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

Scientific Discovery Through Advanced Computing

Presentation to the Advanced Scientific Computing Advisory Committee

Michael Strayer
SciDAC Director
April 5, 2004

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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**

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PI Meeting

SciDAC Scientific Discovery through Advanced Computing

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)

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Applications

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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)

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Integrated Software Infrastructure Centers

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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 Atomics)
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"?)

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Applied Math ISICs

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"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

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APDEC

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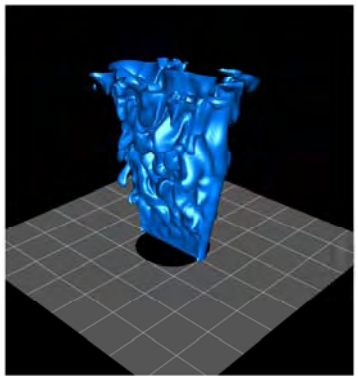
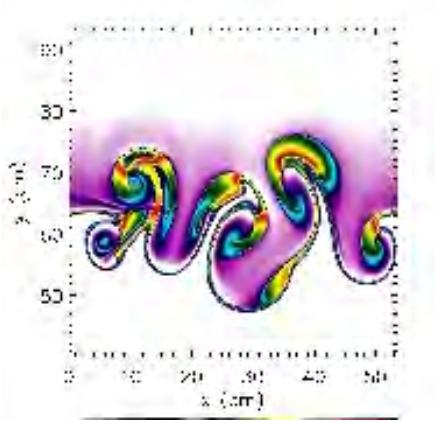
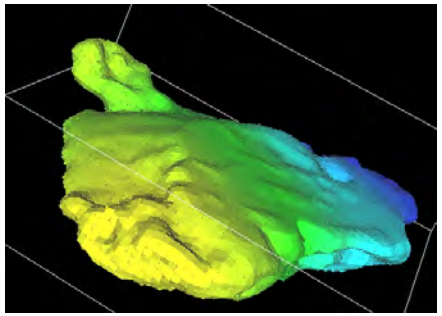
"Developed AMR algorithm for turbulent combustion with detailed chemistry and transport, with high-resolution simulations of laboratory-scale hydrocarbon flames"





"Flame propagation in type 1A supernovae Supernova Science Center"

"Cell modeling (A. Arkin, P. Schwartz, LBNL; D. Adalsteinsson, Univ. of North Carolina)"



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APDEC

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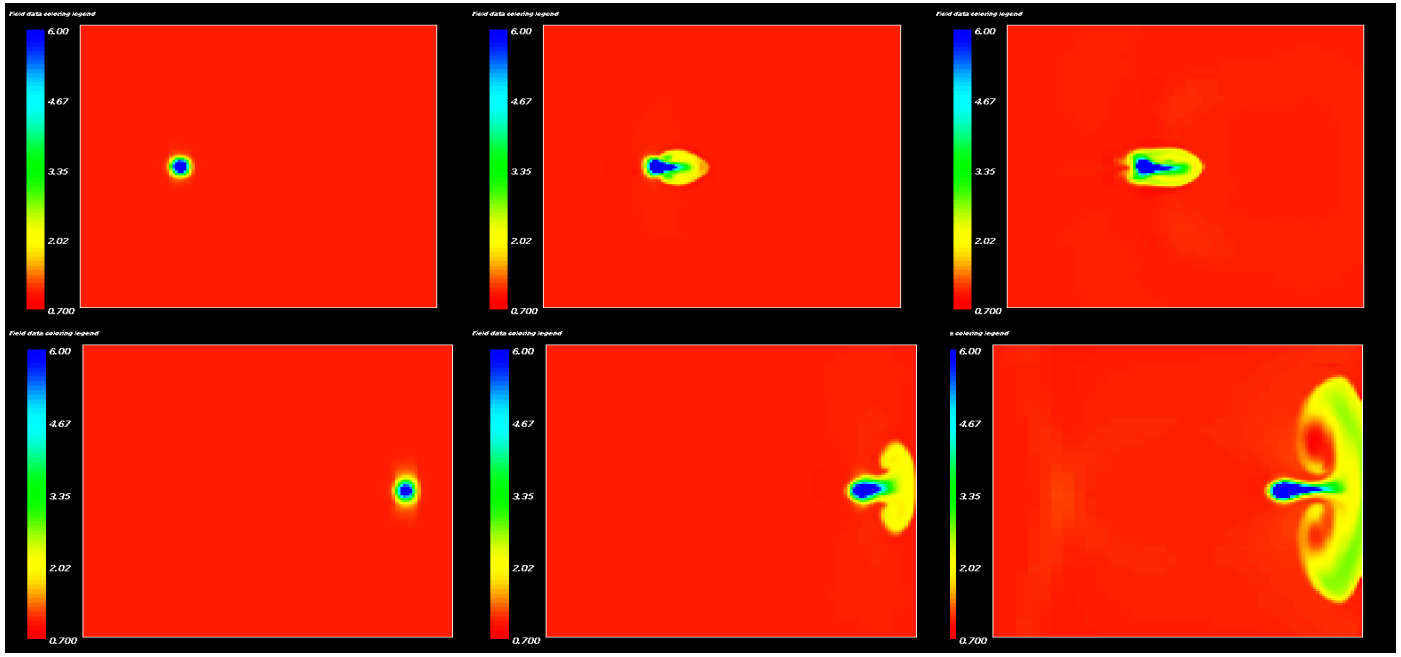
- Detailed 3D AMR simulations of pellet injection using the MHD equations– pellet treated as moving density source
- Pellet ablates with an analytic model
- Instantaneous heating of ablated mass by electrons
- Single fluid MHD equations describe plasma

