BLUE WATERS

SUSTAINED PETASCALE COMPUTING

Blue Waters System Overview

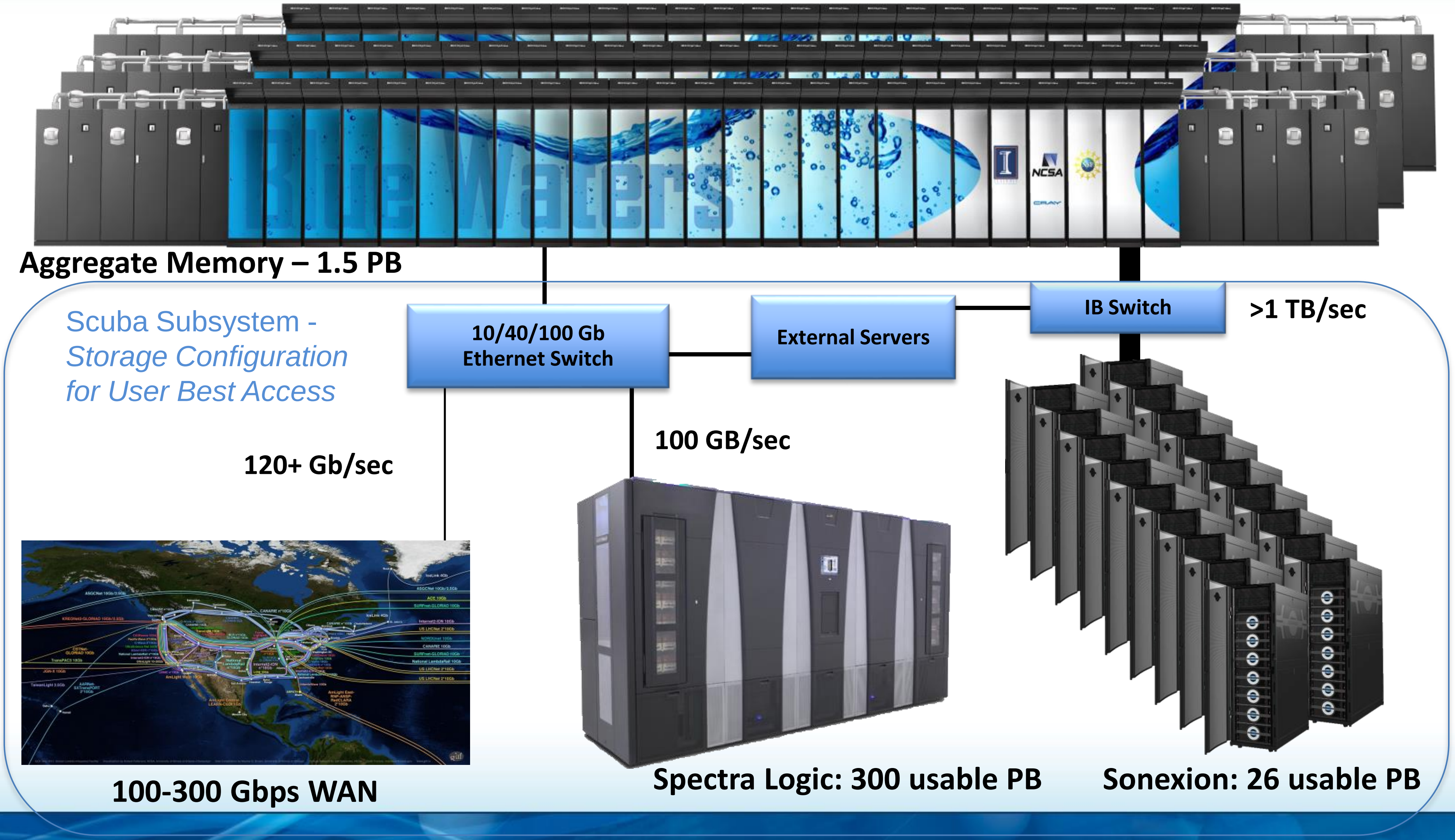
NCSA

NSF

GREAT LAKES CONSORTIUM
FOR PETASCALE COMPUTATION

CRAY

Blue Waters Computing System



Aggregate Memory – 1.5 PB

Scuba Subsystem - Storage Configuration for User Best Access

10/40/100 Gb Ethernet Switch

External Servers

IB Switch

>1 TB/sec

100 GB/sec

120+ Gb/sec

100-300 Gbps WAN

