

# BLUE WATERS

SUSTAINED PETASCALE COMPUTING

## Update on Topology Aware Scheduling (aka TAS)



GREAT LAKES CONSORTIUM  
FOR PETASCALE COMPUTATION

CRAY®

Work done in collaboration with

- J. Enos, G. Bauer, R. Brunner, S. Islam



- R. Fiedler 

- Adaptive Computing 

# When things look good

of 10 largest running jobs on the Gemini torus.

Tue 11.02.2014 at 09:39:51 AM CST

JOBID	USERID
574728	jtao
576980	redwards
576982	redwards
576985	redwards
576987	redwards
589495	yanxinl
590655	yanxinl
588655	wdaughto
592154	leeping
590536	fdm

## What's the problem?

- Efficient job scheduling on a large torus is not easy.
- Over time (between large jobs, reboots) fragmented allocations appear.
- Fragmentation can lead to degraded and variable application performance.

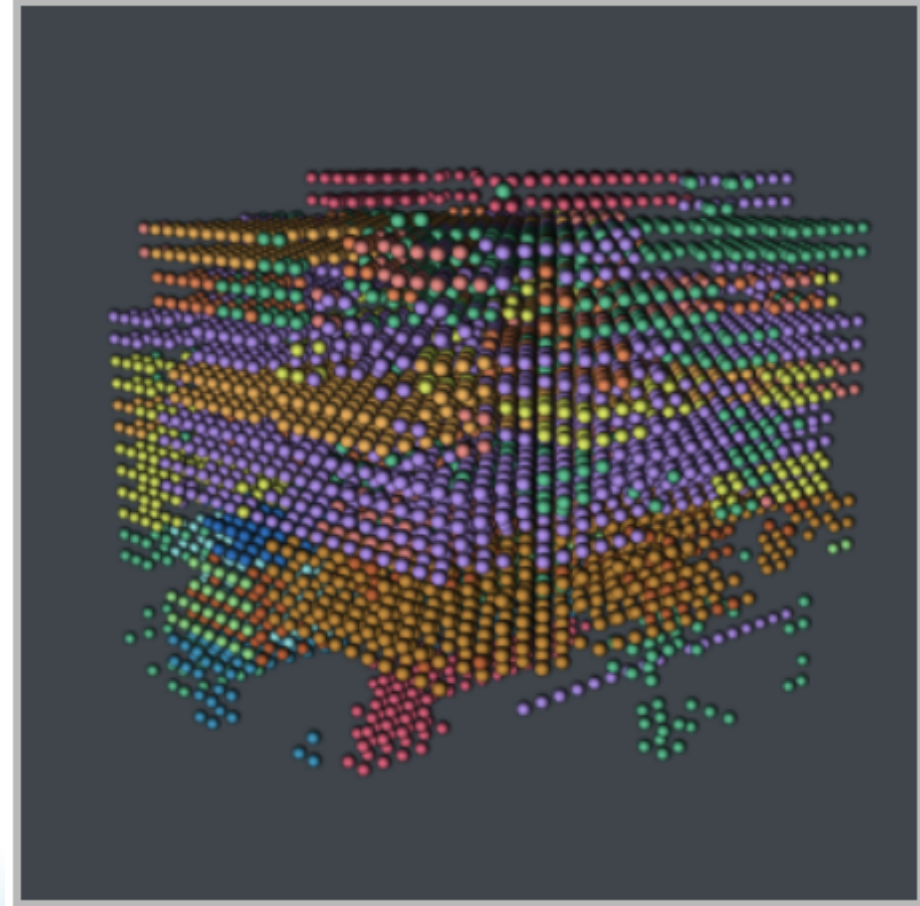
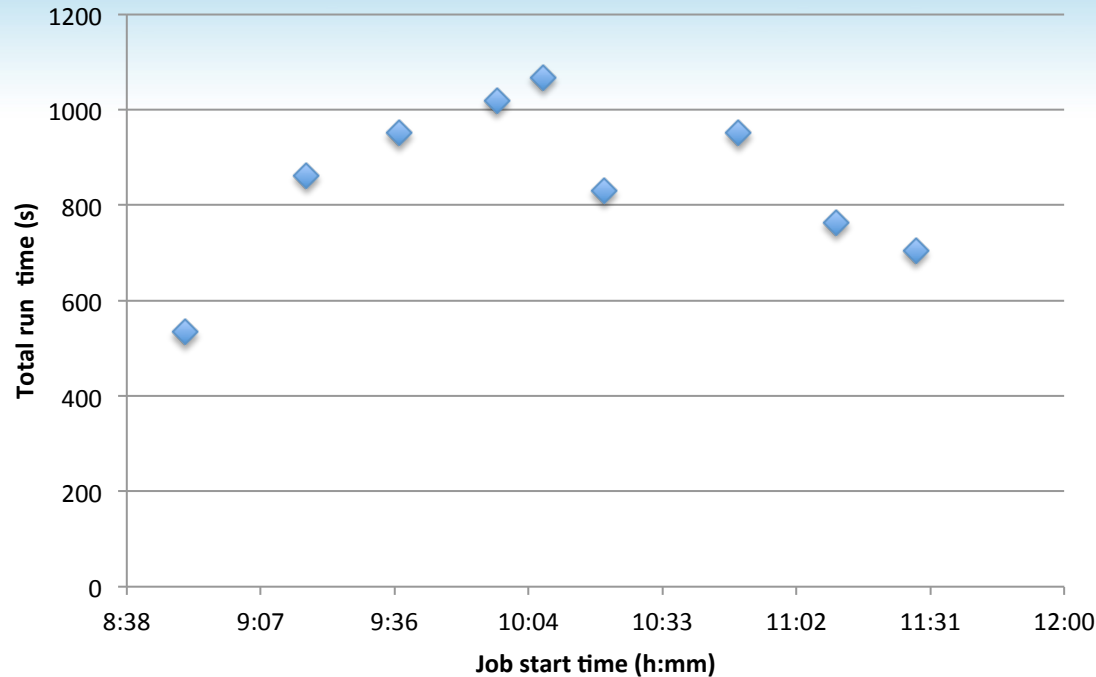


