

Overview of the High Performance Computing Environment at Sandia



The Red Storm Supercomputer

Red Storm Target Environment

SRN

25 GB/s
Network



SCN

25 GB/s
Network



Discom WAN



Black
RoSE
Cluster



HPSS
Archive

Red
RoSE
Cluster

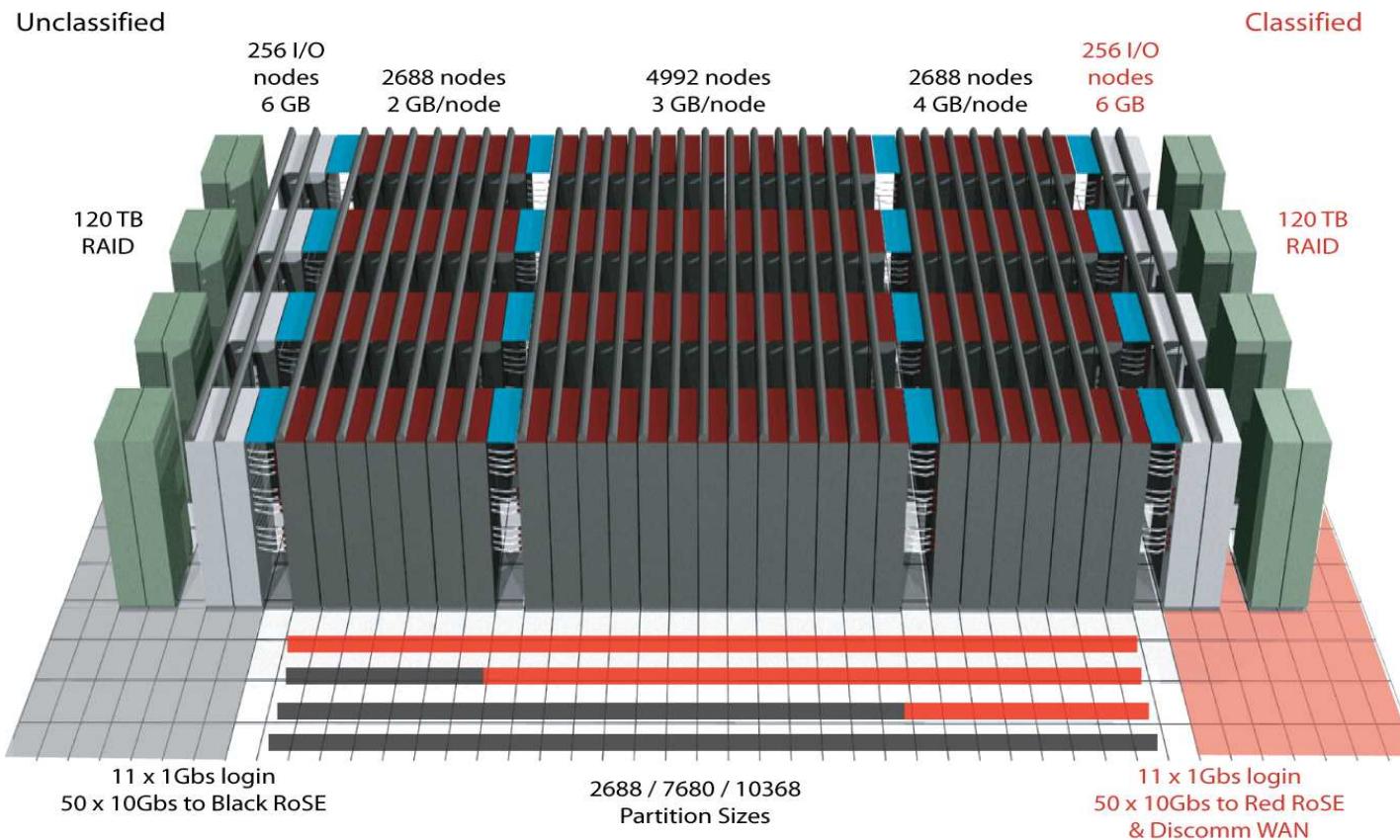


HPSS
Archive



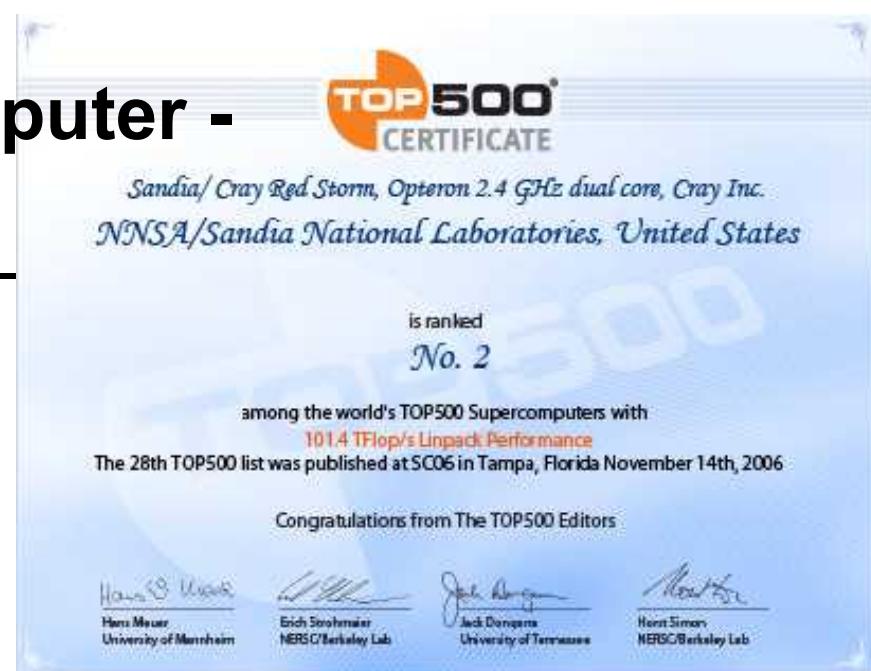


Red Storm System



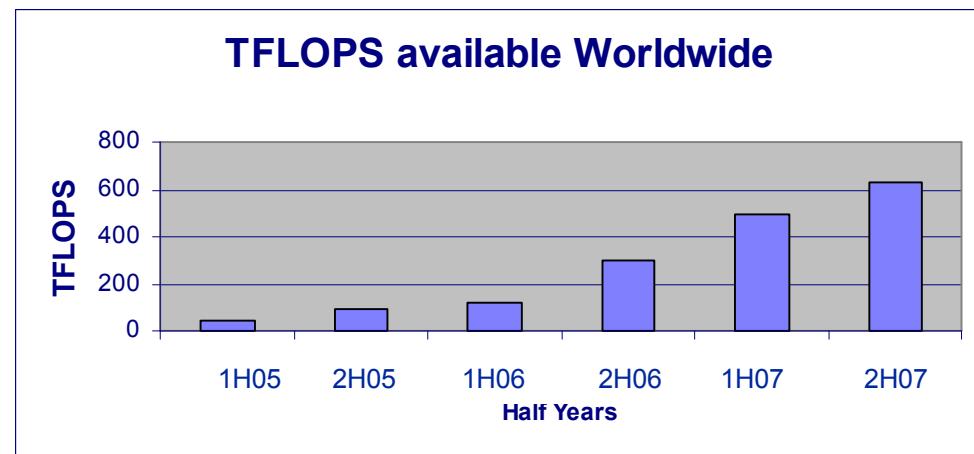
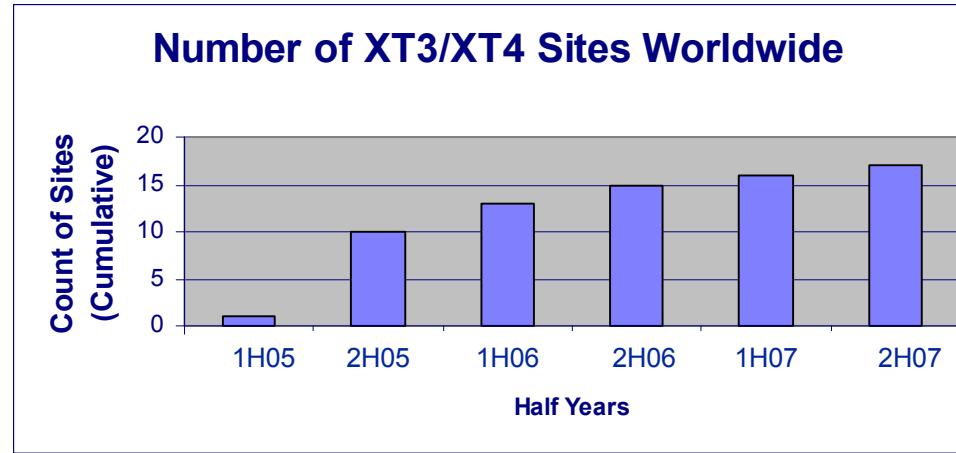
Red Storm Supercomputer - recently upgraded

