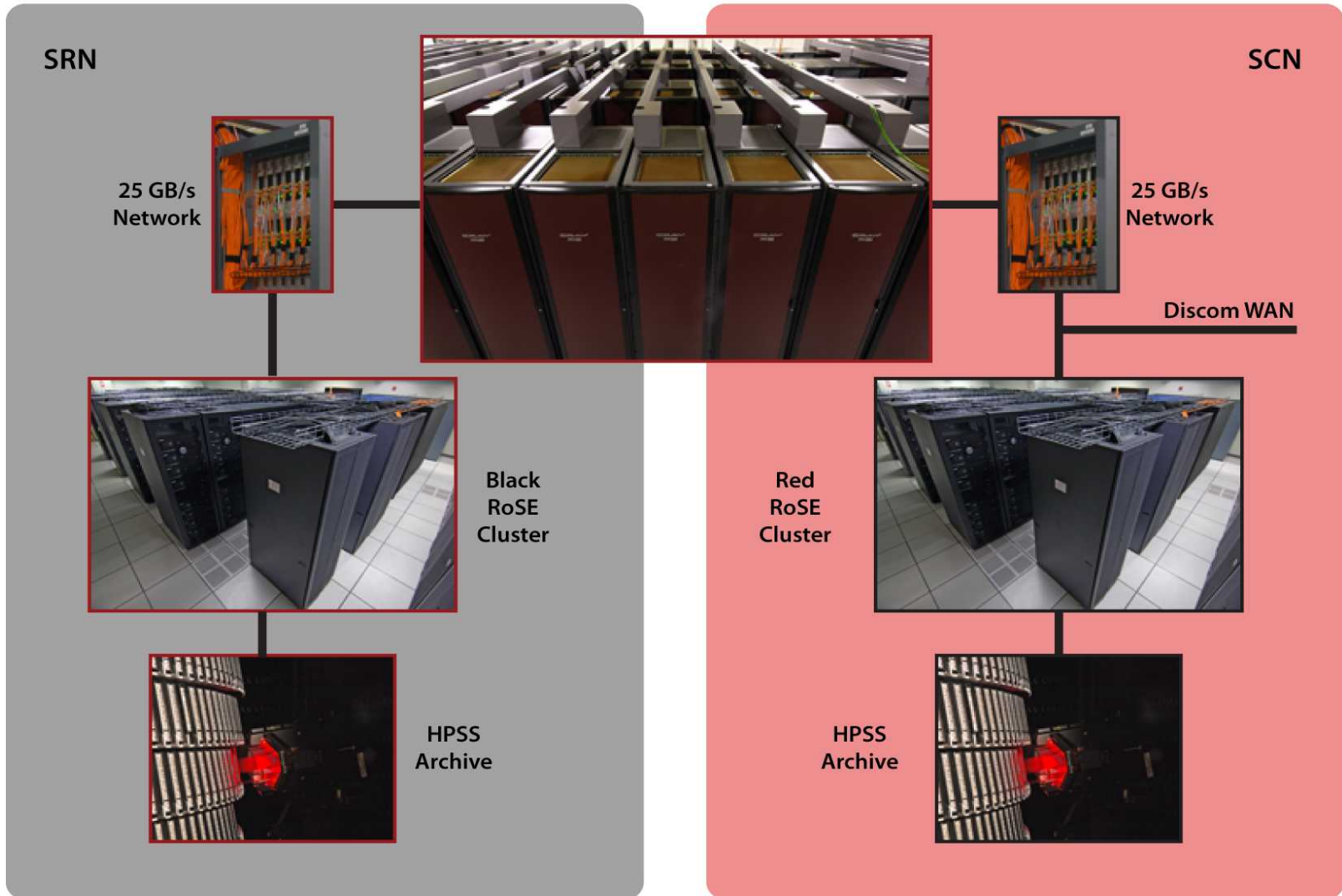


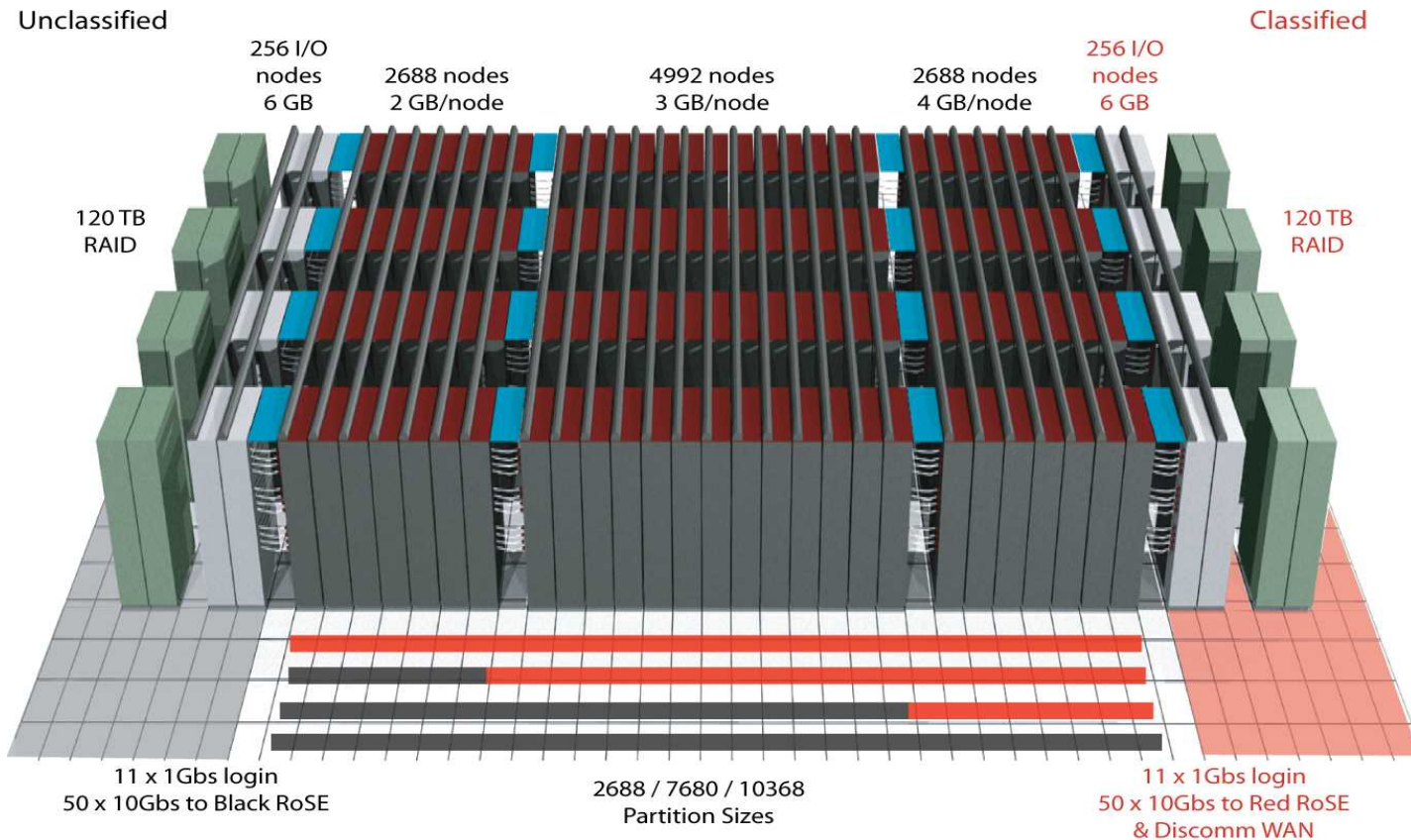
# Overview of the High Performance Computing Environment at Sandia