Spectra Logic: 300 usable PB

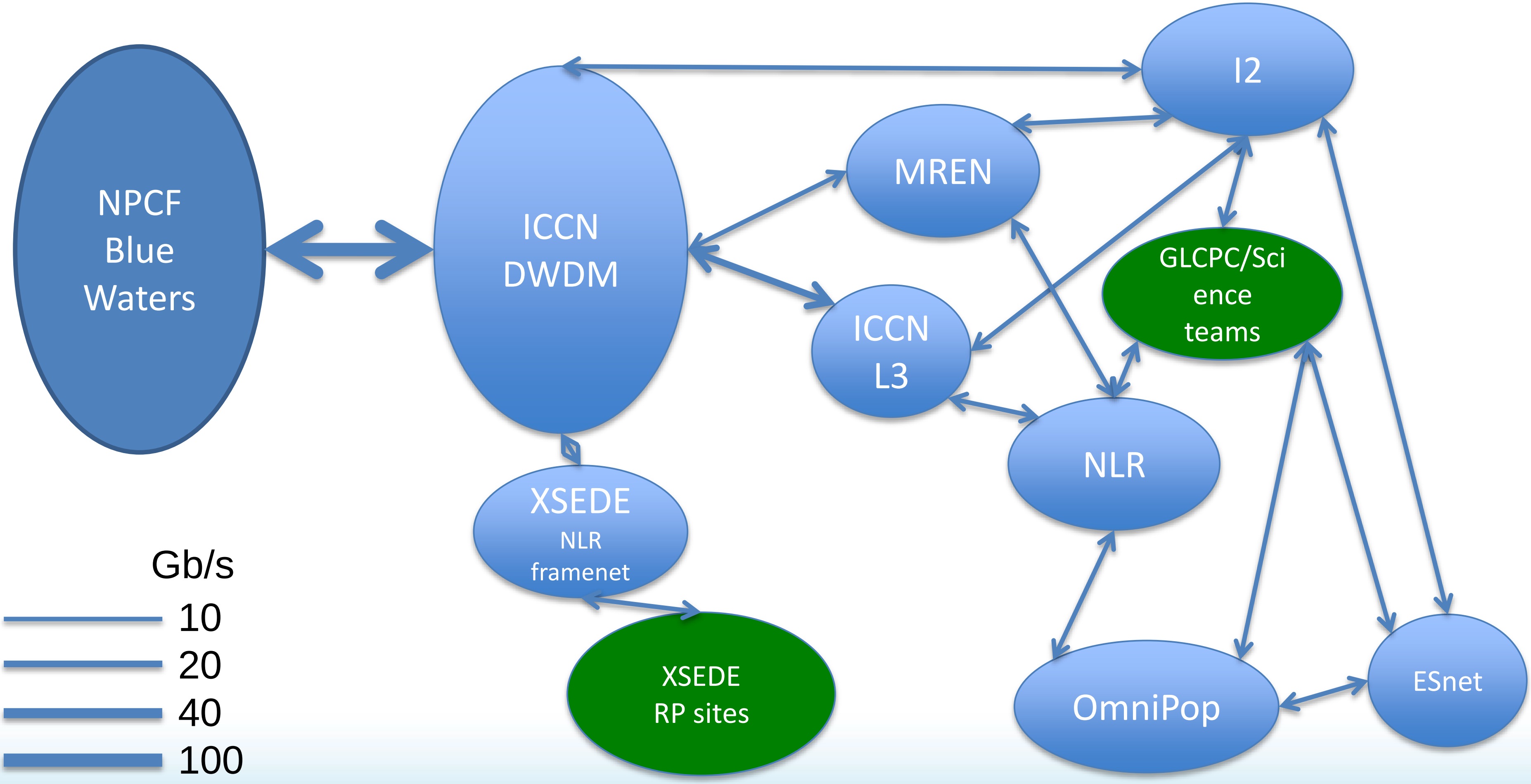
Sonexion: 26 usable PB

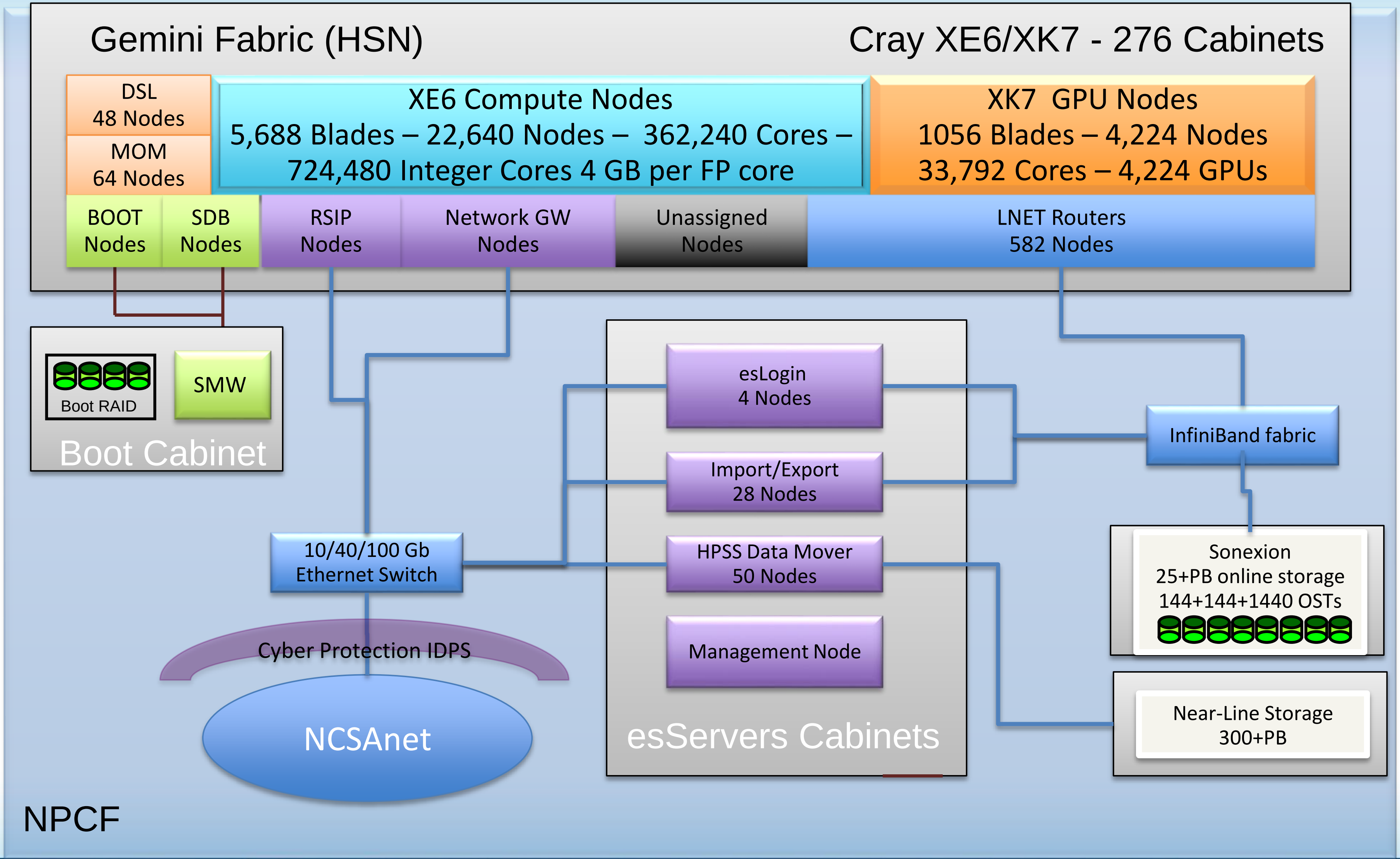
National Petascale Computing Facility

- 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

The Movement of Data





Gemini Fabric (HSN)

Cray XE6/XK7 - 276 Cabinets

DSL
48 Nodes

MOM
64 Nodes

XE6 Compute Nodes
5,688 Blades – 22,640 Nodes – 362,240 Cores – 724,480 Integer Cores 4 GB per FP core