- **SeaStar 2.1 network chips**
 - ↑ Bandwidth
- **5th Row (↑12960 compute nodes)**
- **Dual Core Opterons**
 - ↑ 25920 compute processors (12960 compute nodes)
 - ↑ 2.4 GHz
- **New OS's (Linux 2.6, CVN)**
 - Virtual node model
 - 1PE or 2PE / nodes
- **New File Systems**
 - Lustre 1.4 on Linux 2.6
- **Complete: mid-November, 2006**



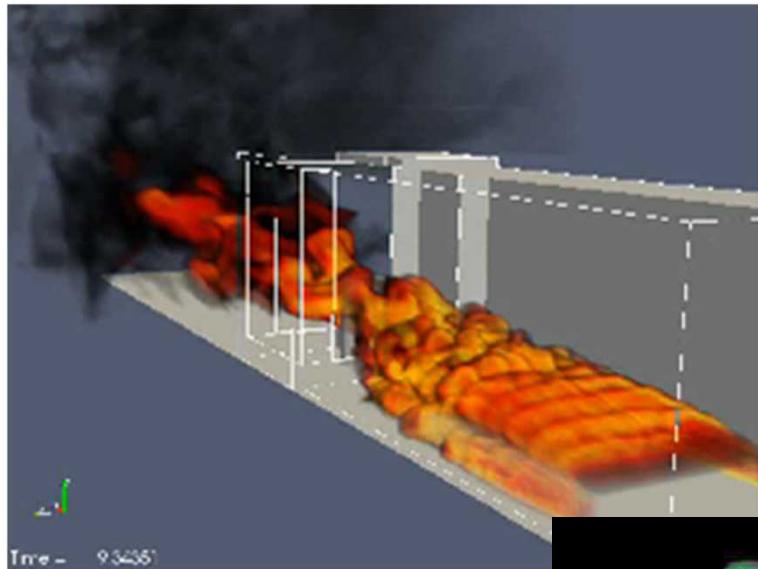
Red Storm technology has resulted in a Cray success story -- there are 17 sites with Cray XT3 or XT4 Computers Worldwide

ARMY/HPCRC
AWE (England)
CSC (Finland)
CSCS (Switzerland)
DOD/ERDC
EPSRC (UK)
JAIST (Japan)
NERSC
ORNL
PITT SC
SNL
SS-634 (non-US)
SS-635
SS-643
SS-661
U OF TOKYO (JST)
U of Western Australia

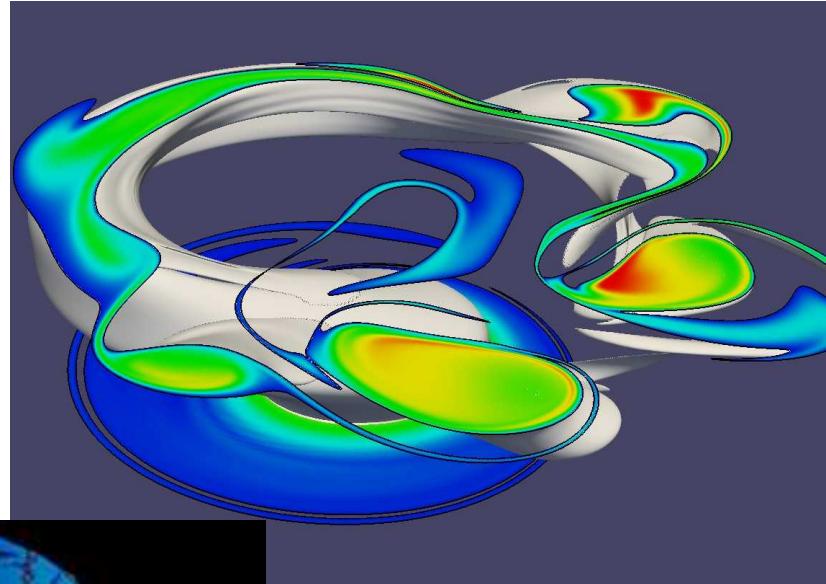




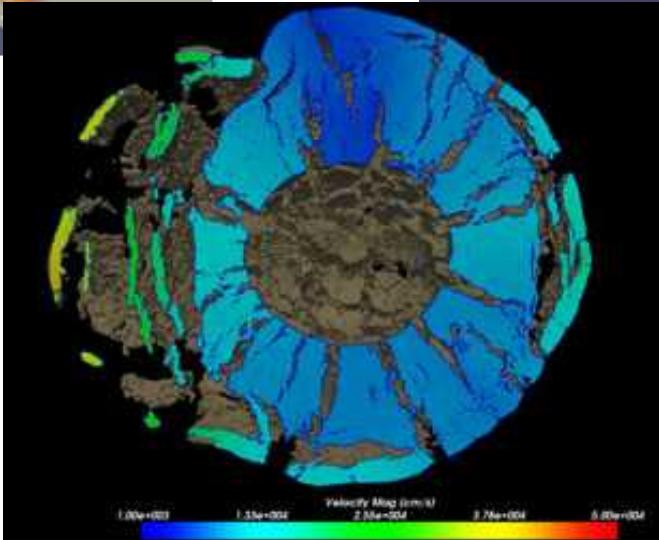
Red Storm Large-scale Simulation Visualizations



Pool Fire Calculation
on Red Storm (2048
proc.).

