BLUE WATERS

SUSTAINED PETASCALE COMPUTING

Blue Waters and Petascale Science

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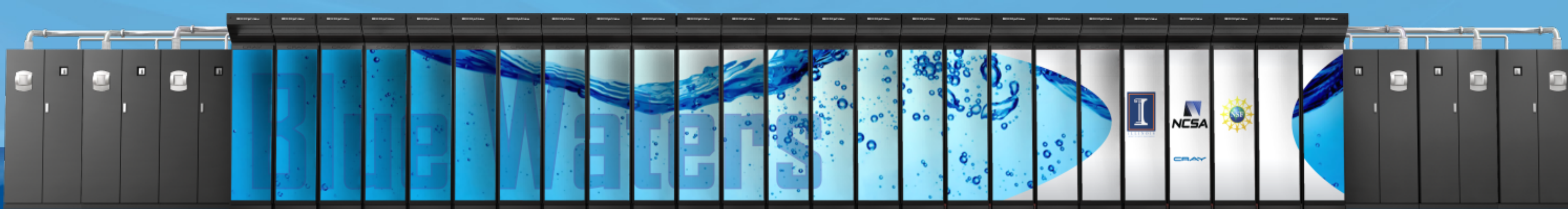


NCSA NSF GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION CRAY

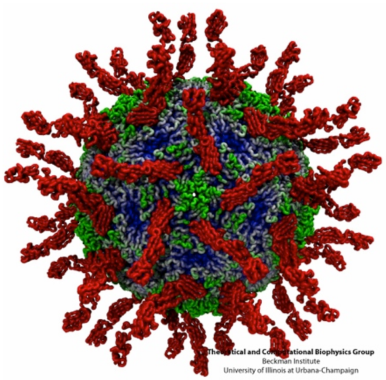
National Center for Supercomputing Applications - NCSA

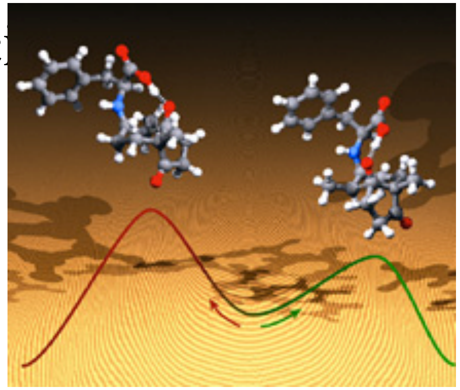
- Established in 1986 as one of the original sites of the National Science Foundation's Supercomputer Centers Program
  - Supported by the state of Illinois, University of Illinois, the National Science Foundation, and grants from others.
- A leader in deploying robust high-performance computing resources and in working with research communities to develop new computing and software technologies.
  - Fielded 30 major HPC computational systems for the national science and engineering community
  - Two major projects (Blue Waters and XSEDE) and many other activities
  - Currently evolving a large strategic focus on Data Driven Science
- NCSA focuses on:
  - Developing and supporting powerful, reliable computing, data, and networking resources that enable researchers to solve demanding science and engineering problems.
    - Develop and explore innovative architectures and techniques to accelerate scientific computing.
  - Working with research communities to help them fully exploit the extraordinary resources available on the Internet (computing systems, data sources and stores, and tools) with cyber environments.
  - Developing software, techniques, and tools to improve national cyber-protection and to help law enforcement better respond to cyberattacks.
  - Providing insights into complex systems and sharing the thrill of scientific discovery with the broadest possible audience through artful visualizations of scientific phenomena.
  - Preparing the next generation of scientists and engineers to effectively use computational tools and techniques.
- PCI – Parallel Computing Institute
- CEC – Center for Extreme Scale Computing

Science & Engineering on Blue Waters

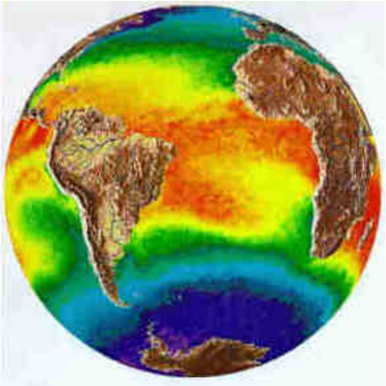
Blue Waters will enable advances in a broad range of science and engineering disciplines. Examples include:

Molecular



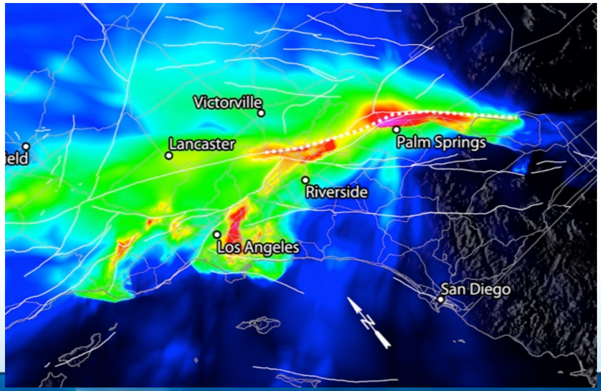


Weather & Climate

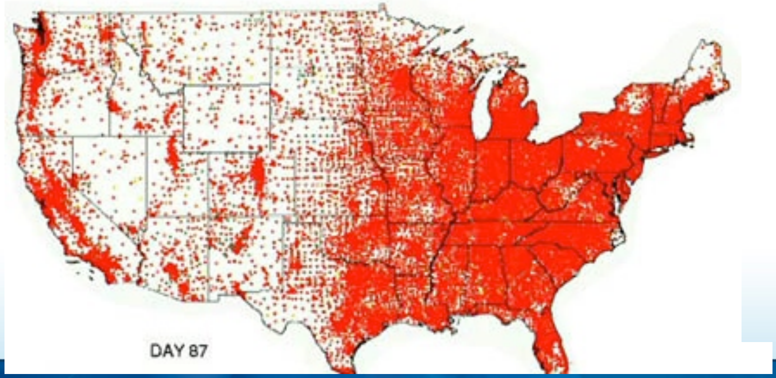


Astrono

Earth



Health



Blue Waters Goals

- **Deploy a computing system capable of sustaining more than one petaflops or more for a broad range of applications**
  - Cray system achieves this goal using a well defined metrics, including most intense I/O sub-system available
- **Enable the Science Teams to take full advantage of the sustained petascale computing system**
  - Blue Waters Team has established strong partnership with Science Teams, helping them to improve the performance and scalability of their applications
- **Enhance the operation and use of the sustained petascale system**
  - Blue Waters Team is developing tools, libraries and other system software to aid in operation of the system and to help scientists and engineers make effective use of the system
- **Provide a world-class computing environment for the petascale computing system**
  - The NPCF is a modern, energy-efficient data center with a rich WAN environment (100-400 usable Gbps) and data archive (>300 usable PB)
- **Exploit advances in innovative computing technology**
  - Proposal anticipated the rise of heterogeneous computing and planned to help the computational community transition to new modes for computational and data-driven science and engineering

The Blue Waters Eco-System

Petascale Education, Industry and Outreach

Petascale Applications
(Computing Resource Allocations)

Petascale Application Collaboration Team Support

Outstanding Full Services
WAN Connections, Science and Engineering Application Support, System Management, Cyber-protection, Operations, …

Great Lakes Consortium for Petascale Computing

Value added hardware (external networking, IDS, nearline storage, import/export, etc) and software (Eclipse, HPSS, Visualization, computational libraries, etc)

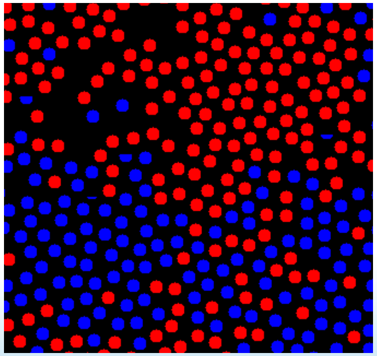
Blue Waters Base System – Processors, Memory, Interconnect, Online Storage, System Software, Programming Environment