# The Red Storm Supercomputer

# Red Storm Target Environment



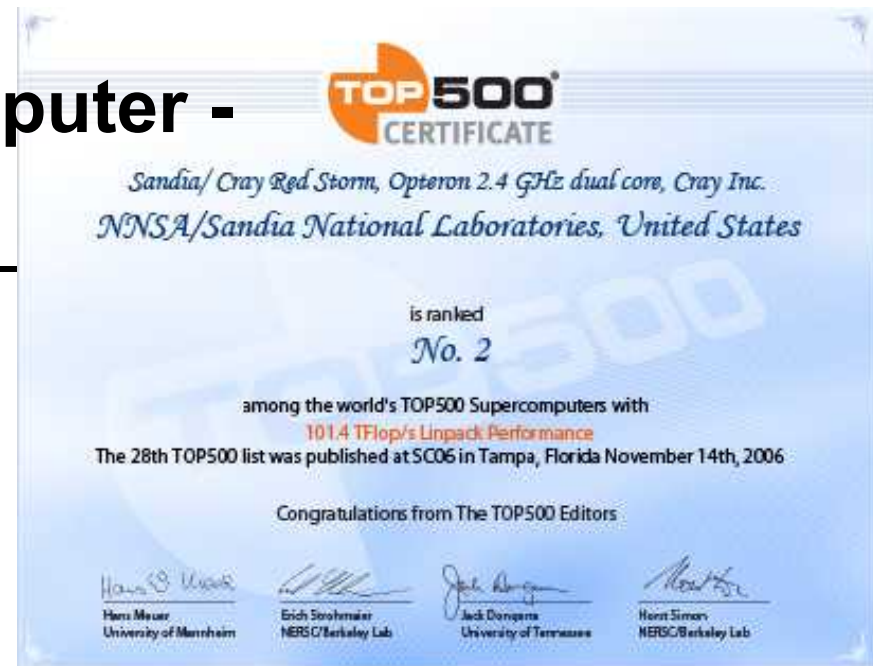
# Red Storm System





# 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

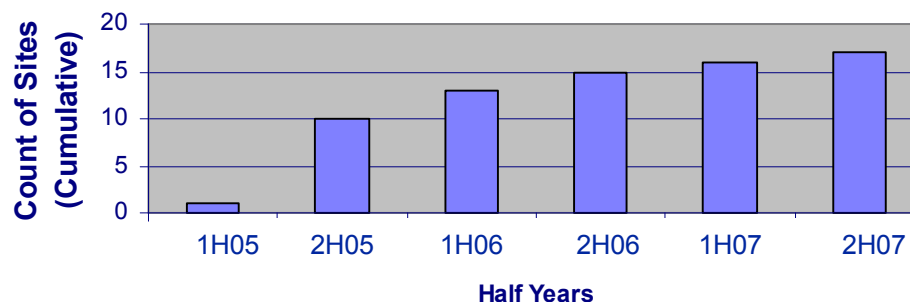
SS-643

SS-661

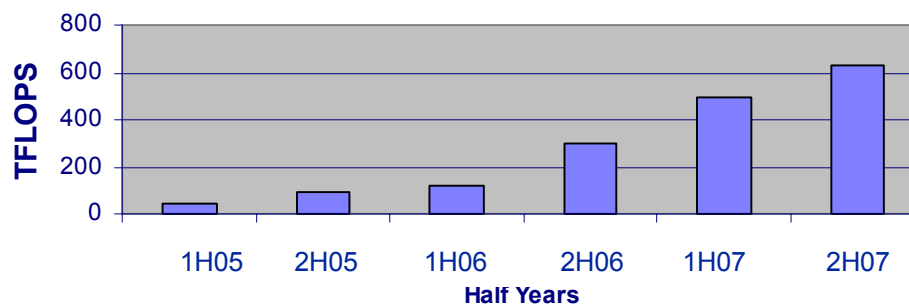
U OF TOKYO (JST)