Image credit: Robert Sisneros



- 4,116 XE node jobs run at different times.
- Run to run variability
  - makes it difficult to assign a reasonable wall clock time.
  - has an impact on job throughput.

## Blue Waters Torus

- 24x24x24 gemini routers, 2 nodes each
- XE nodes not shown
- XK nodes (red) 15x6x24
- XIO nodes (yellow)
- Links along X & Z dimensions 2x faster than links along Y.

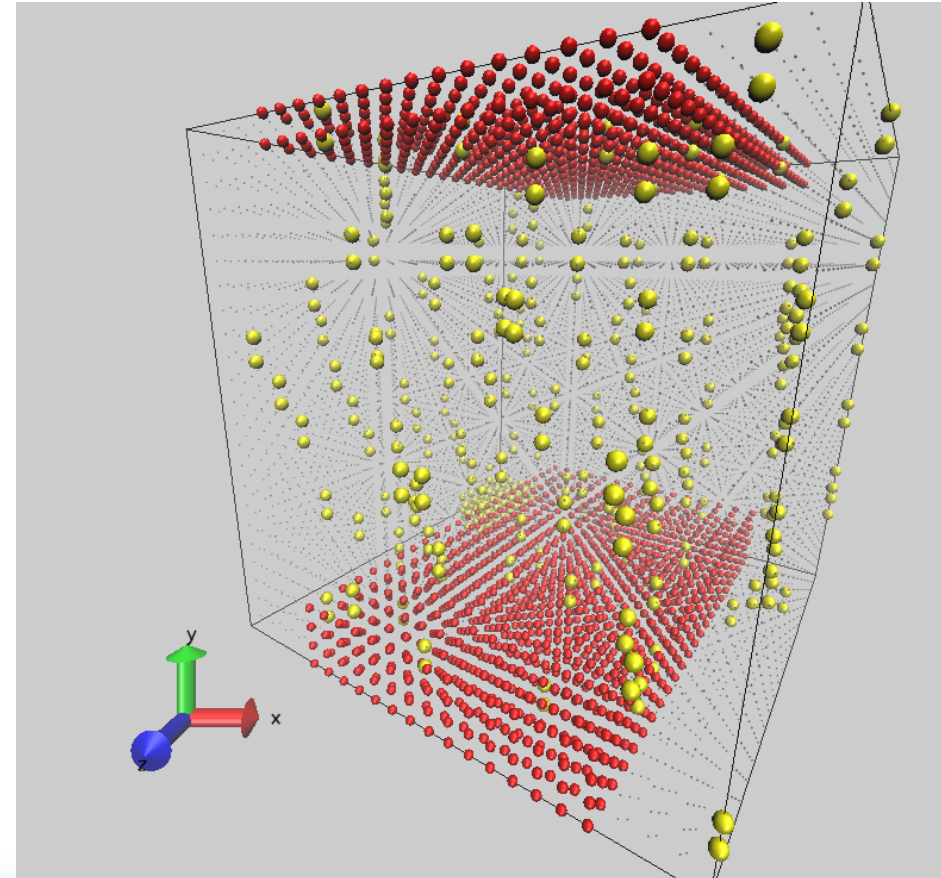
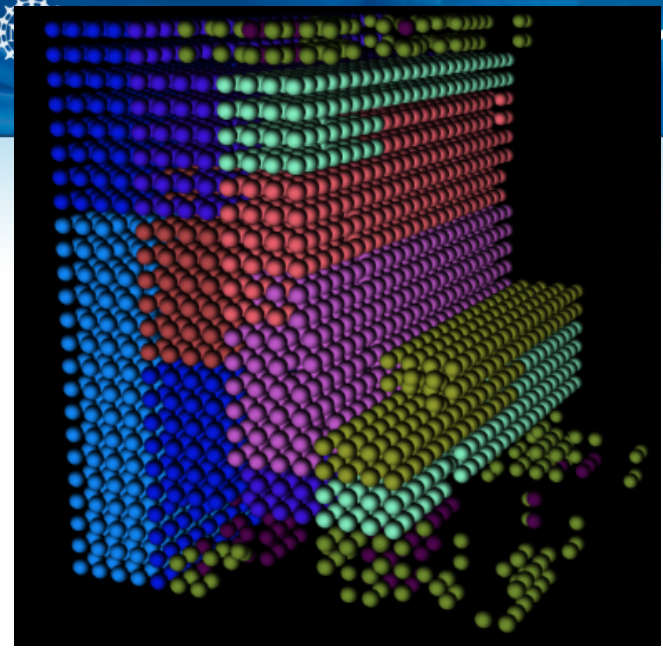


