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Improving Performance and Scaling on Blue Waters Through Topology-Aware Task Placement

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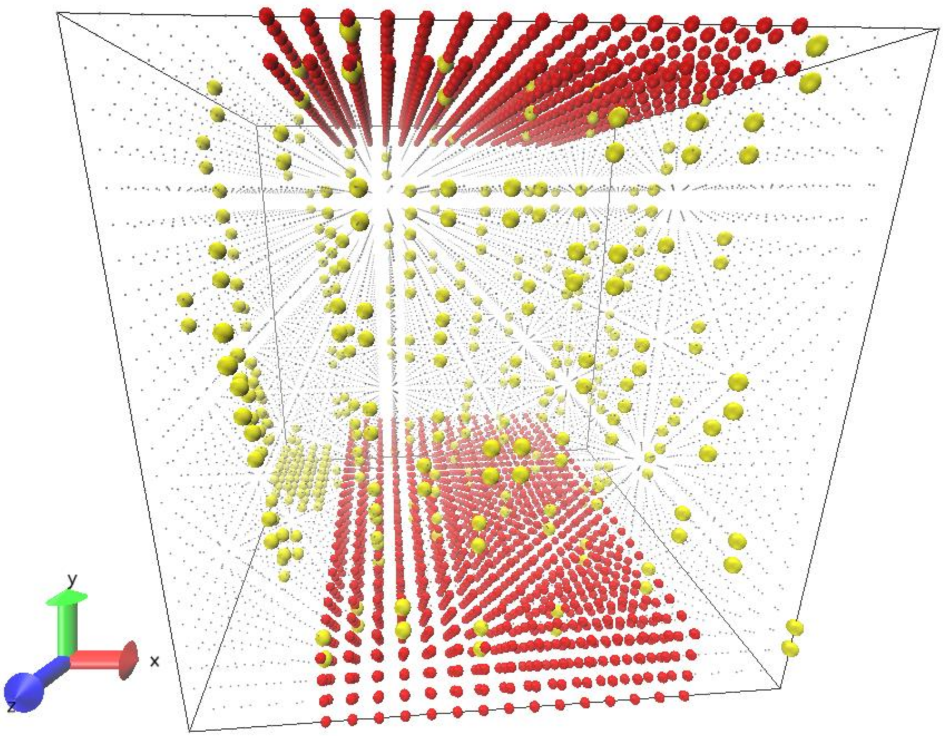
Overview

- **Blue Waters interconnect**
- **Topology-aware scheduling coming soon**
  - Prism-shaped allocations
  - Improves communication performance
  - Minimizes job-job interference
  - Transparent to users
- **Simple task placement strategies**
  - Default method
  - Craypat/grid_order
- **Task placement for Cartesian grid topologies**

Blue Waters Interconnect

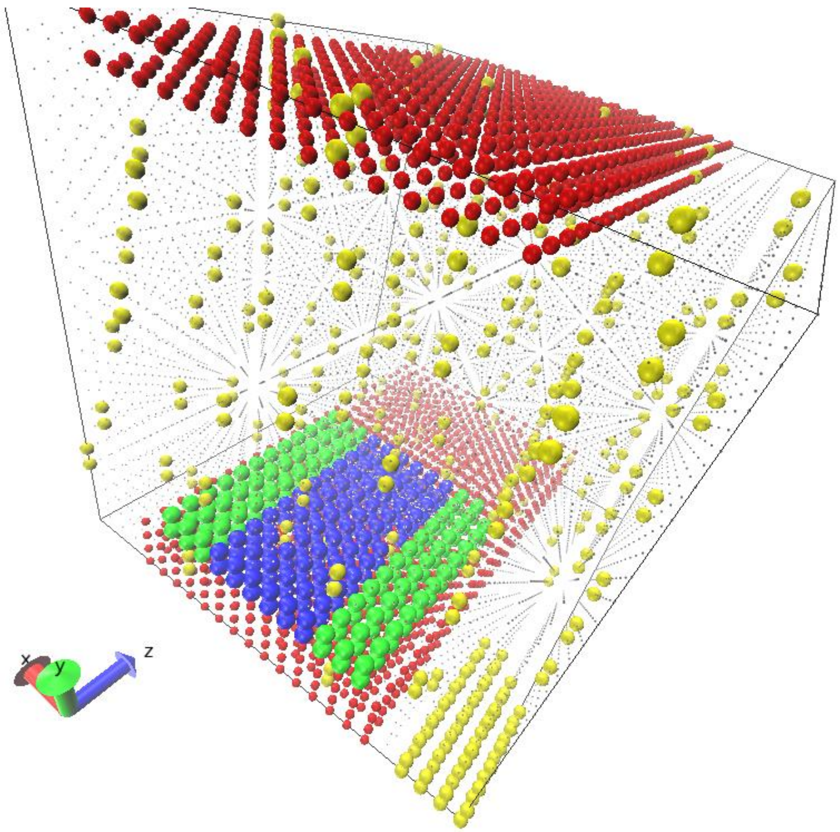
3D Torus

- Topology is 24x24x24 gemini routers
- 2 nodes per gemini
- 15x6x24 contiguous XK geminis (red)
- Service nodes randomly distributed (yellow)
- Blades: 2 geminis along Y
- Y-links between blades have 1/2 bandwidth of X- or Z-links
  - 2 nodes on same gemini don't use interconnect to exchange messages
- Routing algorithm is X, then Y, then Z (static)



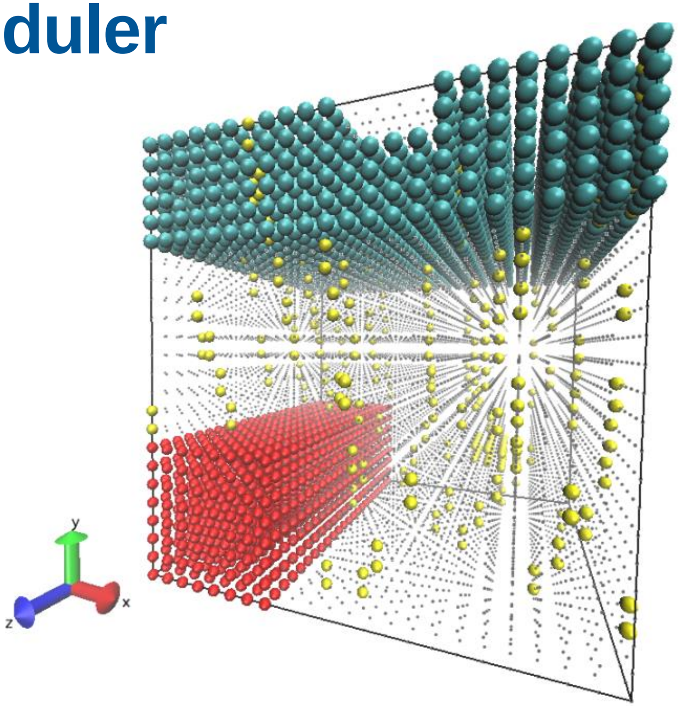
Blue Waters Interconnect (cont'd)

