

12th DOE ACTS Collection Workshop
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Welcome Remarks

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The US Department of Energy (DOE)

- Mission: ensure America's security and prosperity by addressing its energy, environmental and nuclear challenges through transformative science and technology solutions
- National Laboratories
 - Ames Laboratory
 - Argonne National Laboratory
 - Brookhaven National Laboratory
 - Fermi National Accelerator Laboratory
 - Idaho National Laboratory
 - Lawrence Berkeley National Laboratory
 - Lawrence Livermore National Laboratory
 - Los Alamos National Laboratory
 - National Energy Technology Laboratory
 - National Renewable Energy Laboratory
 - Oak Ridge National Laboratory
 - Pacific Northwest National Laboratory
 - Princeton Plasma Physics Laboratory
 - Sandia National Laboratory
 - Savannah River National Laboratory
 - SLAC National Accelerator Laboratory
 - Thomas Jefferson National Accelerator Facility

DOE's Advanced Scientific Computing Research Program

<http://science.energy.gov/ascr>

- Research Division

- Computer Science: innovative advancement in computer performance and computational science techniques
- Applied Mathematics: mathematical and computational research that facilitates the use of the latest high-performance computer systems in advancing our understanding of science and technology
- Next Generation Network for Science: research and development activities to support distributed high-end science in the Office of Science
- Scientific Discovery through Advanced Computing Program (SciDAC): accelerate progress in scientific computing that delivers breakthrough scientific results through partnerships comprised of applied mathematicians, computer scientists, and scientists from other disciplines

- Facilities Division

- Oak Ridge Leadership Computing Facility
- Argonne Leadership Computing Facility
- National Energy Research Scientific Computing Center (NERSC)

Delivering the Science



Scientific Discovery and the Role of High End Computing

<http://science.energy.gov/ascr/news-and-resources/program-documents>



Lawrence Berkeley National Laboratory

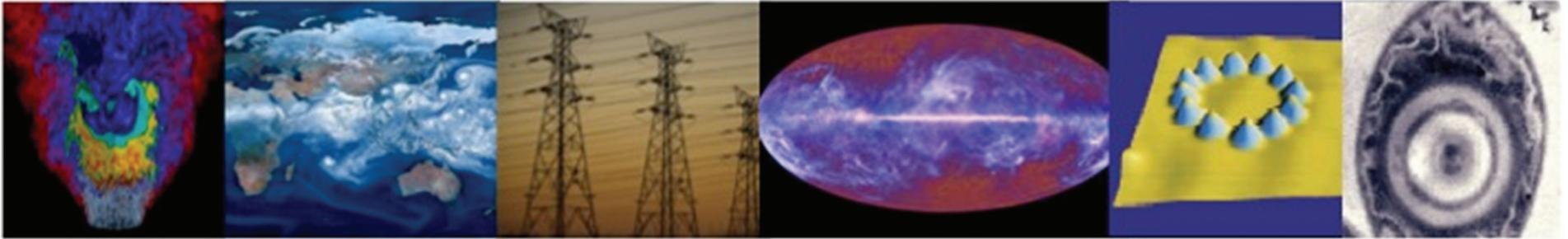
<http://www.lbl.gov>

- Areas of research
 - renewable energy sources such as biofuels and artificial photosynthesis
 - energy efficiency at home, at work, and around the world
 - ability to observe, probe, and assemble materials atom by atom
 - climate change research, environmental science, and the growing connections between them
 - chemistry and physics of matter and force in the universe –from the infinite to the infinitesimal
 - computational science and advanced networking to enable discovery and remote collaborations
 - biological sciences for human health and energy research
- National user facilities
 - Advanced Light Source
 - Energy Sciences Network
 - Joint Genome Institute
 - Molecular Foundry
 - National Center for Electron Microscopy
 - National Energy Research Scientific Computing Center