Image credit: VMD

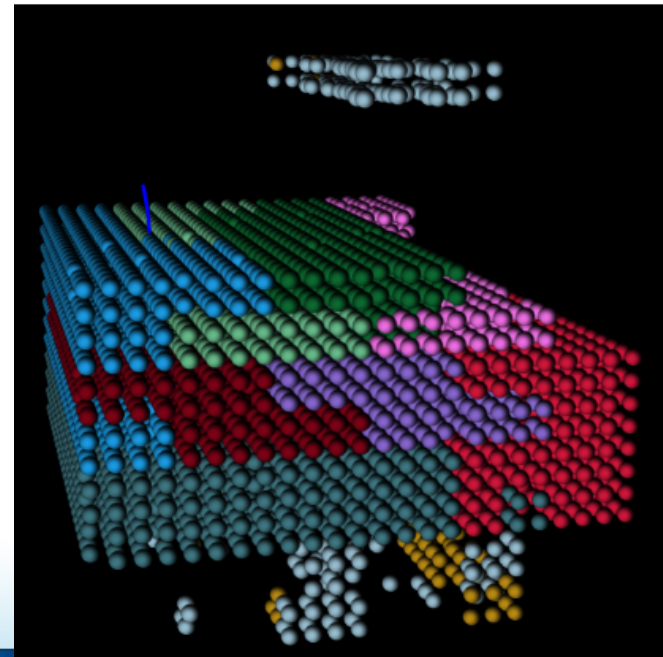


## While waiting for TAS

- Changed default node ordering to favor XZ slabs; improving aggregate interconnect bandwidth and location.
- Workload of MILC, NWCHEM, PSDNS ChaNGa, NAMD, WRF, CESM, DNS\_distuf showed average improvements in runtime of 15% to 25%.
- Change does not address job-job interaction.



before



after

- Experimented with pre-defined moab features (explicit node lists) and nodesets of these features.
- Worked well for some teams to improve performance and limit job-job interference.
- Impacted job throughput (having to wait longer for specific sets of nodes).
- Responsiveness of moab adversely affected.



# Impact of topology aware scheduling

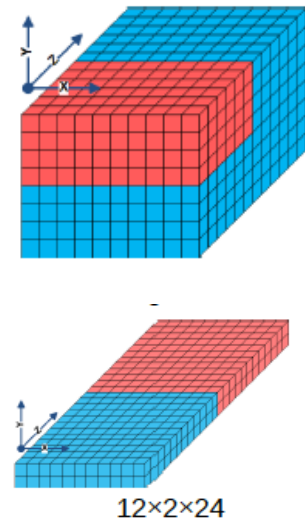
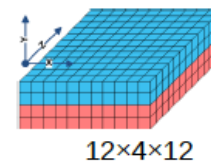
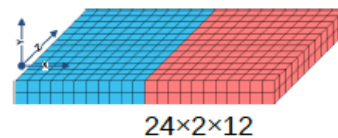
- Important to scientists
  - Reduction in time to solution
  - Reduction of run-to-run variation
  - Get science done
- Important to the project and funder
  - Get Science done
  - System utilization

## How to interact with TAS

- Topology aware user specifications
  - #PBS -l geometry=X×Y×Z with some wild cards
  - Application communication characteristics:
    - #PBS -l comm={high|low}[:{high|low}][:{global|local}]
    - “low” or “high” communication intensity.
      - bi-section bandwidth consideration.
    - “low” or “high” communication sensitivity.
      - allow for fragmented node allocations.
    - “global” or “local” as the dominant communication pattern.
  - Cost function for waiting for shape.