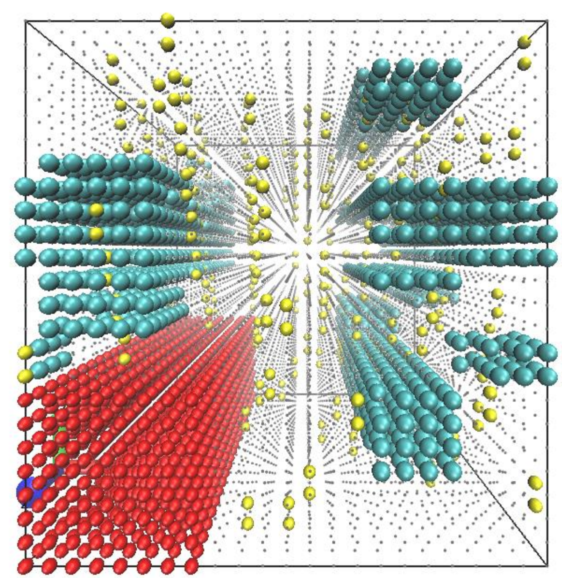
- **Routing takes shortest path**
- **If job spans > 1/2 of given dimension, some communication may wrap around torus through nodes not assigned to job**
- **Jobs share interconnect for application communication, IO**
- **Run times affected by task placement, other running jobs**
  - Figure: job on green geminis passes messages through job on blue geminis



Node Allocations: ALPS & Job Scheduler

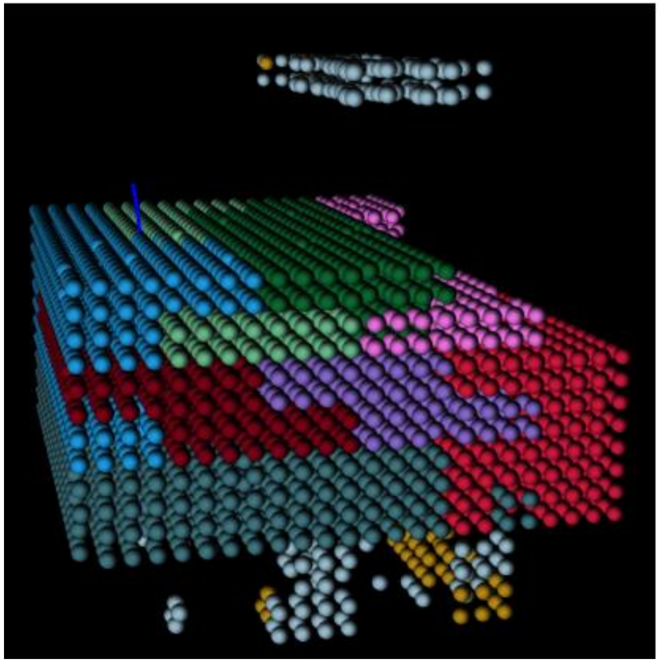
- **ALPS provides the scheduler (Torque/Moab) with list of compute nodes in specific order:**
  - 2x4x2 gemini blocks in space-filling curve
- **Over time, after many jobs start & end, list of available nodes becomes increasingly fragmented**
  - Less compact allocations
  - Longer communication paths
  - More job-job interference
  - Less consistent, longer run times
- **Significant Cray/Adaptive/NCSA efforts underway to provide more compact allocations**
  - Favor XZ slabs & regular prisms
  - Request specified shapes





Task Placement and Interference

- **Applications that perform more communication are often more sensitive to placement and interference**
  - All-to-All communication patterns
  - Bisection bandwidth governs communication time
- **Even if you get a nice prism …**
  - Without careful placement, applications with nearest-neighbor communication actually perform pairwise communication between randomly located nodes
  - Bisection bandwidth governs communication time in this case, too!



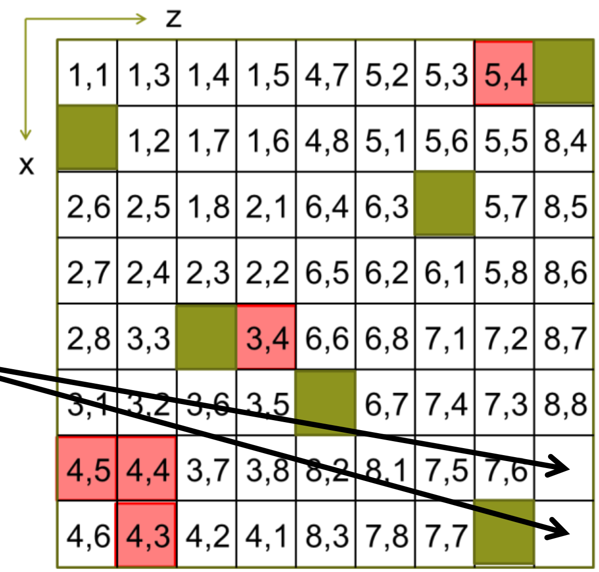
Topology-Aware Scheduling in Moab

- **NCSA/Cray/Adaptive collaboration**
- **Goals**
  - Improve application scaling on Cray XE/XK systems through better-localized job placement
  - Improve application run-time consistency by minimizing job-job interference due to application communication
  - Increase system throughput by maintaining good utilization
- **Approach**
  - Allocate nodes in contiguous prisms
  - Eliminate interference: allocation either spans a torus dimension, or spans half or less of a dimension (avoids torus wrap)
  - Favor xz slabs to maximize bisection bandwidth
  - Boost utilization by more freely placing jobs that are not affected by application communication
  - Allow applications to request specific allocation shapes

T-A Scheduler’s Criteria for Allocation Shape

Job requests N nodes, scheduler picks N_x, N_y, N_z

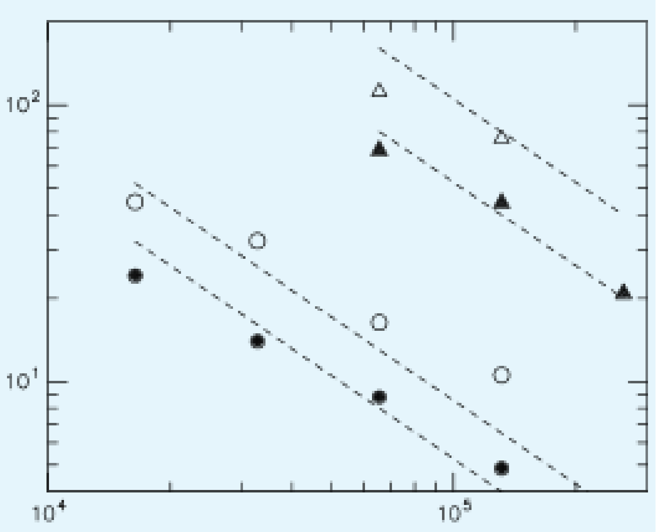
- **Bisection bandwidth per node**
  - Accounts for dateline zones in the torus
- **Prism volume**
- **Max hop count**
- **Number of nodes in prism left idle**
- **Whether candidate N_x, N_y, or N_z > 12 or < 24**
  - Prevents torus wrap through other jobs
- **Which shapes will enable job to run soonest**
- **Etc.**
- **There are site-tunable weight factors for each criterion**
- **Job-job interference possible via I/O only**



Weak Scaling for Application Using All-to-All

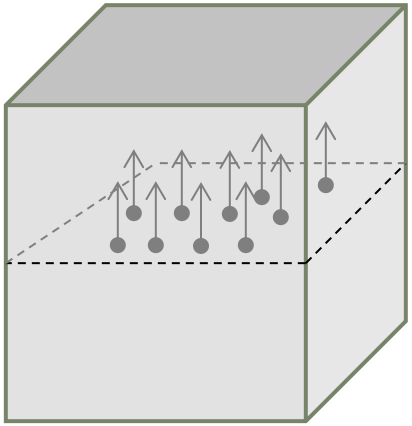
3D FFTs: N^3 grid points, P tasks

- **1D FFT computation time ~ N^3 * (const. + log N)**
- **Transpose communication time ~ All-to-All time**
  - All-to-All time ~ Data volume/bandwidth
    ~ N^3/bandwidth
- **For weak scaling experiments**
  - N^3/P is held constant
  - Computation time grows slowly with P
  - Communication time ~ P/bandwidth
- **Thus, near-ideal weak scaling requires**
  - Bisection bandwidth ~ P
  - i.e., constant per-node bisection bandwidth
- **Minimizing time to solution means maximizing bisection bandwidth per node**