U of Western Australia

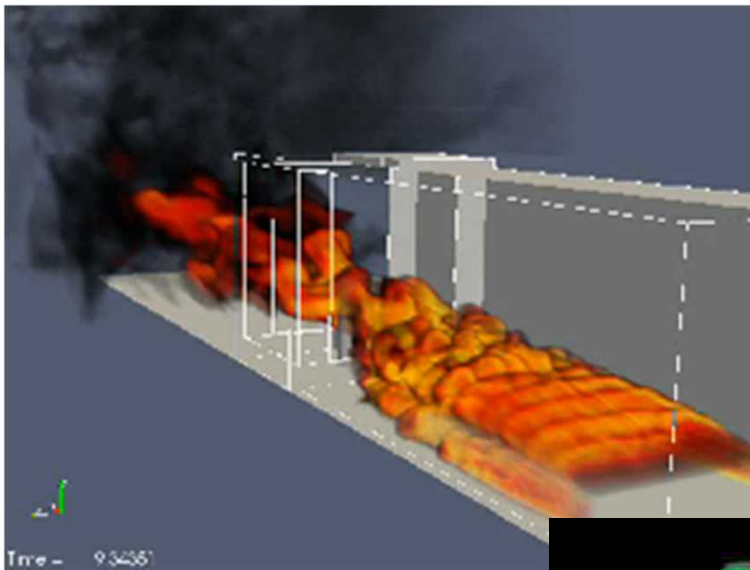
## Number of XT3/XT4 Sites Worldwide



## TFLOPS available Worldwide

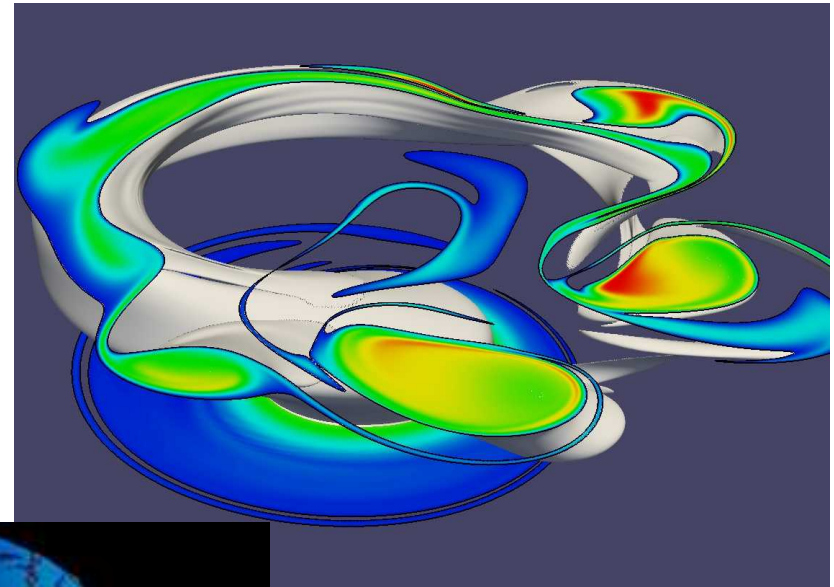
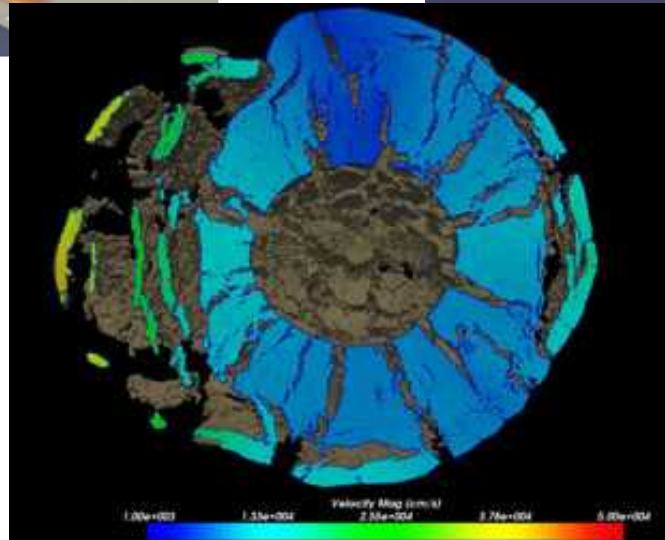


# Red Storm Large-scale Simulation Visualizations



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

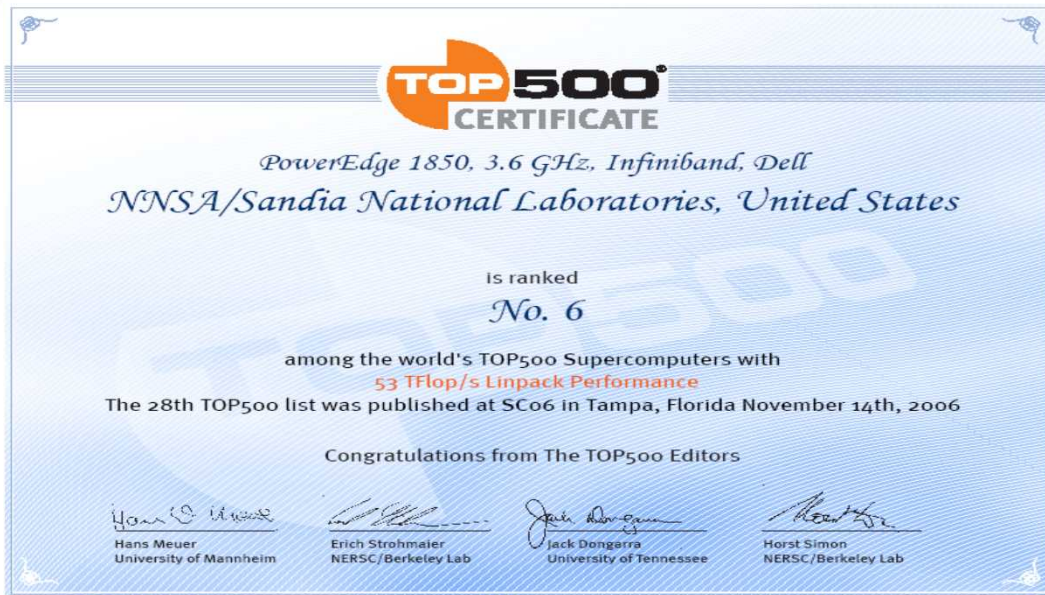
**Golevka Asteroid Destruction,  
simulation of 10 Megaton Blast  
at center of mass (>1 billion  
cells, 15 hrs. on 7200 nodes of  
Red Storm)**



