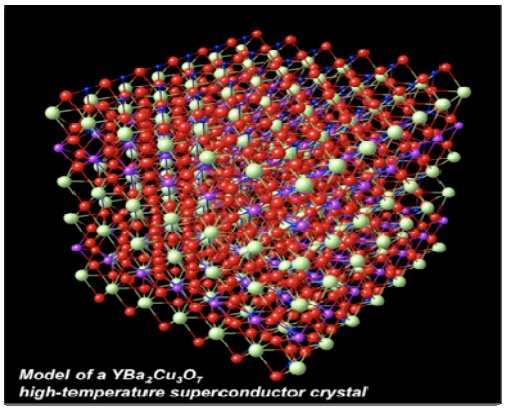
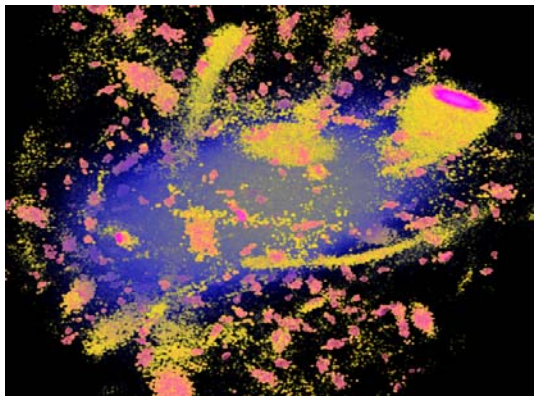
OLCF Scientific Discovery

Advanced Scientific Computing Research Program



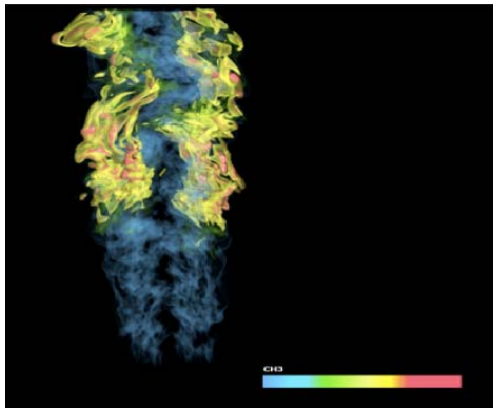
Electron pairing in HTC cuprates*

The 2D Hubbard model emits a superconducting state for cuprates & exhibits an electron pairing mechanism most likely caused by spin-fluctuation exchange. *PRL* (2007, 2008)



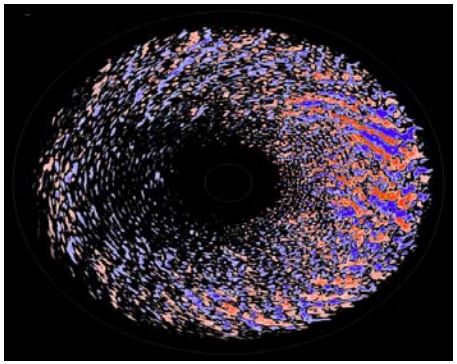
Shining the light on dark matter*

A glimpse into the invisible world of dark matter, finding that dark matter evolving in a galaxy such as our Milky Way remains identifiable and clumpy. Aug 7, 2008 issue of *Nature*



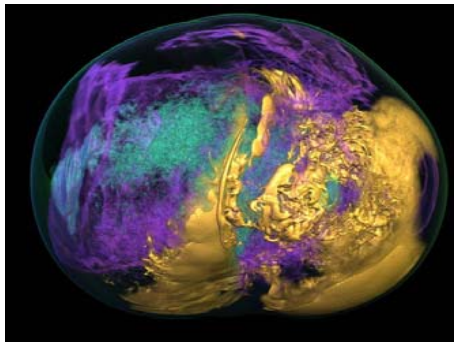
Stabilizing a lifted flame*

Elucidated the mechanisms that allow a flame to burn stably above burners, namely increasing the fuel or surrounding air co-flow velocity *Combustion and Flame(2008)*



Taming turbulent heat loss in fusion reactors*

Advanced understanding of energy loss in tokamak fusion reactor plasmas,. *PRL*(vol 99) and *Physics of Plasmas* (vol 14)



How does a pulsar get its spin?*

Discovered the first plausible mechanism for a pulsar's spin that fit observations, namely the shock wave created when the star's massive iron core collapses. Jan 4, 2007 issue of *Nature*

***on ASCR's 2008 Top 10 Scientific Breakthroughs list**
http://www.science.doe.gov/ascr/ProgramDocuments/Docs/Breakthroughs_2008.pdf

