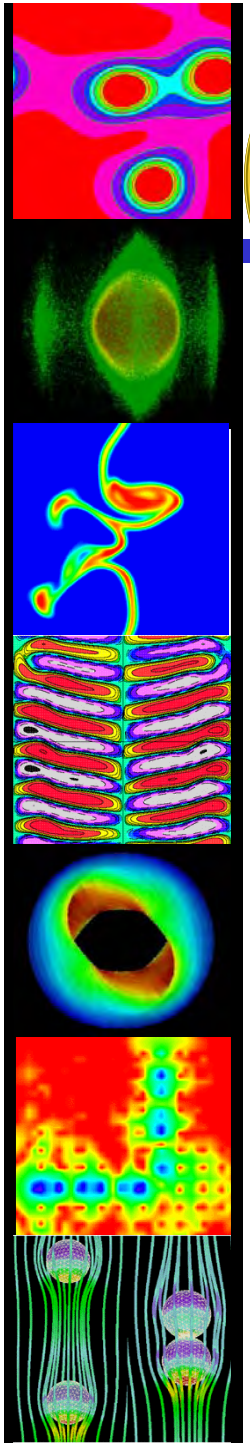


Overview

and

Earth Simulator Response

ASCAC Meeting
Washington, DC
October 17-18, 2002

Ed Oliver/ Walt Polansky

www.science.doe.gov/ASCR/

MICS Activities and Plans

- FY 2002 Activities
  - Conducted a workshop and 8 Town Meetings to evaluate Earth Simulator impact
  - Launched Early Career Principal Investigator activity to strengthen core research program
  - Convened ASCAC-BESAC sponsored workshop on Computational Nanoscience
  - Conducted workshop on networking requirements for future of science
  - Conducted Genomes to Life workshops on applied mathematics and computer science
  - Initiated ESnet backbone upgrade from 622 Mbs (OC12) to 10 Gbs (OC192) to service increased networking requirements for science

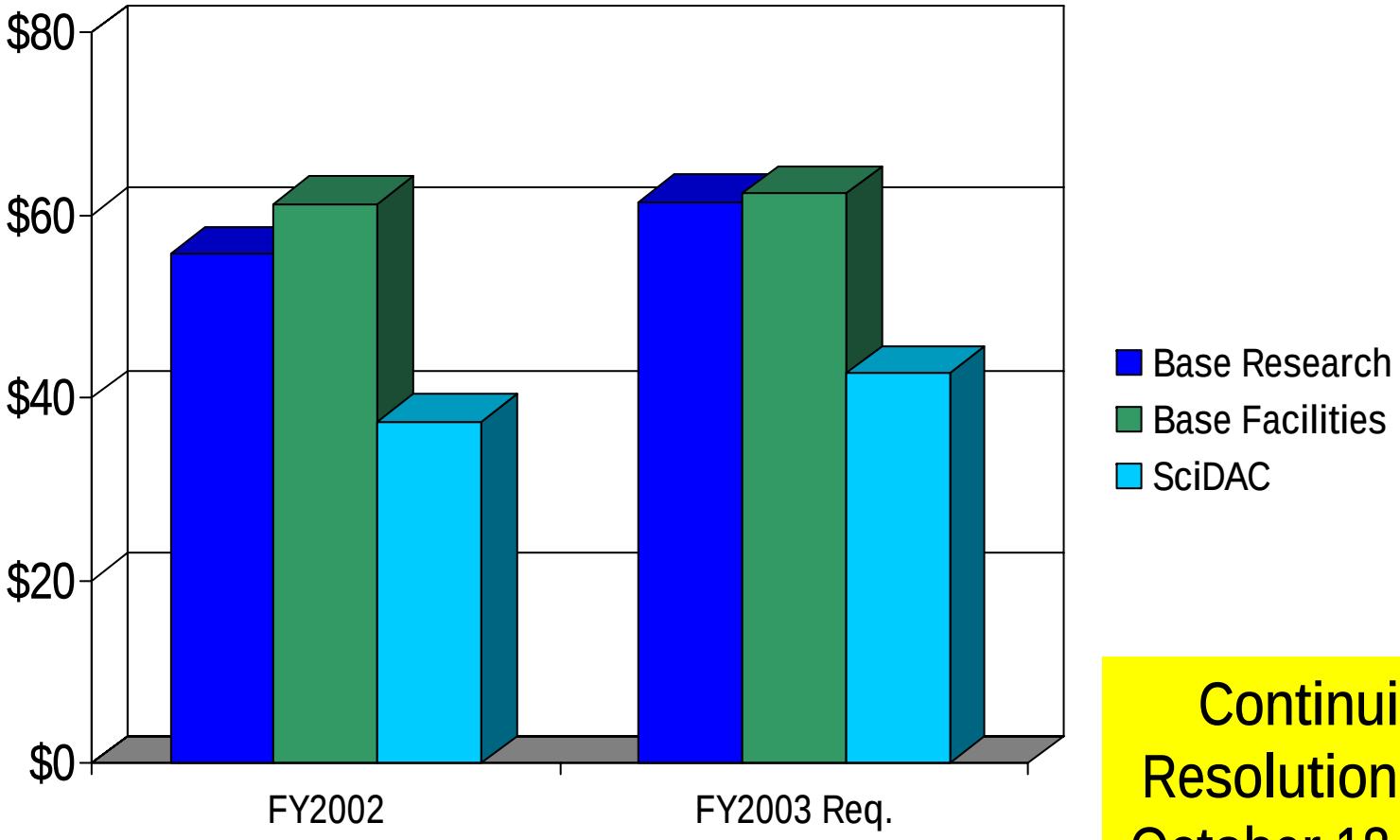
- FY 2003 Plans
  - Initiate reviews of applied mathematics and collaboratory pilot research activities
  - Initiate review of SciDAC portfolio
  - Continue workshops and Town Meetings to assess UltraScale Simulation needs

