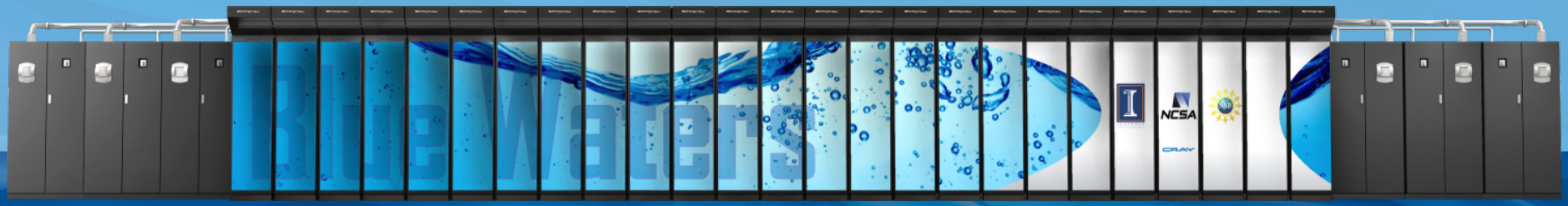
BLUE WATERS

SUSTAINED PETASCALE COMPUTING

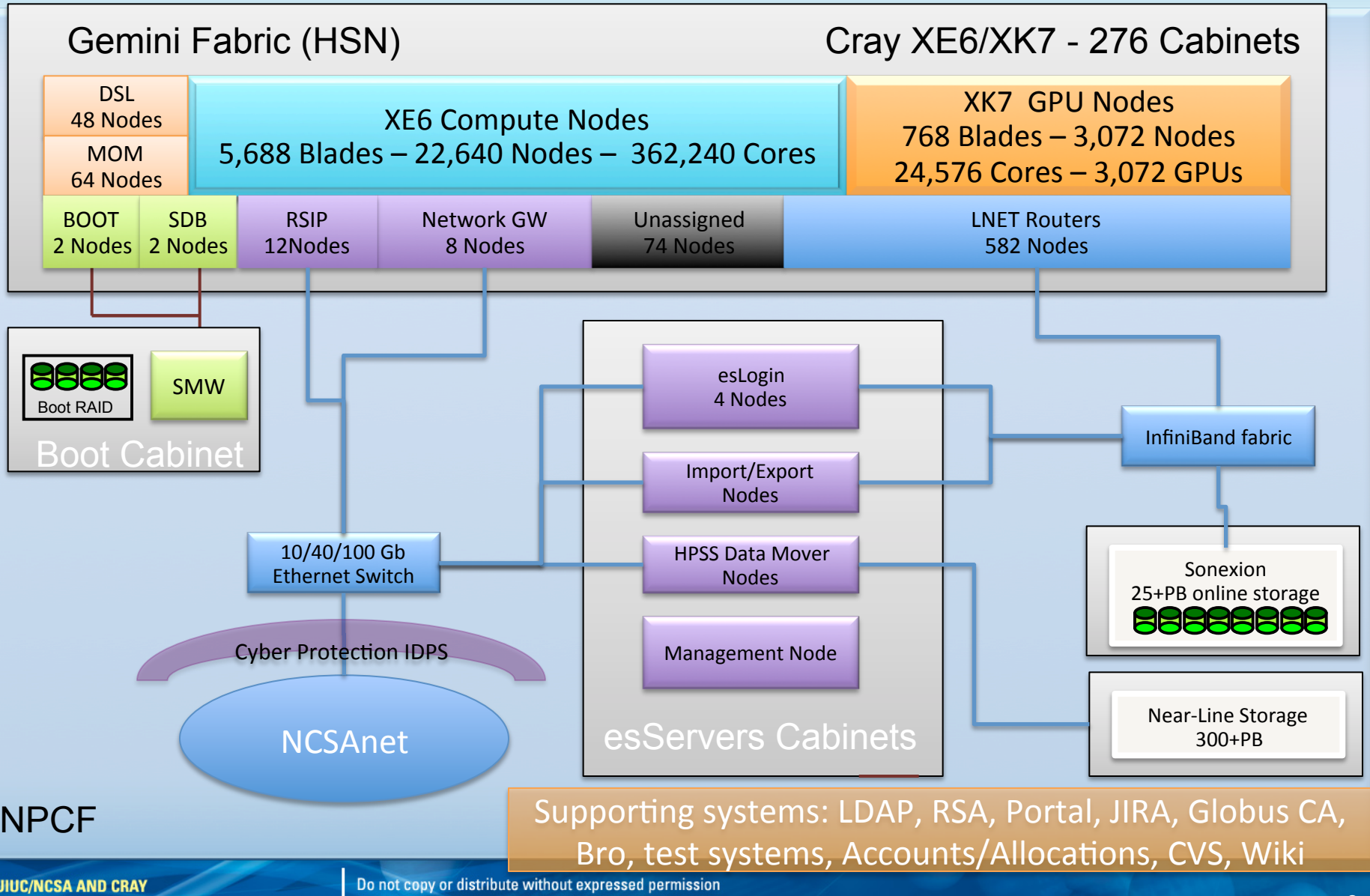
INRIA/UIUC/ANL JLPC – June 2012