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



# The Thunderbird Linux Cluster



## Linpack results:

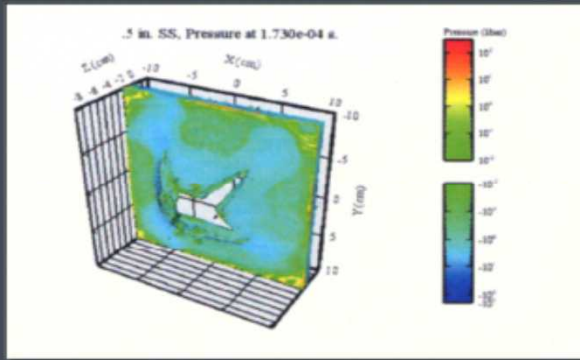
- 53 TFlops
- 84.66% efficiency
- 9.44 hours
- 8654 processors
- Infiniband interconnect  
(Open Fabrics / Open MPI)

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



# TBird Computation & Simulations

## **Thunderbird High Performance Computing** *Computation, Simulation, Analysis, and Visualization*

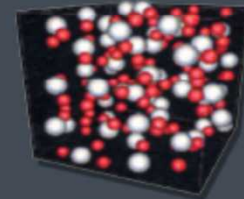


### **Explosive Sheet**

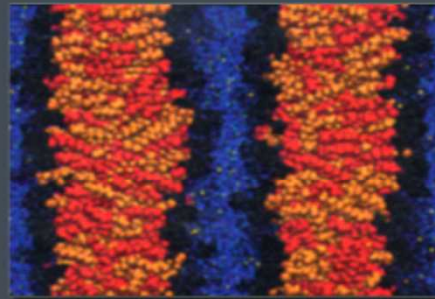
*This simulation models the detonation of an explosive layer atop a metal sheet.*

### **168 Atoms**

*Animation of water molecules.*



-Thomas Mattsson



### **Two Lipid Bilayers**

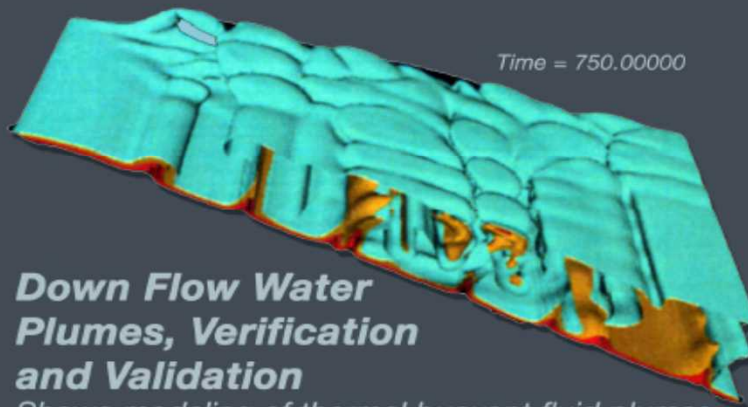
*This biomolecular simulation of two lipid bilayers separated by salt water explores the origins of long-range bilayer interactions.*

-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**

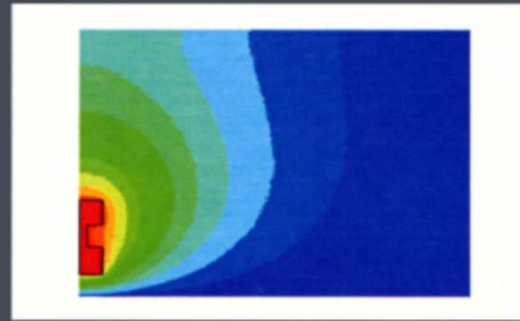
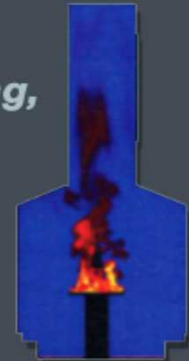
Shows modeling of thermal buoyant fluid plumes as they emerge from a lower heated surface of a transmission channel. The temperature field is tracked as the plumes impinge on a cylinder downstream in the channel.

