Scientific Discovery Through Advanced Computing

Presentation to the Advanced Scientific Computing Advisory Committee

Michael Strayer
SciDAC Director
April 5, 2004
SciDAC

- SciDAC is a $60M program for Computational Science
- Strongly interdisciplinary - involves all of the Offices of Science
- Create a scientific culture to use high-end computers effectively
- Goal of advancing scientific discovery central to the OS research missions
3rd annual PI meeting March 22-24, 2004
Charleston, SC
Theme: Enabling Science

23 Invited Talks, 2 poster Sessions, 1 Panel Discussion

Two Plenary Talks:
System and Application Performance at Extreme-Scale
Adolfy Hoisie (LANL)
The Grid: Essential Infrastructure for DOE Science
Ian Foster (ANL)
Applications

**HEP Applications**
Introduction: Irwin Gaines (Fermilab and DOE/HEP)
Advanced Computing for 21st Century Accelerator Science
  - Kwok Ko (SLAC) / Rob Ryne (LBNL)
Center for Supernova Research
  - Adam Burrows (Univ. of Arizona)

**NP Applications**
Introduction: Sidney Coon (DOE/NP)
Terascale Supernova Initiative
  - Tony Mezzacappa (ORNL)
Lattice QCD from the Nuclear Physics Perspective
  - John Negele (MIT)

**BES Applications**
Introduction: Richard Hilderbrandt (DOE/BES)
Direct Simulations of Flow-Combustion Interactions
  - Arnaud C. Trouvé (Univ. of Maryland)
Advanced Methods for Electronic Structure
  - Robert J. Harrison (ORNL)

**BER Applications**
Introduction: Jeff Amthor (DOE/BER)
Development of an Atmospheric Climate Model with Self-Adapting Grid and Physics
  - Michael Herzog (Univ. of Michigan)
Collaborative Design and Development of the Community Climate System Model for Terascale Computers
  - Phil Jones (LANL)

**FES Applications**
Introduction: Steve Eckstrand (DOE/FES)
Magnetic Reconnection: Applications to Fusion, Space, and Astrophysical Plasmas
  - Amitava Bhattacharjee (Univ. of New Hampshire)
Computational Atomic and Molecular Physics for Transport Diagnostics of Fusion Plasmas
  - Mitch Pindzola (Auburn Univ.)
Modeling of RF Wave Propagation in Plasmas
  - Lee Berry (ORNL)
The CS ISICs
Introduction: Fred Johnson (DOE/ASCR)
Performance Evaluation
  Pat Worley (ORNL)
Scientific Data Management
  Arie Shoshani (LBL)
Scalable Systems Software
  Rusty Lusk (ANL)
Component Technology for Terascale Simulation Software
  David Bernholdt (ORNL)

Collaboratories, Networks, Middleware
Introduction: Mary Anne Scott (DOE/ASCR)
National Fusion Collaboratory
  David Schissel (General Atomic)
DOE Science Grid
  William T.C. Kramer (LBNL)
Networking Research Overview
  Micah Beck (Univ. of Tennessee)

The Math ISICs
Introduction: John van Rosendale (DOE/ASCR)
Algorithmic and Software Framework for Applied PDEs
  Phil Collela (LBNL)
Terascale Simulation Tools and Technologies
  Lori Freitag Diachin (LLNL)
Terascale Optimal PDE Simulations
  David Keyes (Columbia Univ.)

Panel Discussion
  Topic: Is SciDAC changing the culture of computation and simulation in science or is it “business as usual”?)
“Outstanding performance of the three Math ISICs”

Applied Partial Differential Equation Center
LBNL, LLNL

Terascale Simulation Tools and Technologies
BNL, ANL, LLNL, ORNL, PNNL, SNL

Terascale Optimal PDE Solvers
Columbia University, ANL, LBNL, LLNL
“Developed AMR algorithm for turbulent combustion with detailed chemistry and transport, with high-resolution simulations of laboratory-scale hydrocarbon flames”

“Flame propagation in type 1A supernovae
Supernova Science Center”

“Cell modeling (A. Arkin, P. Schwartz, LBNL; D. Adalsteinsson, Univ. of North Carolina)”
- Detailed 3D AMR simulations of pellet injection using the MHD equations—pellet treated as moving density source
- Pellet ablates with an analytic model
- Instantaneous heating of ablated mass by electrons
- Single fluid MHD equations describe plasma
“Using an unstructured mesh, enabled first long-time PEP-II beam heating study maintaining overall good quality in aspect ratios and angle of elements.”

“Understand the behavior of Shewanella microbe flocs in oxygen rich environments.”

Floc geometry built using image reconstruction techniques from a stack of confocal images

Unstructured mesh generated

Solve reaction-diffusion equations to find the concentration of oxygen in the floc
“Optimal mesh generation and adaptive methods reduce error in climate applications.”

“New TSTT adaptive mesh capability has provided extremely accurate solutions for accelerator design eigensolvers.”
TOPS’ PETSc software has been employed in two Bell Prizes in 1999 & 2003

2003 prize: geological parameter estimation problem
Forward PDE: 17 million unknowns
Inverse problem: 70 billion unknowns (over time history)
2048 procs of HPAlphaServer for 24 hours

target
reconstruction
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The program will be recompeted in FY2006

Ongoing discussions with Ray Orbach

Ongoing discussions with BER, BES, FES, HEP, and NP

Call for community input at PI meeting

Preserve the present progress and plan for new initiatives during difficult budget years