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**DOE/Office of Science**

# U. S. Department of Energy – Office of Science

REPORT OF
The Panel on Recent Significant Advancements in Computational Science

BREAKTHROUGHS 2008

applied mathematics, astrophysics, biology, chemistry, combustion, energy science, materials science, computer science, fusion-energy science

BREAKTHROUGHS

## CONTENTS

## 1.3 Petaflops on Scientific Application – 11/08





WORLD'S FASTEST OPEN SCIENCE SUPERCOMPUTER

ALCF

ARGONNE LEADERSHIP COMPUTING FACILITY

JUNE 2008 • SOURCE: 31st TOP500

NITRD

# INCITE - Background

- Initiated at National Energy Research Scientific Computing Center (NERSC) at LBNL in 2004

- 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
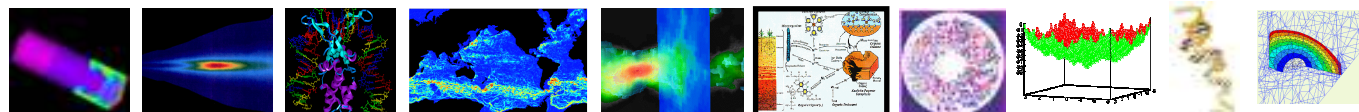
- Peer and computational reviews
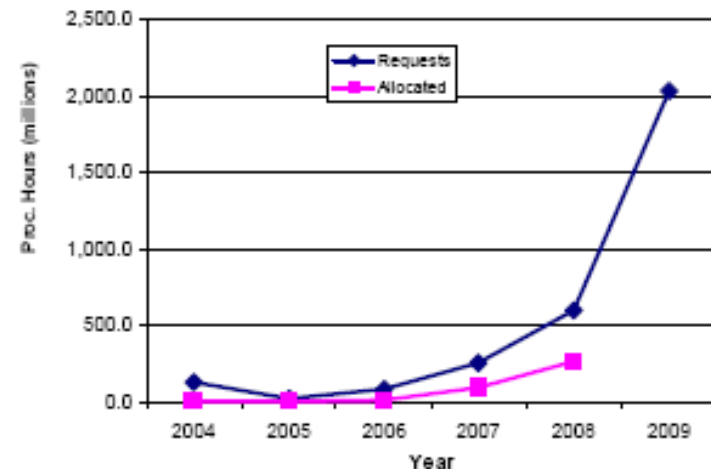
# INCITE - 2009

- 79 unique proposals received from scientific disciplines of accelerator physics, astrophysics, chemical sciences, climate research, computer science, engineering physics, environmental science, fusion energy, life sciences, materials science and nuclear physics

- 21 renewal proposals

- Over **2 Billion processor hours** requested for 2009 from new and renewal proposals

> **Over 600 Million processor hours available for 2009 awards, including renewals**
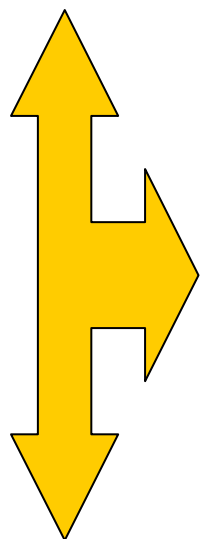
# Scientific Discovery Through Advanced Computing

**Scientific Discovery**



**Applications**

## SciDAC 2

- Accelerator science and simulation          - Astrophysics
- Climate modeling and simulation          - Computational Biology
- Fusion science          - High-energy physics
- Petabyte high-energy/nuclear physics          - Materials science and chemistry
- Nuclear physics          - QCD
- Radiation transport          - Turbulence
          - Groundwater reactive transport modeling and simulation

- Centers for Enabling Technology

- Scientific Applications Partnerships          - Institutes (University-lead)

**Computing/ Networking**
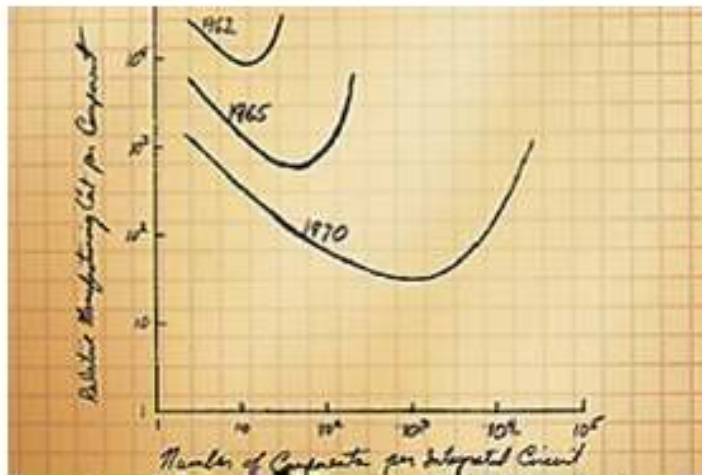
**INCITE NERSC Allocation**

| | | |
|---|---|---|
| Leadership Computing- ANL | 556 TF IBM BG/P | |
| Leadership Computing- ORNL | 263 TF  Cray XT4 | 1 PF Cray XT5 |
| Production Computing- NERSC | 104 TF  Cray XT4 | ~360 TF Cray XT4 |
| ESnet | On path toward Dual rings 40Gbps/ 10 Gbps fault tolerant | |