XK7 GPU Nodes
1056 Blades – 4,224 Nodes
33,792 Cores – 4,224 GPUs

BOOT Nodes

SDB Nodes

RSIP Nodes

Network GW Nodes

Unassigned Nodes

LNET Routers
582 Nodes

Boot RAID

SMW

Boot Cabinet

esLogin
4 Nodes

Import/Export
28 Nodes

HPSS Data Mover
50 Nodes

Management Node

esServers Cabinets

InfiniBand fabric

Sonexion
25+PB online storage
144+144+1440 OSTs

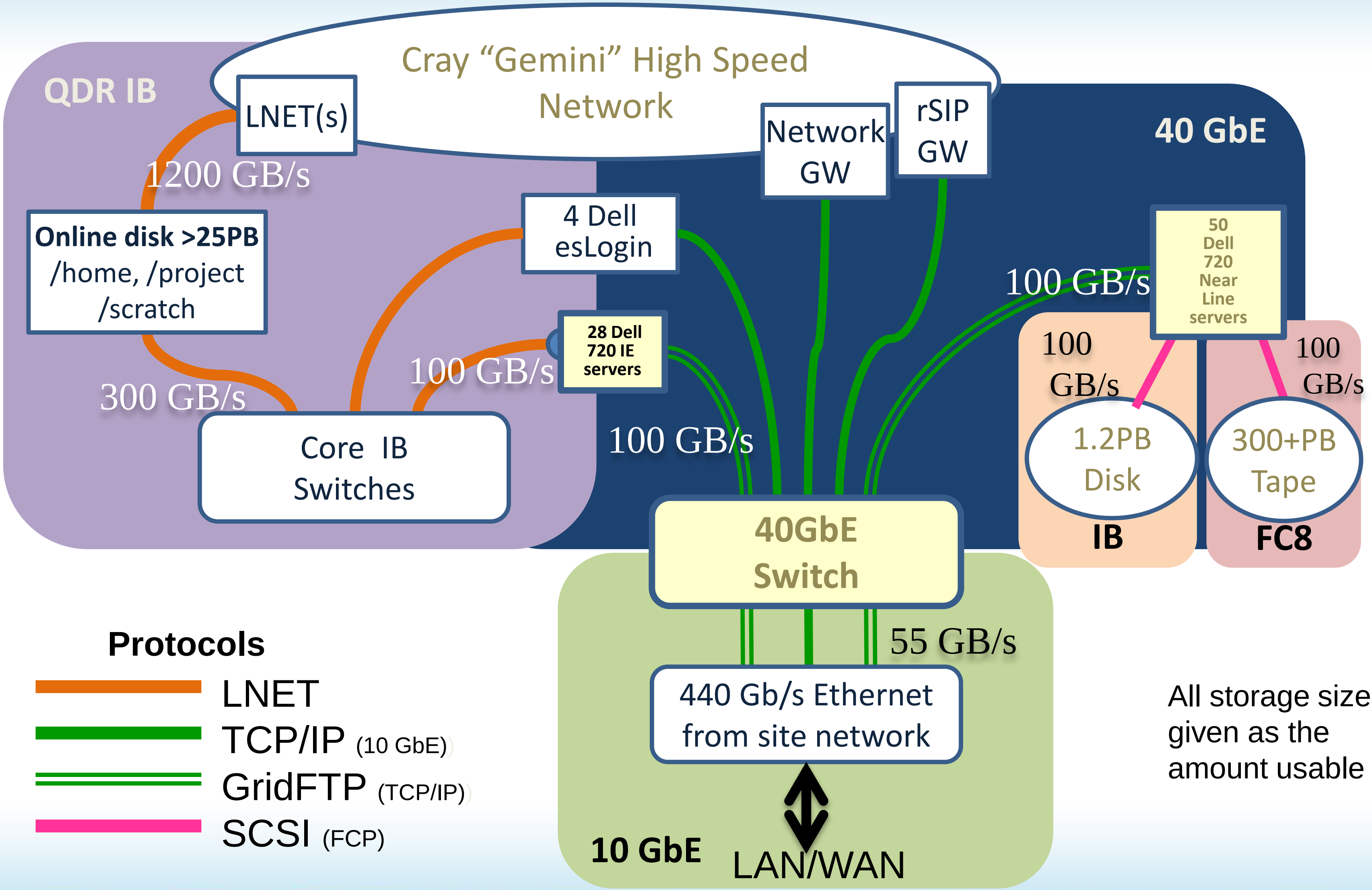
Near-Line Storage
300+PB

10/40/100 Gb Ethernet Switch

Cyber Protection IDPS

NCSAnet

NPCF



Protocols

🟧	LNET
🟩	TCP/IP (10 GbE)
〓	GridFTP (TCP/IP)
🟪	SCSI (FCP)

All storage sizes given as the amount usable

Blue Waters Nearline/Archive System

- Spectra Logic T-Finity
  - Dual-arm robotic tape libraries
  - High availability and reliability, with built-in redundancy
- Blue Waters Archive