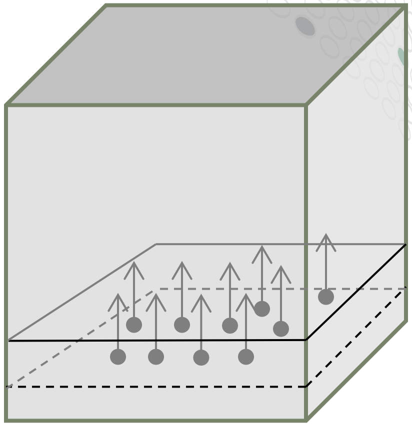


Bisection Bandwidth: Full System

- **Bisection bandwidth of nodes in use determines run time for All-to-All**
- **Bisection bandwidth is defined as lowest bandwidth through any cross-sectional area**
  - BW topology is 24x24x24 geminis
  - Bisection bandwidth through cross section:
    - Normal to X: 24x24*X-link-bw*2 for torus wrap
    - Normal to Y: 24x24*Y-link-bw*2 for torus wrap
    - Normal to Z: 24x24*Z-link-bw*2 for tours wrap
  - Y-link bandwidth ~ 1/2 X-link or Z-link bandwidth
  - Bisection bandwidth normal to Y ~ 24x24*X-link-bw
    - Limits All-to-All
  - Bisection bandwidth per node ~ X-link-bw/48



Bisection Bandwidth: Slab w/N Geminis in Y

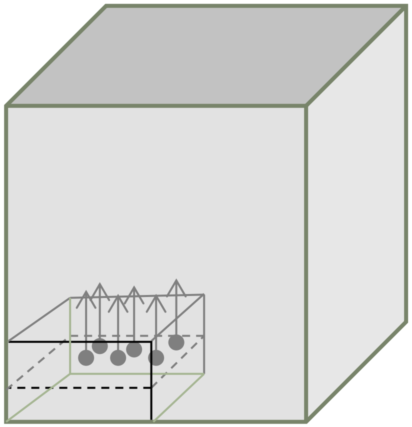


- **Consider subset of nodes: 24xNx24**
- **Bisection bandwidth through cross section:**
  - Normal to X: N*24*X-link-bw*2 for torus wrap ~ 2*Nx24*X-link-bw
  - Normal to Y: 24x24*Y-link-bw * f(N) ~ f(N)*12x24*X-link-bw
  - Normal to Z: 24xN*Z-link-bw*2 for tours wrap ~ 2*Nx24*X-link-bw

- **Bisection bandwidth per node for any N**
  - ~ X-link-bw/24 for N=1 through N=6 [since f(N) = 1 and 2N <= 12]
  - ~ X-link-bw/(4*N) for N=6 through N=12 [since f(N) = 1 and 2N >= 12]
  - ~ X-link-bw*(N-1)/(23*2*N) for N > 12 [since f(N) = 2*(N-1)/(24-1)]

Bisection Bandwidth: Small slab

- **Consider smaller node counts, e.g., 12x6x12 so no wrapping occurs**
  - ~1700 nodes
- **Bisection bandwidth through cross section:**
  - Normal to X: 6*12*X-link-bw ~ 12*6*X-link-bw
  - Normal to Y: 12*12*Y-link-bw ~ 12*6*X-link-bw
  - Normal to Z: 12*6*Z-link-bw ~ 12*6 X-link-bw
- **Bisection bandwidth per node**
  - ~ X-link-bw/24
  - Same good value as for 24x6x24 geminis



T-A Scheduler Allows User-Specified Shapes

Why would one want to specify allocation shape?

1. **Application requires maximum bisection bandwidth**
   - Scheduler should not consider other cost factors
2. **Application communicates more in some dimensions than others**
   - Same amount of communication per grid cell in each direction
   - Per-node tiling with 2M by M by 2M grid cells anticipates 2X faster links along x and z
   - Want cubic allocation, not xz slab
   - Need to provide custom MPI rank order (Craypat or grid_order) to place groups of neighboring ranks on each node
3. **Tasks are to be placed on the torus in near-optimal manner (Topaware)**

Prism Geometry Requests

How to get a particular prism shape instead of allowing the T-A scheduler to choose for you

- **To get a particular prism shape**

  #PBS -l nodes=576:ppn=32:xe
  #PBS -l geometry=12x2x12

- **Multiple geometry choices**

  #PBS -l nodes=576:ppn=32:xe
  #PBS -l geometry=12x2x12/12x4x6/6x4x12

Virtual Topologies and Task Placement

- **Many applications define Cartesian grid virtual topologies**
  - MPI_CartCreate
  - Roll your own (i, j, …) virtual coordinates for each rank
- **Craypat rank placement**
  - Automatic generation of rank order based on detected grid topology
- **grid_order tool**
  - User specifies virtual topology to obtain rank order file
  - Node list by default is in whatever order ALPS/MOAB provide
- **These tools can be very helpful in reducing off-node communication, but they do not explicitly place neighboring groups of partitions in virtual topology onto neighboring nodes in torus**

