SAND2008-0079P

Overview of the High Performance Computing Environment at Sandia

National Nuclear Security Administration

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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The Red Storm Supercomputer

National Nuclear Security Administration

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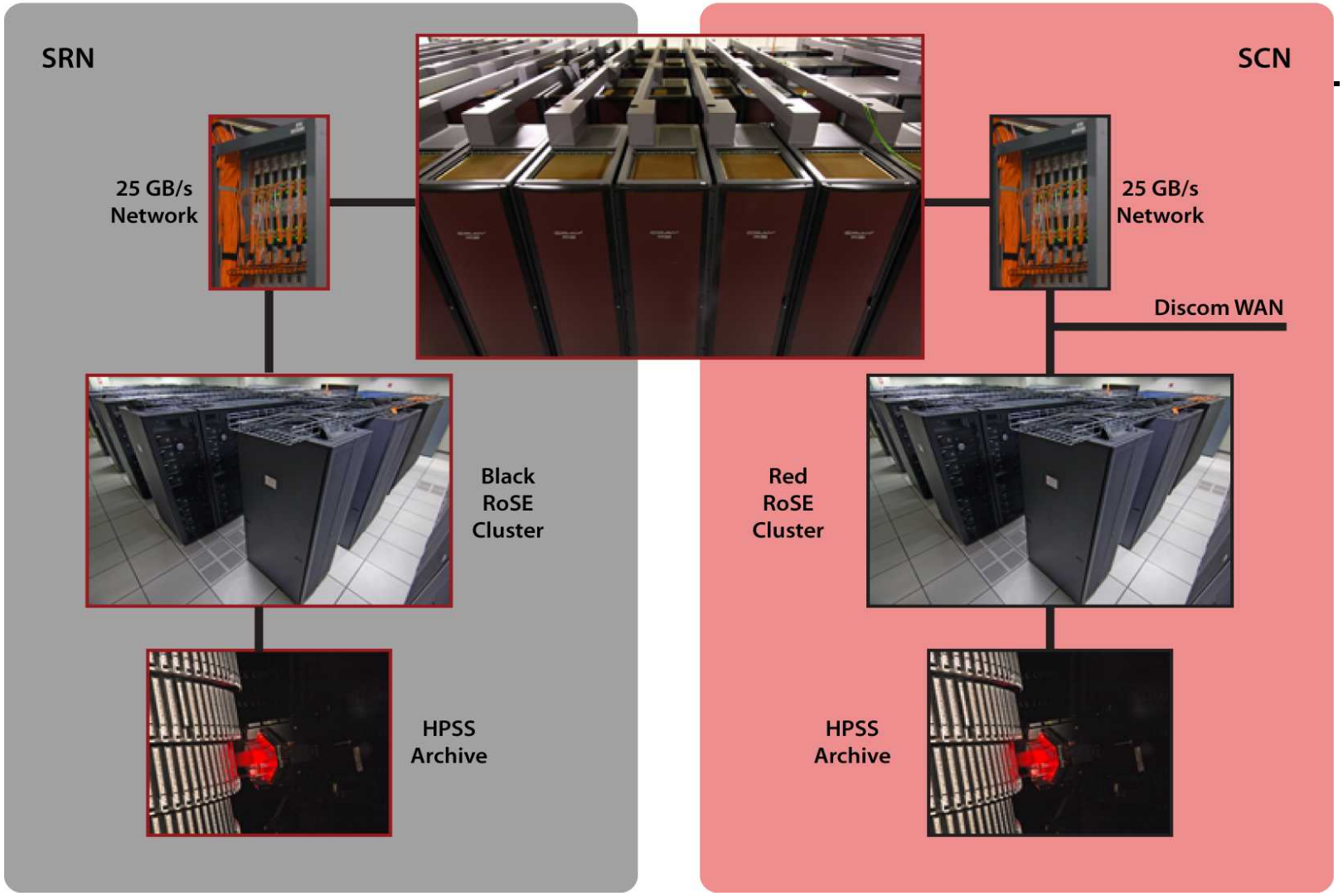
Red Storm Target Environment