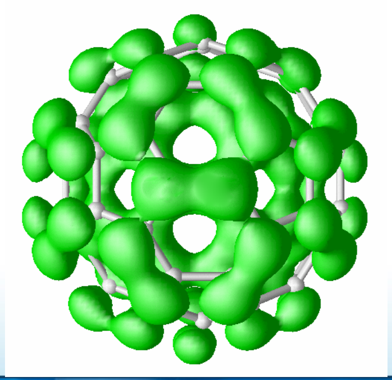
National Petascale Computing Facility

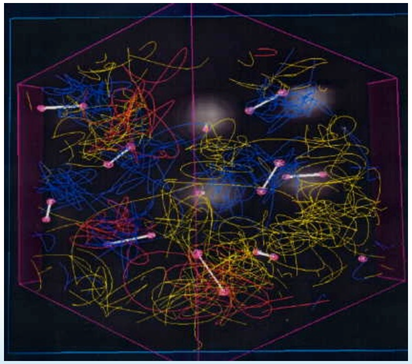
Breakthrough Petascale Quantum Monte Carlo Calcs.

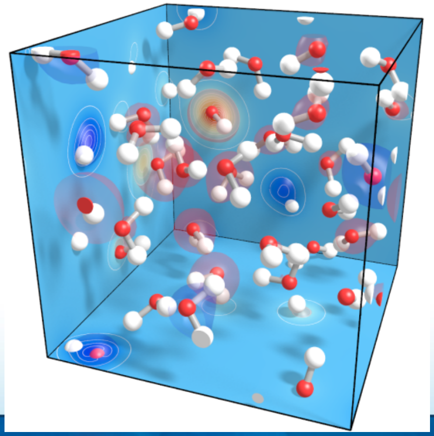
Shiwei Zhang, David Ceperley (UIUC)

- Computational Goals
  - Properties of hydrogen and hydrogen-helium mixtures in astrophysically relevant conditions
  - Electronic & magnetic structures of transition-metal compounds
  - Phases and properties of fermionic atoms in optical lattices
  - Properties of materials for energy conversion
  - Dynamical QMC simulations of liquid water and other disordered materials



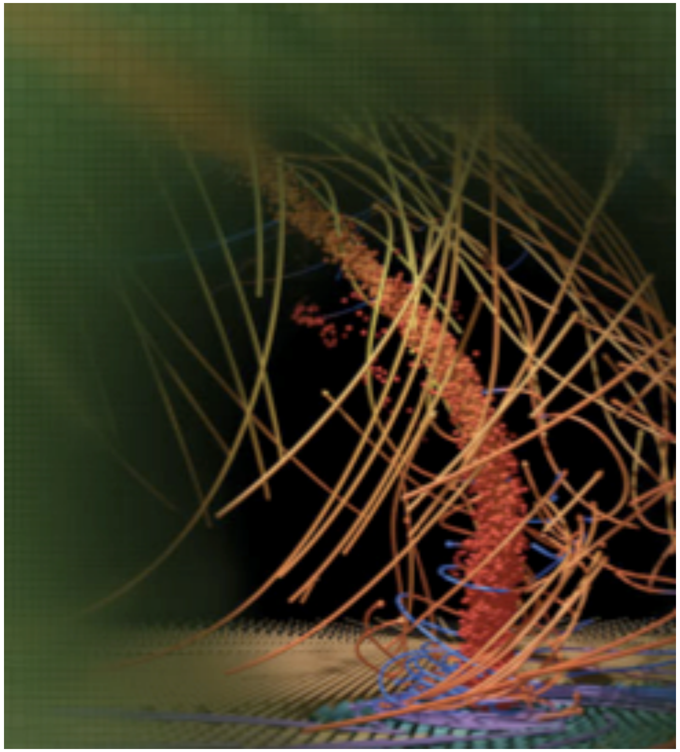






Understanding Tornadoes and Their Parent Supercells Through Ultra-High Resolution Simulation/Analysis

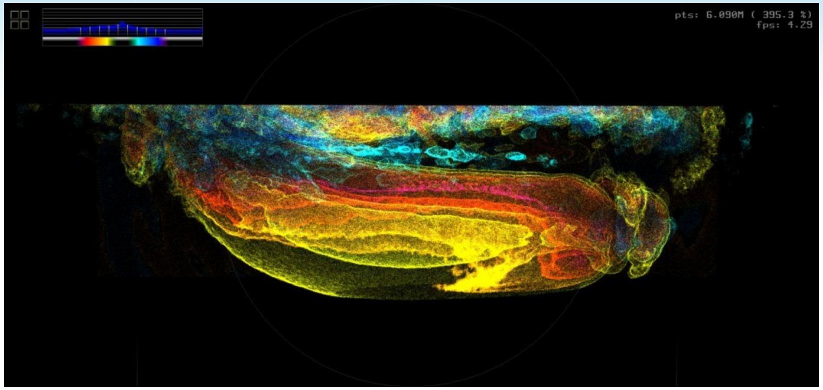
Bob Wilhelmson (UIUC), et al



- Goal
  - Simulate development, structure, & demise of large damaging tornadoes in supercells at resolution sufficient to capture low-level tornado inflow, thin precipitation shaft that forms “hook echo” adjacent to tornado, and other smaller scale structures
- Approach
  - Simulate storms with model that solves (using finite differences) the equations of motion for air and water substances (droplets, rain, ice, …)

Earthquake System Science (PressOn)

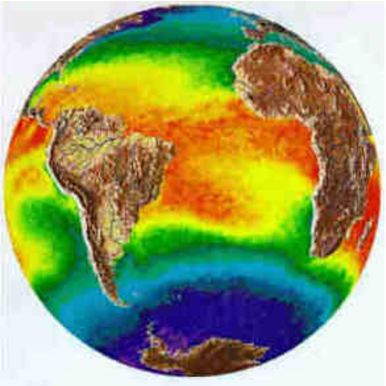
Tom Jordan, Phil Maechling



- Prepare 3 seismic & engineering codes for Blue Waters
  1. AWP-Olsen: finite difference dynamic rupture & wave propagation
  2. Hercules: finite element wave propagation
  3. OpenSees: structure modeling for earthquake engineering
- Science Goals
  - Improve resolution of dynamic rupture simulations by ~10X to investigate realistic friction laws, near-fault stress states, & off-fault plasticity
  - Investigate upper frequency limit of deterministic ground-motion prediction by simulating strong motions up to 3 Hz using realistic 3D structural models for Southern California
  - Improved understanding of engineering response to earthquakes by modeling response of buildings to broadband ground motions

Testing Hypotheses About Climate Prediction

Stan, Kirtman, Large, Randall



- Hypotheses
  - The large errors in current-generation climate models are associated with fundamentally flawed assumptions in the parameterizations of cloud processes and ocean eddy mixing processes
  - Climate predictability, a synthetic quality entirely associated with a given model, increases with increasing model resolution by virtue of the changing representation of atmospheric and oceanic noise
- Target Problems
  - Annual Cycle Experiment using the Co. St. U. Global Cloud-Resolving Atmospheric General Circulation Model
    - Test if annual cycle of physical climate system quantities such as the precipitation and surface temperatures are more accurately reproduced when both cloud processes and the ocean meso-scale are resolved and coupled

Industry S&E Teams

- Industry can participate in the NSF PRAC process
- 5+% allocation can dedicated to industrial use
  - Specialized support by the NCSA Private Sector Program (PSP) staff
  - Blue Waters staff will support the PSP staff as needed
  - Potential to provide specialized services within Service Level Agreements parameters
    - E.g. throughput, extra expertise, specialized storage provisions, etc.

* *

High interest shared by partner companies in the following:

- Scaling capability of a well-known and validated CFD code
- Temporal and transient modeling techniques and understanding.