-Greg Evans

### **Fuego Calore Coupling, V and V**

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

-Amalia Black



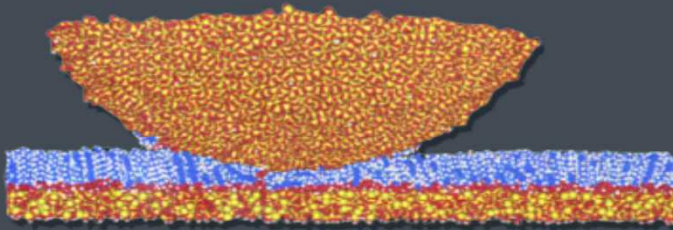
### **Thermal Wave Simulation**

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

-Michael Gallis

# TBird Computation & Simulations

## **Thunderbird High Performance Computing** *Computation, Simulation, Analysis, and Visualization*



### **Micro Electro Mechanical Systems, Coating Friction and Adhesion**

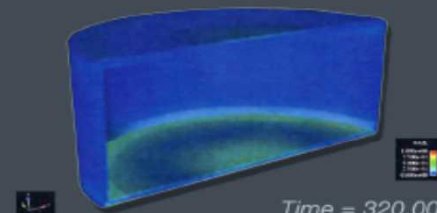
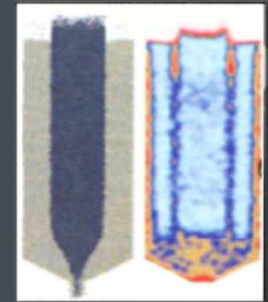
The tip of an Atomic Force Microscopy device interacts with a self-assembled mono-layer coating (blue carbon atoms and white hydrogen atoms) an amorphous Silica substrate (yellow silicon atoms and red oxygen atoms). The experiment measures the coating's tribological properties.

-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**

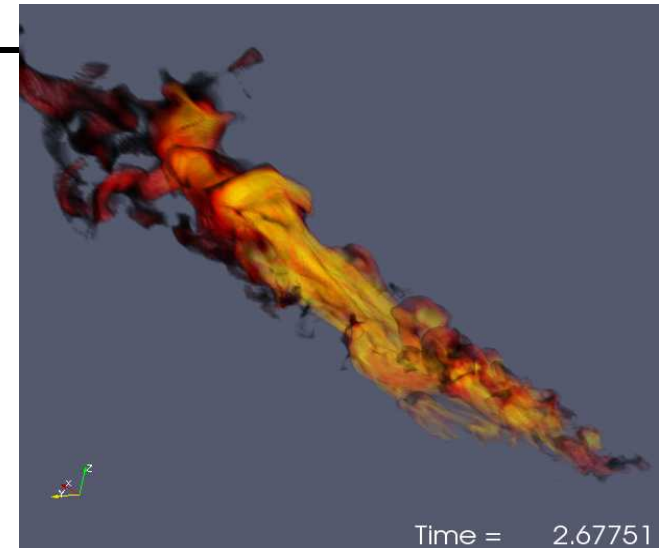
A validation and verification of Thermal Mechanical Coupled Physics showing container failure as a result of chemical pressure loading.