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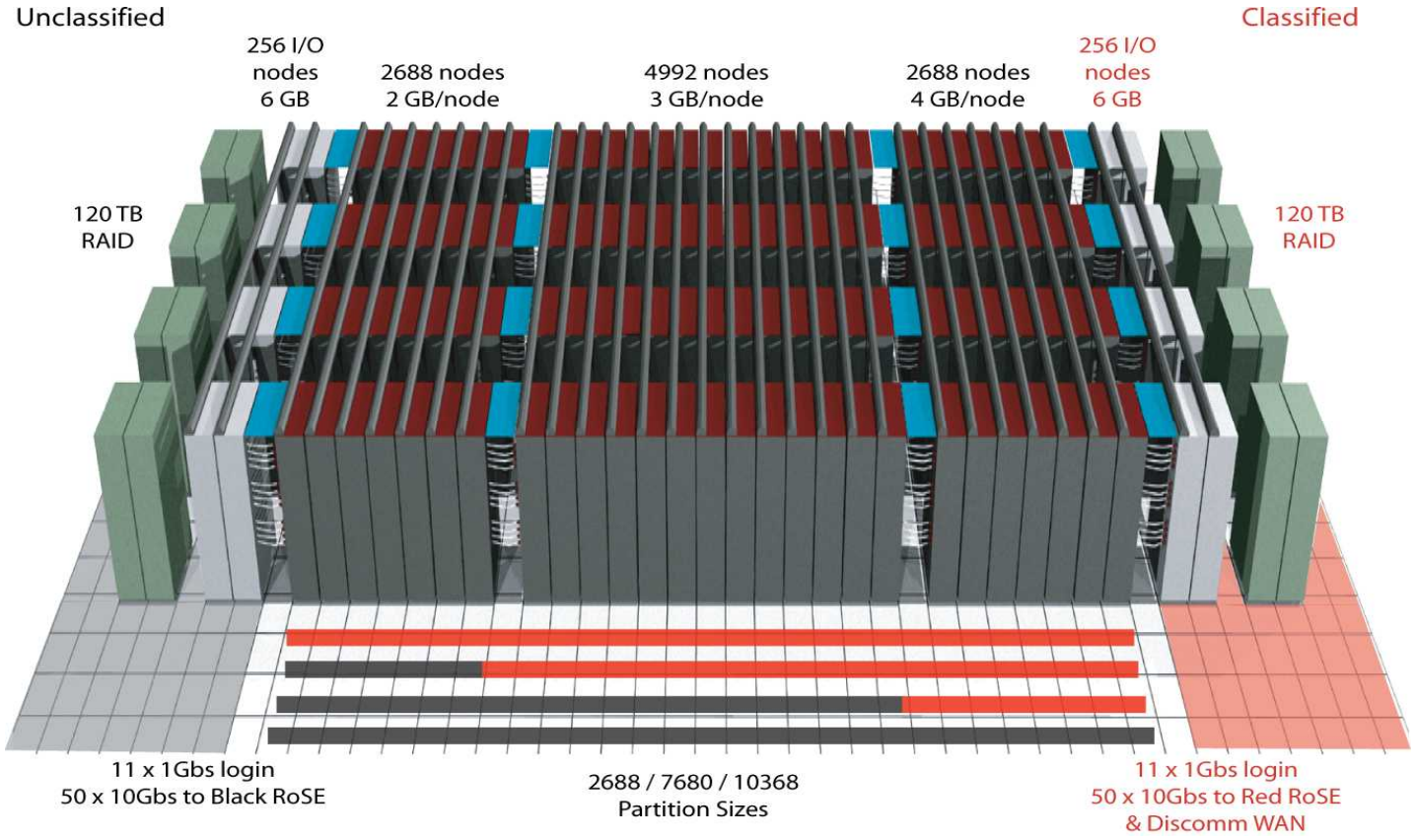
Red Storm System