## Workload Tests

- Initial tests limited to allocate convex shapes to lessen internode communication interference on other jobs (dimension ordered routing).
- The scheduler was able to try different rectangular shapes weighted by aggregate bandwidth.



## Workload Test

- Synthetic workload composed of several applications
  - MILC, PSDNS, NAMD, NWCHEM, ChaNGa, QMCPACK, DNS\_distuf, WRF, SpecFEM3D\_globe.
  - Represents a broad range of communication patterns.
  - Numerous representative node counts and scaled run times based on actual Blue Waters production logs.
  - Initial conditions set by stub jobs.
- 1544 jobs (XE and XK) run in two hour window
- Good scheduler responsiveness
- Good utilization

- Top 10 jobs shown.
- XZ slabs favored.
- Some jobs specified  $X \times Y \times Z$ .

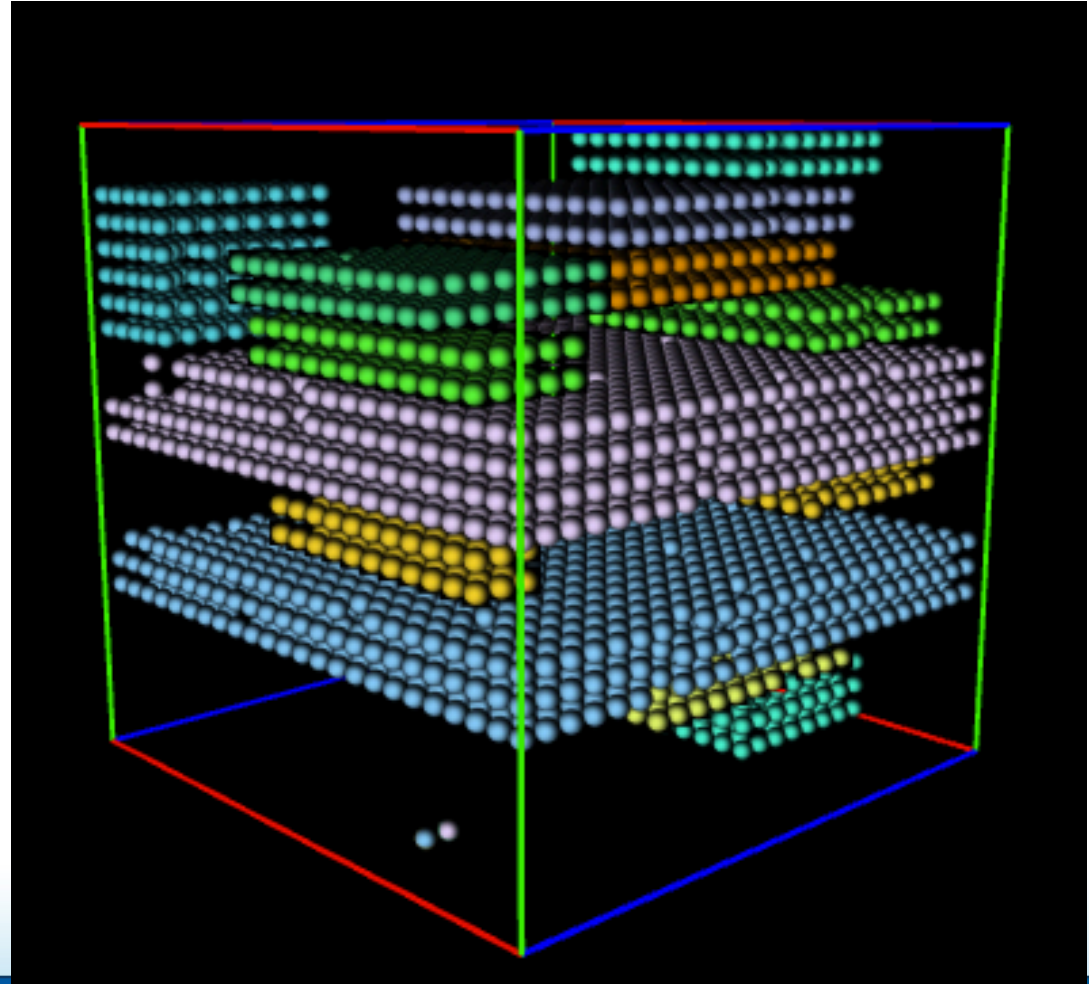
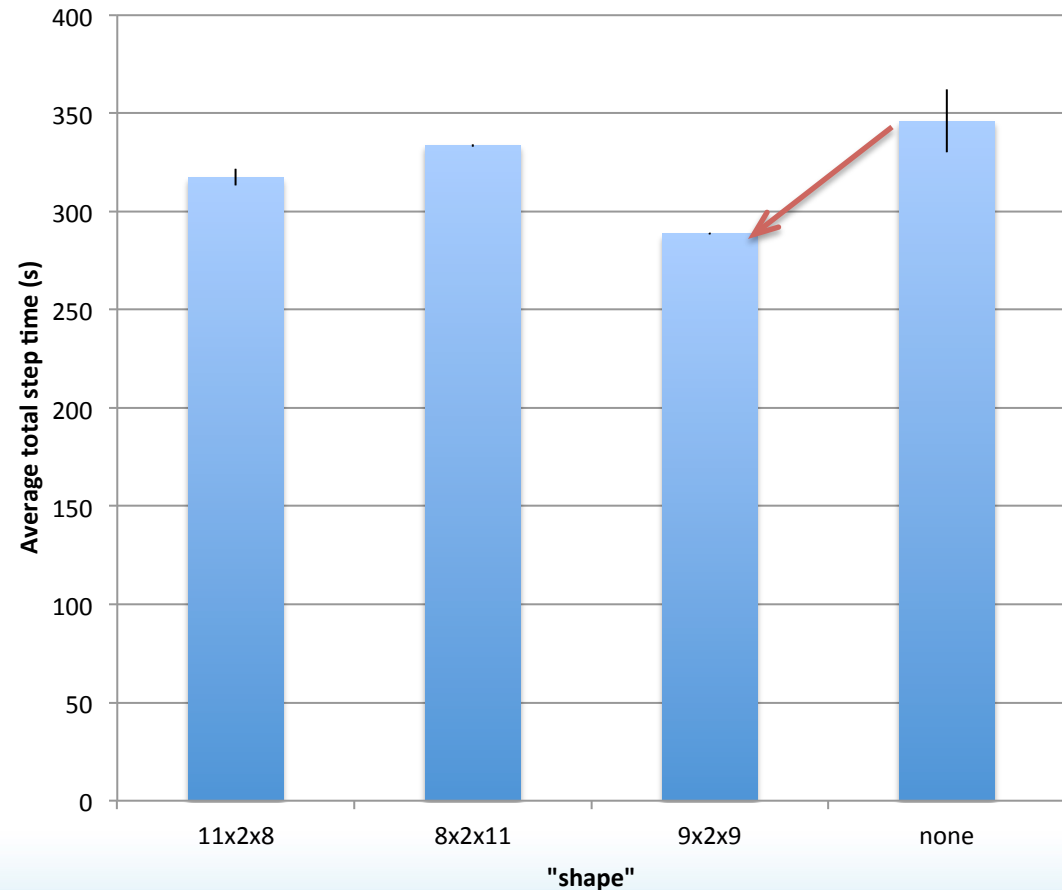