Two example cases under discussion:

- NASA OVERFLOW at scale for CFD flows
- Temporal modeling techniques using the freezing of H_2O molecules as a use case and as a reason to conduct both large-scale single runs and to gain significant insight by reducing uncertainty.

PI	Award Date	Project Title
Sugar	04/15/2009	Lattice QCD on Blue Waters
Bartlett	04/15/2009	Super instruction architecture for petascale computing
Nagamine	04/15/2009	Peta-Cosmology: galaxy formation and virtual astronomy
Bissett	05/01/2009	Simulation of contagion on very large social networks with Blue Waters
O'Shea	05/01/2009	Formation of the First Galaxies: Predictions for the Next Generation of Observatories
Schulten	05/15/2009	The computational microscope
Stan	09/01/2009	Testing hypotheses about climate prediction at unprecedented resolutions on the NSF Blue Waters system
Campanelli	09/15/2009	Computational relativity and gravitation at petascale: Simulating and visualizing astrophysically realistic compact binaries
Yeung	09/15/2009	Petascale computations for complex turbulent flows
Schnetter	09/15/2009	Enabling science at the petascale: From binary systems and stellar core collapse To gamma-ray bursts
Woodward	10/01/2009	Petascale simulation of turbulent stellar hydrodynamics
Tagkopoulos	10/01/2009	Petascale simulations of Complex Biological Behavior in Fluctuating Environments
Wilhelmson	10/01/2009	Understanding tornadoes and their parent supercells through ultra-high resolution simulation/analysis
Wang	10/01/2009	Enabling large-scale, high-resolution, and real-time earthquake simulations on petascale parallel computers
Jordan	10/01/2009	Petascale research in earthquake system science on Blue Waters
Zhang	10/01/2009	Breakthrough peta-scale quantum Monte Carlo calculations
Haule	10/01/2009	Electronic properties of strongly correlated systems using petascale computing
Lamm	10/01/2009	Computational chemistry at the petascale
Karimabadi	11/01/2010	Enabling Breakthrough Kinetic Simulations of the Magnetosphere via Petascale Computing
Mori	01/15/2011	Petascale plasma physics simulations using PIC codes
Voth	02/01/2011	Petascale multiscale simulations of biomolecular systems
Woosley	02/01/2011	Type Ia supernovae
Cheatham	02/01/2011	Hierarchical molecular dynamics sampling for assessing pathways and free energies of RNA catalysis, ligand binding, and conformational change
Wuebbles	04/15/2011	Using petascale computing capabilities to address climate change uncertainties
Gropp	06/01/2011	System software for scalable applications
Klimeck	09/15/2011	Accelerating nano-scale transistor innovation
Pande	09/15/2011	Simulating vesicle fusion on Blue Waters

Science Area	Number of Teams	Codes	Structured Grids	Unstructured Grids	Dense Matrix	Sparse Matrix	N-Body	Monte Carlo	FFT	Significant I/O
Climate and Weather	3	CESM, GCRM, CM1, HOMME	X	X		X		X		
Plasmas/ Magnetosphere	2	H3D(M), OSIRIS, Magtail/UPIC	X				X		X	X
Stellar Atmospheres and Supernovae	2	PPM, MAESTRO, CASTRO, SEDONA	X			X		X		X
Cosmology	2	Enzo, pGADGET	X			X	X			
Combustion/ Turbulence	1	PSDNS	X						X	
General Relativity	2	Cactus, Harm3D, LazEV	X			X				
Molecular Dynamics	4	AMBER, Gromacs, NAMD, LAMMPS			X		X		X	
Quantum Chemistry	2	SIAL, GAMESS, NWChem			X	X	X	X		X
Material Science	3	NEMOS, OMEN, GW, QMCPACK			X	X	X	X		
Earthquakes/ Seismology	2	AWP-ODC, HERCULES, PLSQR, SPECFEM3D	X	X			X			X
Quantum Chromo Dynamics	1	Chroma, MILD, USQCD	X		X	X	X		X	
Social Networks	1	EPISIMDEMICS								
Evolution	1	Eve								
Computer Science	1			X	X	X			X	X

GLCPC

Great Lakes Consortium for Petascale Computing

GLCPC Mission:

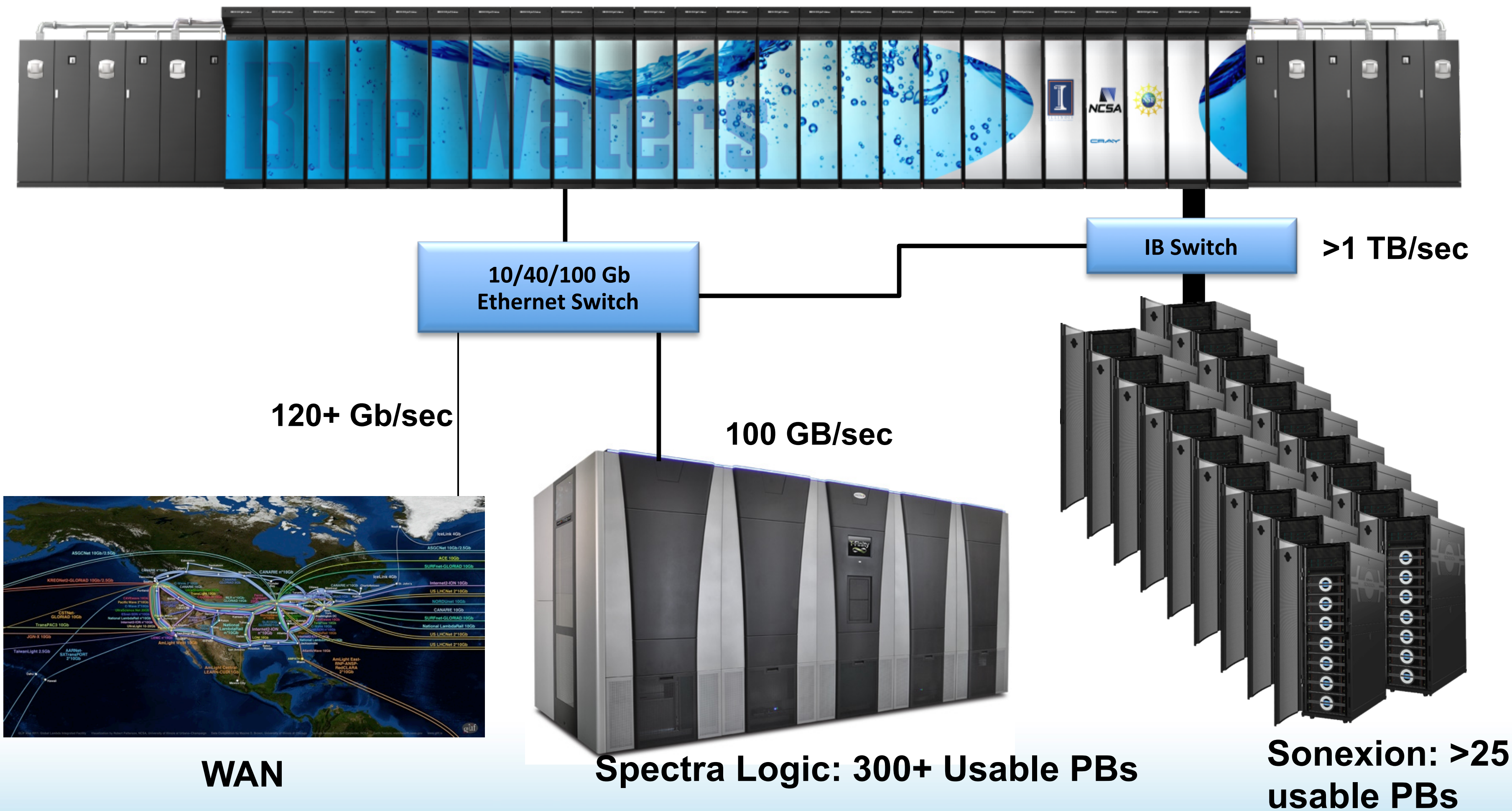
"…facilitate and coordinate multi-institutional efforts to advance computational and computer science engineering, and technology research and education and their applications to outstanding problems of regional or national importance…"