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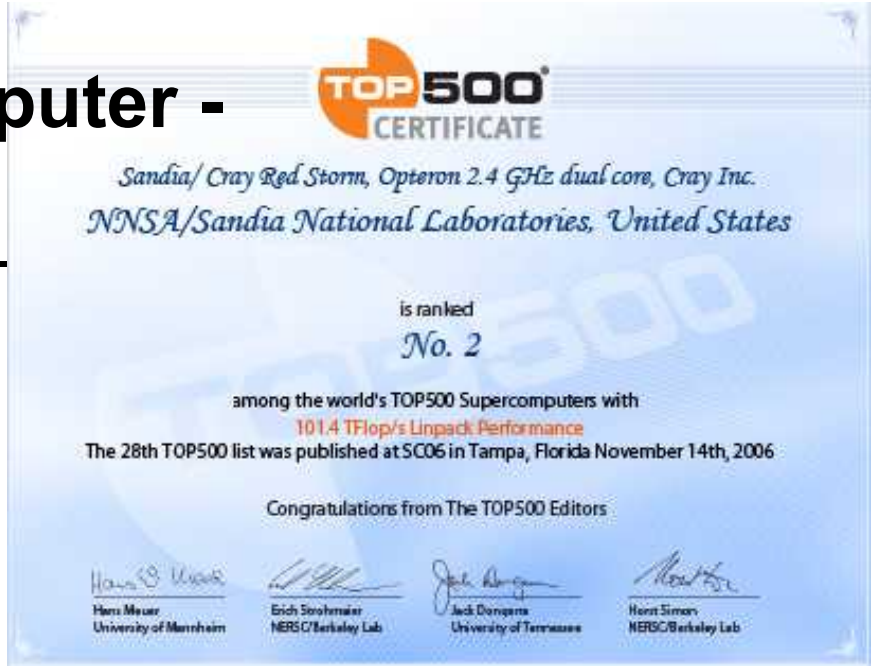
Red Storm Supercomputer - recently upgraded



- 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

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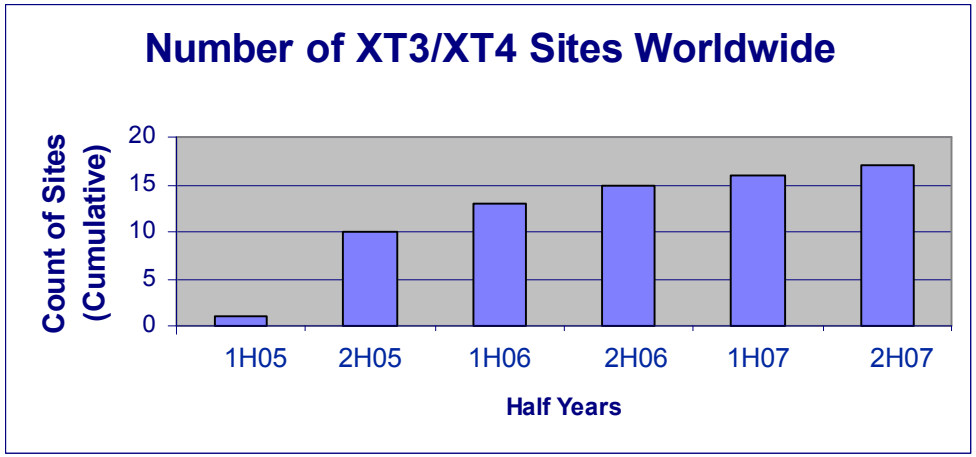
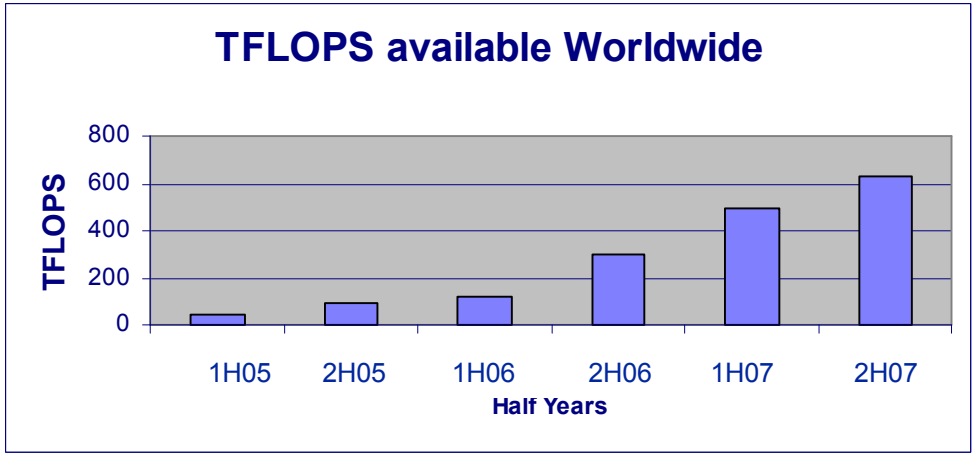
Red Storm technology has resulted in a Cray success story -- there are 17 sites with Cray XT3 or XT4 Computers Worldwide