  - Capacity: 380 PBs (*raw*), 300 PBs (*usable*)
  - Bandwidth: 100 GB/sec (*sustained*)
  - Redundant arrays of independent tapes RAIT for increased reliability.
  - Largest HPSS open production system.

Online Storage

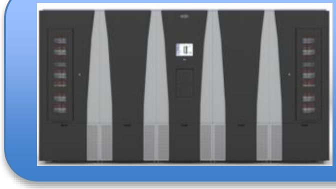
home : 144 OSTs : 2.2 PB useable : 1 TB quota

projects: 144 OSTs : 2.2 PB useable : 5 TB group quota

scratch: 1440 OSTs : 22 PB useable : 500 TB group quota

- Cray Sonexion with Lustre for all file-systems.
- All visible from compute nodes.
- Scratch has 30 day purge policy in effect for both files and directories. Not backed up.
- ONLY home and project file-systems are backed up.

Nearline Storage (HPSS)



home: 5 TB quota

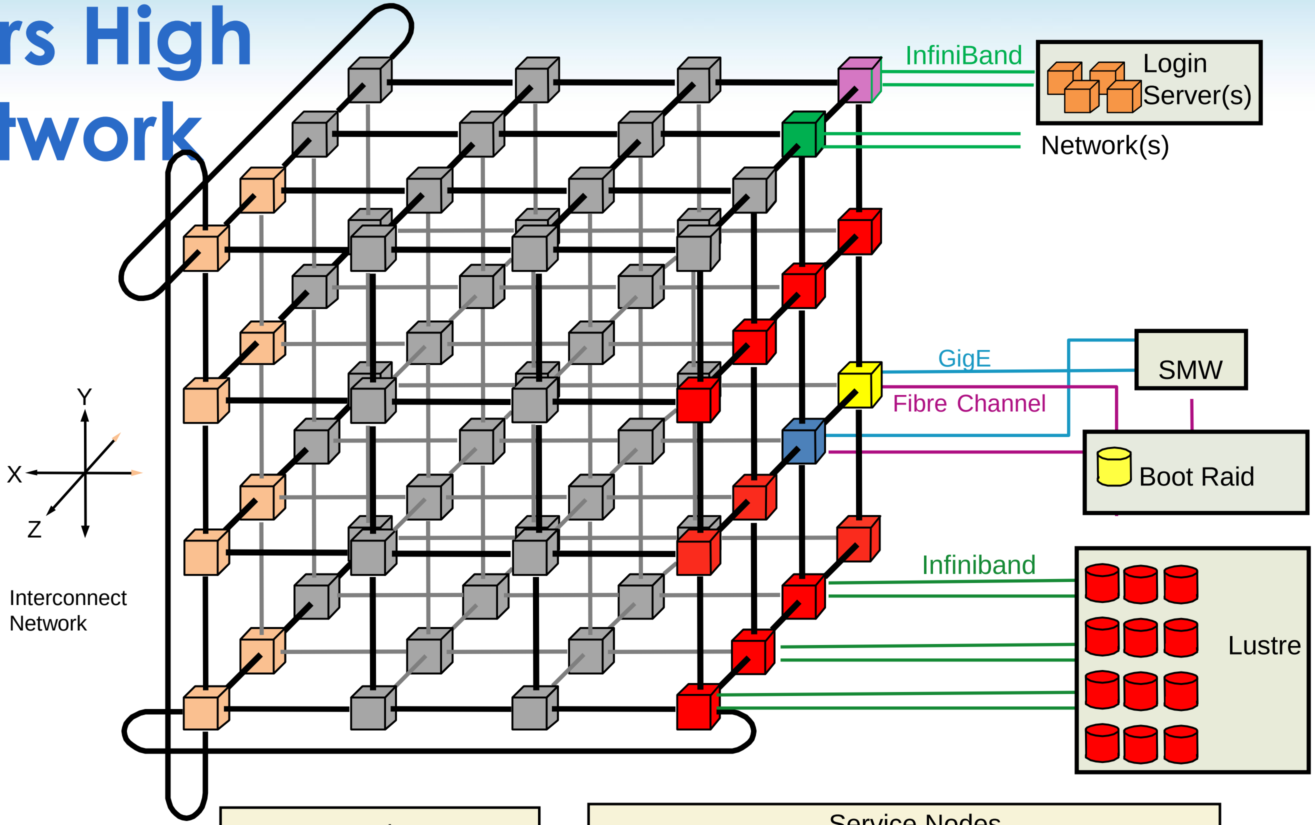
projects: 50 TB group quota

- IBM HPSS + DDN + Spectra Logic.
- Accessed via GO or globus-url-copy.