"Mapping and Scheduling Break Out"

Bill Kramer



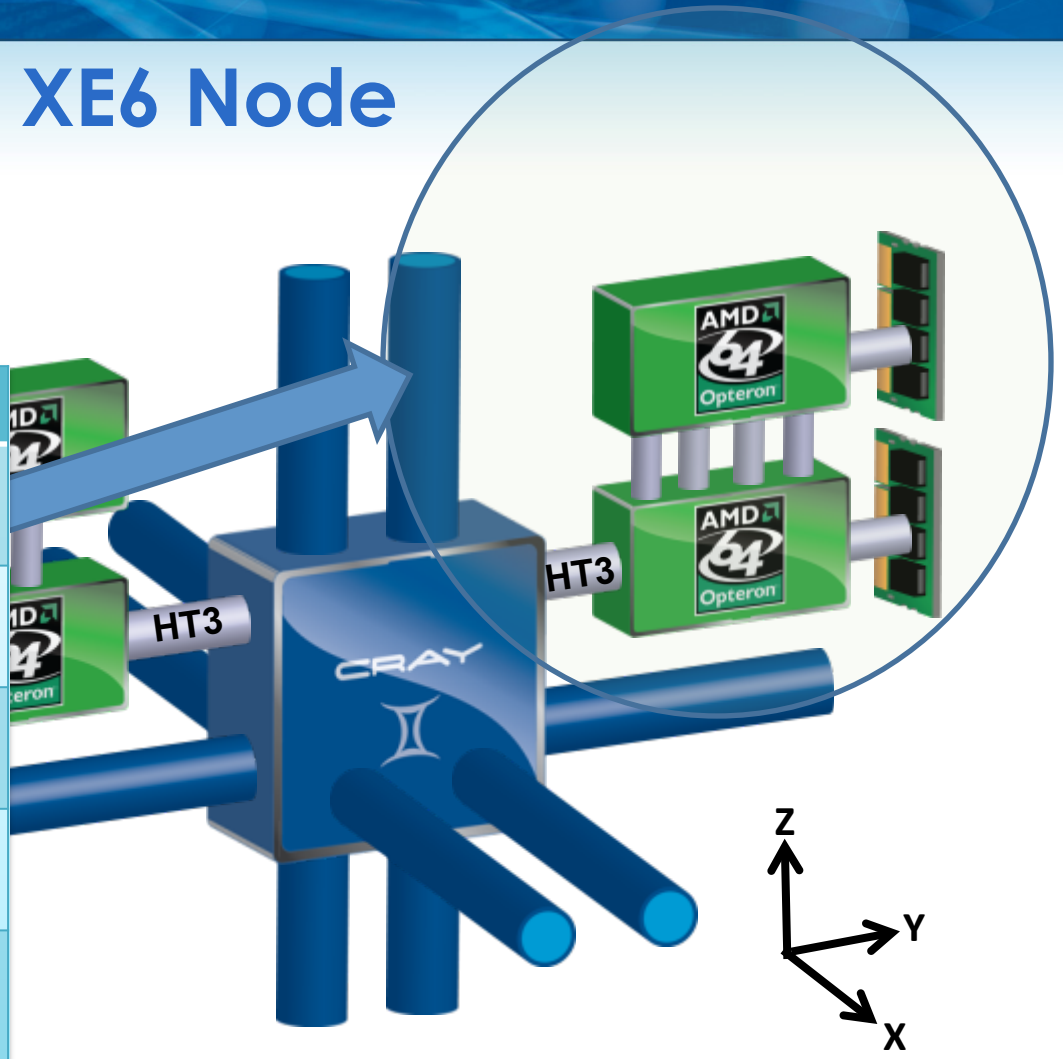
NCSA NSF GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION CRAY