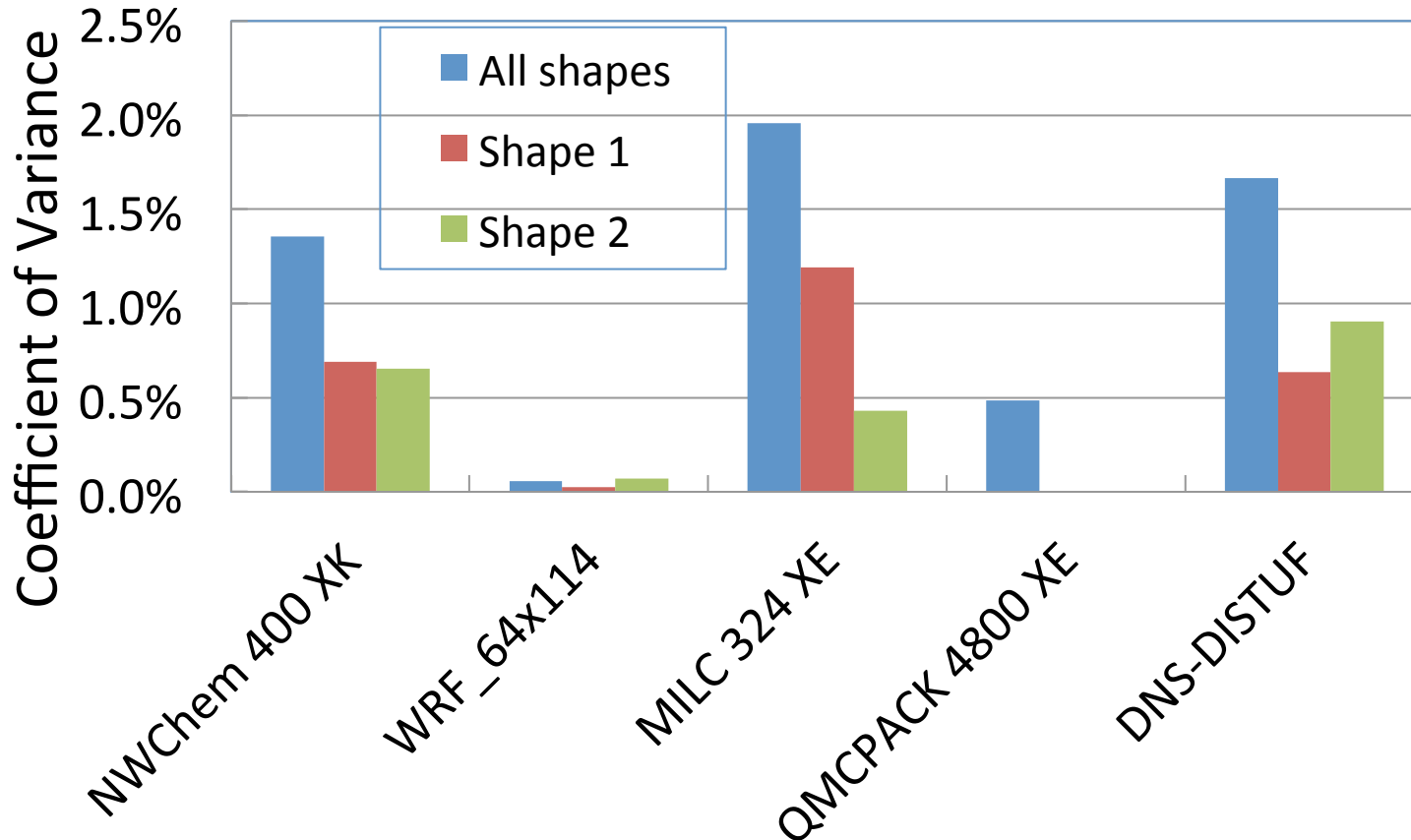
Image credit: Dave Semeraro

## Preliminary Workload Test Results

- 324 nodes - MILC
- 3 shapes used in workload testing.
- “none” collected in batch
- 17% reduction in average runtime
- 10x reduction in CoV.
- Larger impact at larger scales.



