Parallel Computing for Science & Engineering SSC 374/394c

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Instructors:

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TACC Mission & Strategic Approach

To enable discoveries that advance science and society through the application of advanced computing technologies.

- Resources & Services
  - Evaluate, acquire & operate world-class resources
  - Provide expert support via leading technology expertise
- Research & Development
  - Produce new computational technologies and techniques
  - Collaborate with researchers to apply advanced computing technologies in science projects

TACC Technology Focus Areas

- High Performance Computing (HPC)
  - Applications
  - Performance and Architectures
  - Software Tools
- Visualization
  - Scalable Visualization Technologies
  - Visualization Interfaces and Technologies
- Advanced Computing Interfaces
  - Web and Cloud Services
  - Web and Mobile Applications

THE GRAND CHALLENGE EQUATIONS

$$B_i A_i = E_i A_i + \rho_i \sum_j B_j A_j F_{ji}$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{F} = m\,\vec{a} + \frac{dm}{dt}\vec{v}$$

$$dU = \left(\frac{\partial U}{\partial S}\right)_V dS + \left(\frac{\partial U}{\partial V}\right)_S dV$$

$$\nabla \cdot \vec{D} = \rho$$

$$Z = \sum_j g_j\, e^{-E_j/kT}$$

$$F_j = \sum_{k=0}^{N-1} f_k e^{2\pi i jk/N}$$

$$\nabla^2 u = \frac{\partial u}{\partial t}$$

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J}$$

$$p_{n+1} = r\, p_n\, (1 - p_n)$$

$$\nabla \cdot \vec{B} = 0$$

$$P(t) = \frac{\sum_i W_i\, B_i(t)\, P_i}{\sum_i W_i\, B_i(t)}$$

$$-\frac{h^2}{8\pi^2 m}\nabla^2 \Psi(r,t) + V\,\Psi(r,t) = -\frac{h}{2\pi i}\frac{\partial \Psi(r,t)}{\partial t}$$

$$-\nabla^2 u + \lambda\, u = f$$

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\,\vec{u} = -\frac{1}{\rho}\nabla p + \gamma\,\nabla^2 \vec{u} + \frac{1}{\rho}\vec{F}$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f$$

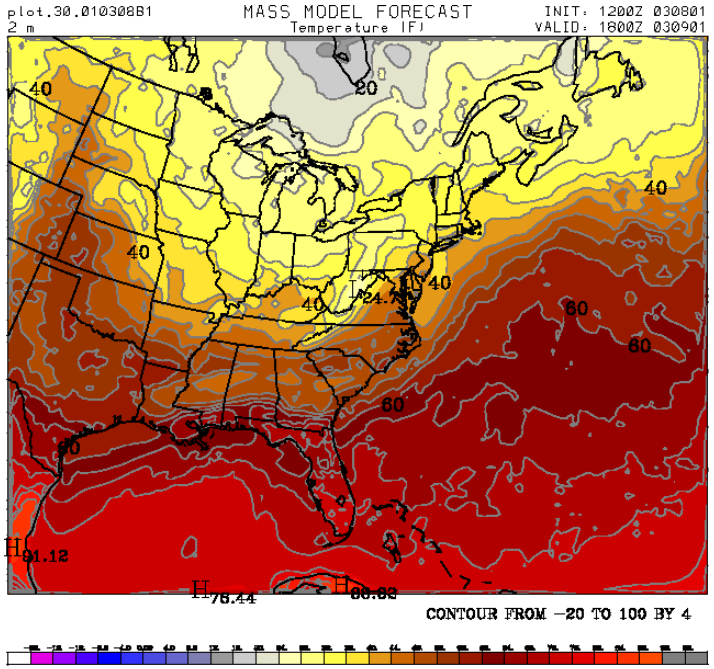
• NEWTON'S EQUATIONS • SCHROEDINGER EQUATION (TIME DEPENDENT) • NAVIER-STOKES EQUATION •
• POISSON EQUATION • HEAT EQUATION • HELMHOLTZ EQUATION • DISCRETE FOURIER TRANSFORM •
• MAXWELL'S EQUATIONS • PARTITION FUNCTION • POPULATION DYNAMICS •
• COMBINED 1ST AND 2ND LAWS OF THERMODYNAMICS • RADIOSITY • RATIONAL B-SPLINE •