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





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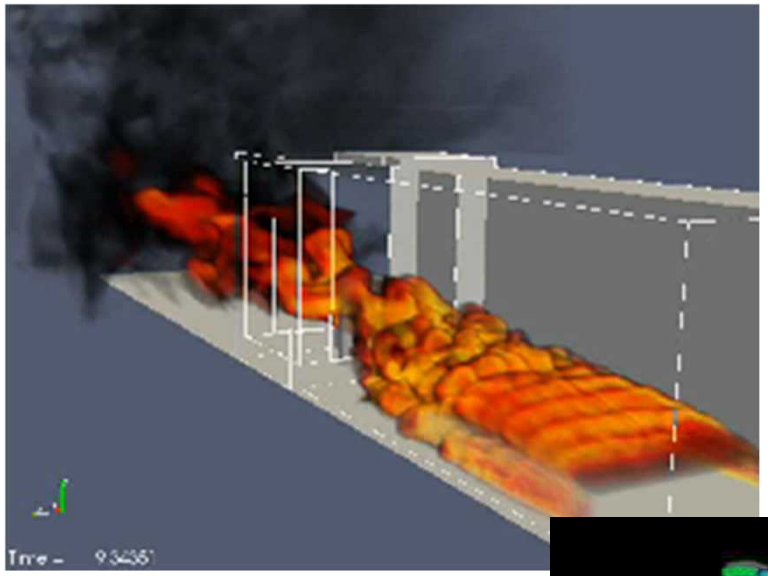
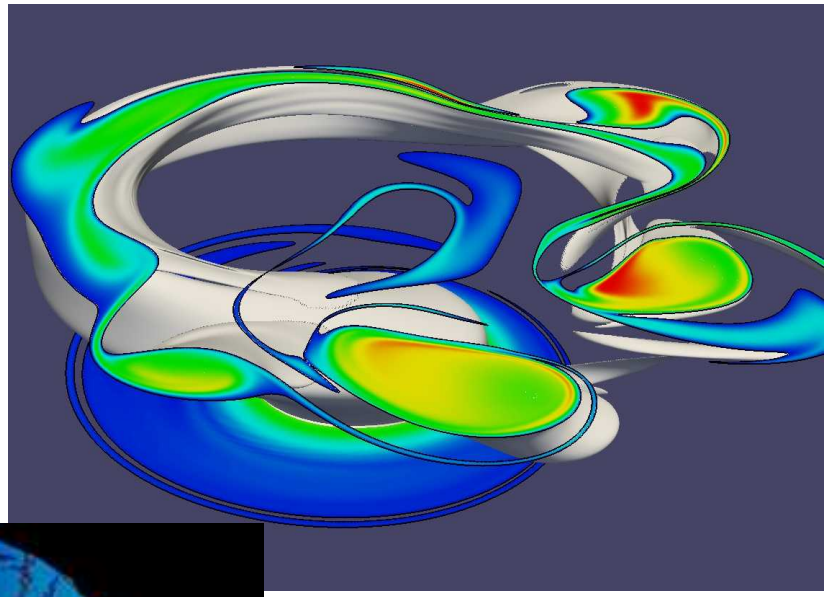
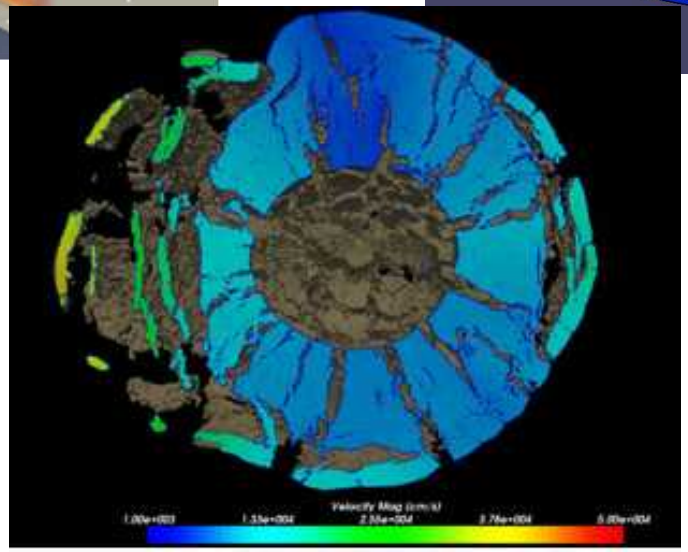
Red Storm Large-scale Simulation Visualizations



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)

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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.