GO with Globus Online

- GridFTP client development for IE and HPSS nodes.
- Enabled data striping with GridFTP.
- Managed file transfers.
- Command line interface.
- Globus connect for sites without GridFTP endpoints.

Blue Waters High Speed Network



Compute Nodes

- ⬜ Cray XE6 Compute
- 🟧 Cray XK7 Accelerator

Service Nodes

Operating System

- 🟦 Boot
- 🟨 System Database

Login/Network

- 🟪 Login Gateways
- 🟩 Network

Lustre File System

- 🟥 LNET Routers

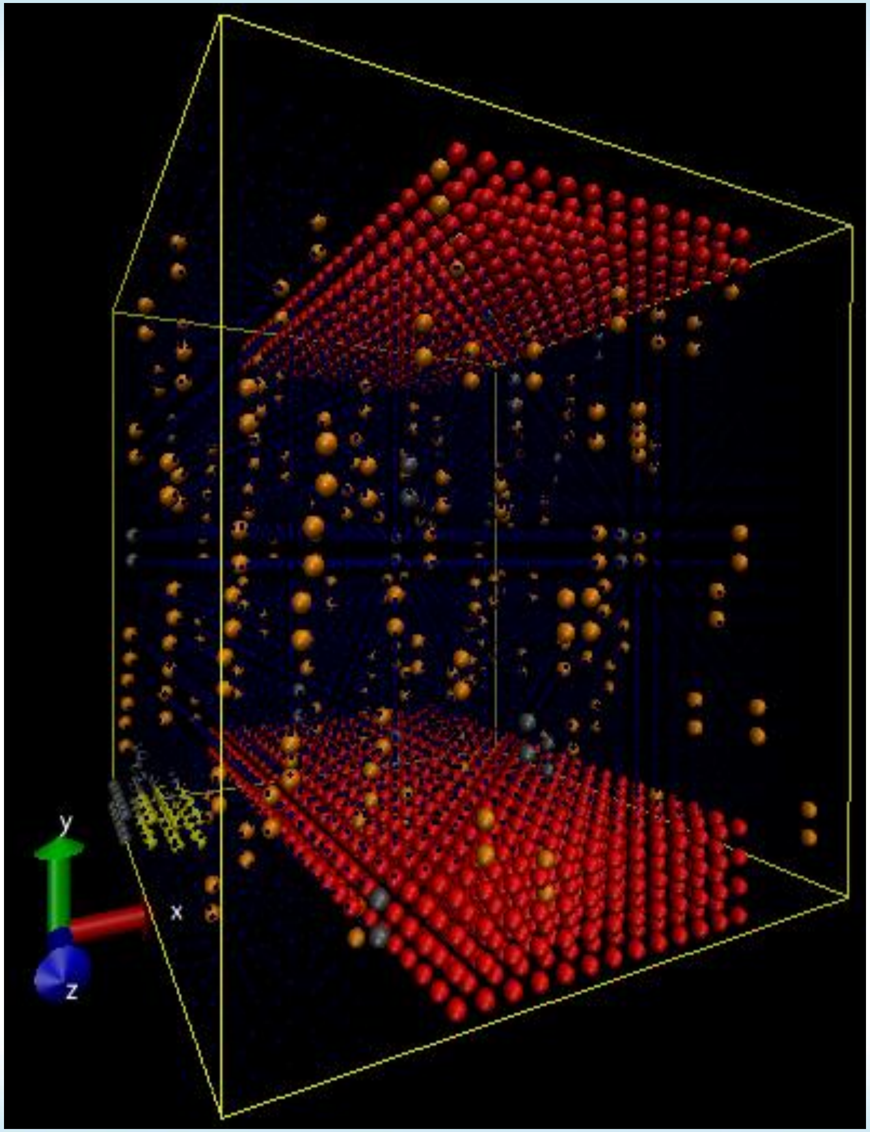
Blue Waters 3D Torus Size
24 x 24 x 24

HSN View

Gemini-node distinction

- Red – XK
- Orange – LNET
- Yellow – MOM
- Gray – Service
- Blue – XE

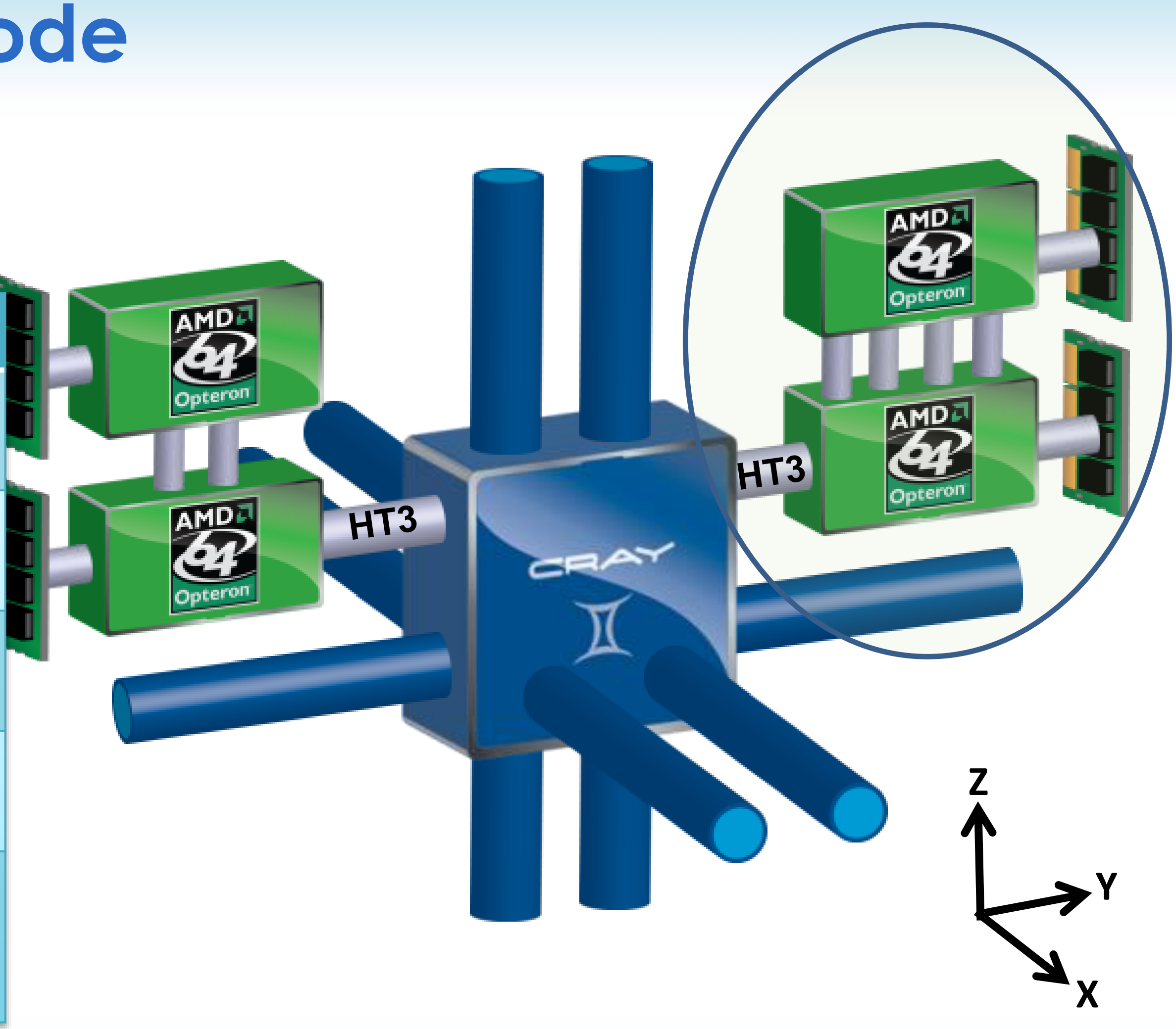
Complicated Topology



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.

XE Node NUMA and core complexity

- 2 sockets per XE node.
- 2 NUMA domains per socket.
- 4 Bulldozer FP units per NUMA domain.
- 2 integer units per FP unit.