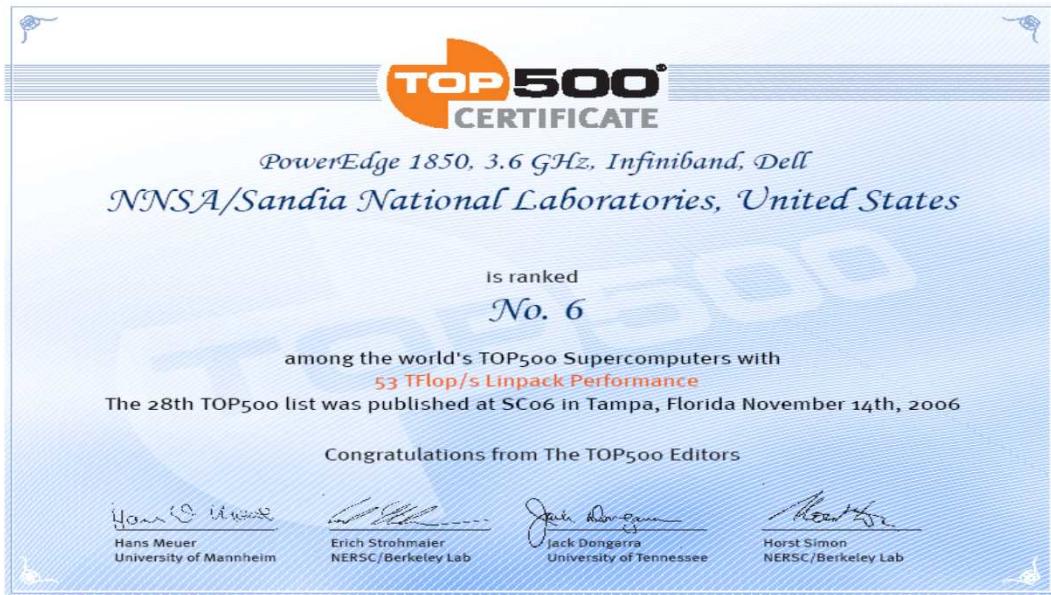


SNL's SEAM Climate Modeling
Results on 7200 proc of Red
Storm (1 billion cells and over
1 terabyte of data)



Golevka Asteroid Destruction,
simulation of 10 Megaton Blast
at center of mass (>1 billion
cells, 15 hrs. on 7200 nodes of
Red Storm)

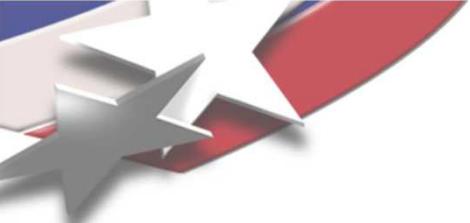
The Thunderbird Linux Cluster



Linpack results:

- 53 TFlops
- 84.66% efficiency
- 9.44 hours
- 8654 processors
- Infiniband interconnect
- (Open Fabrics / Open MPI)

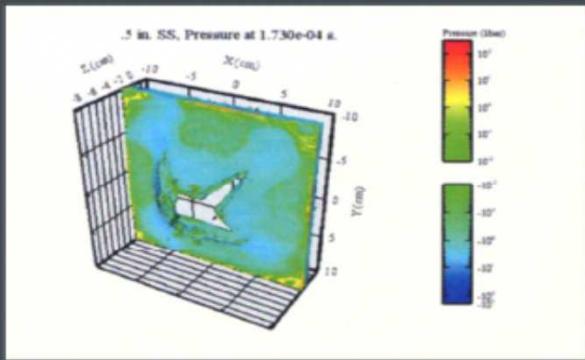
TBird maintained its position as the 6th most powerful supercomputer in the world on November 2006.



TBird Computation & Simulations

Thunderbird High Performance Computing

Computation, Simulation, Analysis, and Visualization



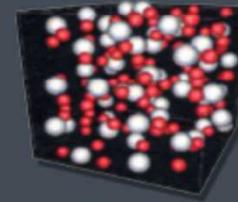
Explosive Sheet

This simulation models the detonation of an explosive layer atop a metal sheet.