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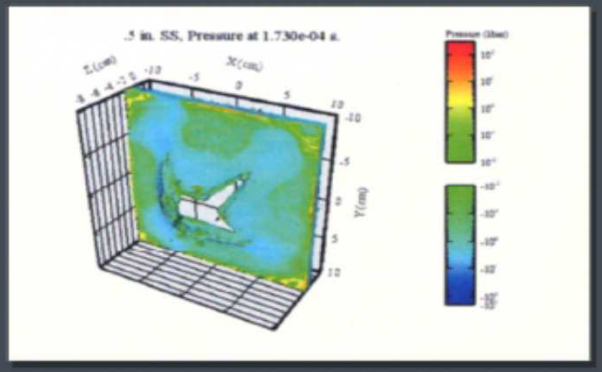
TBird Computation & Simulations

Thunderbird High Performance Computing

Computation, Simulation, Analysis, and Visualization

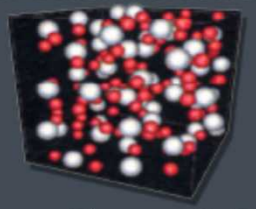


Explosive Sheet

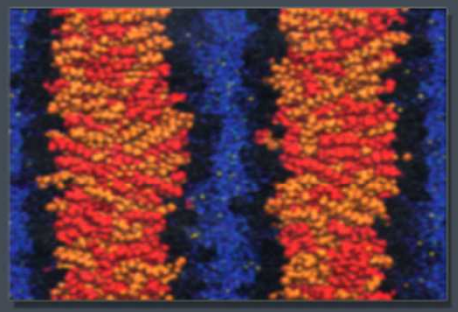
This simulation models the detonation of an explosive layer atop a metal sheet.

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.

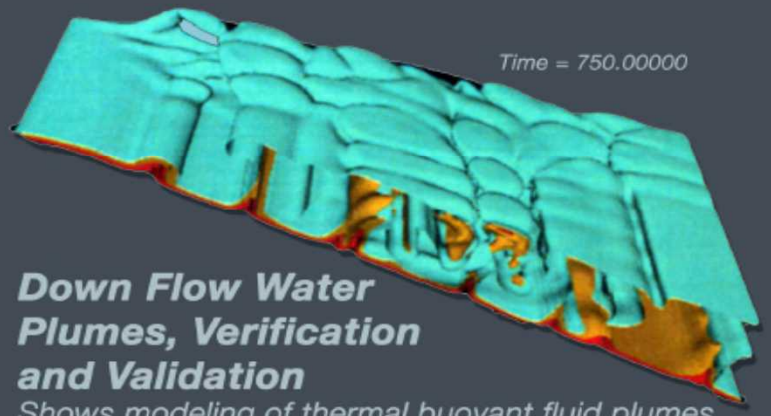
-Paul Crozier

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

TBird Computation & Simulations

Thunderbird High Performance Computing

Computation, Simulation, Analysis, and Visualization



Down Flow Water Plumes, Verification and Validation

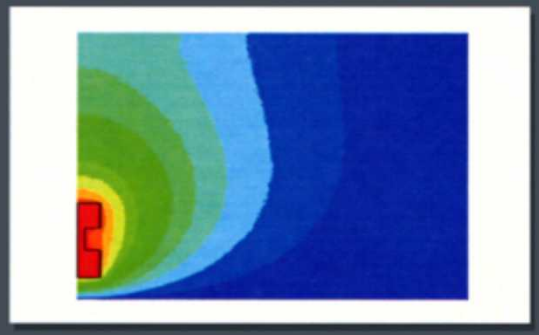
Shows modeling of thermal buoyant fluid plumes as they emerge from a lower heated surface of a transmission channel. The temperature field is tracked as the plumes impinge on a cylinder downstream in the channel.

-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

Visualization and Data, Dept. 4326

NNSA National Nuclear Security Administration

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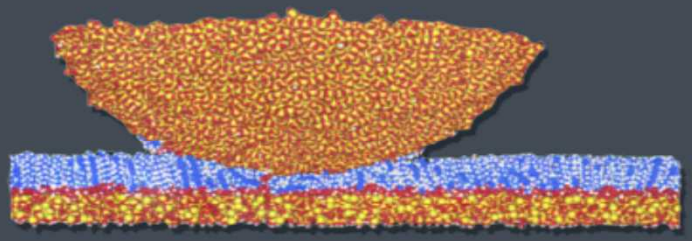
TBird Computation & Simulations

Thunderbird High Performance Computing

Computation, Simulation, Analysis, and Visualization



Micro Electro Mechanical Systems, Coating Friction and Adhesion

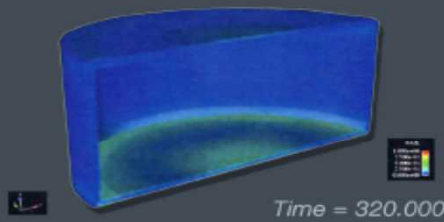
The tip of an Atomic Force Microscopy device interacts with a self-assembled mono-layer coating (blue carbon atoms and white hydrogen atoms) an amorphous Silica substrate (yellow silicon atoms and red oxygen atoms). The experiment measures the coating's tribolgical properties.