-Shane Schumacher

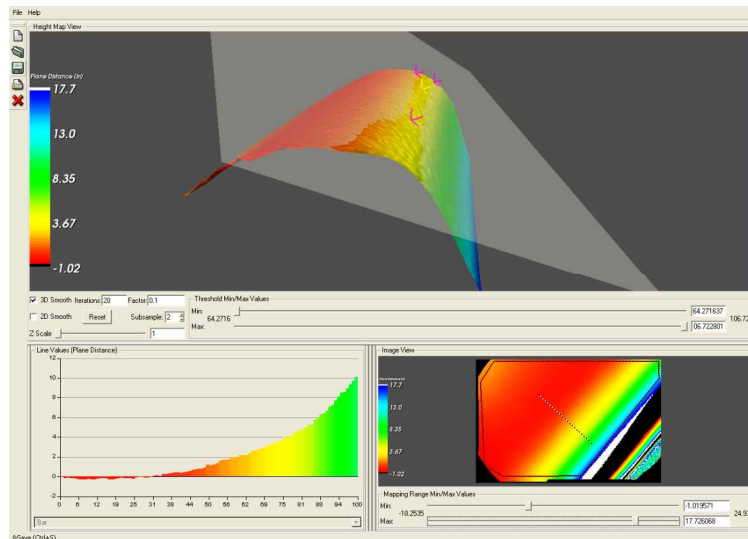
Visualization and Data, Dept. 4326

# Data Analysis / Visualization Capabilities

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



Pool Fire Simulation



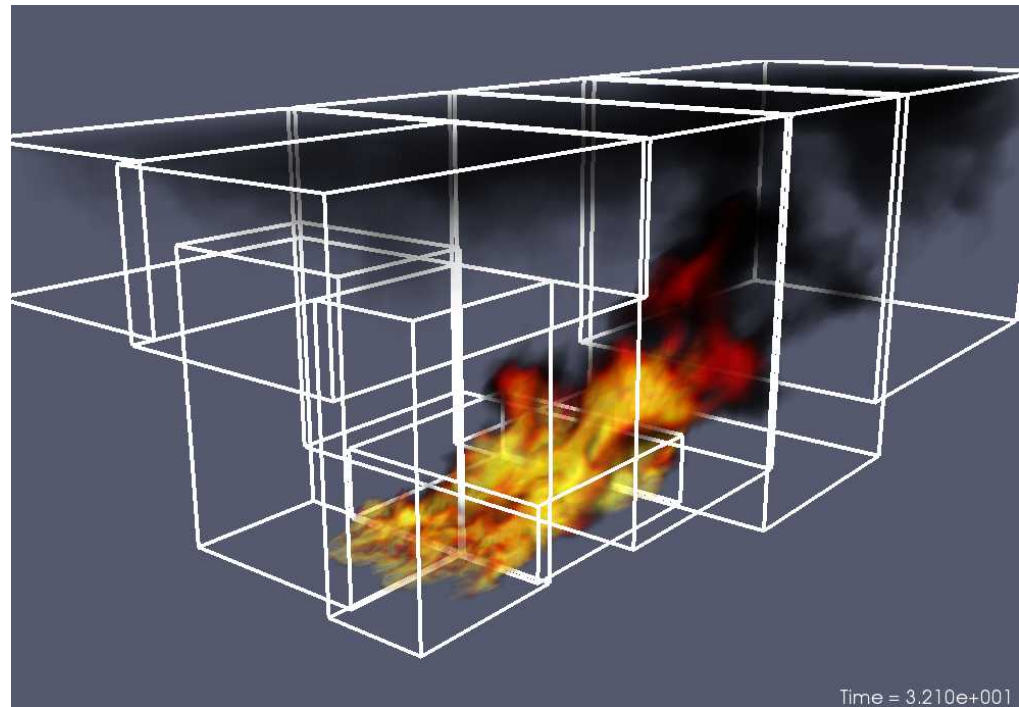
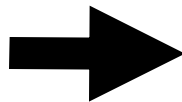
NASA Application

Information Visualization



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

```
0265640 132304 133732 032051 037334 024721 015013 052226 001662
0265660 025537 064663 054606 043244 074076 124153 135216 126614
0265700 144210 056426 044700 042650 165230 137037 003655 006254
0265720 134453 124327 176005 027034 107614 170774 073702 067274
0265740 072451 007735 147620 061084 157435 113057 155356 114603
0265760 107204 102316 171451 045040 120223 001974 030477 046673
0266000 171317 116055 155117 134444 167210 041405 147127 050505
0266020 004137 046472 124015 134360 173550 053517 044635 021135
0266040 070175 047705 113754 175477 105532 076515 177366 056333
0266060 041023 074017 127113 003214 037026 037640 066171 123424
0266100 067701 037406 140000 165341 072410 100032 125455 056646
0266120 006716 071402 055672 132571 105645 170073 050376 072117
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0266560 166410 067251 156160 106406 136770 030516 064740 022032
0266600 142166 123707 175121 071170 076357 037233 031136 015232
0266620 075074 016744 044055 102230 110063 033350 052765 172463
```