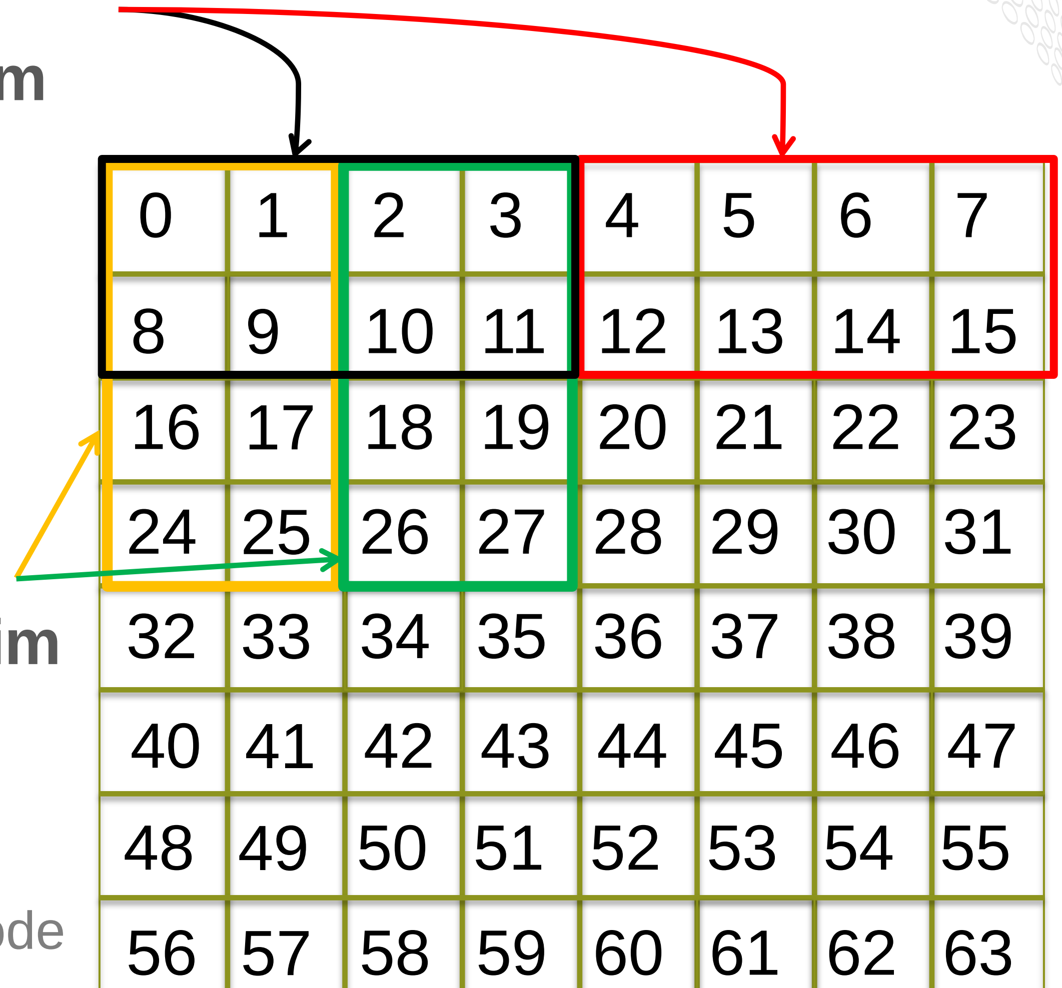
Examples: 2D Virtual topology

grid_order -C -c 4,2 -g 8,8

- **Ranks ordered with 1st dim changing fastest**
- **Nodes get 4x2 partitions**
- **Rank order is**
  - 0,1,2,3,8,9,10,11 on 1st node
  - 4,5,6,7,12,13,14,15 on 2nd
  - Node pair is 8x2

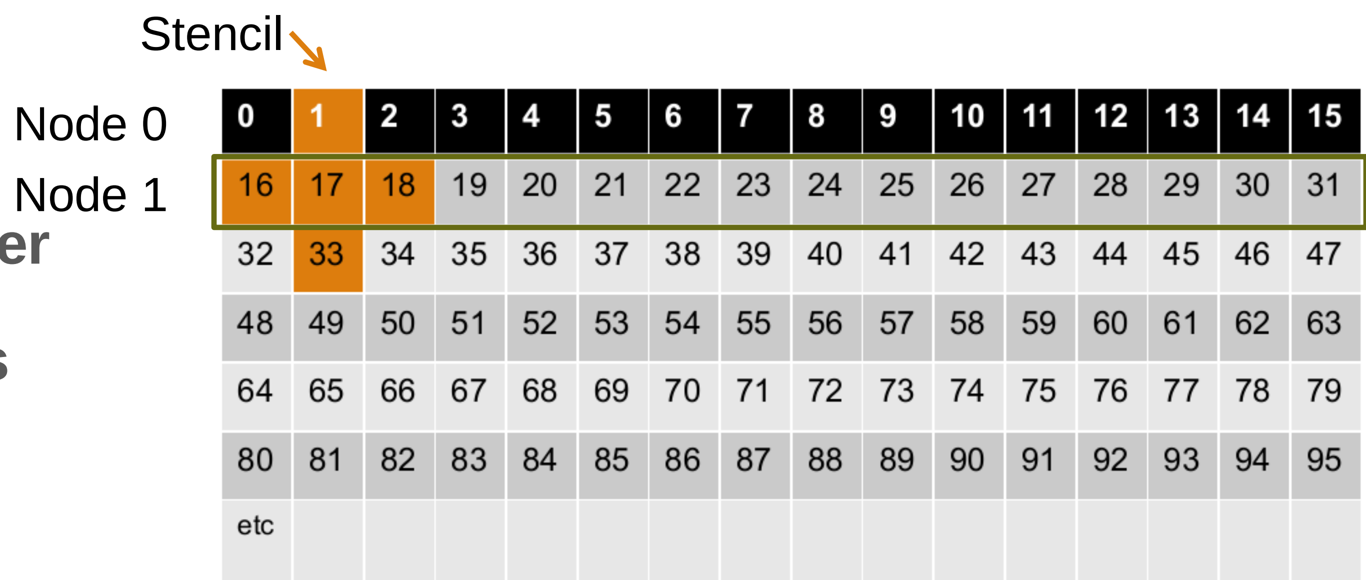
grid_order -R -c 4,2 -g 8,8

- **Ranks ordered with 2nd dim changing fastest (MPI)**
- **Nodes get 2x4 partitions**
- **Rank order is**
  - 0,1,8,9,16,17,24,25 on 1st node
  - 2,3,10,11,18,19,26,27 on 2nd
  - Node pair is 4x4

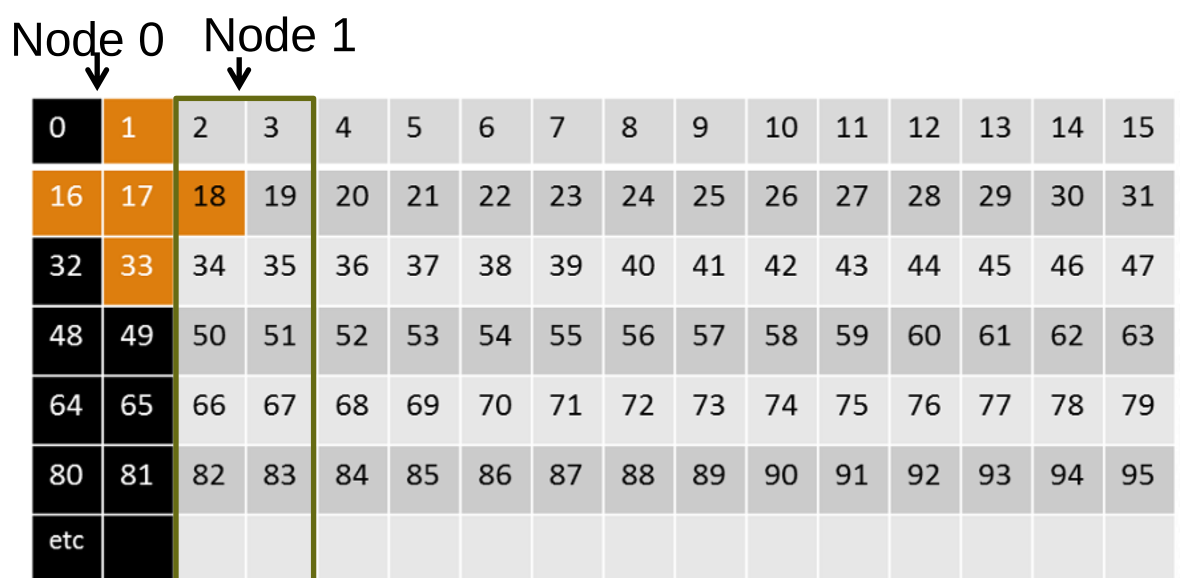


Examples: WRF (2D Virtual Topology)

190x384 partitions



- Default layout
- 16x1 partitions per node
- Every task needs off-gemini communication



- 18% faster using grid_order -C -c 2,8 -g 190,384
- 2x8 partitions per node
- Interior stencils on same gemini
- 8x2 not nearly as good