-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

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National Nuclear Security Administration

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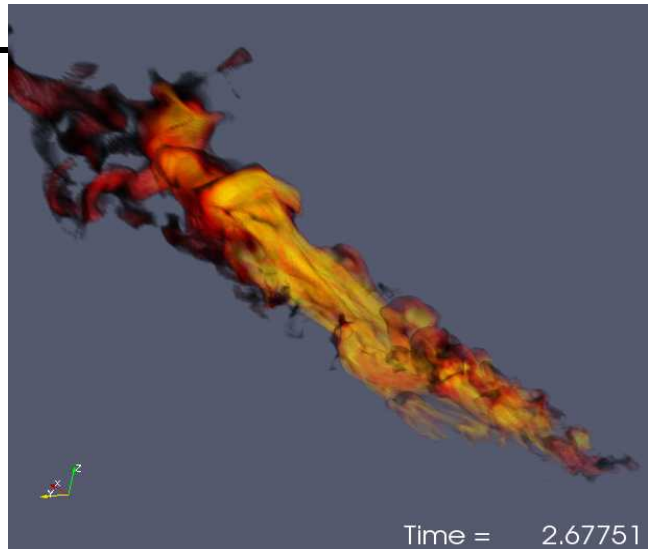
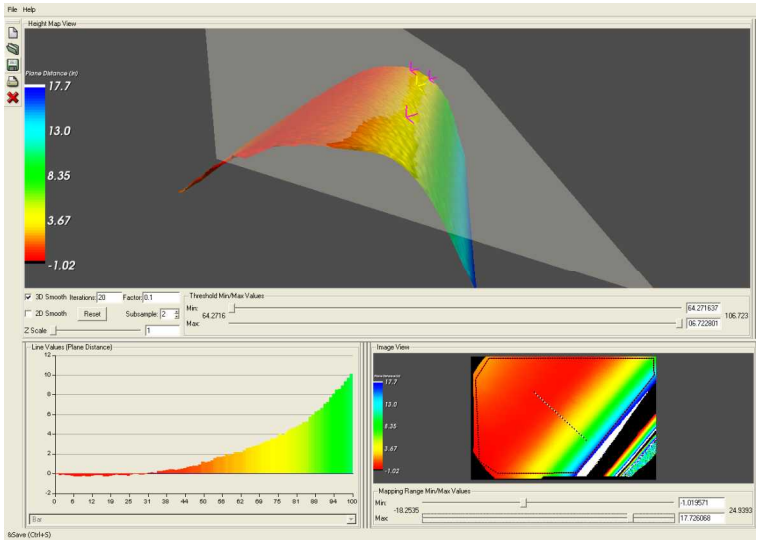
Data Analysis / Visualization Capabilities

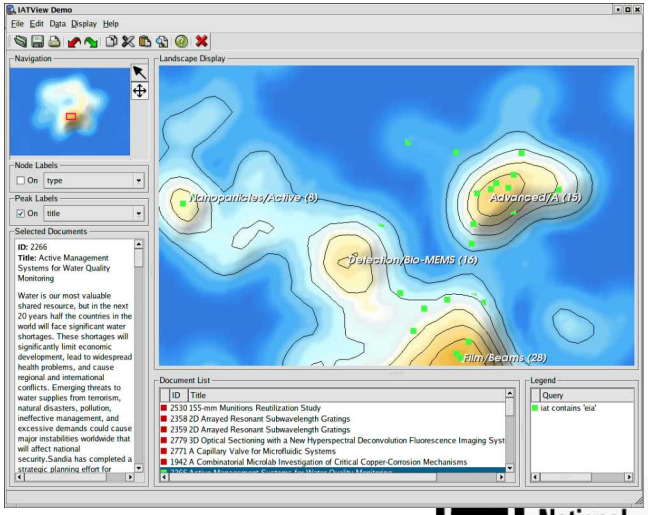
- **Scientific Visualization and Data Analysis**
- **Information Visualization**
- **Image Analysis**