Time = 3.210e+001



# Understanding Simulation Results from Supercomputers

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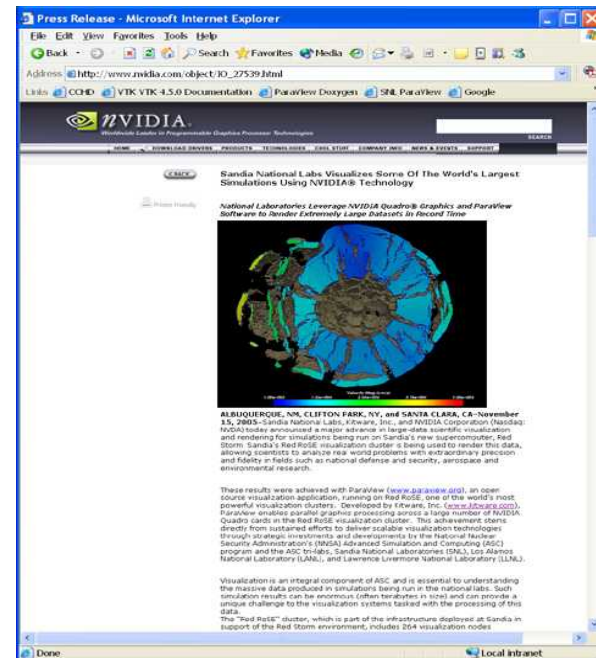
## Key Issues Dealing with Simulation Data at Extreme Scales

- 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.

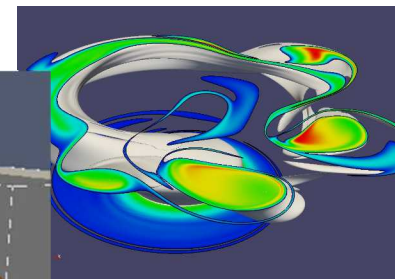
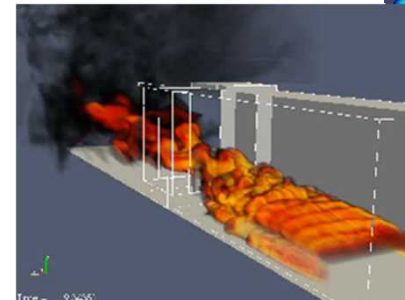
# Delivering advanced capability to enable understanding of simulation results

## ParaView

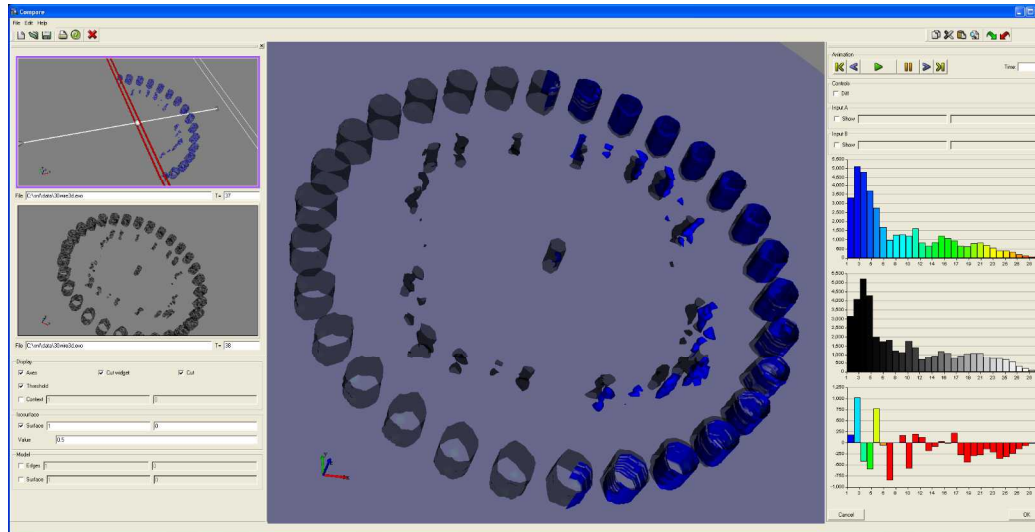
- Open-source parallel visualization and data analysis software toolkit
- Scalable framework for handling all sizes of data
  - From desktop to super computer simulation sizes
  - Scale in Resolution (desktop to power-wall)
  - Interactive data manipulation: probing, queries, etc...
- Enabled by Sandia's 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