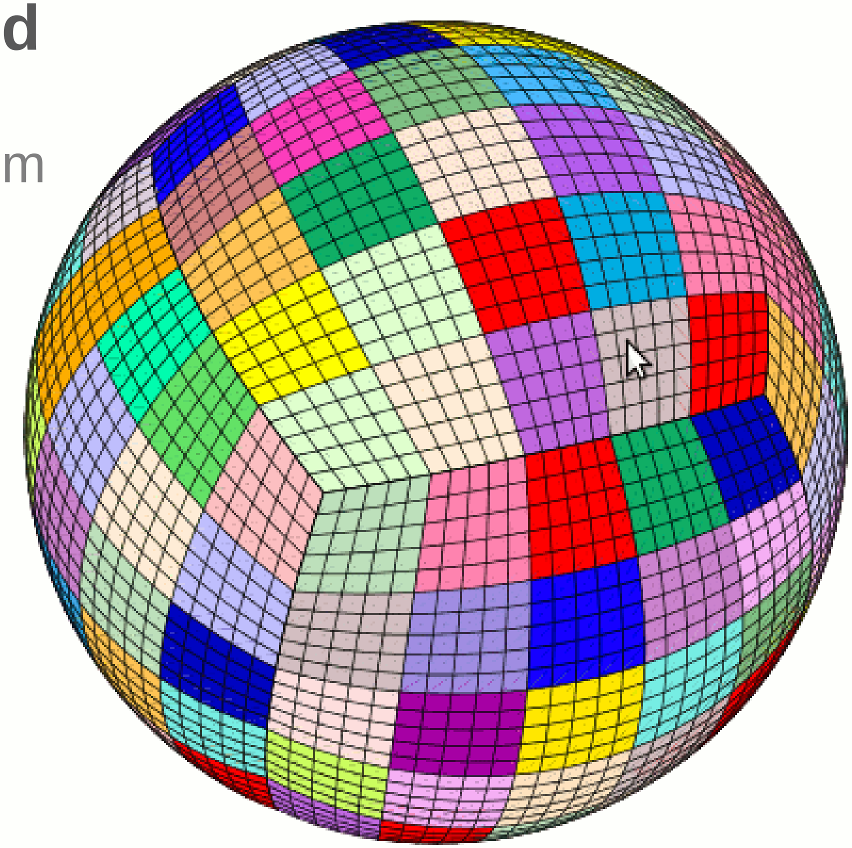
Examples: 3D Cubed Sphere

SPECFEM3D_GLOBE

- **Quad element unstructured grid**
- **5419 nodes, 32 tasks per node**
- **Craypat detected a 1020x170 grid pattern (8 less than # tasks)**
  - On-node 81% of total B/task w/Custom
  - On-node 48% of total B/task w/SMP
- **Found best performance with**

grid_order –R -c 4,1 -g 1020,170

  - Each node gets eight 4x1 patches
  - Also tried –c 8,2, etc.
  - 16% speedup over SMP ordering



Examples: 4D Virtual Topology

MILC – Lattice QCD

- **4D Lattice, 84x84x84x144**
- **4116 nodes, 16 tasks per node, 65856 tasks**
- **6x6x6x6 lattice points per task**
- **Found best performance with**

grid_order –R -c 2,2,2,2 -g 14,14,14,24

  - 1.9X speedup over SMP ordering!
  - Difficult to map 4D virtual topology onto 3D torus using 2x2x2x2 partitions per node
  - Topaware can provide a layout with near-optimal mapping and significantly better performance

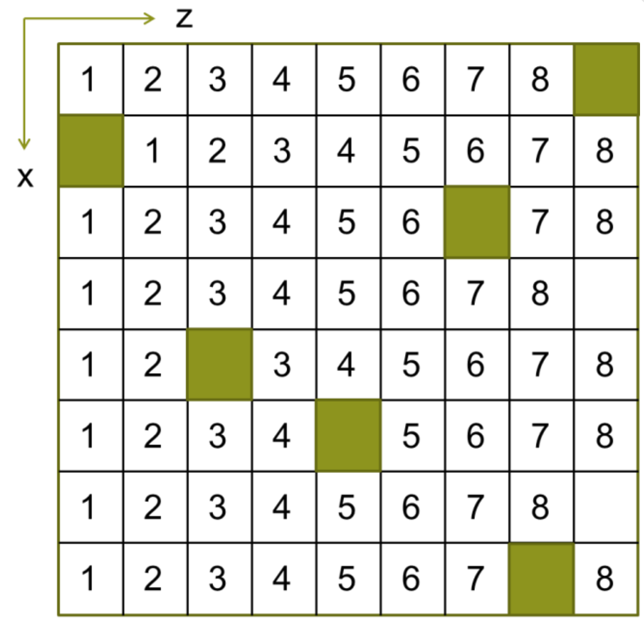
Topaware: Going Beyond Simple Rank Reordering

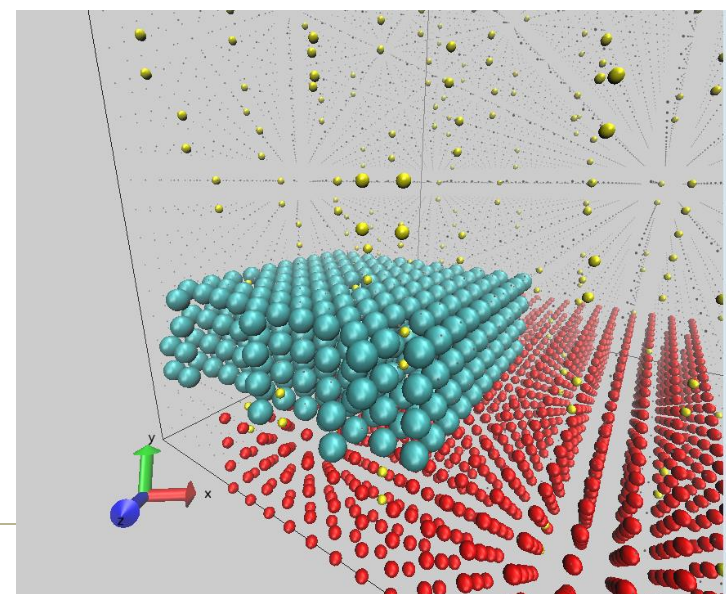
Significant improvement possible

- **Can we place tasks on a given set of nodes so that virtual neighbors are nearby on torus?**
  - Difficult problem for arbitrary node lists
  - Possibly helpful library: Hoefler's LibTopoMap http://htor.inf.ethz.ch/research/mpitopo/libtopomap/
  - Not widely used – steep learning curve, etc.
- **Can we specify size of prism of geminis and directly map virtual topology to torus?**
  - Presence of service & down nodes complicates this
- **T-A scheduler can provide specified number of geminis in each z-pencil through an allocation**
  - This is exactly what Topaware needs to get good layouts
  - With Topaware, NO NEED TO MODIFY APPLICATION!

Topaware Integrated with T-A Scheduler

- **Provides near optimal task mapping for 2, 3, & 4D Cartesian grid virtual topologies**
  - Prism is extended along z by max number of service/down nodes in any z-pencil
  - Determines multiple valid layouts and evaluates layout quality
  - Allows unbalanced layouts
    - Nodes on prism boundaries may have fewer tasks
    - Enables good layouts for more virtual topology sizes
  - Scheduler ensures allocation has required gemini count in each z-pencil