[Courtesy of San Diego Supercomputer Center]

Examples of Scientific Computing
(*it really is everywhere*)

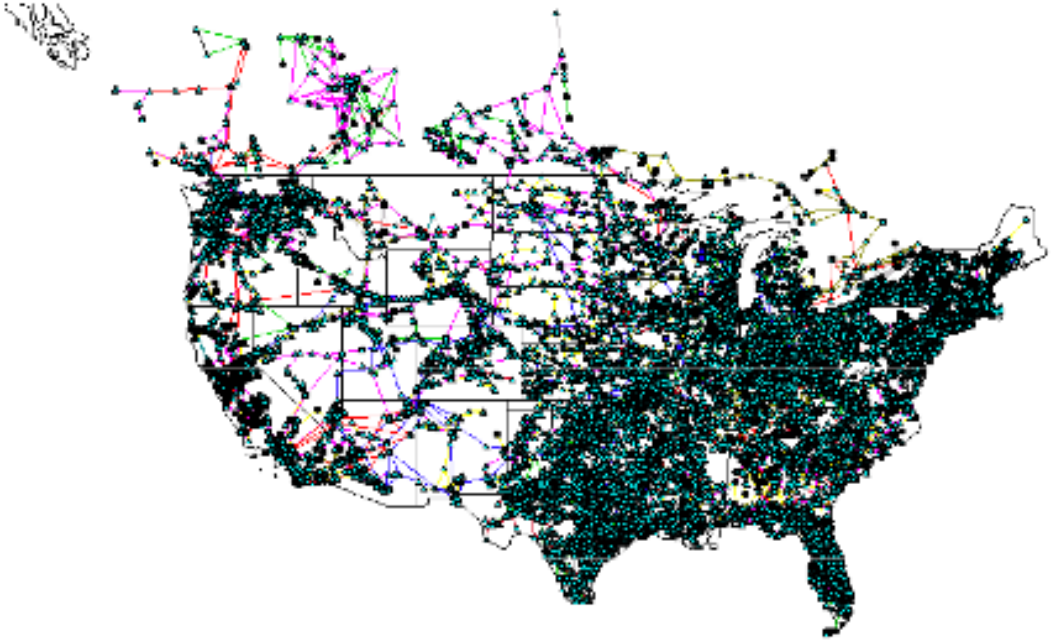
Aerospace

F18 Store Separation



Weather Forecasting

New kinds of computations



The New York Times
Thursday, September 4, 2008

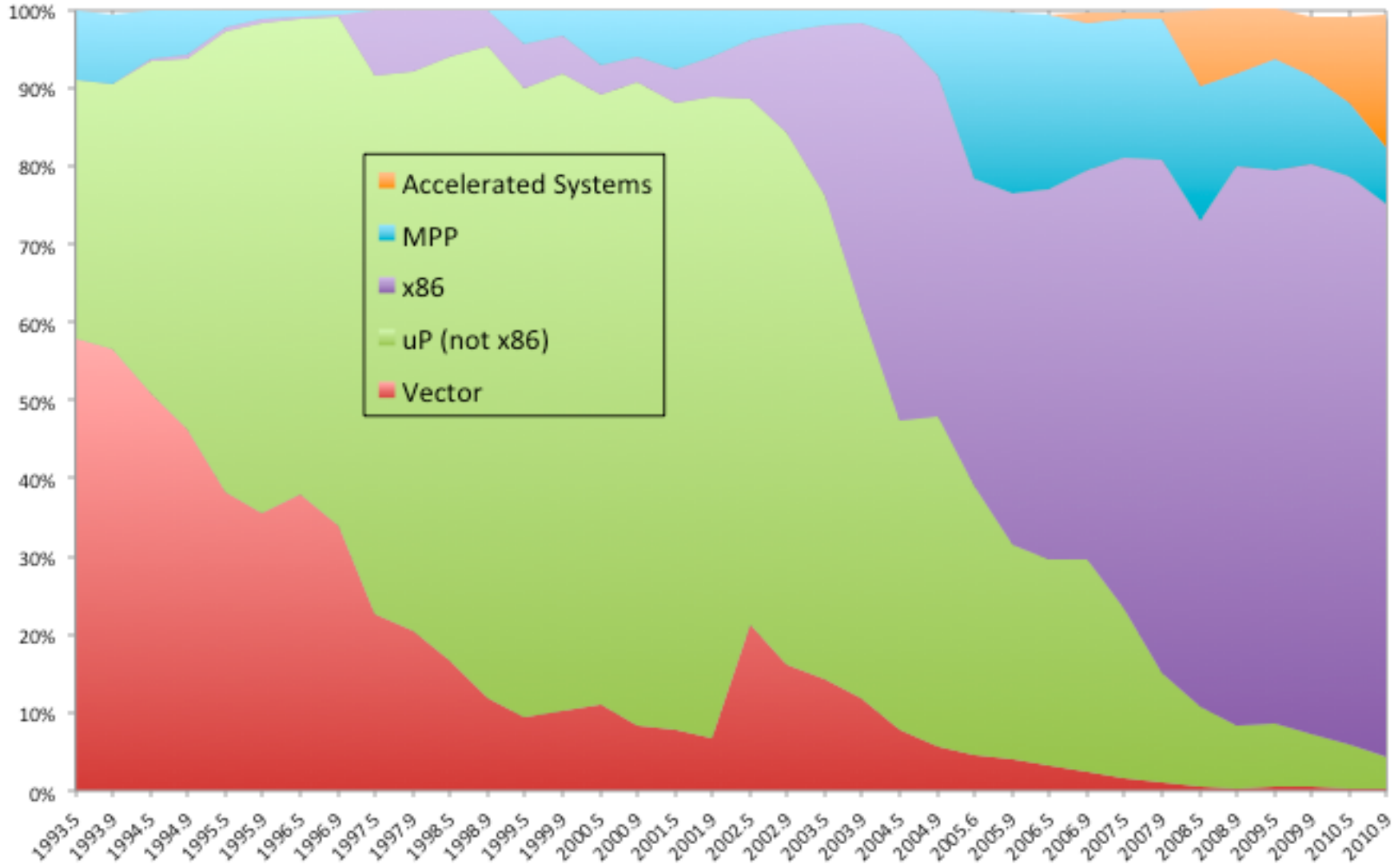
Report on Blackout Is Said To Describe Failure to React

By MATTHEW L. WALD
Published: November 12, 2003

A report on the Aug. 14 blackout identifies specific lapses by various parties, including FirstEnergy's failure to react properly to the loss of a transmission line, people who have seen drafts of it say.