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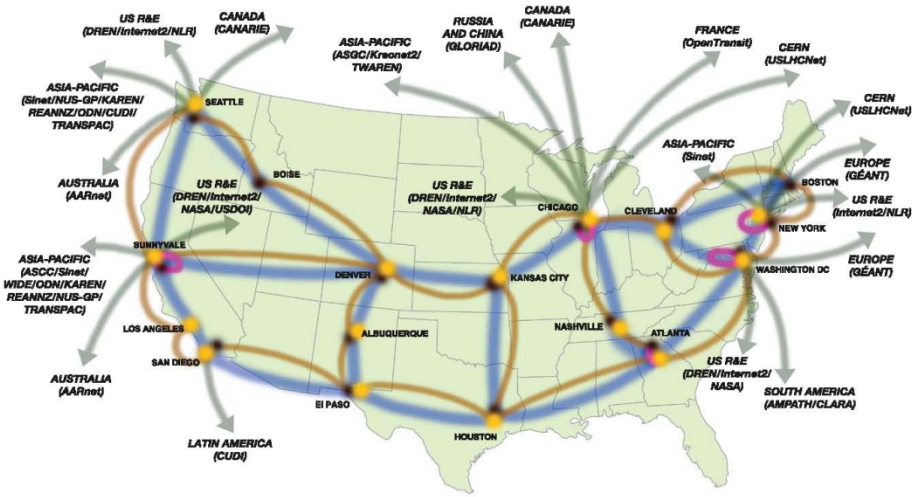
Energy Sciences Network (ESnet)

Advanced Scientific Computing Research Program

- Steve Cotter new head of ESnet
- Close collaboration between ASCR network research and ESnet technology
- ESnet 4 build-out nearing completion (Dec 08)
  - Approx 68k miles of 10G waves
  - Science Data Network (SDN)): 16 of 17 nodes deployed, enabling virtual circuits for high-speed data transfers
  - MANs upgraded prior to LHC coming back on line
- LHC first particle beams Sep 08
  - Largest computer grid in the world
- Extensive international connectivity / collaborations



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2008 Operational Assessments Review

Advanced Scientific Computing Research Program

- August 19-20 operational assessments were performed for: ALCF (ANL), ESnet (LBNL), NERSC (LBNL), OLCF (ORNL) and MSCF (EMSL/PNNL)
- Purpose: Review facility performance and plans for operational phase (as opposed to upgrade projects)
- Reviewers
  - Roy Whitney (JLab) Chair
  - Brad Comes (HPCMO/DoD)
  - Stephane Ethier (PPPL)
  - Lynn Rippe (LBNL)
  - William Turnbull (NOAA)
  - Vicky White (FNAL)
- Positive reviews of Facilities

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“Best Practices” Workshop Series

Advanced Scientific Computing Research Program

- 2008 Workshop focused on Risk Management Techniques and Practices for High-Performance Computing Centers
- Purpose: To assess current and emerging techniques, practices, and lessons learned for effectively identifying, understanding, managing, and mitigating risks associated with acquiring leading-edge computing systems at high-performance computing centers (HPCCs).
- About 70 participants (labs, other agencies, vendors)
- Jointly sponsored by SC and NNSA, hosted by LLNL
- Held September 17-18 in SF (Hotel Nikko)
- Report due in November 2008
- SC08 BOF on Workshop Series Nov. 20, 2008.

Charge Questions & Comments

1. Are the processes for supporting the customers, resolving problems, and communicating with key stakeholders effective?
   - Yes, all of the facilities are very customer focused.
2. Are the facilities maximizing resources consistent with its mission?
   - Yes, the facilities demonstrated that they are aggressive in achieving uptime goals.
   - For DOE
     - SC/ASCR should be very cautious with any increase in the number of INCITE awards as this may negatively impact achieving Leadership science.
     - MTTI and MTTF needs to be consistently defined across all centers.
3. Are the facilities meeting the Department of Energy strategic goal 3.1/3.2?
   - Yes, the facilities are clearly focused on achieving science missions and/or providing resources critical for successfully achieving science.

Charge Questions & Comments

4. Are the costs for the upcoming year reasonable to achieve the needed performance?
   - Yes, all of the facilities demonstrated that they had effective budget plans and understanding of costs for successfully delivering their operations.
5. What innovations have been implemented that have improved the facilities operations?
   - Innovations have been widely shared and most facilities demonstrated how they are both suppliers and consumers of innovations for and from both DOE and non-DOE facilities.
6. Are the facilities effectively managing risk?
   - Yes with a few concerns, the common one being continuity of funding.
7. Do the facilities have a valid [cyber security] authorities to operate?
   - Yes, all of the facilities have valid authorities to operate.