CHANGES Workshop

Advancing Scientific Computing through Global Partnerships

Thom Dunning

National Center for Supercomputing Applications
Institute for Advanced Computing Applications & Technologies
University of Illinois at Urbana-Champaign

ACCESS to CHANGES

A productive partnership between CNIC and NCSA for advancing scientific computing has now been extended to include JSC.

CNIC-NCSA Partnership Established in 2009

- **Areas of Mutual Interest**
  - High performance computing
  - Data-intensive/data-driven computing
  - Scientific visualization
  - Cyberinfrastructure and *e*-Science


September 2009


August 2010
欢迎
ACCESS10


The American-Chinese Cyberinfrastructure and E-Science workShop
VIsualization and Visual Analytics (ACCESS|VIVA) Aug 15-17, 2011 Xi'an, China


NCSA


erican-Chinese Cyberinfrastructur


ACCESS09 | HPC
2009中美科研信息化研讨会|高性能计算
2009 American-Chinese Cyberinfrastructure and E-Science workShop | HPC
Powering Cyber-research in the 21st Century

Jülich Supercomputing Centre
Forschungszentrum Jülich

Welcome to the partnership!

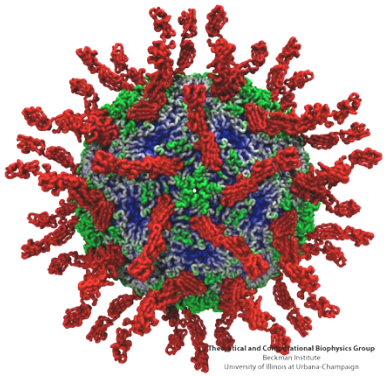
Update on Blue Waters

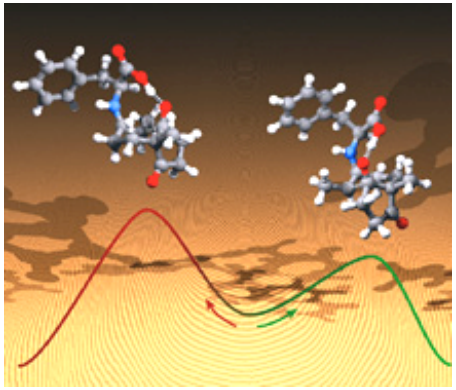
Deployment of a sustained petascale computing system

Advancing Science and Engineering

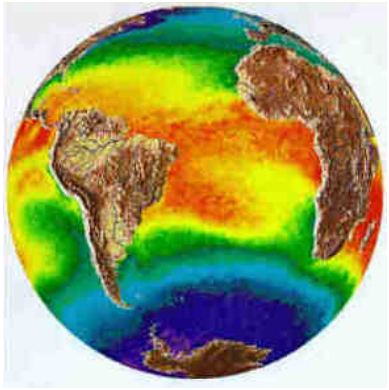
Advances in a broad range of science and engineering disciplines will be enabled by sustained petascale computers:

Molecular Science



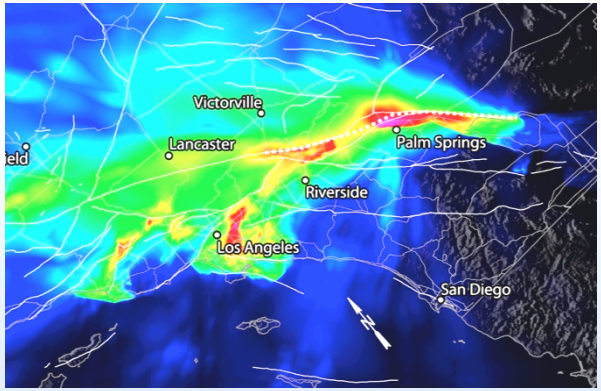


Weather & Climate Forecasting

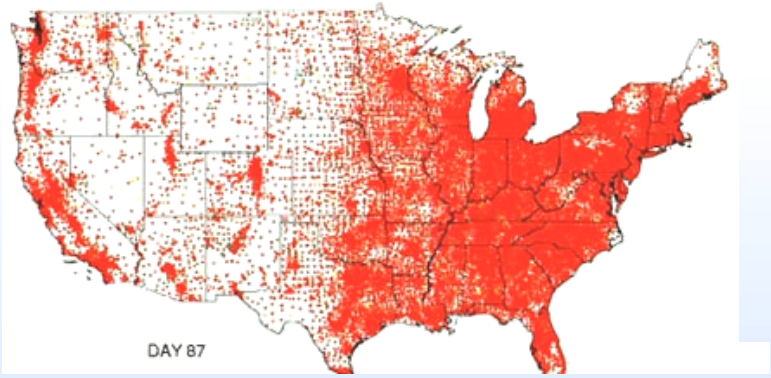


Astronomy

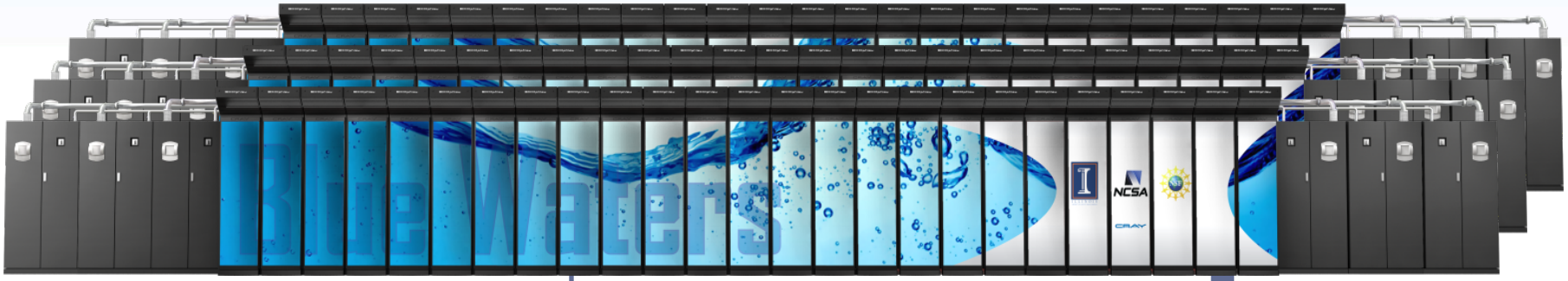
Earth Science



Health



Blue Waters Computing System



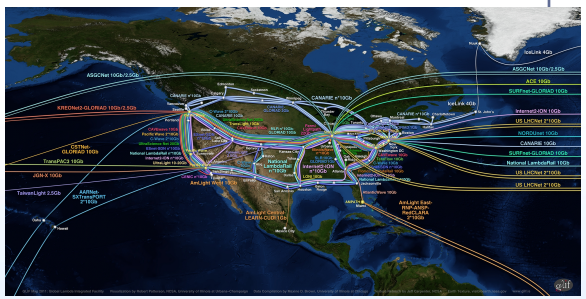
10/40/100 Gb Ethernet Switch

IB Switch

>1 TB/sec

120+ Gb/sec

100 GB/sec



WAN

Spectra Logic: 300 PBs

Sonexion: 26 PBs

Blue Waters & Sequoia Computing Systems

System Attribute	NCSA Blue Waters	LLNL Sequoia (#1)
Vendor(s)	Cray/AMD/NVIDIA	IBM
Processors	Interlagos/Kepler	PowerPC A2
Total Peak Performance (PF)	11.6	20.1
Total Peak Performance (CPU/GPU)	7.6/4.0	20.1/0.0
Number of CPU Chips (8, 16 cores/chip)	48,352	98,304
Number of GPU Chips	3,072	0
Amount of CPU Memory (TB)	1,518	1,572
Interconnect	3-D Torus	5-D Torus
Amount of On-line Disk Storage (PB)	26	50(?)
Sustained Disk Transfer (TB/sec)	>1	0.5-1.0
Amount of Archival Storage	300	?
Sustained Tape Transfer (GB/sec)	100	?