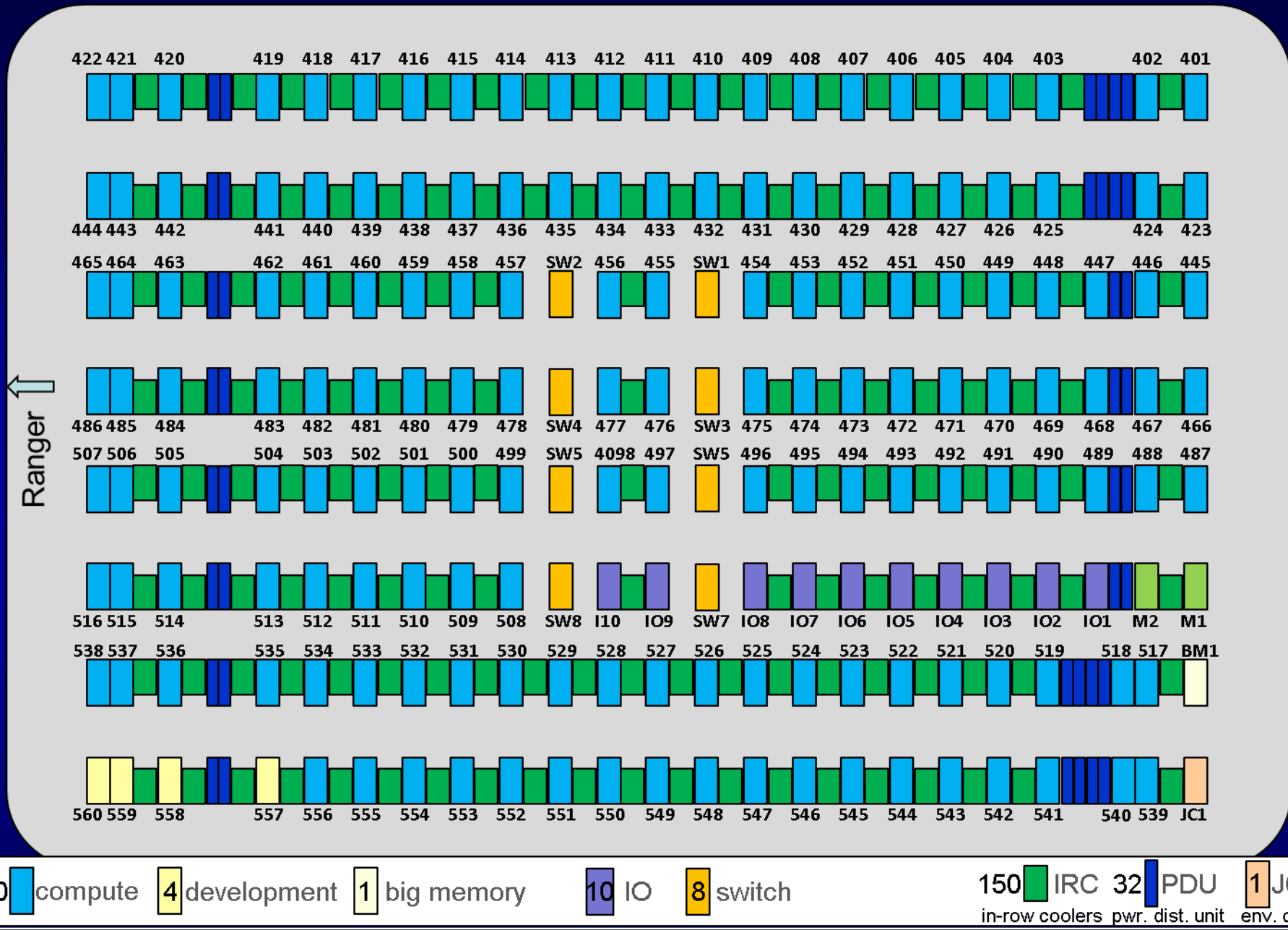
A working group of experts from eight states and Canada will meet in private on Wednesday to evaluate the report, people involved in the

Top500 by Overall Architecture



Stampede

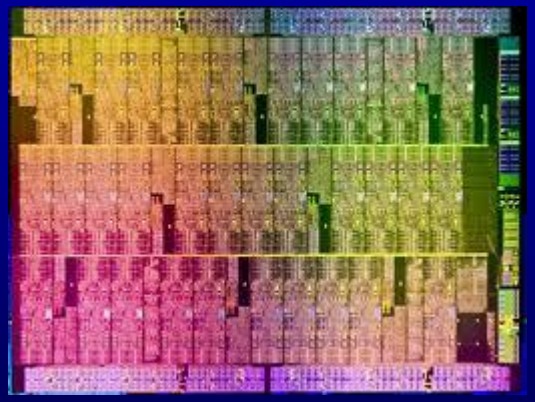
- NSF 11-511: “High Performance Computing System Acquisition: Enhancing the Petascale Computing Environment for Science and Engineering”
- Enable sustained petascale computational and data-driven science and engineering and provide an “innovative component”