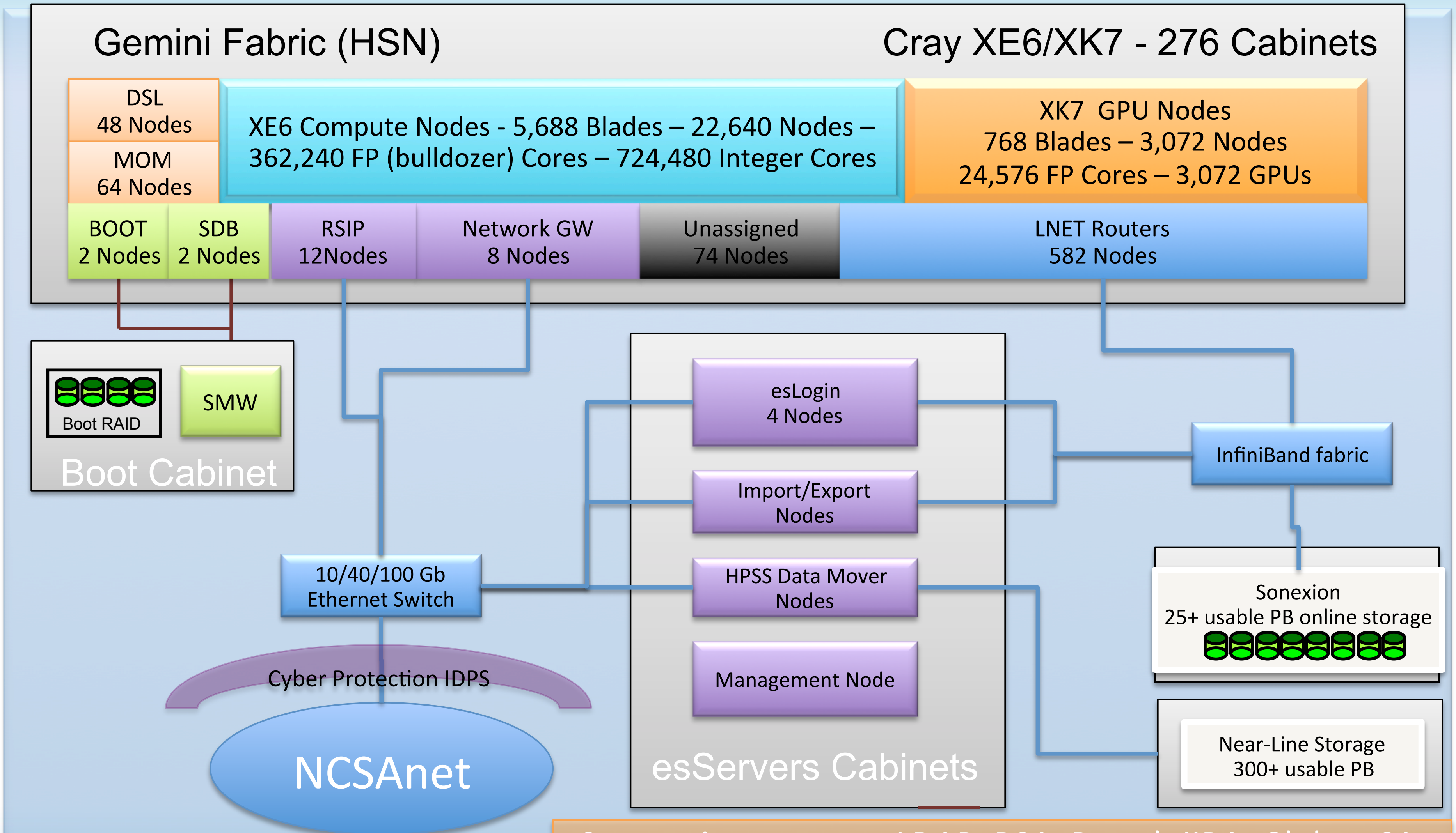
- 2% allocation
- 501c3 Organization*
- 28 Charter members**
- Executive Committee
- Allocations Committee
- Education Committee

* State 501c3 filing complete, federal filing in progress

** 28 Charter members represent over 80 universities, national laboratories, and other education agencies

Blue Waters Computing Super-system





Supporting systems: LDAP, RSA, Portal, JIRA, Globus CA, Bro, test systems, Accounts/Allocations, CVS, Wiki

Blue Waters Software Environment

Languages
- Fortran
- C
- C++
- Python
- UPC

Performance Analysis
- Cray Performance Monitoring and Analysis Tool
- PAPI
- PerfSuite
- Tau

Compilers
- Cray Compiling Environment (CCE)
- PGI
- GNU

Debuggers
- Allinea DDT
- lgdb

Prog. Env.
- Eclipse
- Traditional

Programming Models
- Distributed Memory (Cray MPT)
  - MPI
  - SHMEM
- Shared Memory
  - OpenMP 3.0
- PGAS & Global View
  - UPC (CCE)
  - CAF (CCE)

IO Libraries
- NetCDF
- HDF5
- ADIOS

Resource Manager
- Adaptive COMPUTING

Visualization
- VisIt
- Paraview
- YT

Tools
Environment setup
- Modules

Debugging Support Tools
- Fast Track Debugger (CCE w/ DDT)
- Abnormal Termination Processing
- STAT
- Cray Comparative Debugger#

Data Transfer
- globus online
- HPSS

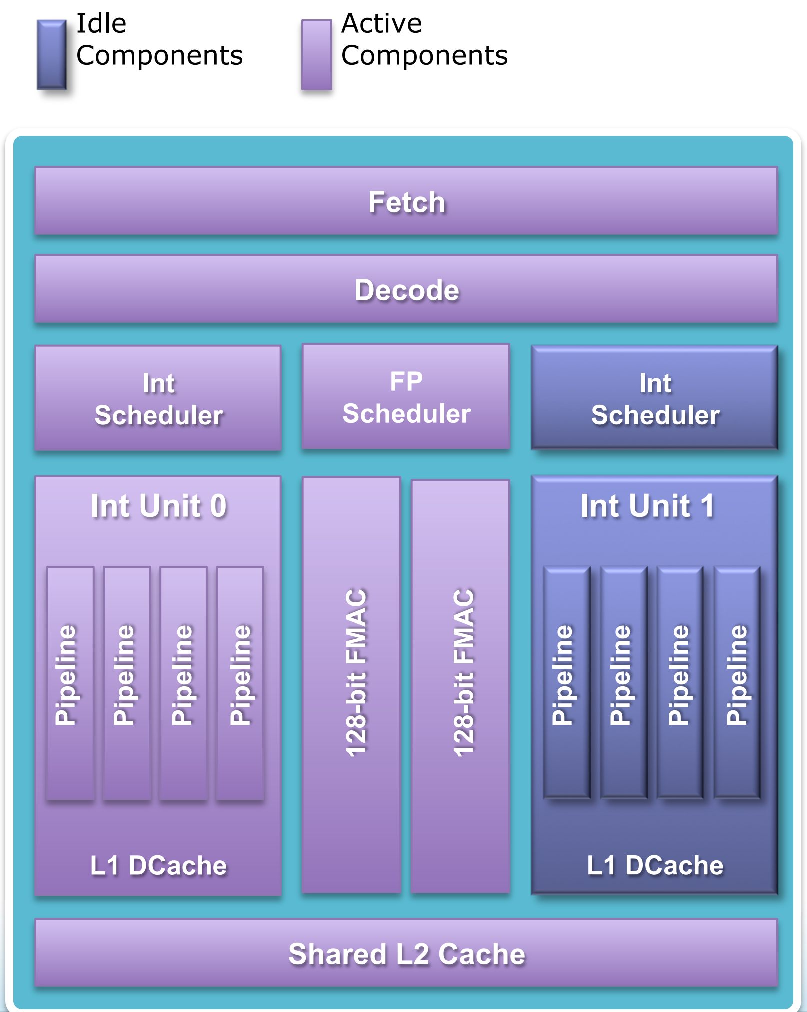
Optimized Scientific Libraries
- LAPACK
- ScaLAPACK
- BLAS (libgoto)
- Iterative Refinement Toolkit
- Cray Adaptive FFTs (CRAFFT)
- FFTW
- Cray PETSc (with CASK)
- Cray Trilinos (with CASK)