LAYOUT EXAMPLE: 2D Virtual Topology

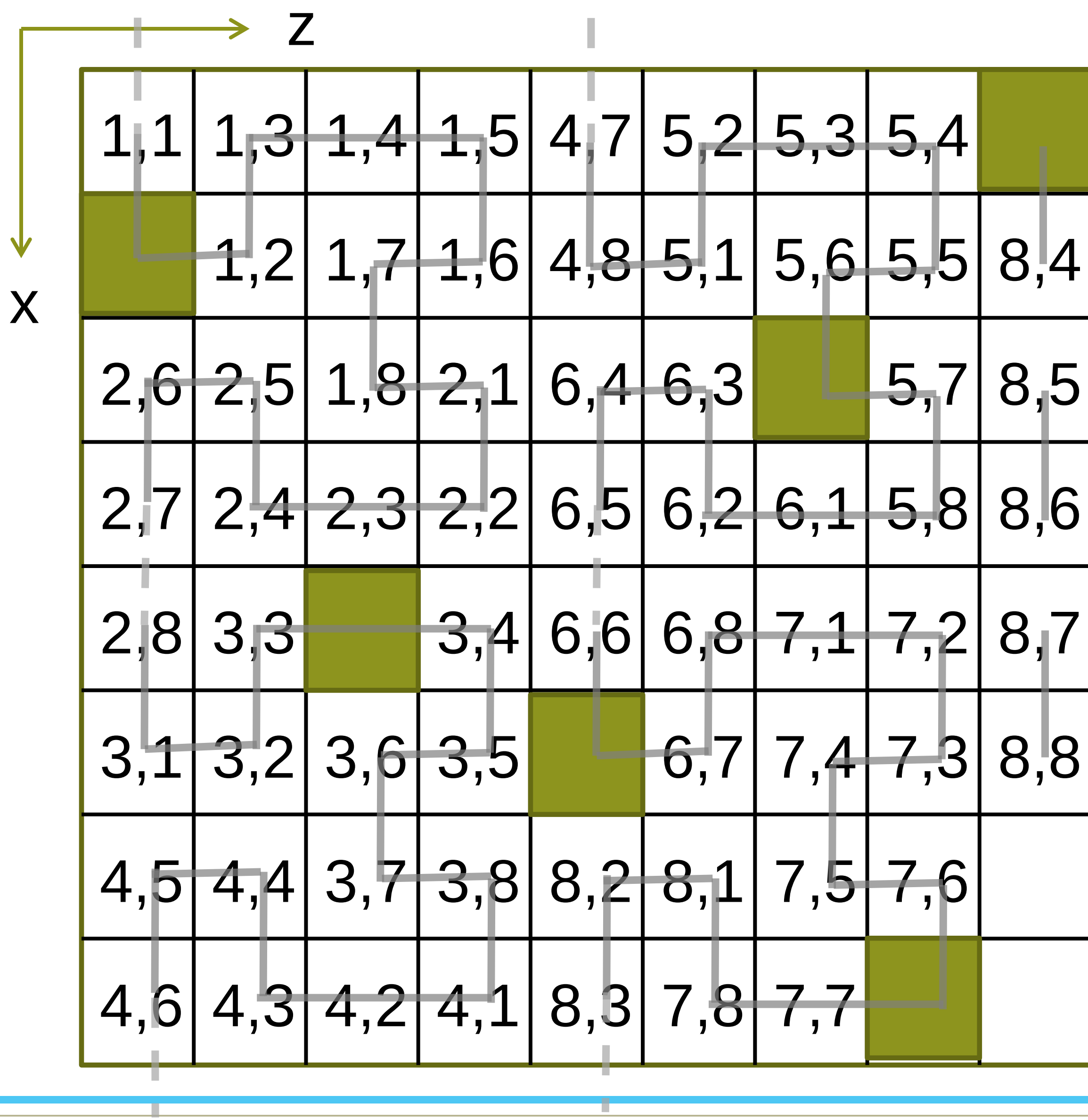
z →

x ↓

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

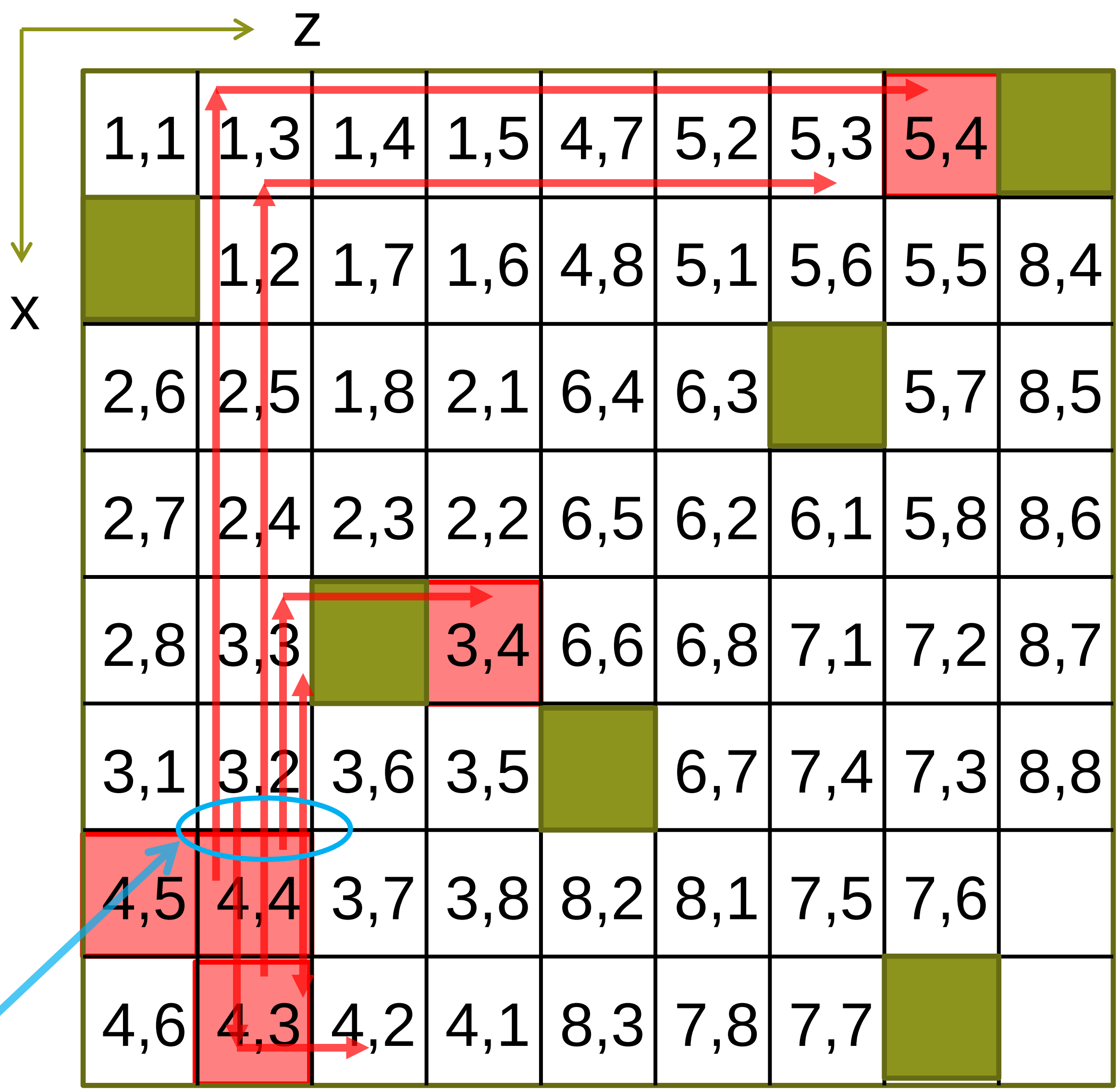
Ideal 8x8 layout on ideal system, 1 rank per router (!)