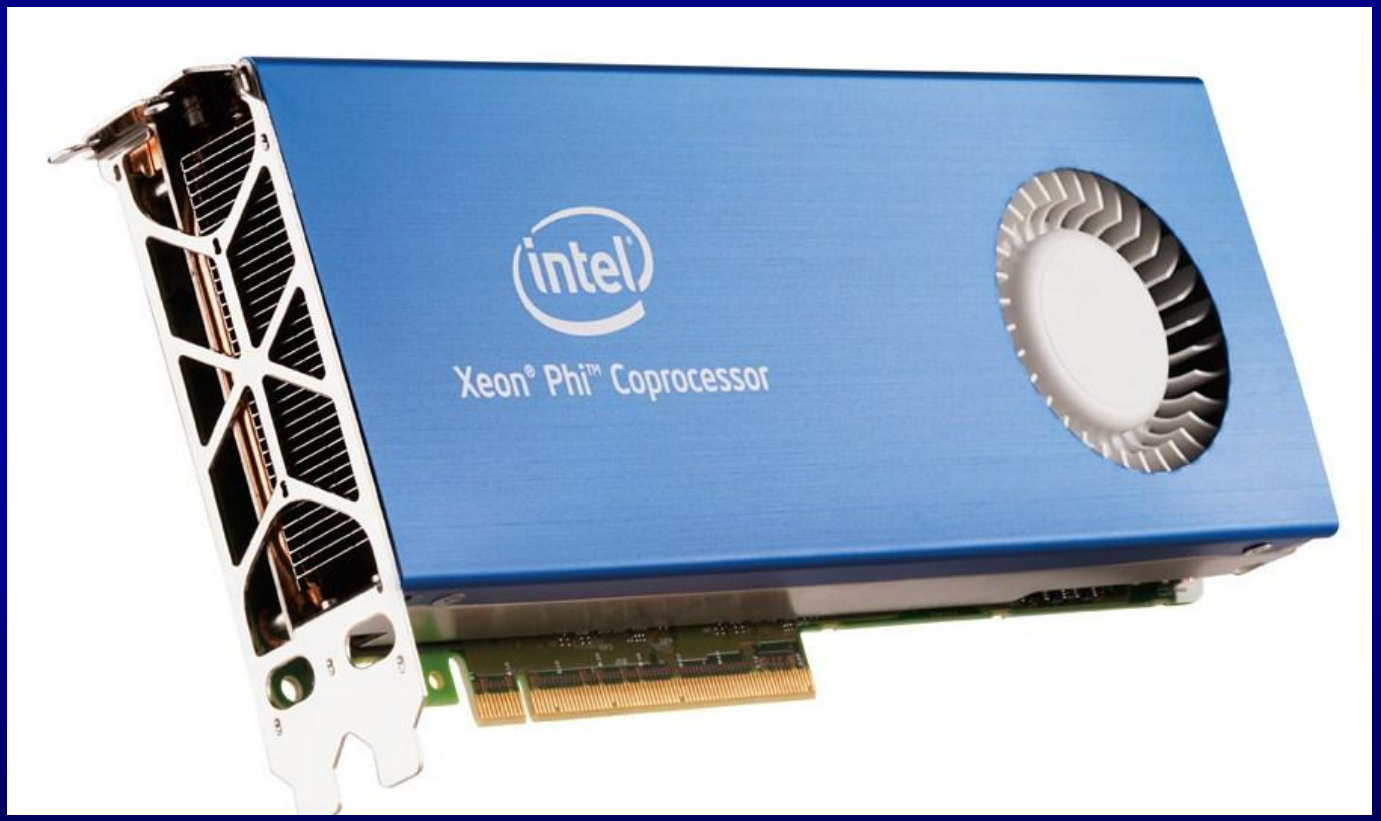


Stampede consists of 182 48U cabinets.