Cray Linux Environment (CLE)/SUSE Linux

Cray developed	3rd party packaging
Under development	NCSA supported
Licensed ISV SW	Cray added value to 3rd party

Defining a Core - AMD Wide AVX mode

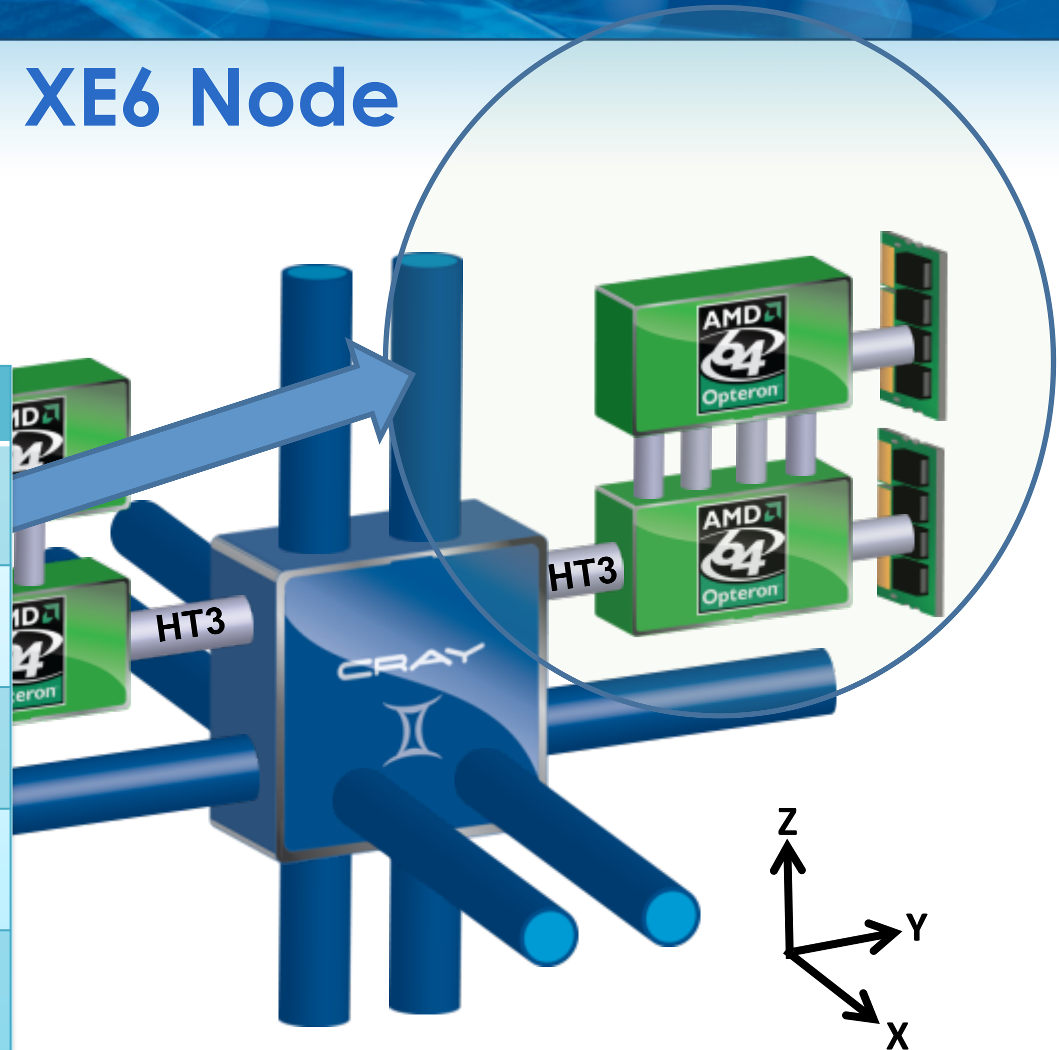
- In this mode, only one integer scheduler unit is used
  - Most common mode for S&E applications
    - Code is Floating Point dominated and makes use of AVX instructions
    - Code needs more memory per MPI rank
- Implications
  - This core has *exclusive* access to the 256-bit FP unit and is capable of 8 FP results per clock cycle
  - The core has twice the memory capacity
  - The core has twice the memory bandwidth
  - The L2 cache is effectively twice as large
  - The peak performance of the chip is not reduced
- AMD refers to this as a “Core Module”



Blue Waters XE6 Node

Blue Waters contains 22,640 XE6 compute nodes

Node Characteristics	
Number of Core Modules*	16
Peak Performance	313 Gflops/sec
Memory Size	64 GB per node
Memory Bandwidth (Peak)	102 GB/sec
Interconnect Injection Bandwidth (Peak)	9.6 GB/sec per direction