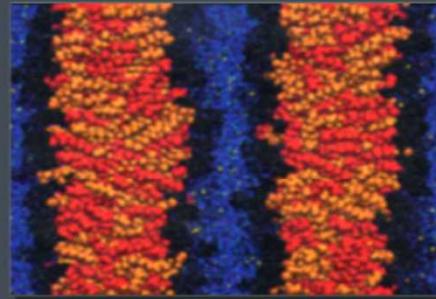
Applications reporting 18-20% performance speedup on Thunderbird since the switch to the new Open IB-based software stack.

168 Atoms

Animation of water molecules.



-Thomas Mattsson



Two Lipid Bilayers

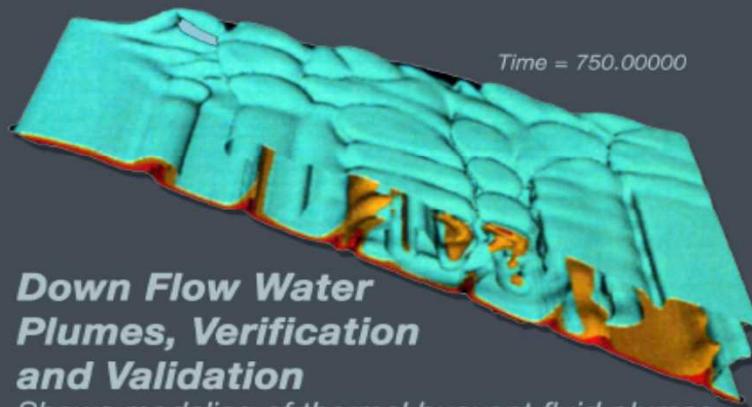
This biomolecular simulation of two lipid bilayers separated by salt water explores the origins of long-range bilayer interactions.

-Paul Crozier

TBird Computation & Simulations

Thunderbird High Performance Computing

Computation, Simulation, Analysis, and Visualization



Down Flow Water Plumes, Verification and Validation

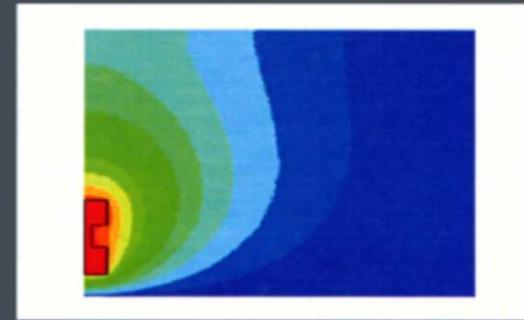
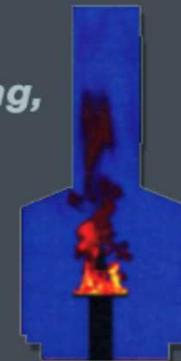
Shows modeling of thermal buoyant fluid plumes as they emerge from a lower heated surface of a transmission channel. The temperature field is tracked as the plumes impinge on a cylinder downstream in the channel.

-Greg Evans

Fuego Calore Coupling, V and V

A 2.4 million element mesh simulation of an abnormal thermal environment, 1024 processors.

-Amalia Black



Thermal Wave Simulation

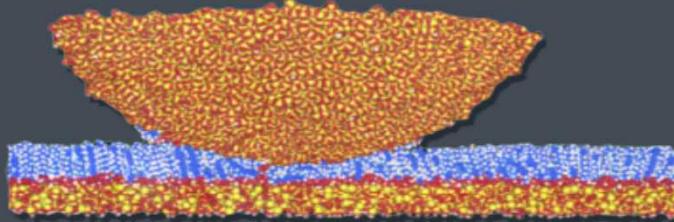
This data shows thermal waves from a gas flow around an I-shaped microbeam. This is a non-equilibrium simulation.

-Michael Gallis

TBird Computation & Simulations

Thunderbird High Performance Computing

Computation, Simulation, Analysis, and Visualization



Micro Electro Mechanical Systems, Coating Friction and Adhesion

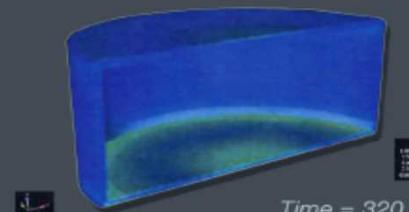
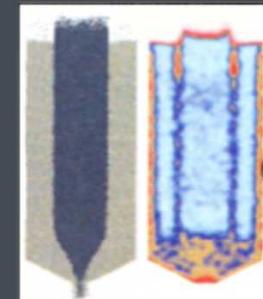
The tip of an Atomic Force Microscopy device interacts with a self-assembled mono-layer coating (blue carbon atoms and white hydrogen atoms) an amorphous Silica substrate (yellow silicon atoms and red oxygen atoms). The experiment measures the coating's tribological properties.