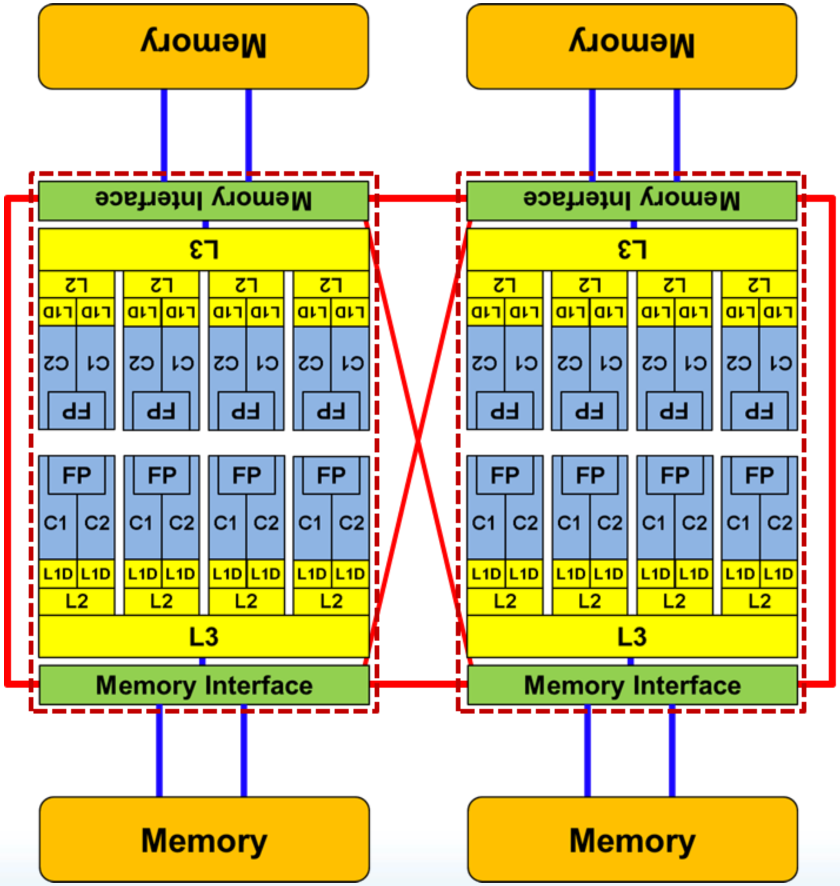


Image courtesy of Georg Hager http://blogs.fau.de/

CPU Node Comparison

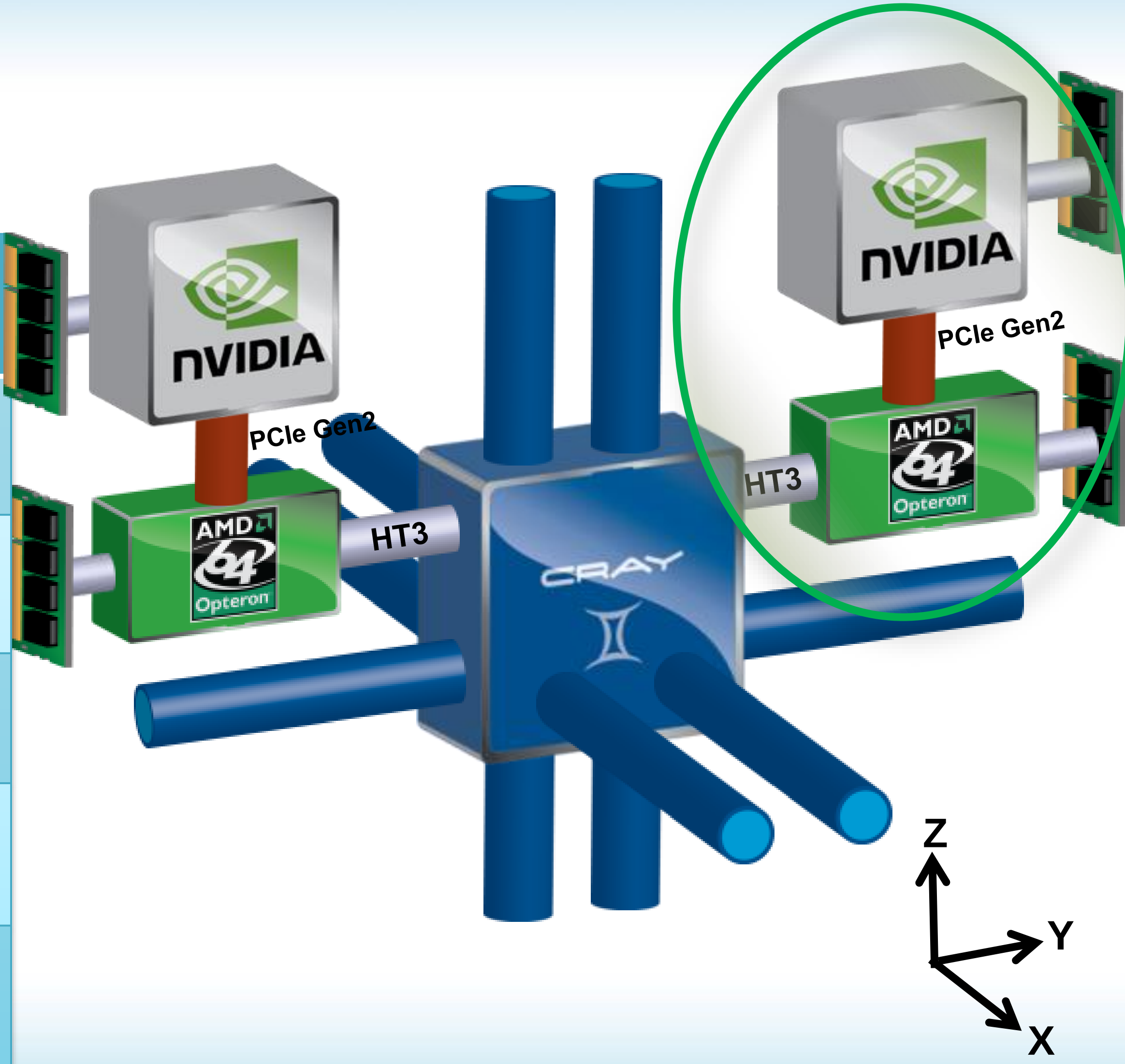
Node	Processor type	Nominal Clock Freq. (GHz)	FPU cores	Peak GF/s	Peak GB/s
Blue Waters Cray XE	AMD 6276 Interlagos	2.45	16*	313	102
NICS Kraken Cray XT	AMD Istanbul	2.6	12	125	25.6
NERSC Hopper XE	AMD 6172 MagnyCours	2.1	24	202	85.3
ANL IBM BG/P	POWERPC 450	0.85	4	13.6	13.6
ANL IBM BG/Q	IBM A2	1.6	16*	205	42.6
NCAR Yellowstone	Intel E5-2670 Sandy Bridge	2.6	16*	333	102
NICS Darter Cray XC30	Intel E5-2600 Sandy Bridge	2.6	16*	333	102

An * indicates processors with 8 flops per clock period.