MICS Subprogram Budget Evolution

$ in millions

FY2002 Approp. - $154.400

FY2003 Request- $166.625



Continuing Resolution until October 18, 2002

UltraScale Simulation Challenges and Opportunities...

... for leadership in computational sciences

- Earth Simulator has revolutionized field of scientific simulation
  - "Global Atmospheric Simulation with the Spectral Transform Method"- 26.58 Tflops
  - "Three-dimensional Fluid Simulation for Fusion Science with High Performance Fortran"- 12.5 Tflops
  - "Direct Numerical Simulation of Turbulence by Fourier Spectral Method"- 12.4 Tflops

- Without robust response to Earth Simulator, U.S. is open to losing its leadership in defining and advancing frontiers of computational science as new approach to science. This area is critical to both our national security and economic vitality. (Advanced Scientific Computing Advisory Committee – May 21, 2002).

UltraScale Simulation Calendar of Events

April 20, 2002	**New York Times**	**"Japanese Computer Is World's Fastest, as U.S. Falls Back"**
May 15-16,2002	**Earth Simulator Rapid Response Meeting**	**ES performance a credible threat to US computational science leadership**
June 12, 2002	**IBM/ORNL/NCAR meeting**	
June 14, 2002	**OSTP Meeting (Marburger)**	**Possible need for interagency response**
June 20, 2002	**Cray/ORNL/NCAR meeting**	
June 19-20, 2002	**Visit to NASA Ames**	
June 21, 2002	**Visit to Silicon Graphics, Inc.**	
July 8, 2002	**SIAM Mini-Symposium**	**Presentation of ES challenge**
July 17, 2002	**SAC Meeting**	**Overviews of ES and challenge to SC**
July 22, 2002	**DOE visit to the Earth Simulator**	**Yokohama, Japan**
August 5-30, 2002	**Discussions with Fusion, Chemistry, Astrophysics, Accelerator Design, Network, Nano-materials communities**	
Sept. 5- 17 2002	**Discussions with NERSC Users, Biologists**	

...driven by the science to be enabled.

Typical questions posed during Town Meetings

- How can this science be advanced through simulations ?
- Why are these advances important to the field ? ...to the Office of Science and the DOE ?
- What breakthrough simulations need to be performed ? What knowledge will result ? What would be the benefit to the Office of Science and the DOE ?
- What computational and networking resources would be needed to perform breakthrough simulations ? When would you be ready to utilize those resources ?
- What challenge does the Earth Simulator pose to your field of science ?

Expected Outcomes from Town Meetings

- Discussions among peers about opportunities presented by ultrascale computing.
- Self-assessments of the influence the Earth Simulator may have on simulations of physical, chemical and biological systems.
- Contribution(s) to “Building the Science Case for Ultra Scale Simulation”, http://www.ultrasim.info
- Further dialog.