-Mike Chandross

Pebble Bed Nuclear Reactor

A dramatically safer, economical, and more efficient reactor design that utilizes an inert or semi-inert gas to cool and directly drive the turbine.

-Gary Grest



Time = 320.00000 (sec)

Calagio Code Simulation

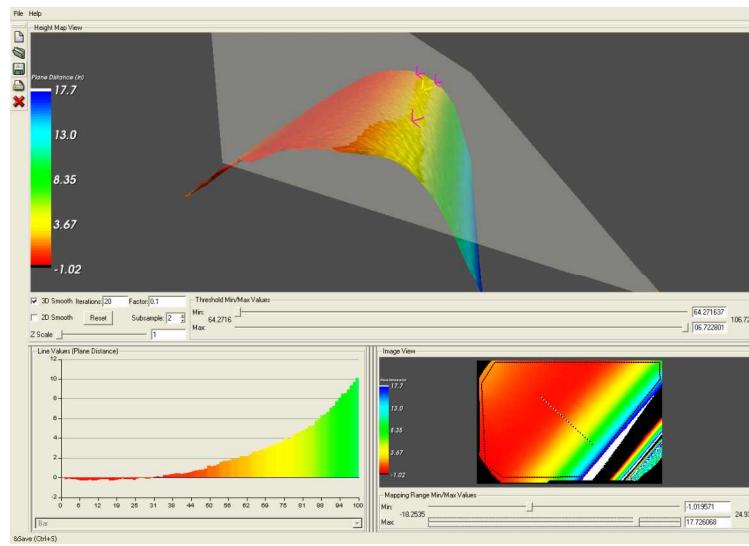
A validation and verification of Thermal Mechanical Coupled Physics showing container failure as a result of chemical pressure loading.

-Shane Schumacher

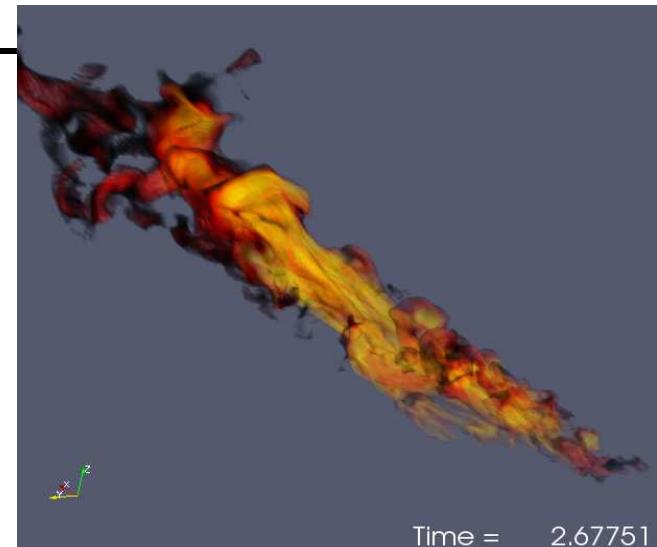
Visualization and Data, Dept. 4326

Data Analysis / Visualization Capabilities

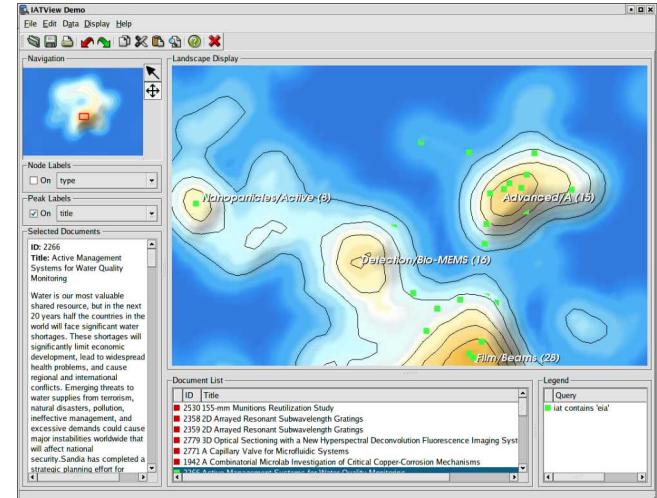
- Scientific Visualization and Data Analysis
- Information Visualization
- Image Analysis