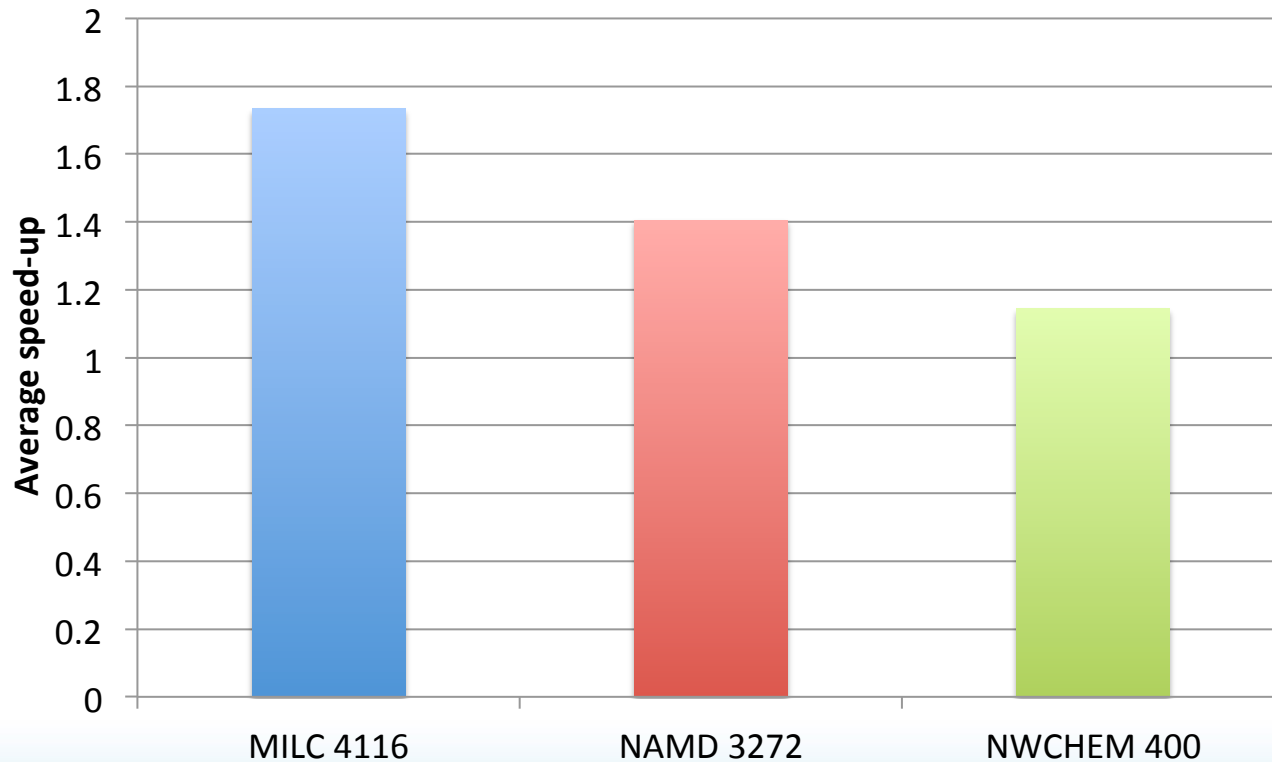
# Preliminary Workload Test Results



- Worst Application run time CoV is less than 2%
- Worst 'Per Shape' Application CoV is less than 1.25%

# Preliminary Workload Test Results

- Speed-up from using topology aware scheduling

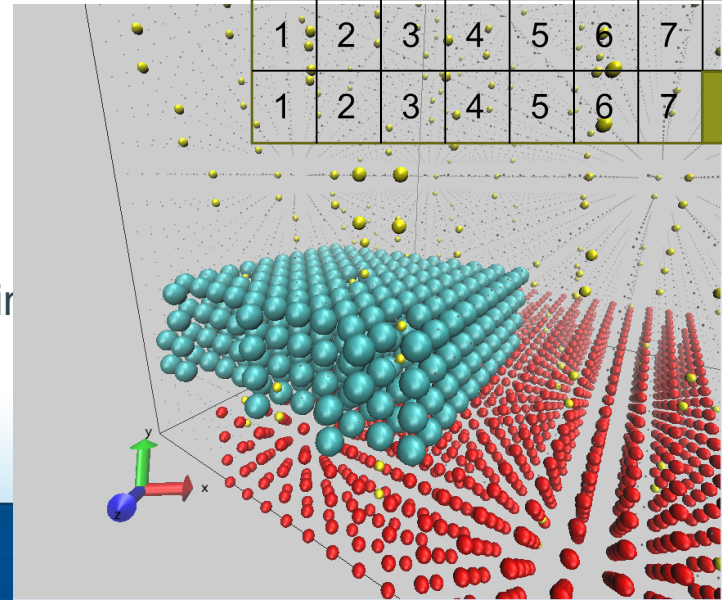




# Node Selection and Task Layout

- Most codes will need to consider MPI rank ordering to take full advantage of nodes provided by topology aware scheduler.
- Topoaware: Provides task mapping for 2, 3, & 4D Cartesian grid virtual topologies.
  - Developed by Bob Fiedler, Cray.
  - In each z-pencil, extends set of selected geminis along z if needed to skip unavailable nodes
  - Determines multiple valid layouts and evaluates layout quality
  - Allows unbalanced layouts
    - Nodes on prism boundaries may have fewer tasks
    - Enables more good layouts for more virtual topology sizes
  - Scheduler ensures allocation has desired gemini count in each z-pencil

1	2	3	4	5	6	7	8	
	1	2	3	4	5	6	7	8
1	2	3	4	5	6		7	8
1	2	3	4	5	6	7	8	
1	2		3	4	5	6	7	8
1	2	3	4		5	6	7	8
1	2	3	4	5	6	7	8	
1	2	3	4	5	6	7		8



# Topaware tests: Halo exchange

- Virtual topology: 32x32x32
- 10x improvement possible.
- Hop count not the only story.
- Reduction in congestion and improved bandwidth important.
- grid\_order provided by Cray to order communication between nearest neighbors in a grid.

Placement	Iter time (ms)	Max hops
Default 8x8x8	11.315	9
Grid_order 8x8x8	7.722	16
Topaware 8x8x8	2.771	2
Topaware 11x6x11 (unbalanced)	1.287	2
Topaware 11x8x8 (unbalanced)	1.147	2
Topaware 8x8x11 (unbalanced)	1.214	2
Topaware 11x7x8 (unbalanced)	1.782	2
Topaware 8x7x11 (unbalanced)	1.737	2
Topaware 11x8x7 (unbalanced)	1.580	2
Topaware 7x8x11 (unbalanced)	1.690	2

## Topaware tests: MILC

- MILC
  - Virtual topology 21x2x21x24
  - 1764 nodes, 12 tasks each
  - 21x2x21 geminis
  - 2.2x faster with Topaware than with grid\_order -c 2,2,2,2 on same nodes
  - grid\_order can provide 2x over not using grid\_order.
  - See [Topology Consideration](#) talk at December 2013 workshop.