2D Virtual Topology: Default Layout



Space-filling curve orders nodes on real XE/XK system

2D Virtual Topology: Default Layout



Stencil scattered; 6 communication paths share this x link

2D Virtual Topology: Topaware Layout

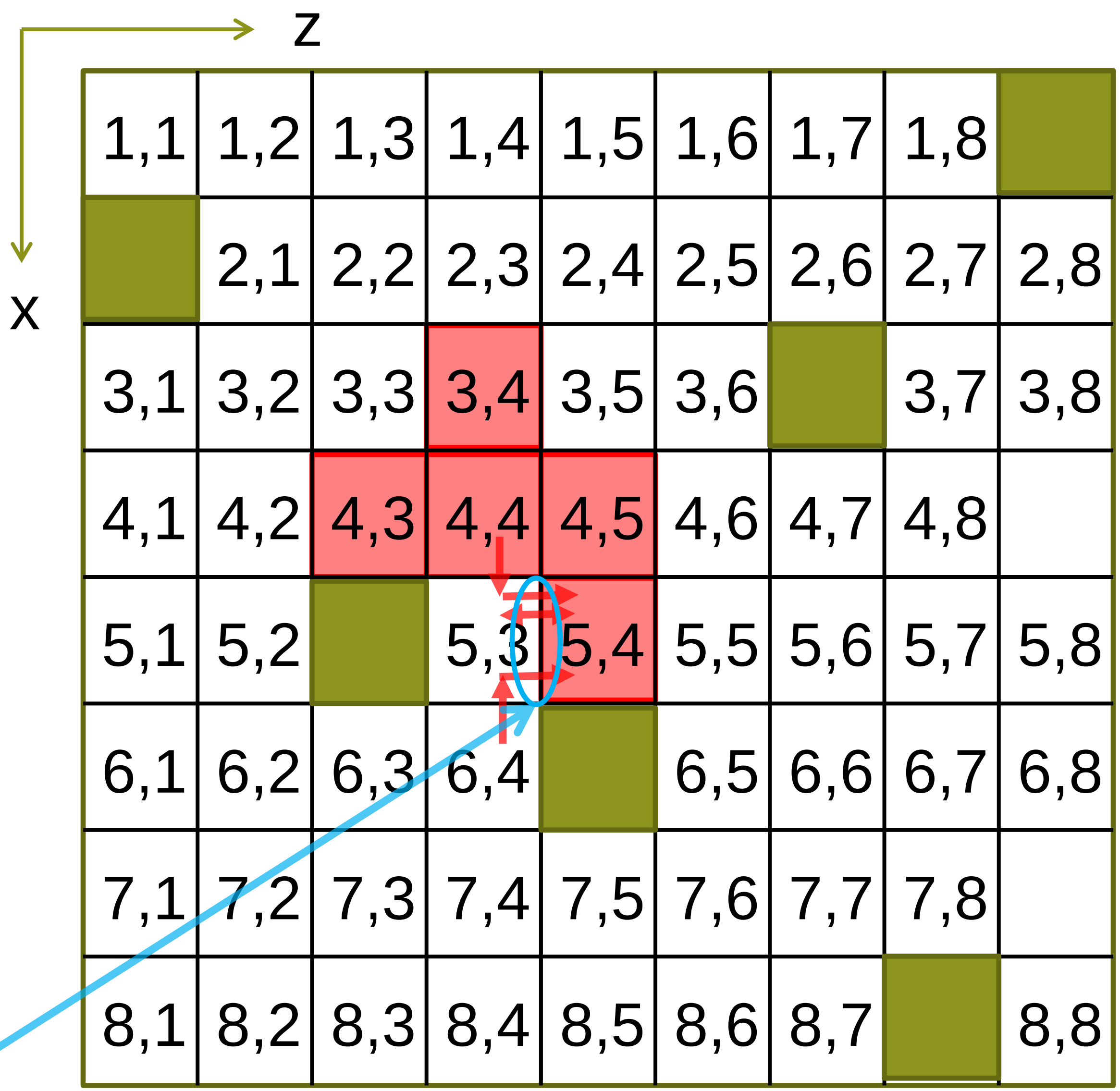
z →

x ↓

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

Topaware keeps ranks in desired z-pencils

2D Virtual Topology: Topaware Layout



Stencil remains localized; only 4 paths share this x link

Topware 2.0: Practical Near-Optimal Layouts

- **Helps you choose prism geometries/node counts that will accommodate your decomposed problem**
- **At run time, provides near-optimal layout matching the allocated prism**
- **Steps**
  1. Run Topaware on login node to find desirable geometries
  2. Submit batch job requesting those geometries
  3. Invoke Topaware again within batch job to place tasks on nodes in that allocation
  4. Use aprun to launch job using node order and custom rank order generated by Topaware

Example of Topaware Use

- **Suppose problem has 4000x3000x2500 grid cells.**
  - If each partition has 100x100x100 cells to use desired memory:
  - Virtual topology has 40 partitions in x, 30 in y, 25 in z (30,000 tasks)
  - To run on xe nodes, expect to use no more than 32 tasks per node
- **Invoke Topaware from a login node:**

  ~fiedler/bin/pick_nodes.x –g 40,30,25 –c 32 > top_out

  - -g 40,30,25 describes virtual topology
  - -c 32 says to use (3/4 to 1) * 32 tasks per node
- **Topaware finds many viable layouts, ordered by quality**

```
Layout  10 nt =  10  5 10 np =   4   3   5 splitdim =   1 map = 231 balanced  94
Layout   7 nt =  20  5   5 np =   2   6   5 splitdim =   2 map = 123 balanced  90
Layout  14 nt =    5  5 20 np =   2   6   5 splitdim =   2 map = 231 balanced  90
Layout   8 nt =  20  5   6 np =   2   5   5 splitdim =   1 map = 132 balanced  88
Layout   9 nt =  20  6   5 np =   2   5   5 splitdim =   1 map = 123 balanced  88
Layout  13 nt =    6  5 20 np =   2   5   5 splitdim =   1 map = 231 balanced  88
Layout  15 nt =    5  6 20 np =   2   5   5 splitdim =   1 map = 321 balanced  88
```

Using Topaware to Find Good Layouts

- **Topaware layouts for 40x30x25 topology**

```
Layout  10 nt =  10  5 10 np =   4   3   5 splitdim =   1 map = 231 balanced  94
Layout   7 nt =  20  5   5 np =   2   6   5 splitdim =   2 map = 123 balanced  90
Layout  14 nt =   5  5 20 np =   2   6   5 splitdim =   2 map = 231 balanced  90
Layout   8 nt =  20  5   6 np =   2   5   5 splitdim =   1 map = 132 balanced  88
Layout   9 nt =  20  6   5 np =   2   5   5 splitdim =   1 map = 123 balanced  88
Layout  13 nt =   6  5 20 np =   2   5   5 splitdim =   1 map = 231 balanced  88
Layout  15 nt =   5  6 20 np =   2   5   5 splitdim =   1 map = 321 balanced  88
```

Valid BALANCED layout 10 has map = 231 ppn = **30** numnodes = **1000**

dims(p2v(1)) nt(1) np(p2v(1)) =   30   10   3 ← Dim 2 on 10 geminis in torus x

dims(p2v(2)) nt(2) np(p2v(2)) =   25   5   5 ← Dim 3 on 5 geminis in torus y

dims(p2v(3)) nt(3) np(p2v(3)) =   40   10   4 ← Dim 1 on 10 geminis in torus z

percent_used is 100 ← Uses 100% of nodes in prism

bal_metric is 100 ← All nodes get same number of active tasks (“balanced”)

ppn_metric is 93 ← Uses 30/32 integer cores per node

p2c_metric is 80 ← per node pair “volume to surface ratio” compared to cube

qual_metric is 94 ← Geometric mean of above factors

Prism Geometry Requests

How to get a particular prism shape instead of allowing the T-A scheduler to choose for you

- **For Topaware, also specify number of geminis required in each dimension plus maximum acceptable prism size along z**
  - Max z should be a few greater than the minimum required, in order to allow for service/down nodes

  #PBS -l nodes=1000:ppn=32:xe

  #PBS -l geometry=10x5x10:maxz=12

- **Multiple geometry choices with Topaware**

  #PBS -l nodes=1000:ppn=32:xe

  #PBS -l geometry=10x5x10:maxz=12/20x5x5:maxz=6/5x5x20:maxz=24

  - All layouts in request must require same node count
  - Order indicates Topaware's quality metric (94, 90, 90)
  - Scheduler will prefer 10x5x10 since no torus wrap, then 5x5x20, then 20x5x5