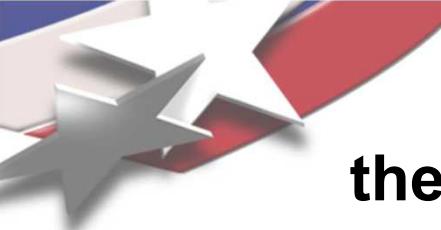
NASA Application



Pool Fire Simulation

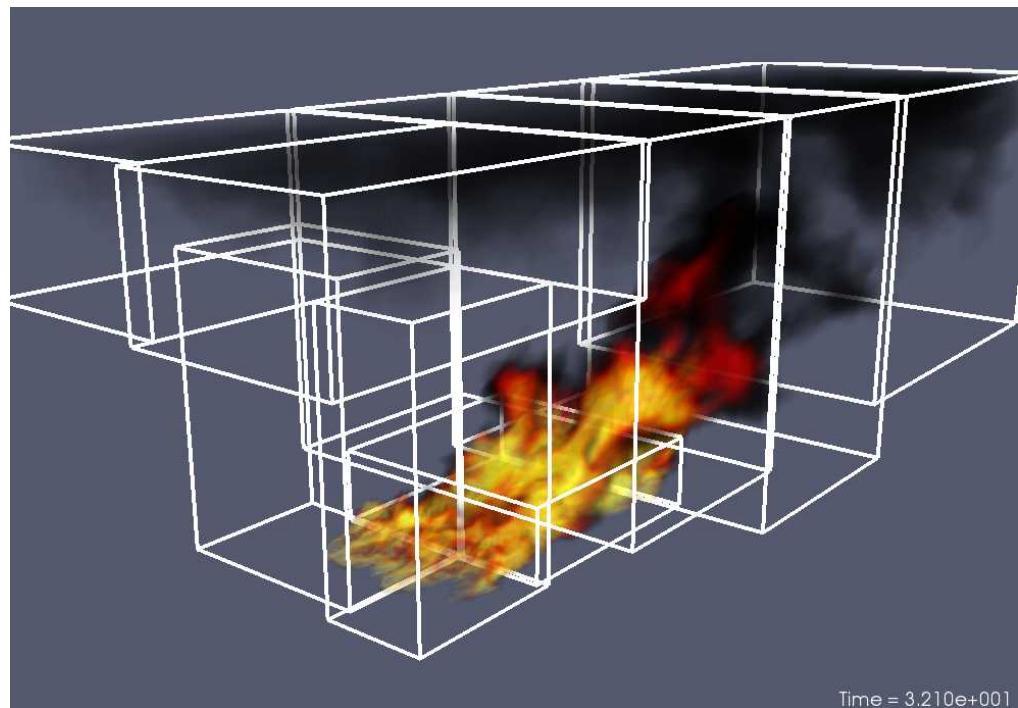
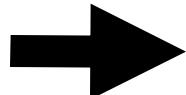


Information Visualization



Much like for large-scale simulations themselves, visualizing the results generally means applying parallel techniques

```
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0265660 025537 064663 054606 043244 074076 124153 135216 125614
0265700 144210 056425 044700 042650 165230 137037 003655 006254
0265720 134453 124327 176005 027034 107514 170774 073702 067274
0265740 072451 007235 147620 061064 152435 113057 155356 114603
0265760 107204 102315 171451 046040 120223 001774 030477 045673
0266000 171317 116055 155117 134444 167210 041405 147122 050505
0266020 004132 046472 124015 134360 178350 053517 044635 021135
0266040 070176 047705 113754 175477 105532 076515 177366 056333
0266060 041023 074017 127113 003214 037026 087640 066171 123424
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0266620 075074 016744 044055 102230 110063 033350 052765 172463
```



Time = 3.210e+001



Understanding Simulation Results from Supercomputers

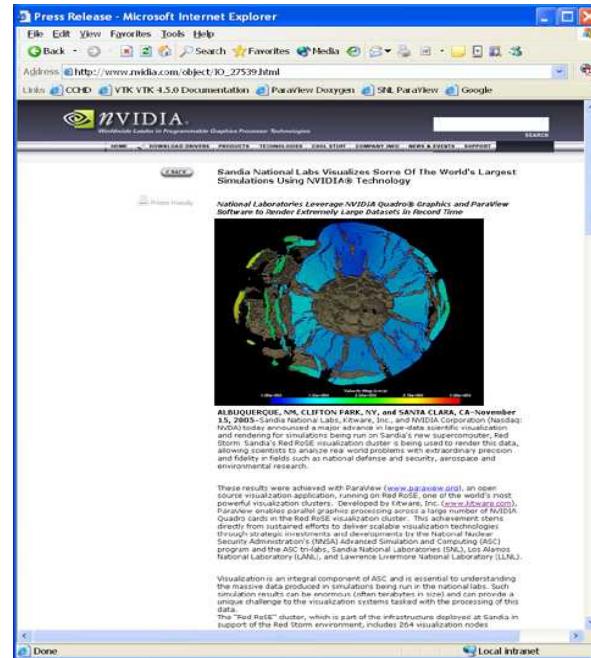
Key Issues Dealing with Simulation Data at Extreme Scales

