
# U.S. Department of Energy's Office of Science

**Advanced Scientific Computing Research Program**

# ASCR High Performance Computing Facilities and Testbeds

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**301-903-3127**

# Presentation Overview

- **Review of ASCAC Facilities Report, April 2004**
- **Facilities Portfolio**
  - NERSC
  - Leadership Computing Facilities
  - Research and Evaluation Testbeds
- **Discussion of Facilities Report Recommendations**
  - Funding
  - Allocations
  - Performance Metrics

# ASCAC Facilities Report
## April 2004



- **Conclusions**
  - Current Office of Science high-end computer and networking facilities are among the best in the world
  - Current and expected near-term Office of Science high-end computing resources are far from adequate to meet the anticipated needs of its science and engineering missions and associated scientific communities.
- **Recommendations**
  - Investment decisions in high-end computing should be guided by the science drivers
  - Over a three-year time frame, substantial investments are required to begin to return the United States to leadership in high-end computing.
  - The Office of Science should manage its advanced computing resources as a single, coordinated facility

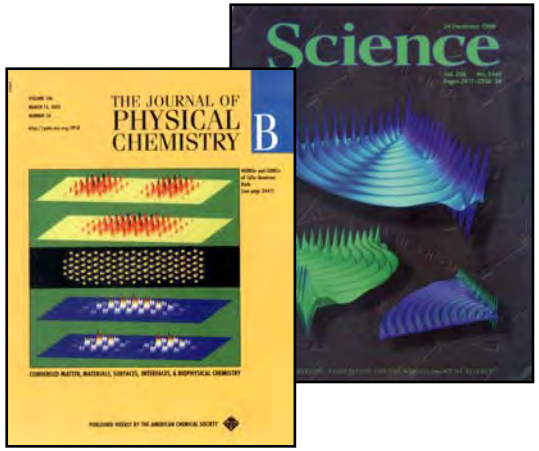
# Current Facilities Portfolio

- **High Performance Production Computing Facility (NERSC)**
  - Delivers high-end capacity computing to entire DOE SC research community
  - Large number of projects (200 – 300)
  - Medium- to very-large-scale projects that occasionally need a very high capability
  - Annual allocations
- **Leadership Computing Facilities**
  - Delivers highest computational capability
  - Small number of projects (10 – 20)
  - Multiple year allocations