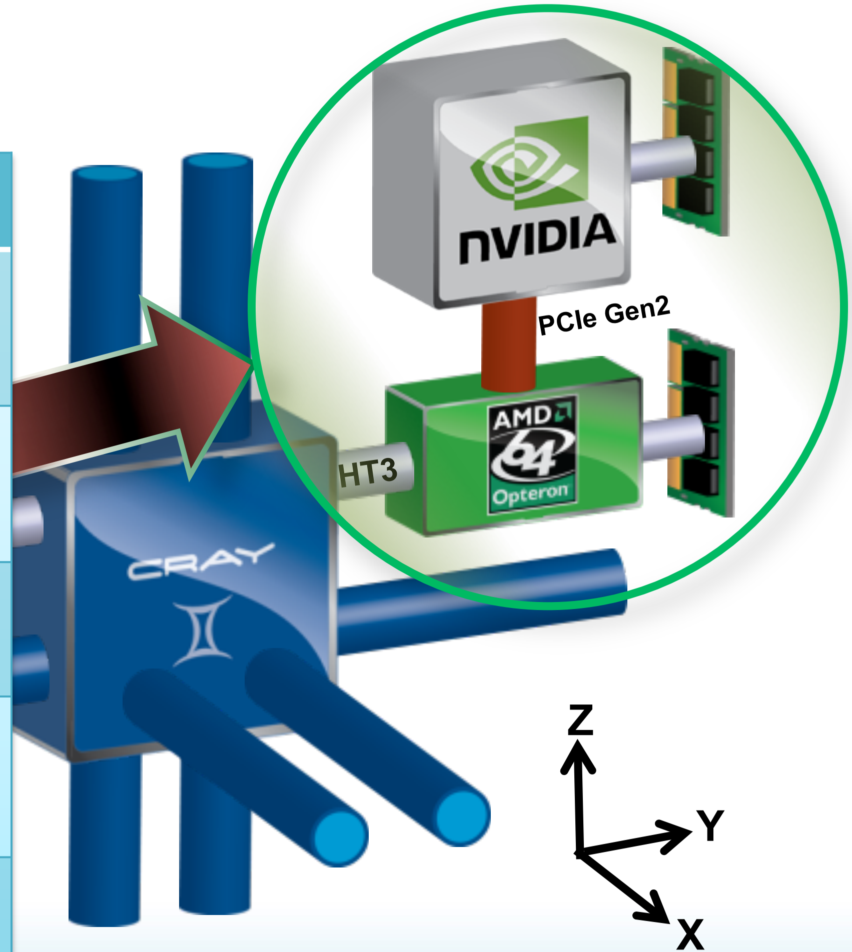


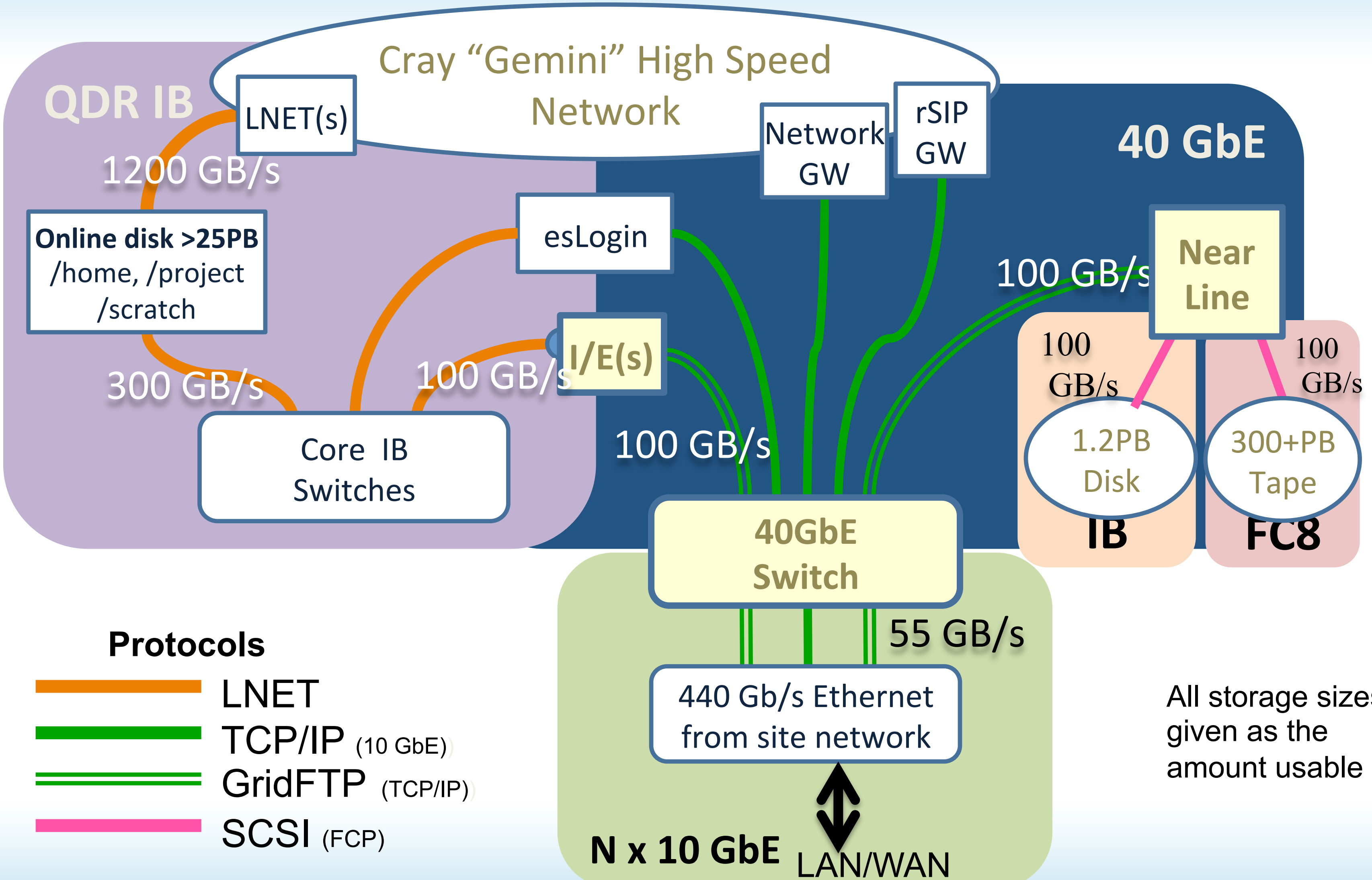
**Each core module includes 1 256-bit wide FP unit and 2 integer units. This is often advertised as 2 cores, leading to a 32 core node.*

Cray XK7 and a Path to the Future

Blue Waters contains 3,072 NVIDIA Kepler (GK110) GPUs

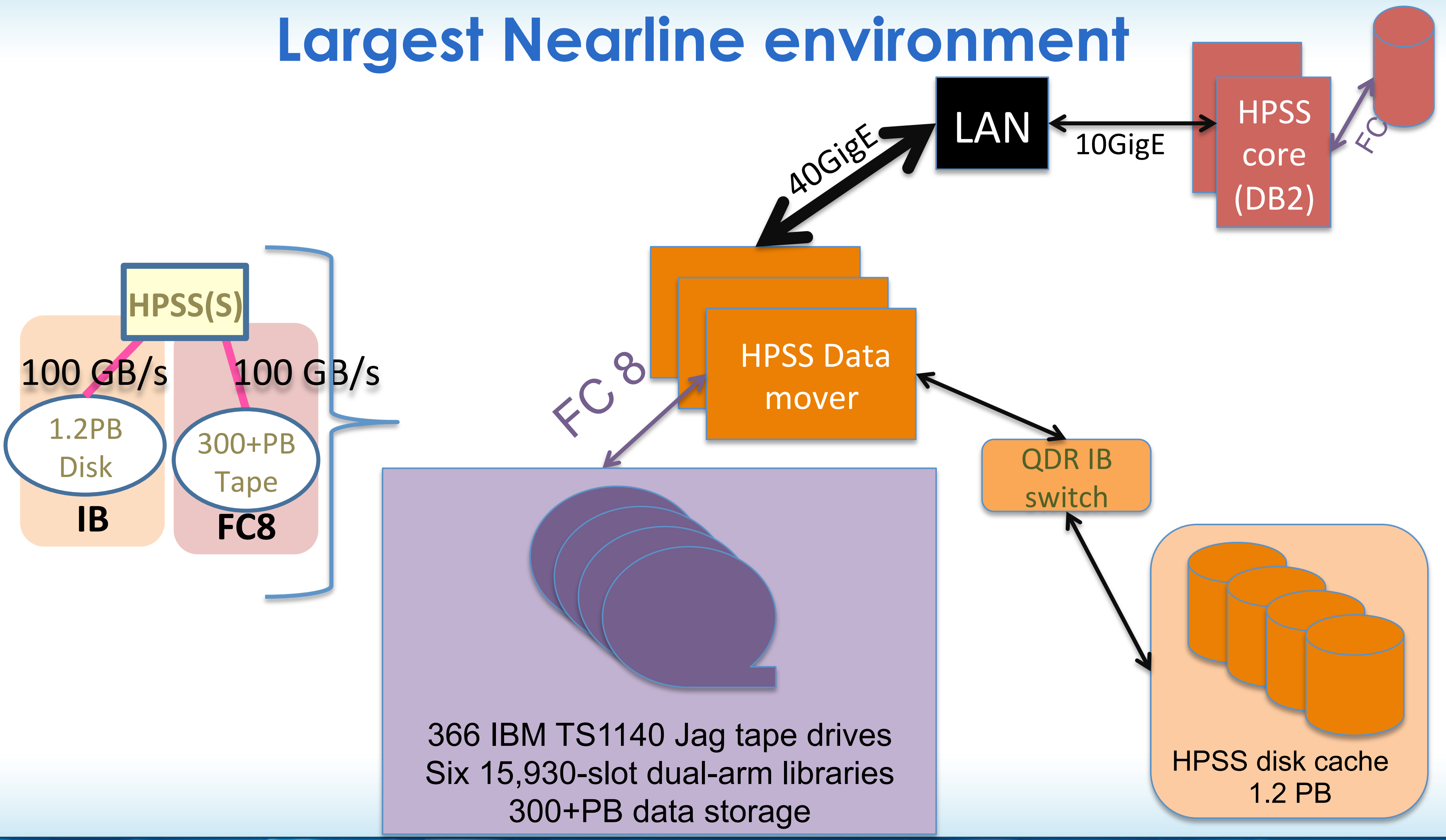
XK7 Compute Node Characteristics	
Host Processor	AMD Series 6200 (Interlagos)
Host Processor Performance	156.8 Gflops
Kepler Peak (DP floating point)	1.4 Tflops
Host Memory	32GB 51 GB/sec
Kepler Memory	6GB GDDR5 capacity 180 GB/sec