Pool Fire Simulation



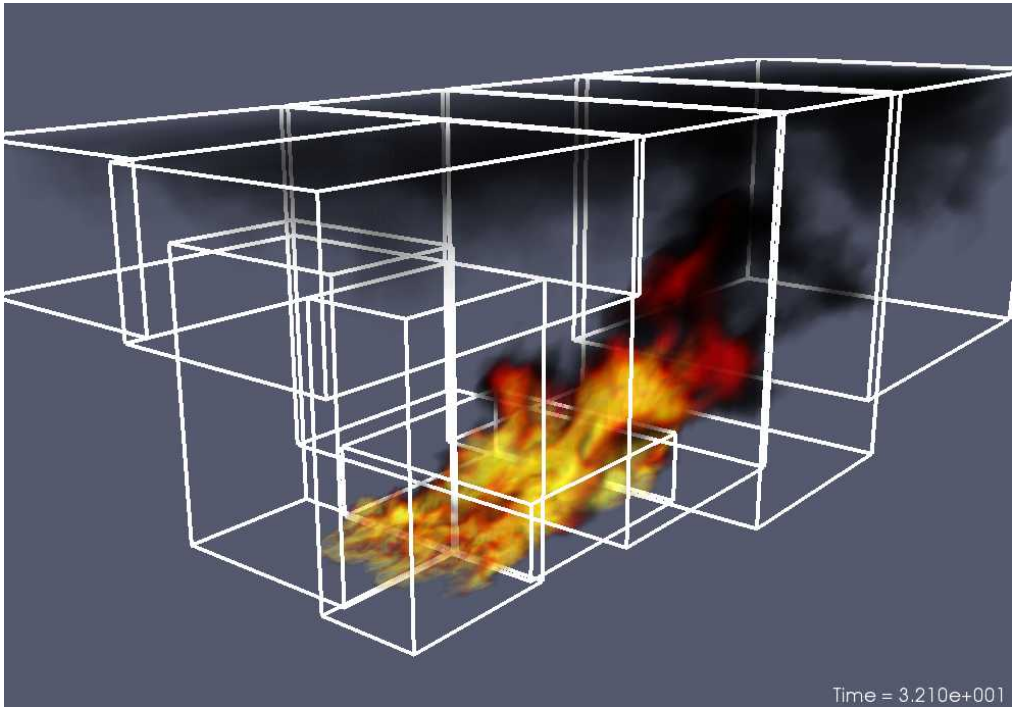
NASA Application



Information Visualization

National Laboratories

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



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Understanding Simulation Results from Supercomputers

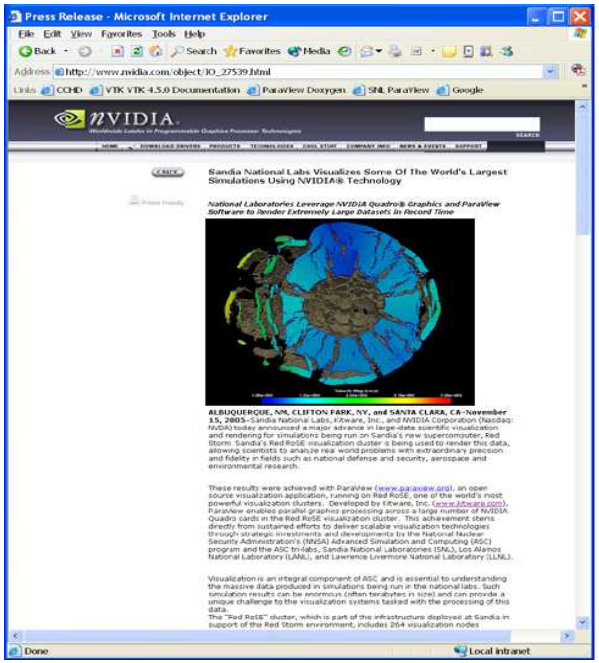
Key Issues Dealing with Simulation Data at Extreme Scales

- 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.

