

**13<sup>th</sup> DOE ACTS Collection Workshop**  
**August 14-17, 2012**

# Welcome Remarks

Osni Marques  
Lawrence Berkeley National Laboratory  
*OAMarques@lbl.gov*

# 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>



# Computational Research Division

## Computational Science



Combustion

Climate

Energy &  
Environment

Cosmology &  
Astrophysics

Nanoscience

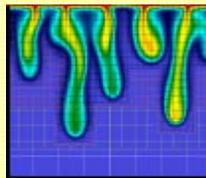
Genomics

### Applied Mathematics

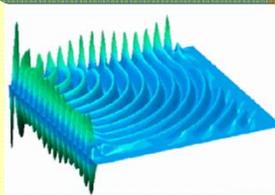
### Computer Science



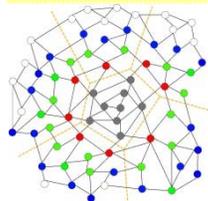
Mathematical Models



Adaptive Mesh Refinement

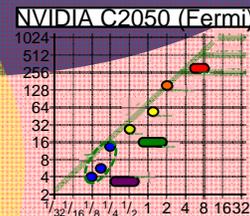


Libraries and Frameworks



Linear Algebra

Interface Methods



Performance & Autotuning

Cloud, grid & distributed computing



HPC architecture, OS, and compilers



Visualization and Data Management



# National Energy Research Scientific Computing Center (NERSC)

## Large-Scale Computing Systems

### Hopper (NERSC-6): Cray XE6

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



### Midrange

140 Tflops total



#### Carver

- IBM iDataplex cluster
- 9884 cores; 106TF

#### PDSF (HEP/NP)

- ~1K core cluster

#### GenePool (JGI)

- ~5K core cluster
- 2.1 PB Isilon File System

### NERSC Global Filesystem (NGF)

Uses IBM's GPFS

- 8.5 PB capacity
- 15GB/s of bandwidth



### HPSS Archival Storage

- 240 PB capacity
- 5 Tape libraries
- 200 TB disk cache



### Analytics & Testbeds



#### Euclid

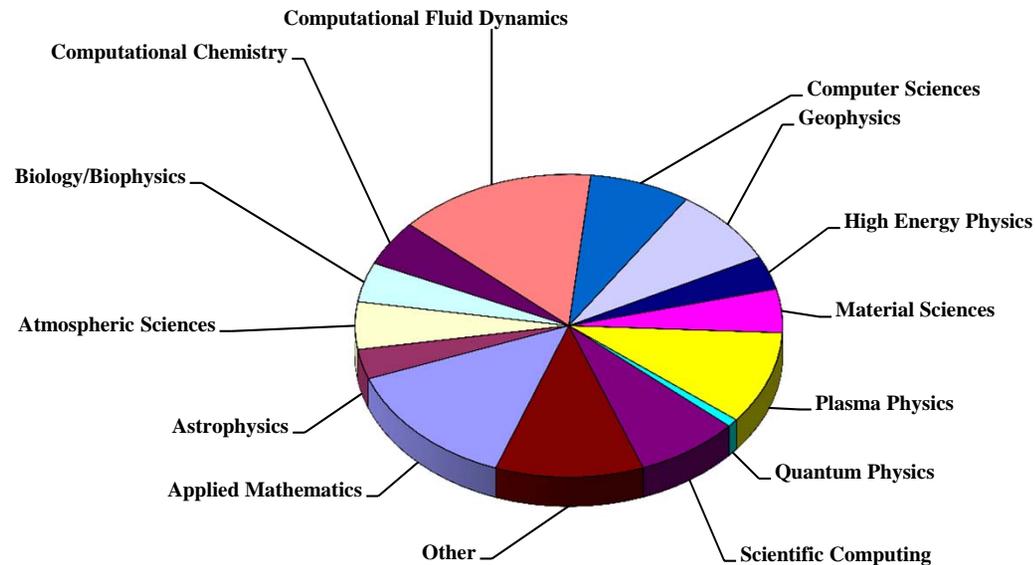
(512 GB shared memory)

**Dirac** 48 Fermi GPU nodes

**Magellan** Hadoop

# 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

<http://acts.nersc.gov/events/Workshop2012/surveyform.html>

August 2011 ACTS Workshop Short Survey - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://acts.nersc.gov/events/Workshop2011/surveyform.html

August 2011 ACTS Workshop Short Survey



[Tools](#)  
[News](#)  
[Project](#)  
[Home](#)

## The DOE ACTS Collection Workshop

### Short Survey

#### General Information

Name (optional):	<input type="text"/>
Field of research/work/study:	<input type="text"/>
High performance computers you have used (other than carver and magellan during the hands-on sessions):	<input type="text"/>

#### About The DOE ACTS Collection

Please list the ACTS tools that you are currently using (if any).

Please list the applications in which you are using ACTS tools (if any).

If you think that some of the ACTS tools presented in this workshop could be used in your application, please list them.

If you think that there are computational features (numerical, computational infrastructure, etc) that are not currently supported by ACTS but that could be useful in your research, please list them.

Secure Search McAfee

# Who uses HPC?

---

courtesy of Richard Gerber (<http://www.nersc.gov/about/nersc-staff/user-services-group/richard-gerber>)

- Scientists and engineers
  - climate prediction
  - protein folding simulations
  - oil and gas discovery
  - defense and aerospace work
  - automotive design
  - financial forecasting
  - ⋮
- Corporations
  - customer records
  - inventory management
  - employee details
  - ⋮

# Why Use Supercomputing?

courtesy of Richard Gerber (<http://www.nersc.gov/about/nersc-staff/user-services-group/richard-gerber>)

Length (m)	Phenomena
$10^{-18}$ - $10^{-15}$	quarks, strings
$10^{-15}$ - $10^{-12}$	proton, neutron
$10^{-12}$ - $10^{-9}$	gamma rays, X rays, hydrogen atom
$10^{-9}$ - $10^{-6}$	DNA, virus, optical light
$10^{-6}$ - $10^{-3}$	bacteria, fog, human hair
$10^{-3}$ - $10^0$	mosquito, golf ball, football
$10^0$ - $10^3$	people, football field, Eiffel tower
$10^3$ - $10^6$	Mt. Everest, Panama Canal, asteroid
$10^6$ - $10^9$	Moon, Earth, light-second
$10^9$ - $10^{12}$	Sun, light-minute, Earth's orbit
$10^{12}$ - $10^{15}$	Solar System
$10^{15}$ - $10^{18}$	light-year, nearest star
$10^{18}$ - $10^{21}$	galactic arm
$10^{21}$ - $10^{24}$	Milky Way, distance to Andromeda galaxy
$10^{24}$ - $10^{26}$	visible universe

Direct Human Experience

# Why Use Supercomputing?

courtesy of Richard Gerber (<http://www.nersc.gov/about/nersc-staff/user-services-group/richard-gerber>)

Time Scale (s)	Phenomena
$10^{-44}$	Planck time
$10^{-24}$	light crosses nucleus
$10^{-15}$	atomic vibration, visible light
$10^{-12}$	IBM SiGe transistor
$10^{-9}$	1 Gz CPU
$10^{-6}$	protein folding, lightning bolt
$10^{-3}$	hard disk seek time, blink of an eye
$10^0$	earthquakes
$10^2$	tornadoes
$10^5$	hurricanes
$10^7$	year
$10^9$	human life span
$10^{10}$	deep ocean mixing time
$10^{12}$	first homo sapiens
$10^{15}$	Milky Way rotation period
$10^{17}$	age of universe

Direct Human Experience