All storage sizes given as the amount usable

Largest Nearline environment



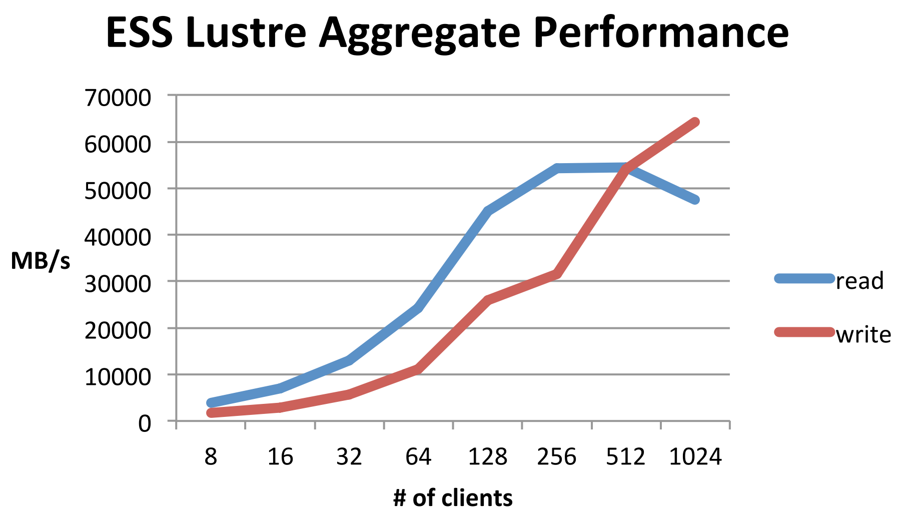
Blue Waters Early Science System

- BW-ESS Configuration
  - 48 cabinets, 4,512 XE6 compute nodes, 96 service nodes
  - 2 PBs Sonexion Lustre storage appliance
- Access through Blue Waters Portal
  - https://bluewaters.ncsa.illinois.edu/

- Current 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

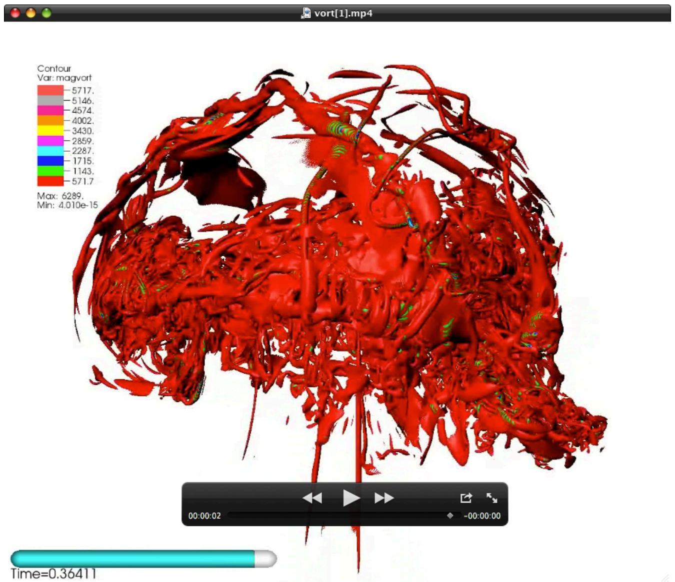
Initial Impressions

- Storage Results
    - Good Performance - “zippy”
        - Initial expectation was 35GB/s and reached 61GB/s for write at full scale
        - 18,000 creates/second
    - Failover worked.
        - MDS failure to hot “spare” work without taking down the file system
        - OSS failure to hot “spare” work without taking down the file system
- System Reliability
    - Good – only modest number of issues
    - Utilization > 90%
- Computational performance
    - Better than required at this stage

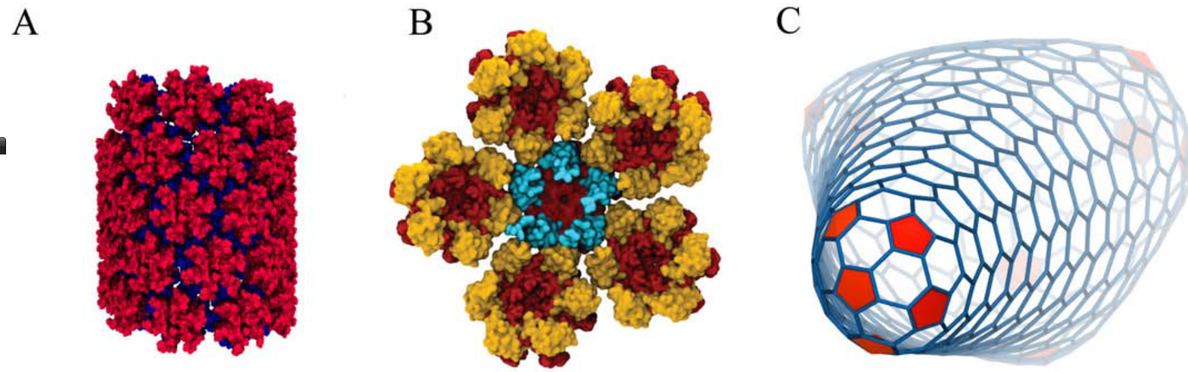


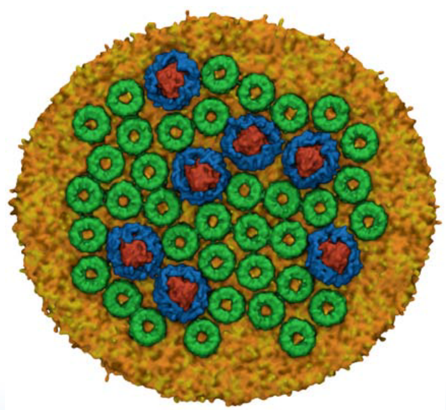
Early Results

Vorticity for a turbulently burning nuclear fusion flame experiencing various instabilities, inside an exploding white dwarf.- Woosley

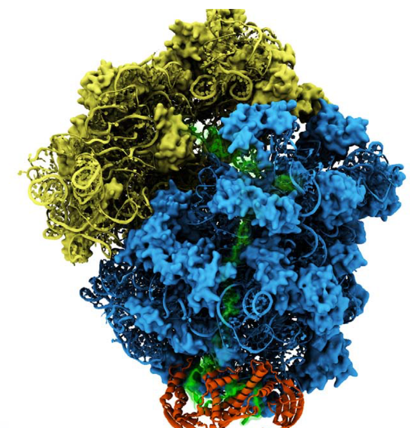


Molecular mechanisms of HIV infection Shulten





Simulation of a Photosynthetic Membrane - Shulten



Ribosome-trigger factor complex - Shulten

National Petascale Computing Facility

- Modern Data Center
  - 90,000+ ft^2 total
  - 30,000 ft^2 6 foot raised floor
    20,000 ft^2 machine room gallery with no obstructions or structural support elements
- Energy Efficiency
  - LEED certified Gold
  - Power Utilization Efficiency, PUE = 1.1–1.2
  - 24 MW current capacity – expandable
  - Highly instrumented

Accomplishments

- All circuits are instrumented – able to verify utility reading are consistent
- Used external water economization
- No operational issues

