Advanced Scientific Computing Research

-- An Introduction --

Ice Sheet Modeling
Principal Investigator Workshop
Annapolis, MD
September 16-17, 2009

Walter M. Polansky
Office of Advanced Scientific Computing Research
FY09: $4.8B
ARRA: $1.6B
FY10 (Req): $4.9B

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SSO
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FY09: $368M
ARRA: $157M
FY10 (Req): $409M
Deliver Petascale Science Today
- Continue to make the Leadership Computing Facilities available to the very best science through Innovative and Novel Computational Impact on Theory and Experiment (INCITE).
- Continue to work with Pioneer Applications to deliver scientific results from day one.

Build the Intellectual Foundation for the Future
- Nuture –
  - World class mathematics and computer science research efforts
  - Applications critical to DOE missions through Scientific Discovery through Advanced Computing (SciDAC).
- Provide direct support for “bleeding-edge” research groups willing to take on the risk of working with emerging languages and operating systems.
- Foster innovative research at the ever blurring boundary between Applied Mathematics and Computer Science.

Realize the Promise of Extreme Scale
- Work with key science applications to identify opportunities for new research areas only possible through extreme scale computing.
- Support innovative research on advanced architectures and algorithms that accelerates the development of hardware and software that is well suited to extreme scale computational science.

http://www.sc.doe.gov/ascr/index.html
Advancing Science through large-scale data, modeling and simulation


- Centers for Enabling Technology: Address mathematical and computing systems software issues

- Institutes: Assist Scientific Applications teams and foster next generation computational scientists

http://www.scidac.gov
SciDAC Model

Scientific Discovery

Applications

Computing/Networking

- Accelerator science and simulation
- Climate modeling and simulation
- Fusion science
- Petabyte high-energy/nuclear physics
- Nuclear physics
- Radiation transport
  - Groundwater reactive transport modeling and simulation

- Centers for Enabling Technology
- Scientific Applications Partnerships
- Institutes (University-lead)

Leadership Computing-
ANL 556 TF IBM BG/P

Leadership Computing-
ORNL > 1 PF Cray XT5

Production Computing-
NERSC ~360 TF Cray XT4

ESnet On path toward Dual rings 40Gbps/10 Gbps fault tolerant

http://www.sc.doe.gov/ascr/Facilities/Facilities.html
Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program started in 2004.

– Small number of computational intense, high impact projects
– Open to national and international researchers, including industry
– No requirement of DOE or Office of Science funding or topic area
– Peer and computational reviews

2009 INCITE Allocations

Approximately 890 million processors awarded in 2009
Ice Sheets Are Important

- A relatively recent, natural event illustrates why:
  - About 19,000 years ago, ice sheets started melting in North America and Eurasia
  - In 2,000 years, the melting glaciers dumped so much fresh water into the North Atlantic the overturning ocean circulation stopped
  - Greenland cooled.
  - 2,500 years later, the freshwater flow ceased.
  - Greenland’s temperature rose by 15 deg C, sea levels rose 5 meters!

Recent simulations on Jaguar and Pheonix at ORNL show deglaciation during the Bølling-Allerød, Earth’s most recent period of natural global warming. Courtesy NCCS

Ice sheet dynamics can be abrupt; Climate changes can be significant
Ice Sheet Modeling

- **Models**
  - Improve models for ice sheet dynamics and interaction between ice sheet and land/ocean
  - Understand the dynamical properties of ice sheet (e.g., crack formation and propagation)
  - Implement these models on HPC

- **Opportunities**
  - Develop data assimilation techniques for incorporating actual data into new models
  - Establish credibility of models and simulations: verification, validation, and uncertainty quantification

- **Computational Algorithms**
  - Scalable algorithms for extreme-scale simulations
  - Adaptive algorithms to focus on important small-scale phenomena
  - Appropriate numerical methods for the simulation of ice sheet dynamics (high-order, non-Newtonian fluid, heat conduction, etc)

- **Infrastructure**
  - Leadership-class high-performance computers for high-fidelity, high-resolution simulations
  - Analysis, visualization, and storage of simulation results – large data sets!
  - Collaboration: data and model exchange
“Perhaps the most significant applications of scientific computing come not in the solution of old problems, but in the discovery of new phenomena through numerical experimentation.”

*Lax Report on Large Scale Computing in Science and Engineering, 1982*