# NERSC Scientific Impact

Advanced Scientific Computing Research Program

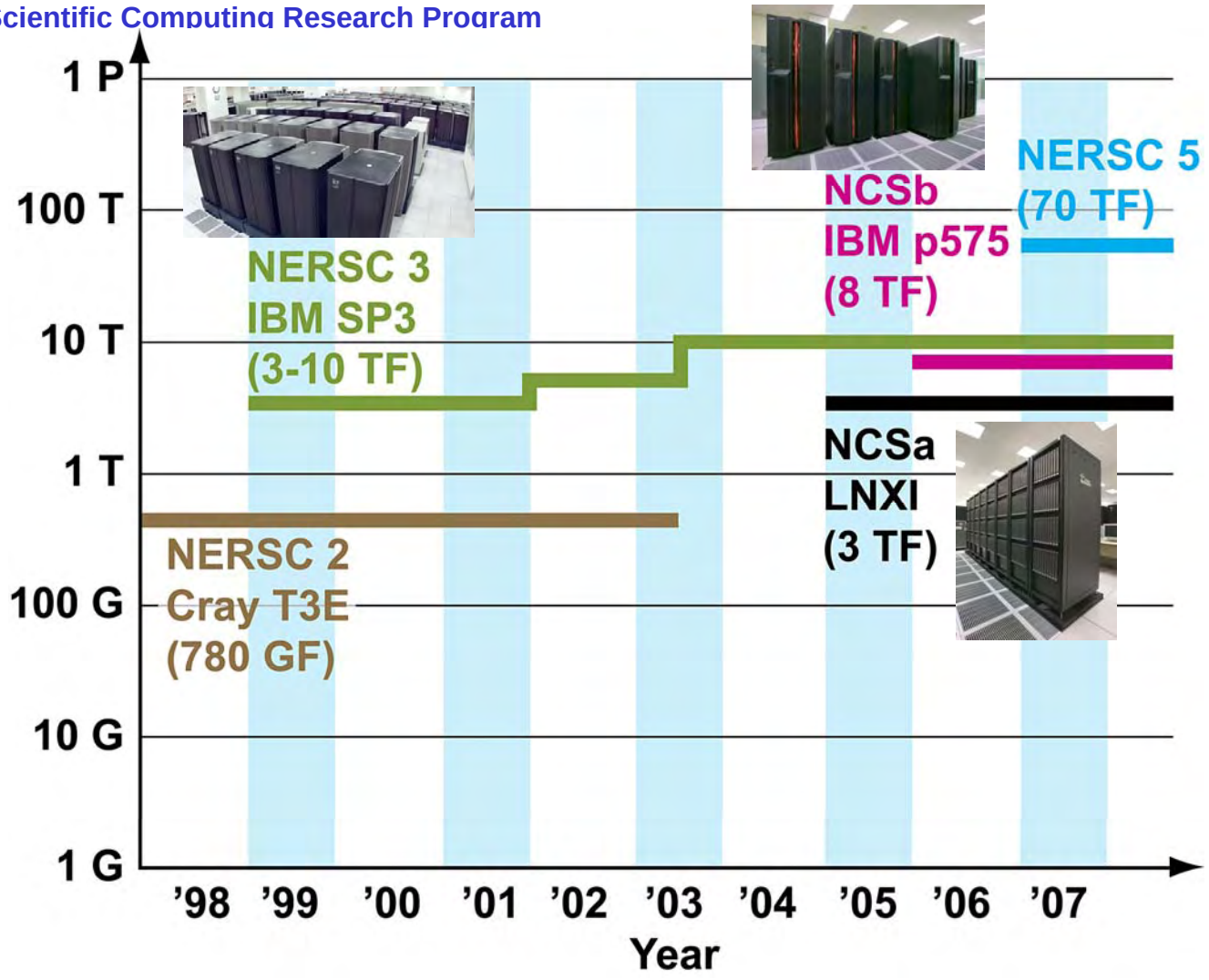

**The mission of the National Energy Research Scientific Computing Center (NERSC) is to accelerate the pace of scientific discovery by providing high performance computing, information, data, and communications services for research sponsored by the DOE Office of Science (SC).**




**In 2005, NERSC users reported the publication of more than 1200 papers that were based wholly or partly on work done at NERSC.**

# NERSC Facilities

Advanced Scientific Computing Research Program



# NERSC-5

- **Acquisition of NERSC-5 to alleviate the current backlog of meritorious requests for high-performance production computing resources**
  - 100-150 Teraflops peak performance
  - 7.5 to 10 Sustained Teraflop/s averaged over 3 years
  - RFP completed
  - Delivery scheduled for FY 2007

# Leadership Class Computing Facilities (LCF)




- **November, 2003**: Then Secretary Abraham announces 20 Year Science Facility plan: #2 Near Term Priority – UltraScale Scientific Computing Capability
- **February, 2004:** DOE Office of Science issued to SC laboratories a call for proposals to provide Leadership Class Computing Capability for Science with funding profile of $25M/year for five years in February, 2004.
- **May 12, 2004:** Following a peer review, then Secretary Abraham announces the establishment the Leadership Computing Facility at Oak Ridge National Laboratory in Tennessee

U.S. Department of Energy

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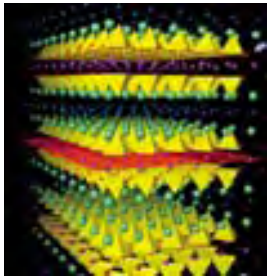
# LCF Resources

**Advanced Scientific Computing Research Program**

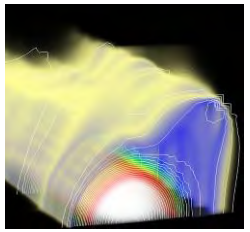

**18.5 Teraflop Cray X1E (Phoenix)**

**25 Teraflop Cray XT3 (Jaguar)**

Results from Early Users



**Resolving Material Disputes**
A recent *Nature Materials* article used the results from simulations on Jaguar to resolve long-standing discrepancies between phenomenological models, widely used to describe properties of new semiconductor materials, and first-principles electronic structure descriptions of magnetic semiconductors.



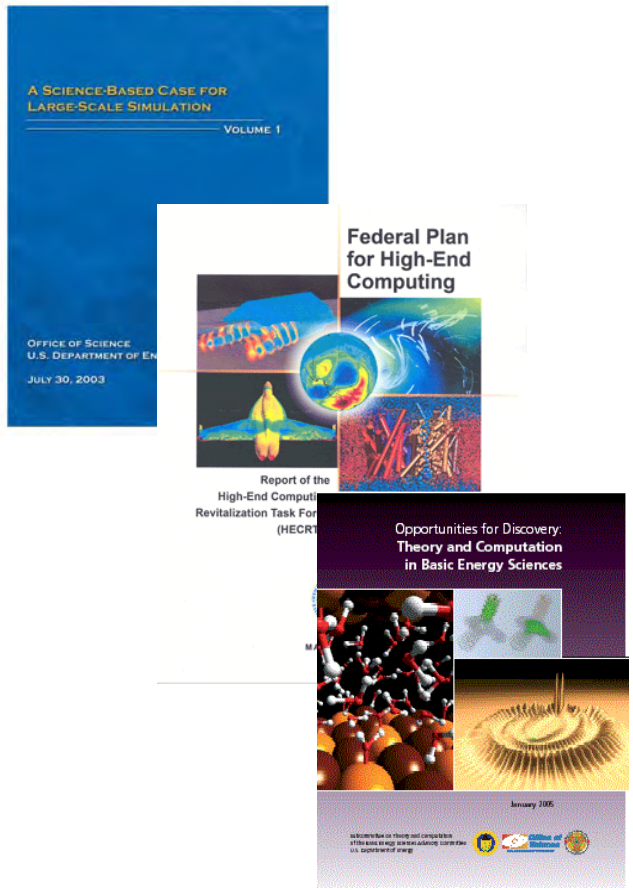
**Plasma Turbulence**
Simulations of the turbulence and flow of plasma is critical for developing tools to harness and use the power from fusion reactions and to address astrophysical challenges such as solar-coronal mass ejections.