How to judge Sustained Performance

- Original NSF Benchmarks
  - Full Size – QCD (MILC), Turbulence (PNSDNS), Molecular Dynamics (NAMD)
  - Modest Size – MILC, Paratec, WRF
- SPP Application Mix (details available)
  - 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 two SPP benchmarks run at full scale

Effective Use of Complex Systems

- Additional effort by the science and engineering teams needed to achieve full potential of Blue Waters (and similar) systems, with all its advanced technology
- Increasing performance requires dramatic increases in parallelism that then generates complexity challenges for science and engineering teams
  - **Scaling applications to large core counts on general-purpose CPU nodes**
  - **Effectively using accelerators and "many-core" processors**
  - **Using homogeneous general purpose and heterogeneous (accelerated) nodes in a single, coordinated simulation**
  - **Effectively using parallel IO systems for data-intensive applications and Innovative storage and data paradigms**
  - **Effectively using limited bandwidth of interprocessor network**
  - **Enhancing application flexibility to increasing effective, efficient use of systems**

Performance and Scalability

- The problem is fewer applications are able to scale in the face of limited bandwidths. Hence the need to work with science teams and technology providers to
  - Develop better process-to-node mapping using for graph analysis to determine MPI behavior and usage patterns.
  - Topology Awareness in Applications and in Resource Management
  - Improve use of the available bandwidth (MPI implementations, lower level communication, etc.).
  - Consider new algorithmic methods
  - Considering alternative programming models that improve efficiency of calculations

Performance and Scalability

- Use of heterogeneous computational units
  - While more than ½ of the science has some GPU based investigations, only a few are using GPUs in production science
    - Many applications are GPUized only in a very limited way
    - Few are using GPUs at scale (more GPU resources are relatively small scale with limited networks)
  - Help the science teams to make more effective use of GPUs consists of two major components.
    - Introduce compiler and library capabilities into the science team workflow to significantly reduce the programming effort and impact on code maintainability.
      - OpenACC support is the major path to more general acceptance
    - Load balancing at scale
- Storage Productivity
  - Interface with improved libraries and middle ware
  - Modeling of I/O
  - On-line and Near-line transparent interfaces

Application Flexibility

- Using both XE and XK nodes in single applications
  - For multi-physics applications that provide a natural decomposition into modules is to deploy the most appropriate module(s) different computational units.
  - For applications use the Charm++ adaptive runtime system, heterogeneity can be handled without significant changes to the application itself.
  - Some applications naturally involve assigning multiple blocks to individual processors include multiblock codes (typically in fluid dynamics), and the codes based on structured adaptive mesh refinement.
  - The application-level load balancing algorithms can be modified to deal with the performance heterogeneity created by the mix of nodes.
- Malleability
  - Understanding topology given and maximizing effectiveness
  - Being able to express desired topology based on algorithms
  - Mid ware support

Flexibility - Application Based Resiliency

- Application Based Resiliency
  - Multiple layers of Software and Hardware have to coordinate information and reaction
  - Analysis and understanding is needed before action
  - Correct and actionable messages need to flow up and down the stack to the applications so they can take the proper action with correct information
  - Application Situational Awareness - need to understand circumstances and take action
  - Flexible resource provisioning needed in real time
  - Interaction with other constraints so sub-optimization does not adversely impact overall system optimization

Current State of Enhanced Approaches

- Blue Waters has redirected up to 10% of its hardware funding to support enhanced intellectual services
- Blue Waters is providing direct funding to current science teams to improve their applications in ways that would not normally take place
  - Some are dramatically re-engineering their applications
- Expanding educational and outreach efforts
  - Expanded virtual school classes, internships and fellowships
  - Expanding community engagements
- Matching technology providers with technology consumers
  - New methods and techniques that directly improve the sustained performance of one or more science teams.

Observations on Co-Design

- Blue Waters has been doing co-design before co-design was a term
- Focus on Interconnect and SW – not processors
- Much different process for vendors – many vendor workers do not understand co-design
- Independent co-design teams is counter productive
  - Competing inputs – now resolution path
- Transparency in cost tradeoffs has to be much better
- Much better and more application modeling
- Resourcing and risk management is very key
- Most of the burden of re-design is still on applications not the system providers
- Need to explicitly fund application teams for co-design and modeling or they will not be able to pay enough attention

Blue Waters Sustaining Goals

- Deploy a capable, balanced system of sustaining more than one petaflops or more for a broad range of applications
- Enable Science Teams to take full advantage of sustained petascale systems
- Enhance the operation and use of the sustained petascale system
- Provide a world-class computing environment for the petascale system
- Exploit advances in innovative computing technology
- Provide National Leadership

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Individual Contributions From

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- Cristina Beldica, Brett Bode, Michelle Butler, Greg Bauer, Mike Showerman, John Melchi, Scott Lathrop, Merle Giles
- Sanjay Kale, Steve Lumetta, Ravi Iyer, David Padua
- The Blue Waters Project Team and our partners
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PI	Award Date	Project Title
Sugar	04/15/2009	Lattice QCD on Blue Waters
Bartlett	04/15/2009	Super instruction architecture for petascale computing
Nagamine	04/15/2009	Peta-Cosmology: galaxy formation and virtual astronomy
Bissett	05/01/2009	Simulation of contagion on very large social networks with Blue Waters
O'Shea	05/01/2009	Formation of the First Galaxies: Predictions for the Next Generation of Observatories
Schulten	05/15/2009	The computational microscope
Stan	09/01/2009	Testing hypotheses about climate prediction at unprecedented resolutions on the NSF Blue Waters system
Campanelli	09/15/2009	Computational relativity and gravitation at petascale: Simulating and visualizing astrophysically realistic compact binaries
Yeung	09/15/2009	Petascale computations for complex turbulent flows
Schnetter	09/15/2009	Enabling science at the petascale: From binary systems and stellar core collapse To gamma-ray bursts

PI	Award Date	Project Title
Woodward	10/01/2009	Petascale simulation of turbulent stellar hydrodynamics
Tagkopoulos	10/01/2009	Petascale simulations of Complex Biological Behavior in Fluctuating Environments
Wilhelmson	10/01/2009	Understanding tornadoes and their parent supercells through ultra-high resolution simulation/analysis
Wang	10/01/2009	Enabling large-scale, high-resolution, and real-time earthquake simulations on petascale parallel computers
Jordan	10/01/2009	Petascale research in earthquake system science on Blue Waters
Zhang	10/01/2009	Breakthrough peta-scale quantum Monte Carlo calculations
Haule	10/01/2009	Electronic properties of strongly correlated systems using petascale computing
Lamm	10/01/2009	Computational chemistry at the petascale
Karimabadi	11/01/2010	Enabling Breakthrough Kinetic Simulations of the Magnetosphere via Petascale Computing
Mori	01/15/2011	Petascale plasma physics simulations using PIC codes

PI	Award Date	Project Title
Voth	02/01/2011	Petascale multiscale simulations of biomolecular systems
Woosley	02/01/2011	Type Ia supernovae
Cheatham	02/01/2011	Hierarchical molecular dynamics sampling for assessing pathways and free energies of RNA catalysis, ligand binding, and conformational change
Wuebbles	04/15/2011	Using petascale computing capabilities to address climate change uncertainties
Gropp	06/01/2011	System software for scalable applications
Klimeck	09/15/2011	Accelerating nano-scale transistor innovation
Pande	09/15/2011	Simulating vesicle fusion on Blue Waters

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PRAC PI Institutions

Note – UIUC is only institution leading more than one PRAC (4)
UIUC has Co-PIs on several others

Computational Microscopy

Klaus Schulten (UIUC)

- Simulations of 4 different biological systems
  - Protein elongation in the ribosome
  - Structural transitions in poliovirus entry
  - Sculpting cellular membranes by BAR domains
  - Energy conversion by the chromatophore organelle
- NAMD molecular dynamics code
  - System size will exceed 100M atoms for the first time