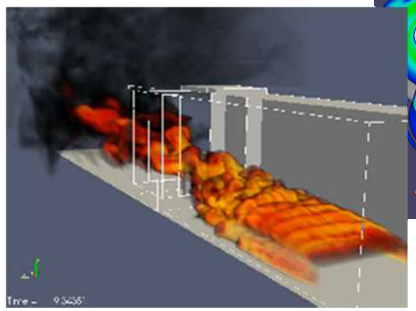
Delivering advanced capability to enable understanding of simulation results

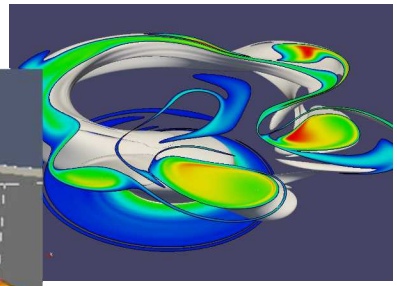
ParaView

- 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





Advanced Simulation & Computing™

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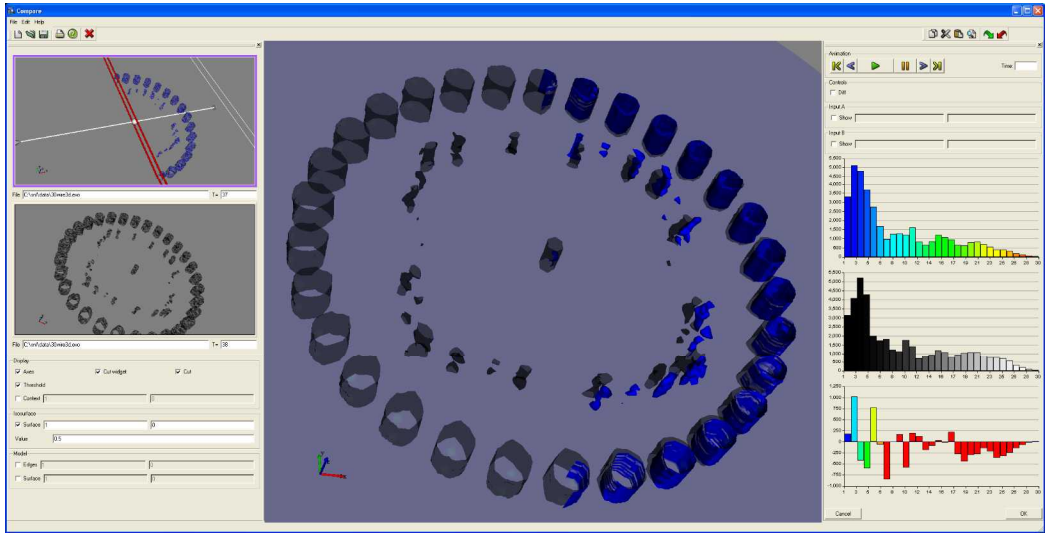
What's Next for Understanding Simulation Results?



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

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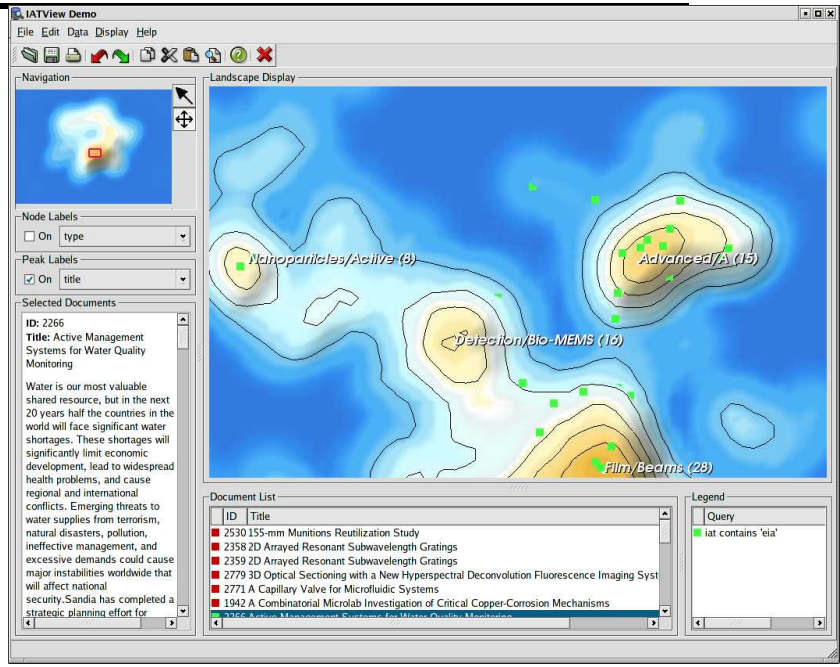
Discovery and Understanding of Data

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



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