- Data is always getting larger
 - Big jobs today are tomorrow's norm
- To understand data: data manipulation, queries, probes must work interactively
 - Should not inhibit discovery and questioning
 - Same functionality that exists for smaller data sets must exist at the extremes
- Visualization is important, but Data is central
 - Must provide means for quantitative analysis.

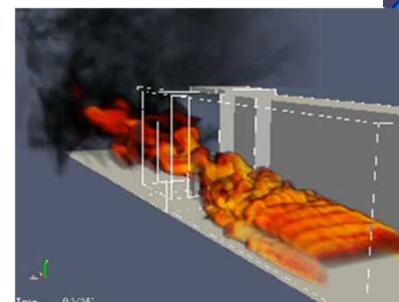
Delivering advanced capability to enable understanding of simulation results

ParaView

- Open-source parallel visualization and data analysis software toolkit
- Scalable framework for handling all sizes of data
 - From desktop to super computer simulation sizes
 - Scale in Resolution (desktop to power-wall)
 - Interactive data manipulation: probing, queries, etc...
- Enabled by Sandia's parallel visualization R&D
 - World rendering record: 8 billion triangles/second
 - Tested with over 256 parallel visualization nodes on Sandia's Red Rose Visualization Cluster
- Over 15,000 downloads/year around the world

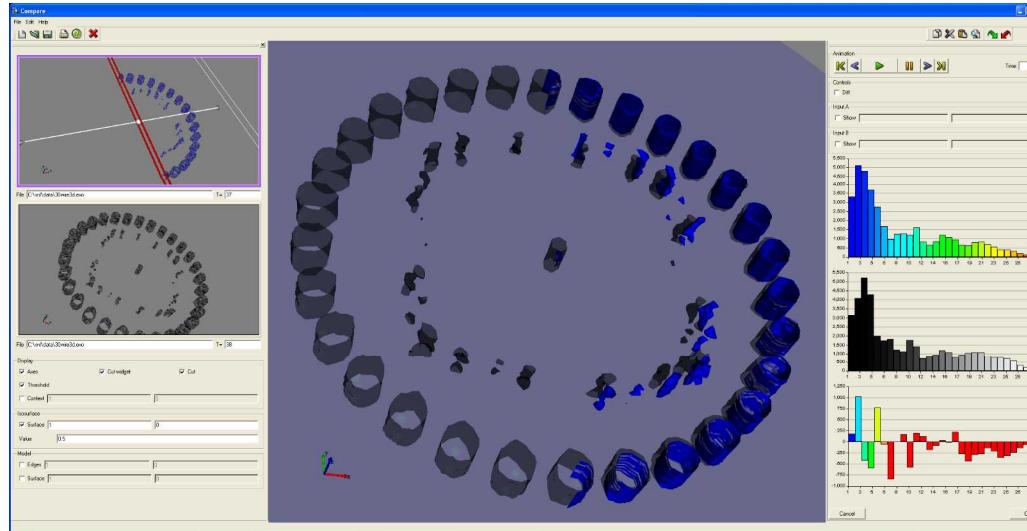


Joint NVIDIA and SNL Press Release





What's Next for Understanding Simulation Results?



Prototype next generation multi-view work for comparing multiple simulations and performing qualitative analysis

- **Data Drill Down Key for Scientists**
 - Improved methods for understand single element data values while maintaining contextual information about global simulation results.
- **Qualitative/Quantitative visualization integration**
 - Understanding data uncertainty
 - Representing thousands of calculation results as a single simulation
 - Integrating multiple sources of data including experimental and statistical results with simulation data

All while Maintaining and Improving Scalability

Discovery and Understanding of Data

Information Visualization

- Understanding large pieces of unstructured information
 - Clustering similar data entries
 - Text, reports, images, sound, movies, executables, etc.
 - **Example: Sandia strategically invests each year in its own portfolio of R&D. Is this investment working? Is it diverse? Are there Gaps? Trends?**
 - **Example: Homeland security. Who is talking to who? Where are they located? Similar information in different reports?**
- Using same scientific visualization infrastructure to achieve scalability
 - **Homeland security needs looking at Peta-bytes per day**