Cray XK7

Blue Waters contains 4,224 NVIDIA K20x (GK110) GPUs

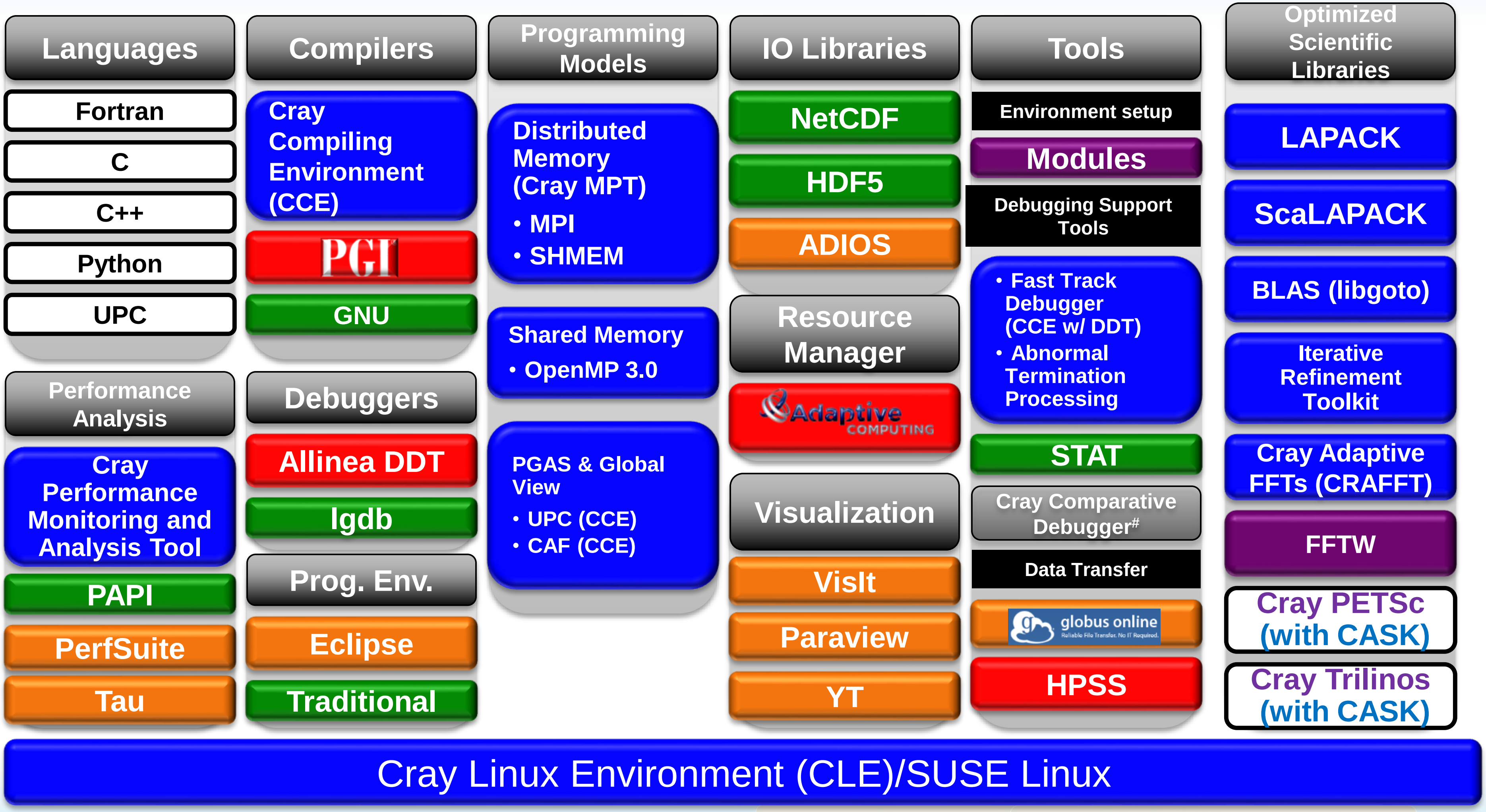
XK7 Compute Node Characteristics	
Host Processor	AMD Series 6200 (Interlagos)
Host Processor Performance	156.8 Gflops
K20x Peak (DP floating point)	1.32 Tflops
Host Memory	32GB 51 GB/sec
K20x Memory	6GB GDDR5 capacity 235GB/sec ECC



XK Features

- Hardware accelerated OpenGL with an X11 server. Not standard support by vendor.
- GPU operation mode flipped to allow display functionality (was compute only).
- X server enabled/disabled at job start/end when specified by user.
- Several teams use XK nodes for visualization to avoid transferring large amounts of data, shortening workflow.

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

Reliability

- We provide to the user a checkpoint interval calculator based on the work of J. Daly, using recent node and system interrupt data. User inputs number of XE and/or XK nodes, and the time to write a checkpoint file.
- September data
  - 22,640 XE nodes MTTI ~ 14 hrs.
  - 4,224 XK nodes MTTI ~ 32 hrs.
  - System interrupts MTTI ~ 100 hrs.
- Checkpoint intervals on the order of 4 – 6 hrs. at full system (depending on time to write checkpoint).

Summary

- Outstanding Computing System
    - The largest installation of Cray's most advanced technology
    - Extreme-scale Lustre file system with advances in reliability/maintainability
    - Extreme-scale archive with advanced RAIT capability
- Most balanced system in the open community
    - Blue Waters is capable of addressing science problems that are memory, storage, compute, or network intensive or any combination.
    - Use of innovative technologies provides a path to future systems
- Illinois/NCSA is a leader in developing and deploying these technologies as well as contributing to community efforts.