Cooling and Electrical Infrastructure

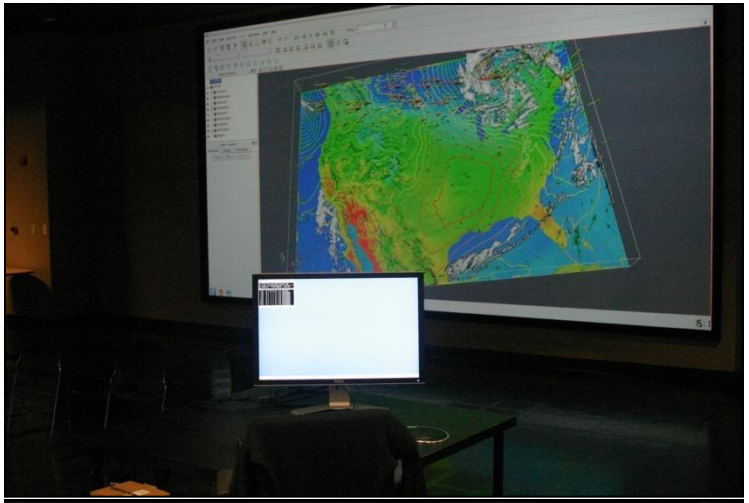
MIC Details





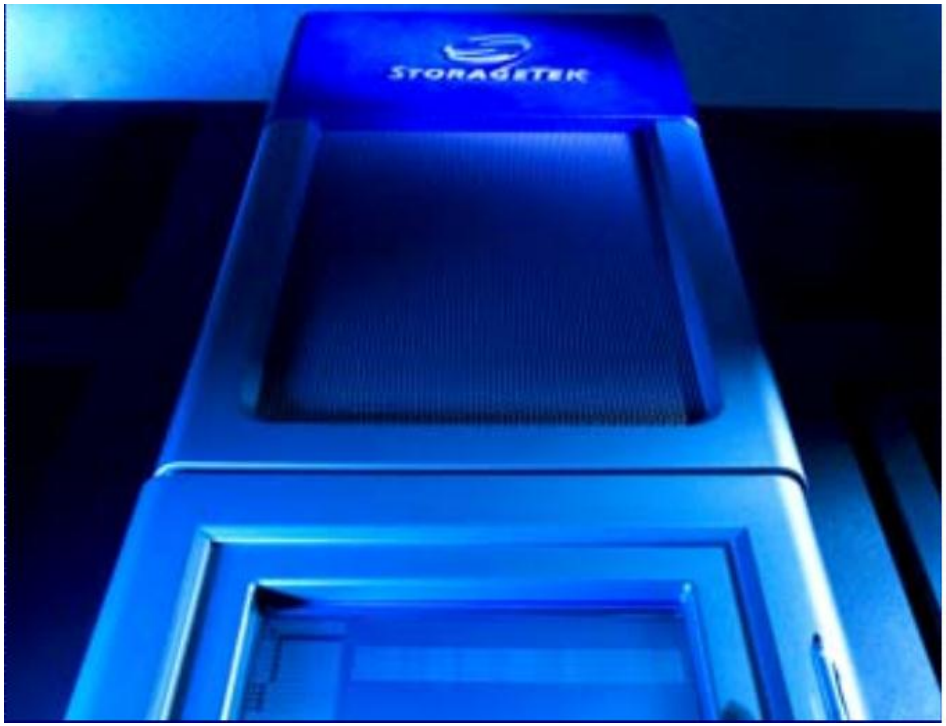
TACC Advanced Visualization Systems

- Upgraded ACES Vislab
  - 16x5 Tiled Display Wall, 328 MPixels, Nvidia GPUs
  - SONY 9MPixel Projector, 20ft x 11ft display
  - High-end Dell Workstations
  - Collaboration/conference room
  - Tiled touch display
- Integrated visualization for remote sessions
  - Ranger: 7 GPU-based systems
  - Lonestar: 16 GPU nodes
  - Stampede: 128 GPU nodes + 16 large shared memory nodes with GPUs
- Longhorn
  - 256-node, 512-GPU system for remote vis and HPC on GPUs



Ranch Archival System

- Sun StorageTek Silo
  - 10,000 - T1000B tapes
  - 6,000 - T1000C tapes
  - ~40 PB total capacity
  - Used for long-term storage



Corral

- 6PB DataDirect Networks online disk storage
- 8 Dell 1950 servers
- 8 Dell 2950 servers
- 12 Dell R710 servers
- High Performance Parallel File System
  - Multiple databases
  - iRODS data management
  - Replication to tape archive
- Multiple levels of access control
- Web and other data access available globally

TACC Support Services

- Technical documentation
  - http://www.tacc.utexas.edu/ (user guides!)
- Training
  - http://www.tacc.utexas.edu/services/training/
  - Taught on-site, sign up at TACC User Portal

- Or – Everything through the TACC Portal (consulting)
  - http://portal.tacc.utexas.edu/