Computational Research Division

Computational Science



Combustion

Climate

Energy &
Environment

Cosmology &
Astrophysics

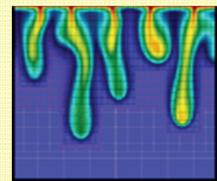
Nanoscience

Genomics

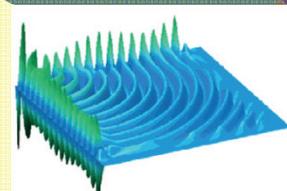
Applied Mathematics



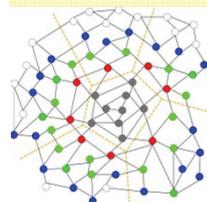
Mathematical
Models



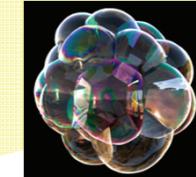
Adaptive Mesh
Refinement



Libraries and
Frameworks

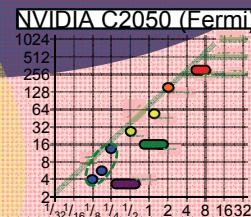


Linear
Algebra



Interface
Methods

Computer Science



Performance
& Autotuning



HPC architecture,
OS, and compilers



Cloud, grid &
distributed
computing



Visualization
and Data
Management

NERSC Systems

Large-Scale Computing Systems

Franklin (NERSC-5): Cray XT4

- 9,532 compute nodes; 38,128 cores
- ~25 Tflop/s on applications; 356 Tflop/s peak



Hopper (NERSC-6): Cray XE6

- 6,384 compute nodes, 153,216 cores
- 120 Tflop/s on applications; 1.3 Pflop/s peak

Clusters

140 Tflops total



Carver

- IBM iDataplex cluster

PDSF (HEP/NP)

- ~1K core cluster

Magellan Cloud testbed

- IBM iDataplex cluster

GenePool (JGI)

- ~5K core cluster

NERSC Global

Filesystem (NGF)



Uses IBM's GPFS

- 1.5 PB capacity
- 5.5 GB/s of bandwidth

HPSS Archival Storage



- 40 PB capacity

- 4 Tape libraries

- 150 TB disk cache

Analytics

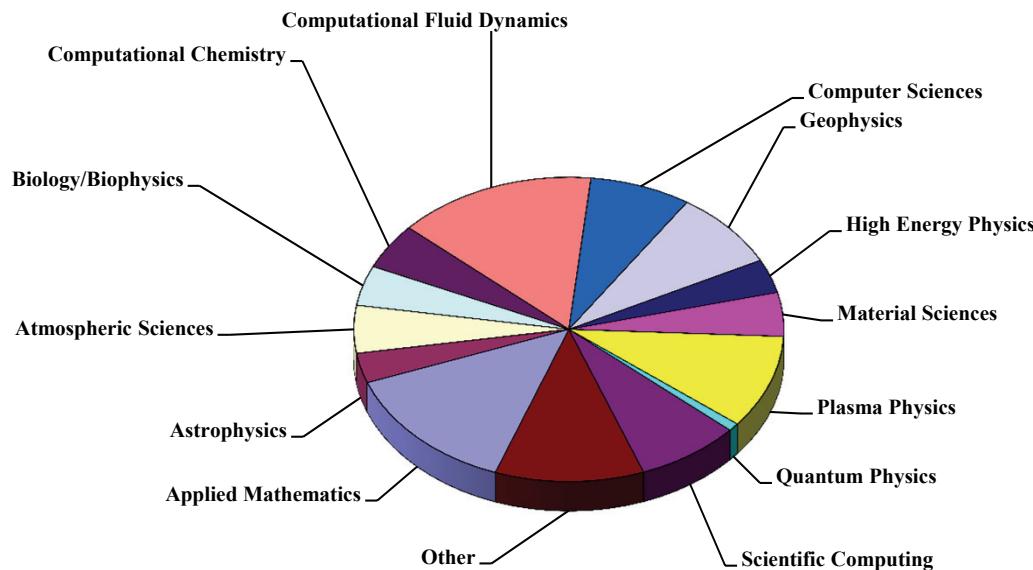


Euclid

(512 GB shared memory)

Dirac GPU testbed (48 nodes)

ACTS Workshop Participants



- fast-track the development of efficient, high-performance applications
- workshop participants are exposed to software technologies that may not be part of regular syllabuses
- workshop participants have an opportunity to engage with tool developers and eventually add functionality to the tools