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

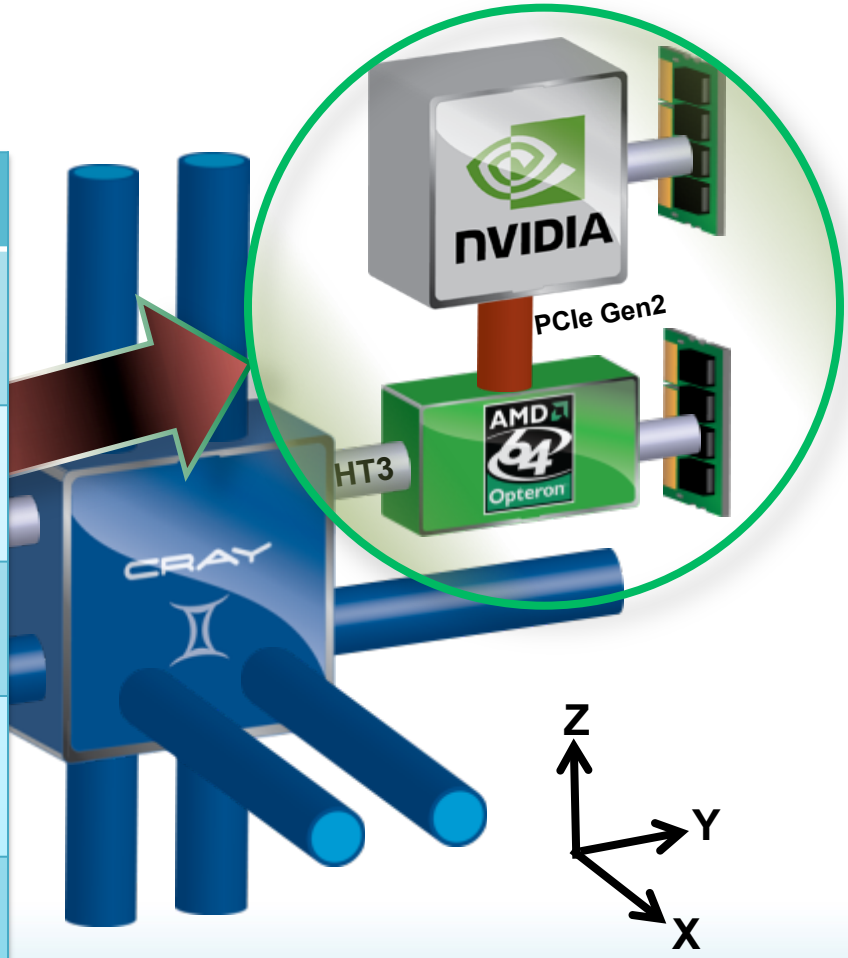


*Each core module includes 1 256-bit wide FP unit and 2 integer units. This is often advertised as 2 cores, leading to a 32 core node.