Blue Waters & Titan Computing Systems

System Attribute	NCSA Blue Waters	ORNL Titan
Vendor(s)	Cray/AMD/NVIDIA	Cray/AMD/NVIDIA
Processors	Interlagos/Kepler	Interlagos/Kepler
Total Peak Performance (PF)	11.6	>20
Total Peak Performance (CPU/GPU)	7.6/4.0	3/17
Number of CPU Chips (8 cores/chip)	48,352	18,688
Number of GPU Chips	3,072	14,592
Amount of CPU Memory (TB)	1,518	688
Interconnect	3-D Torus	3-D Torus
Amount of On-line Disk Storage (PB)	26	20(?)
Sustained Disk Transfer (TB/sec)	>1	0.4–0.7
Amount of Archival Storage	300	15-30
Sustained Tape Transfer (GB/sec)	100	7

Petascale Computing Facility

Partners

EYP MCF/
Gensler
IBM
Yahoo!

- **Modern Data Center**
  - 90,000+ ft^2 total
  - 30,000 ft^2 raised floor
    20,000 ft^2 machine room gallery
- **Energy Efficiency**
  - LEED certified Gold
  - Power Utilization Efficiency = 1.1–1.2

Blue Waters Early Science System

- **BW-ESS Configuration**
  - 1.4+ PFs (peak)
    - 48 cabinets (4,512 XE6 compute nodes)
    - 96 service nodes
  - 2 PBs Sonexion Lustre storage appliance

- **BW-ESS Projects**
  - **Biomolecular Physics**—K. Schulten, University of Illinois at Urbana-Champaign
  - **Cosmology**—B. O'Shea, Michigan State University
  - **Climate Change**—D. Wuebbles, University of Illinois at Urbana-Champaign
  - **Lattice QCD**—R. Sugar, University of California, Santa Barbara
  - **Plasma Physics**—H. Karimabadi, University of California, San Diego
  - **Supernovae**—S. Woosley, University of California Observatories
  - **Severe Weather**—R. Wilhelmson, University of Illinois
  - **High Resolution/Fidelity Climate**—C. Stan, Center for Ocean-Land-Atmospheric Studies (COLA)
  - **Complex Turbulence**—P. K. Yeung, Georgia Tech
  - **Turbulent Stellar Hydrodynamics**—P. Woodward, University of Minnesota

Build Status of Blue Waters

- All compute cabinets (276) installed
- Majority of disks (33 racks) delivered (with 1300 controller); remainder (3 racks) at Cray for testing 1600 controller
- Near- line storage: one Spectra Logic library (with 4000 slot for 4TB media slots) installed and being used for HPSS and Cray software testing

Validating Sustained Petascale Performance

- **Sustained Petascale Performance (SPP) Metric**
  - Similar to NERSC Sustained System Performance metric
  - Time-to-solution metric for end-to-end problem (pre/post processing, processing, I/O, …)
  - Coverage of representative science areas, algorithmic methods and core counts
- **Details**
  - Original NSF Benchmarks
    - Full Size – QCD (MILC), Turbulence (PNSDNS), Molecular Dynamics (NAMD)
    - Modest Size – MILC, Paratec, WRF
  - Science Teams Applications
    - NAMD – molecular dynamics
    - MILC, Chroma – Lattice Quantum Chromodynamics
    - VPIC, SPECFEM3D – Geophysical Science
    - WRF – Atmospheric Science
    - PPM – Astrophysics
    - NWCHEM, GAMESS – Computational Chemistry
    - QMCPACK – Materials Science
  - At least three Science Team benchmarks must run at full scale
  - XK nodes must add ≥15% to SPP

Illinois' Blue Waters Team

PI & Co-PIs


Dunning


Kramer


Snir

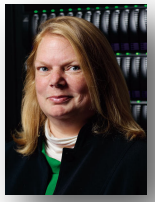

Gropp


Hwu

Task Leads


Beldica
Proj. Mgmt.


Bode
Software


Butler
Storage


Glotzer
Virtual School

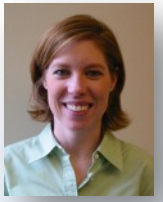

Cappello
Reliability

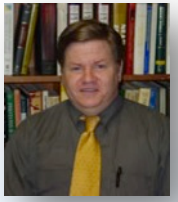

Kale
Apps Simulations


Lathrop
Education


Durbin
Facilities


Giles
Industry


Olson
Proj. Mgmt.


Panoff
UG Education


Semeraro
Visualization


Enos
Ops Transition


Thank You!