# LCF in FY 2007 and Beyond

**Advanced Scientific Computing Research Program**

- **Upgrade LCF at ORNL**
  - Jaguar upgraded
    - 100 Teraflops in FY 2006
    - 250 Teraflop 2007
  - 1 Petaflop system by end of FY 2008

- **Provide architectural diversity with the establishment of LCF at ANL in FY 2007**
  - 100 Teraflop IBM Blue Gene P
  - Expected to accelerate scientific understanding in areas that include materials science, catalysis, protein/DNA complexes, and advanced designs of nuclear reactors.
  - Low power consumption



# Research and Evaluation Prototypes

- **FY 2006**
  - Request for proposals out shortly
- **FY 2007**
  - Coordinate ASCR's effort with the National Nuclear Security Administration (NNSA)
  - Focus on the Defense Advanced Research Projects Administration (DARPA) High Productivity Computing Systems (HPCS) program partnership.

# External Reviews

- **Diverse committees with representatives from scientific disciplines, other DOE Labs and, Federal Agencies**
  - NERSC – May 17-19, 2005
    - Identified as a strong, productive and responsive science-driven center
    - NERSC-5 a much needed and justified acquisition
  - LCF at ORNL – March 7-8, 2006
  - LCF at ANL -- May 23-25, 2006

# Funding Profiles

| | FY 2005 $(000) | FY 2006 ($000) | FY2007 ($000) |
|---|---|---|---|
| NERSC | $37,868 | $37,489 | $54,790 |
| LCF at ORNL | $48,600 | $53,702 | $80,000 |
| LCF at ANL | — | — | $22,504 |
| R & E Prototypes | $13,028 | $12,959 | $13,000 |

# Allocation of Resources



- **85% -- Office of Science mission related**
  - Common Call for proposals issued for NERSC and LCF resources
  - Dr. Orbach establishes allocations for Program Offices
  - Associate Directors or their designees review proposals in their area and determine final allocations

- **10% --Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program**
  - Provides Office of Science computing resources to a small number of computationally intensive research projects of large scale, that can make high-impact scientific advances through the use of a large allocation of computer time and data storage
  - Open to national and international researchers, including industry
  - No requirement of DOE Office of Science funding
  - Peer-reviewed
  - Expanded in FY 2006 to include resources at ANL, LBNL, ORNL, PNNL

- **5% -- Reserved for Director, Office of Science**
  - Allocation at NERSC for Army Corps of Engineers and FEMA to analyze hurricane coastal surges in Louisiana and the Gulf Coast

# Performance Metrics

- **FY 2006 Facilities Target** -- Focus usage of the primary supercomputer at NERSC on capability computing.

  *"40% of the computing time used that is accounted for by computations that require at least 1/8 (768 processors) of the total resource"*

# Top 2005 NERSC Users Now

| 05 Used | 06 Award | ORNL Award | Project Type | Science | PI | Org |
|---|---|---|---|---|---|---|
| 4.5 M | 1.5 M | 2.3 M | SciDAC | fusion | Lee | PPPL |
| 3.5 M | 0.4 M | 3.6 M | INCITE | combustion | Chen | Sandia CA |
| 2.5 M | 0.3 M | | INCITE | astrophysics | Cattaneo | U. Chicago |
| 2.4 M | 0.7 M | | INCITE | biology | Daggett | U. Wash. |
| 2.3 M | 1.5 M | | DOE | fusion | Cohen | LLNL |
| 2.1 M | 0.9 M | | SciDAC | fusion | Pindzola | Auburn U. |
| 2.1 M | 1.8 M | | DOE | QCD | Toussaint | U. Arizona |
| 1.4 M | 0.8 M | | SciDAC | combustion | Bell | LBNL |
| 1.3 M | 1.1 M | 3.0 M | SciDAC | astrophysics | Woosley | UCSC |
| 1.2 M | 0.5 M | | DOE | climate | Randall | Colorado St |
| 1.1 M | 1.4 M | | SciDAC | accelerator physics | Ryne | LBNL |
| 1.0 M | 0.9 M | 4.2 M | SciDAC | astrophysics | Mezzacappa | ORNL |



Courtesy of Francesca Verdier, NERSC

# Challenges

- **To deliver petascale high performance computing hardware by the end of FY 2008 for scientific discover**
- **To revise performance metrics to reflect the differences between capability and capacity computing facilities**
- **To define an coherent allocation strategy**