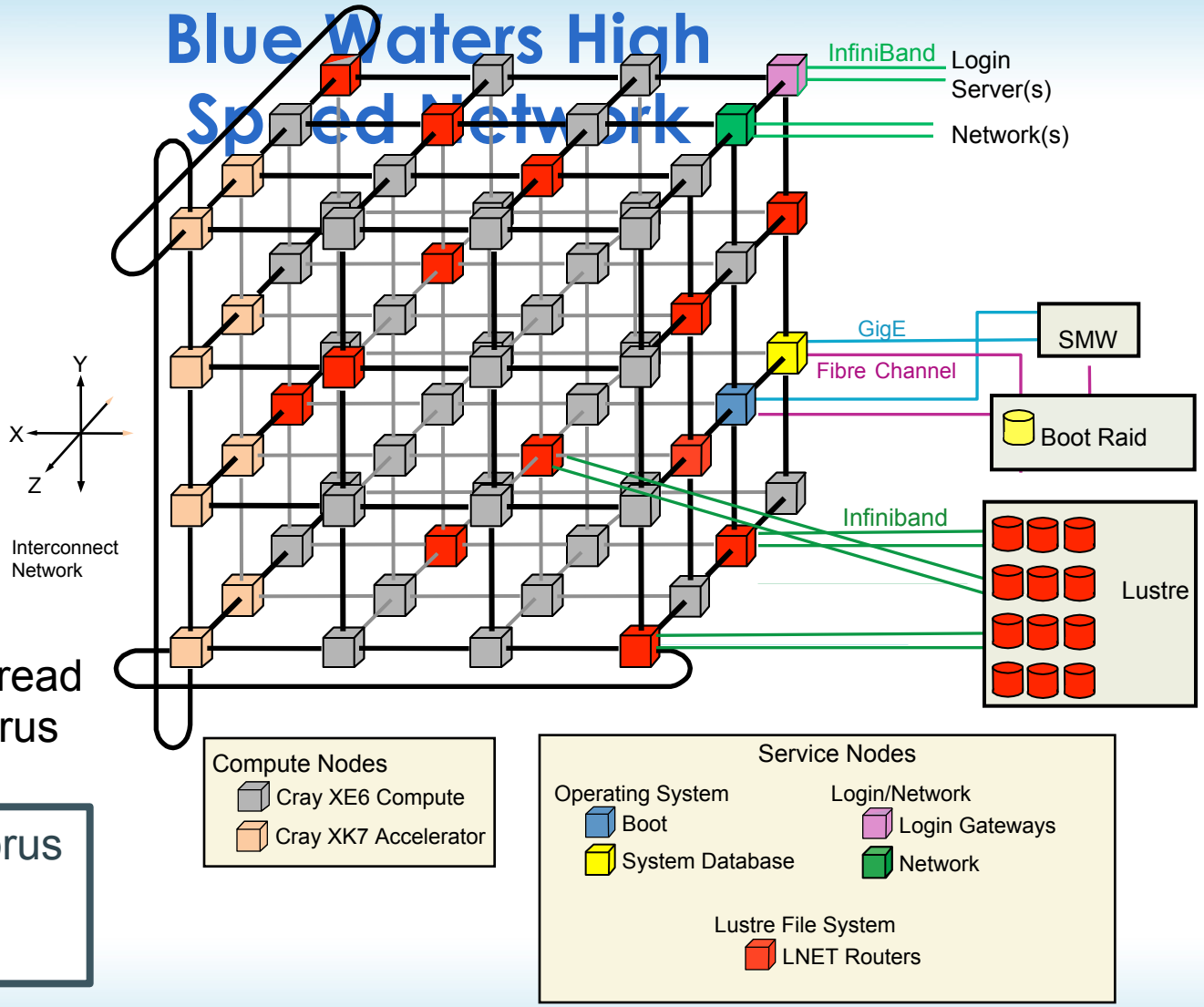
Cray XK7 and a Path to the Future

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



Blue Waters High Speed Network



Service Nodes spread Throughout the torus

Blue Waters 3D Torus Size
23 x 24 x 24

BW Sustained Petascale Performance Measures

- Original NSF Benchmarks
  - Full Size – QCD (MILC), Turbulence (PNSDNS), Molecular Dynamics (NAMD)
  - Modest Size – MILC, Paratec, WRF
- SPP – is a time to solution metric that is using the planned applications on representative parts of the Science team problems
  - Represents end to end problem run including I/O, pre and post phases, etc.
  - Coverage for science areas, algorithmic methods, scale
- SPP Application Mix (details and method 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 three SPP benchmarks run at full scale
- XK nodes have to add 15% more SPP

BW Benchmarks Benefit from Topology Awareness

- Original NSF Benchmarks
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- At least three SPP benchmarks run at full scale
- **Bold** = codes known to benefit from topology optimization

Effective Use of Complex Systems

- Only a small subset of BW applications use Charm++ (sorry Sanjay). The vast majority are MPI or MPI/OpenMP
- Increasing performance requires dramatic increases in parallelism that then generates complexity challenges for science and engineering teams
- Goals that require improved topology mapping and scheduling
  - **Scaling applications to large core counts on general-purpose CPU nodes**
  - **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

- 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

Application Topology Challenges - Opportunities

- Deciding best/improved topology layout for major applications
  - Project Improvements in run time
- Interface and adjustments for MPI task topology
- Improved monitoring/measurement of communication and performance as topology changes
- Flexibility expressing desired topology – can not over specify and expect to have good throughput
- Visualization of layouts and traffic

System Topology Challenges - Opportunities

- Ability to express both logical and physical topology layout/options
  - Current resource manager just presents a logical list of available nodes – not related to logical or physical topology
- Estimating overhead and increase wait time to accumulate better topologies.
- Providing interfaces for different topology aware scheduling algorithms
  - With multidimension weighting
- Schedule for I/O performance/topology
- Visualization of layouts

Topology Awareness and Scheduling Summary

- Topology aware use and scheduling is critical to improving application performance for current and future architectures
- Application and System challenges have to be overcome at multiple levels
- Deterministic solutions are not likely except in small scale or dedicated time
  - More likely there will be flexible “proximity” refinements