Placement	Run Time (10 iterations)
Grid_order	254.0
Topaware	116.4

## Conclusions and Next Steps

- From initial tests with topology aware scheduling we see
  - improvements in overall performance and run-to-run variability
  - promising utilization numbers
- Further tests coming and then deployment.

- What we like to see on Blue Waters ...

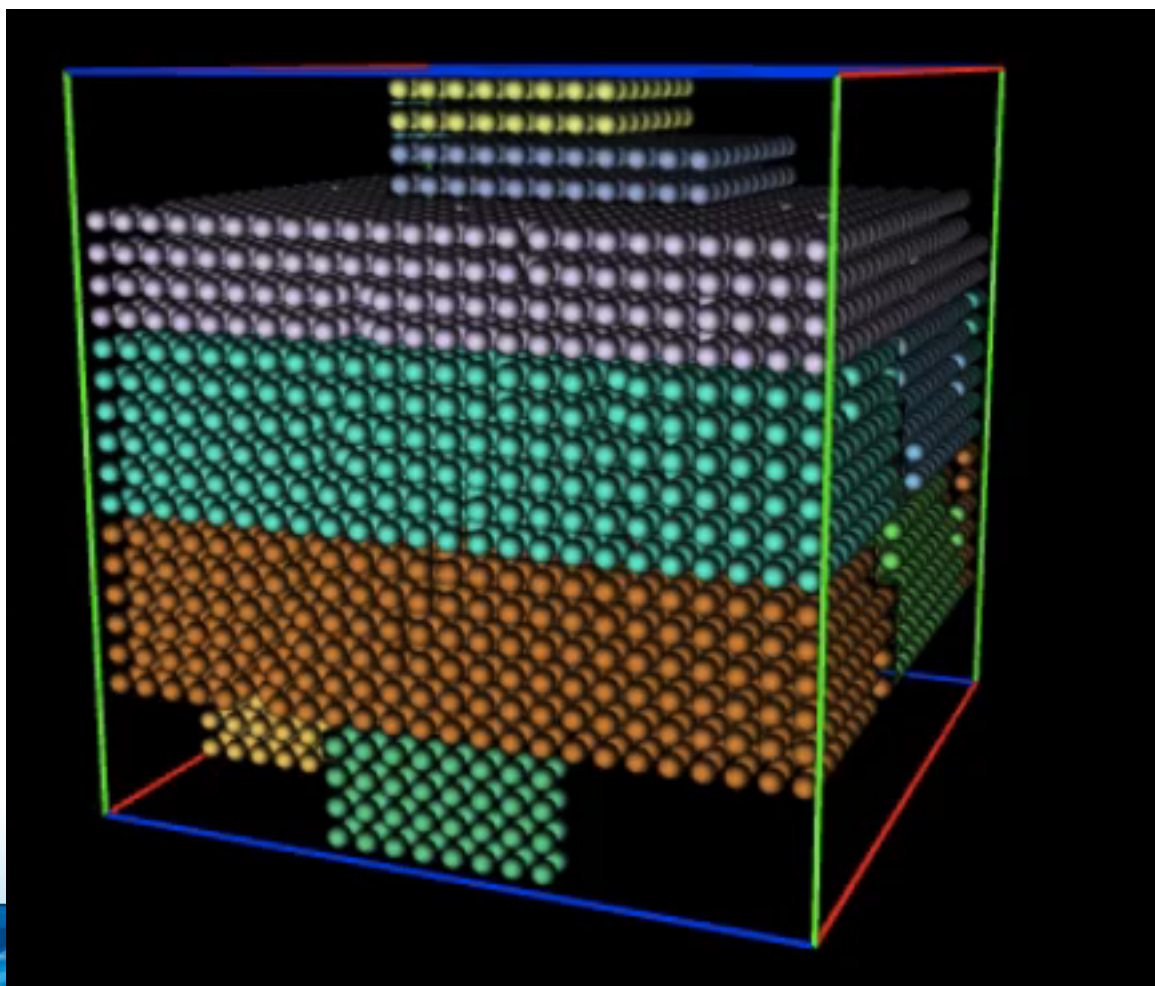


Image credit: Dave Semeraro