Running Batch Jobs Using Topaware

- Suppose we requested 10x5x10 geminis (only)

```
# Get the node list to confine Topaware's scans
cat $PBS_NODEFILE | uniq | tr '\n' ',' | sed -e 's/,$/\n/' > node_list

# Invoke topaware in batch mode using this node list
 ~fiedler/bin/pick_nodes.x -M 2 -U node_list -g 40,30,25 -c 32 >& top_out

# Scan top_out for the first successful layout, where it says:
# SUCCESS Layout  10 nt =  10  5 10 np =    4   3   5 splitdim =   1 map = 231 balanced  94
# The node list has been written to a file called nodes-10-1000_10_5_10_4_3_5
# The rank list has been written to a file called
# MPICH_RANK_ORDER-10-1000_10_5_10_4_3_5_1
…
# Set up to use custom rank order
cp MPICH_RANK_ORDER-1000_10_5_10_4_3_5_1 MPICH_RANK_ORDER
export MPICH_RANK_REORDER_METHOD=3

# Run application using Topaware's node list, plus task affinity and core specialization
aprun -l nodes-10-1000_10_5_10_4_3_5 -n 30000 -N 30
-cc 0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30 -r 1
./my_app.exe
```

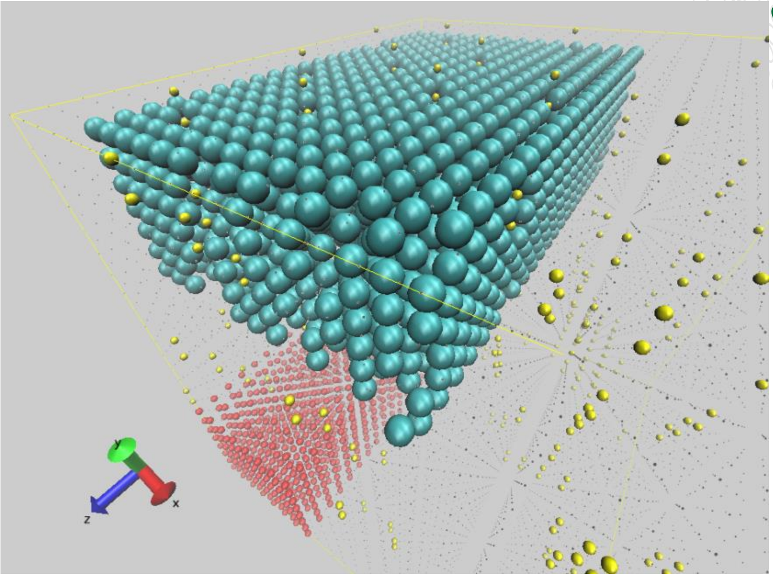
Examples: 4D Halo Exchanges

Compare default ordering, grid_order, and Topaware on <u>same set of nodes</u> (selected by Topaware).

- **4D Lattice, 144x144x144x288 points**
- **12x16x16x16 partitions**
- **1536 nodes, 32 tasks per node, 49152 tasks**
- **12x9x9x18 lattice points per task**
- **Topaware: each node gets 1x2x2x8 tasks**
- **Prism: 24x2x24 geminis**

- **Run times**
  - Default placement (SMP): 0.0240 s
  - grid_order -C -g 12,16,16,16 -c 2,2,2,4: 0.0245 s (worse than default!)
  - Topaware: 0.0127 s (1.9X < default!!)

Application Results on Blue Waters



MILC – Lattice QCD

- **4D Lattice, 84x84x84x144**
- **4116 nodes, 16 tasks per node**
- **6x6x4x9 lattice points per task**
- **Entire 4th dimension on each node pair**
  - Remaining 3 dimensions mapped like any 3D virtual topology
  - 14x7x21 geminis (in 14x7x23 prism from T-A scheduler)
  - 1x2x1x16 partitions per node pair
- **3.7X faster than default SMP placement**
  - 2.1X faster than when using grid_order –c 2,2,2,2 on same geminis!

Results on Blue Waters for Cybershake

- Seismic waves
- 3D virtual topology
- http://hypocenter.usc.edu/research/BlueWaters/XtremeS_CyberShake_final.pdf

Table 1: Topology tuning with Topaware tool improved strong scaling efficiency for fixed 45B mesh point AWP-SGTc benchmark calculation with 64, 512, and 4096 nodes

#nodes	Default	Topaware	Speedup	Efficiency ↑
64	4.006	3.991	0.37%	100% → 100%
512	0.572	0.554	3.15%	87.5% → 90%
4096	0.119	0.077	35.29%	52.6% → 81%

Topaware Unbalanced Layouts

- Virtual topology: 32 by 32 by 32, up to 32 tasks per node

Layout	4	nt =	8	8	8	np =	4	4	4	splitdim =	1	map =	123	balanced	90
Layout	2	nt =	11	8	8	np =	3	4	4	splitdim =	2	map =	123	unbalanced	81
Layout	3	nt =	8	8	11	np =	4	4	3	splitdim =	1	map =	123	unbalanced	81
Layout	1	nt =	11	8	7	np =	3	4	5	splitdim =	2	map =	123	unbalanced	80
Layout	5	nt =	7	8	11	np =	5	4	3	splitdim =	2	map =	123	unbalanced	80

- For 11x8x8, node pairs in first 10 yz planes get 3*4*4 = 48 active tasks (total of 30720/32768 tasks)
- Node pairs in 11^{th} yz plane get 2*4*4 = 32 active tasks (total of 2048/32768 tasks)
- If load were balanced, each node would do 32768 tasks / (11*8*8*2 nodes) = 23.3 units of work
- Unbalanced layout puts 24 units of work (only 3% more!) on most nodes

Topaware Unbalanced Layouts: Results

- **Halo exchanges for virtual topology: 32 by 32 by 32**
  - For < 32 tasks per node, core specialization enables overlap of communication and copying data to/from message buffers

Placement	Communication time (ms)	Tasks per node	Per node speedup
Default 8x8x8	11.315	32	1
Grid_order 8x8x8	7.722	32	1.5
Topaware 8x8x8	2.771	32	4.1
Topaware 11x8x8 (unbalanced)	1.147	24	7.4
Topaware 8x8x11 (unbalanced)	1.214	24	7.0
Topaware 11x8x7 (unbalanced)	1.580	30	6.7
Topaware 7x8x11 (unbalanced)	1.690	30	6.3

Topaware Unbalanced Layouts: What's Needed

- **aprun will create same number of tasks on every node**
  - N total tasks in MPI_COMM_WORLD communicator
- **Application needs modification**
  - Determine M, the number of partitions in desired virtual topology
  - M < N
  - Use MPI_COMM_SPLIT to create new communicator with M ranks
  - Solve the problem using only ranks in the smaller communicator
- **Topaware puts the idle ranks on the node pairs along the appropriate surface(s) of the prism**

Concluding Remarks

- **We hope to deploy the new Topology-Aware scheduler in the Blue Waters production environment soon**
  - Excellent results obtained so far in scale tests
- **Expect most applications to benefit without user effort**
  - Allocates jobs in prisms of gemini routers
  - Better, more consistent run times
  - Improved scaling
  - Limited impact on queue wait times
- **Applications with grid topologies can leverage Topaware**
  - Provides near-optimal task layouts for most decompositions
  - Automatically selects appropriate prism sizes & node counts
  - May improve communication/computation overlap
  - Unbalanced layouts may be surprisingly efficient

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