LFS

HFS



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TSTT

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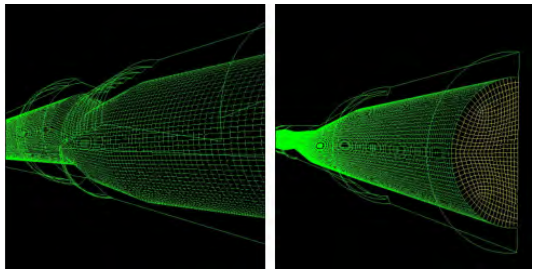
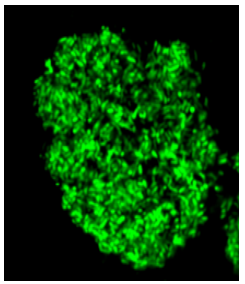
"Using an unstructured mesh, enabled first long-time PEP-II beam heating study maintaining overall good quality in aspect ratios and angle of elements."



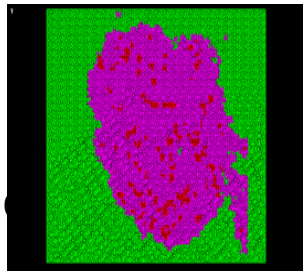
"Understand the behavior ofShewanella microbe flocs in oxygen rich environments."

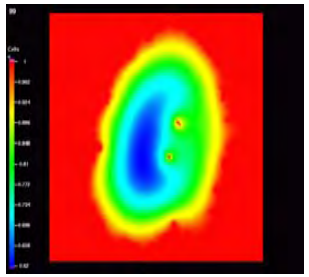


Floc geometry built using image reconstruction techniques from a stack of confocal images

Unstructured mesh generated

Solve reaction-diffusion equations to find th concentration of oxygen in the floc





TSTT

"Optimal mesh generation and adaptive methods reduce error in climate applications."

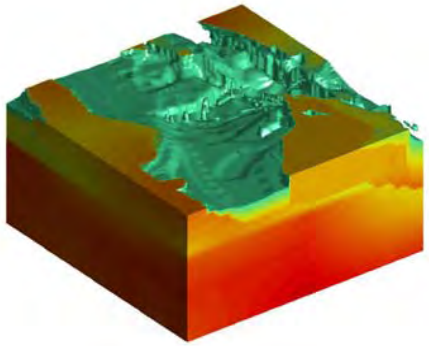
"New TSTT adaptive mesh capability has provided extremely accurate solutions for accelerator design eigensolvers."

TOPS

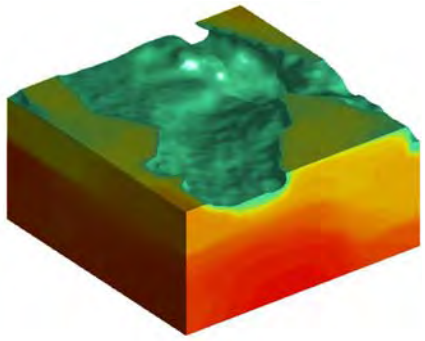
TOPS' PETSc software has been employed in two Bell Prizes in 1999 & 2003

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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TOPS Software

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Collaboration	Current	Future
APDEC	Hypre	
ASCTKD	PETSc	
AST	PARPACK/SuperLU	Veltisto/PETSc
CCTTSS	TAO*, SUNDIALS**	PETSc/Hypre
CEMM	PETSc/Hypre, SUNDIALS	
CMRS	PETSc/Hypre	
CLGT		Hypre, PARPACK
PERC	PETSc	
SSC		PETSc/Hypre
TSI	custom	PETSc/Hypre, SUNDIALS
TSTT	TAO	

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Future of SciDAC

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The program will be recompeted in FY2006

Ongoing discussions with Ray Orbach

Onging 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