# Applied Mathematics Research

♦ **FY 08 Budget:** Approximately 75% Labs, 25% Universities

♦ **Chart Allocations by Area**
  - **Based on $23.6M (FY08)**
  - **Does not include**
    - **Computational Science Graduate Fellowship Program ($5M)**
    - **New Multiscale Mathematics and Optimization awards**
    - **Potential new FY 09 initiatives:**
      - Mathematics for Analysis of Petascale Data
      - Joint Applied Mathematics-Computer Science Institutes
      - High Risk / High Payoff Technologies

### FY 2008



Legend:
- ■ Advanced Linear Algebra
- ■ Discretization & Meshing
- ■ Multiscale, Multiphysics
- ■ Uncertainty & Error Analysis
- ■ Optimization
- ■ Other research
- □ Fellowships & Workshops
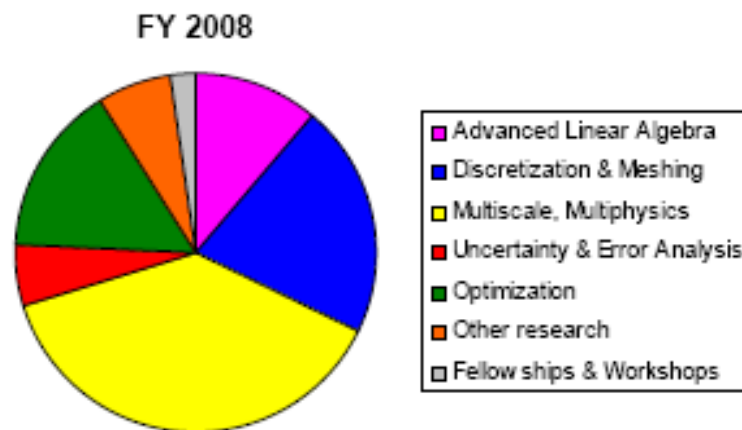
# Computer Science Challenges



Moore's original graph predicting Moore's Law in 1965. Chip capacity will double every 2 yrs.
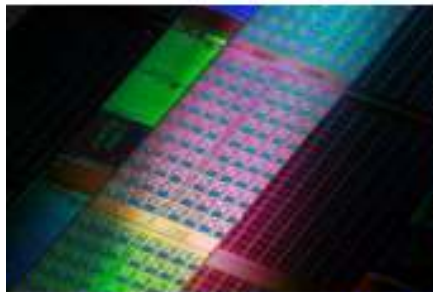


Intel Teraflops Research Chip    IBM Stacked Chip

- Unpredictable evolution of hardware
- Multilevel and heterogeneous parallelism; memory hierarchies
- Programming models must work at scale (numbers of cores, lines of code, numbers of components)
- Managing data, simulation, experimental and observed
- Communications:
  synchronous → asynchronous
- Reliability

*It's not just extreme scale, it's also extreme complexity*

NITRD
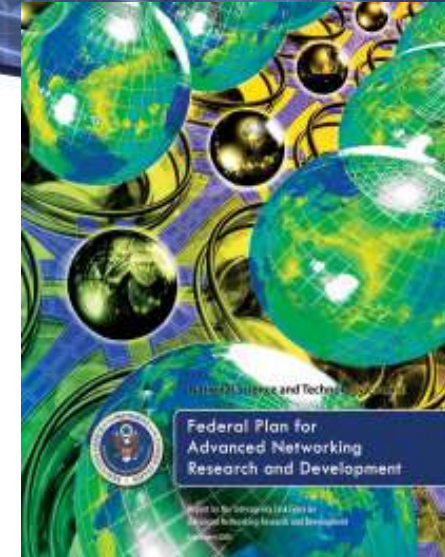
- ◆ **Staffing Changes**
  - ▪ Susan Turnbull - detailee from GSA, Team Lead

- ◆ **Program elements:**
  - ▪ **Network research** - core network research
  - ▪ **Middleware research** – Grid technologies

- ◆ **The next-generation program**
  - ▪ Supports R&D activities to develop advanced networks to enable distributed high-end science
  - ▪ Coordinates with ESnet to develop and deploy networks that enable scientists to push the limits of today's networks

- ◆ Next-generation network technologies have enabled the efficient and rapid distribution of massive data generated by the LHC experiment and climate modeling

- ◆ Major activities in FY09: Network research program announcement