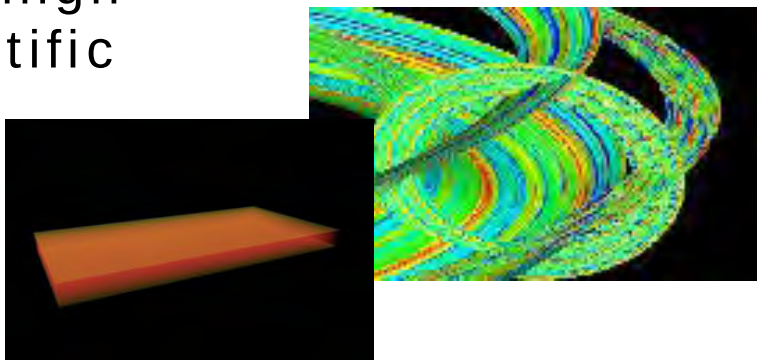
Simulation Capability Needs

FY2004-05 Timeframe

Application	Simulation Need	Performance Improvement Factor	Significance
Climate Science	Calculate chemical balances in atmosphere, including clouds, rivers, and vegetation.	> 50	Provides U.S. policymakers with leadership data to support policy decisions. Properly represent and predict extreme weather conditions in changing climate.
Magnetic Fusion Energy	Optimize balance between self-heating of plasma and heat leakage caused by electromagnetic turbulence.	> 50	Underpins U.S. decisions about future international fusion collaborations. Integrated simulations of burning plasma crucial for quantifying prospects for commercial fusion.
Combustion Science	Understand interactions between combustion and turbulent fluctuations in burning fluid.	> 50	Understand detonation dynamics (e.g. engine knock) in combustion systems. Solve the “soot “ problem in diesel engines.
Environmental Molecular Science	Reliably predict chemical and physical properties of radioactive substances.	> 100	Develop innovative technologies to remediate contaminated soils and groundwater.
Astrophysics	Realistically simulate the explosion of a supernova for first time.	>> 100	Measure size and age of Universe and rate of expansion of Universe. Gain insight into inertial fusion processes.

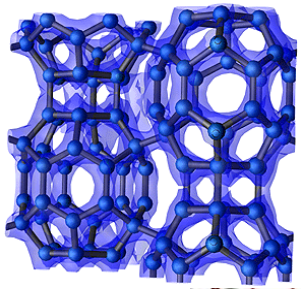
Ultrascale Scientific Computing…

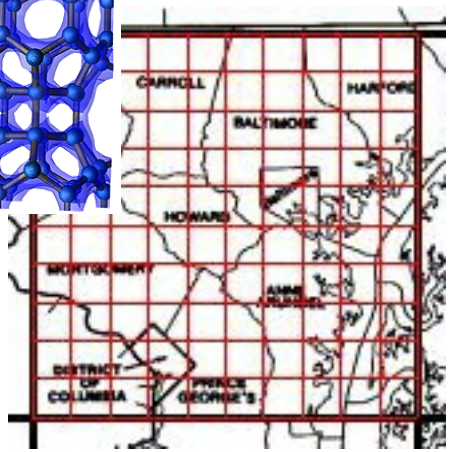
…essential for U.S. leadership in high performance computing for scientific simulation



Issues:

- Deliver leadership class computers for science.
- Couple applications scientists with computer architects, engineers, and semiconductor researchers.
- Partner with industry on applications.
- Partner with domestic vendors.



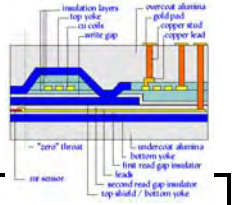


Advanced Computing and Networking Critical to Office of Science Mission

Scientific problems of strategic importance typically:

- Involve physical scales that range over 5-50 orders of magnitude;
- Couple scientific disciplines, e.g., chemistry and fluid dynamics to understand combustion;
- Must be addressed by teams of mathematicians, computer scientists, and application scientists; and
- Utilize facilities that generate millions of gigabytes of data shared among scientists throughout the world.

The Scale of the Problem



Two layers of Fe-Mn-Co containing 2,176 atoms corresponds to a wafer with dimensions approximately fifty nanometers (50x 10^{-9}m) on a side and five nanometers (5 x 10^{-9}m) thick. A simulation at NERSC of the properties of this configuration lasted for 100 hrs. , a calculation rate of 2.46 Teraflops (one trillion floating point operations per second). To explore material imperfections, the simulation would need to be at least 10 times more compute intensive.

Early Career Principal Investigator Activity

- Purpose- Identify exceptionally talented researchers early in their careers and interest them in research programs relevant to DOE missions.

- Eligibility- Tenure-track regular faculty position, U.S. academic institution, 5 years or less after receiving Ph.D. or after completing postdoctoral position

- In FY2002, 132 applications; 17 awards ($1.6M/yr. for 3 years)
  - applied mathematics: 7
  - computer science: 8
  - high-performance networks: 2

Notice for FY2003 ECPI Grant Applications in preparation.

Links

Mathematical, Information and Computational Sciences Program
http://www.sc.doe.gov/ascr/mics/index.html

Genomes to Life
http://www.doegenomestolife.org/

Nanoscale Science, Engineering, and Technology Research
http://www.sc.doe.gov/production/bes/NNI.htm

UltraScale Simulation Planning
http://www.ultrasim.info/

Earth Simulator Home Page
http://www.es.jamstec.go.jp/esc/eng/

Status of FY2003 Appropriations Bills
http://thomas.loc.gov/home/approp/app03.html