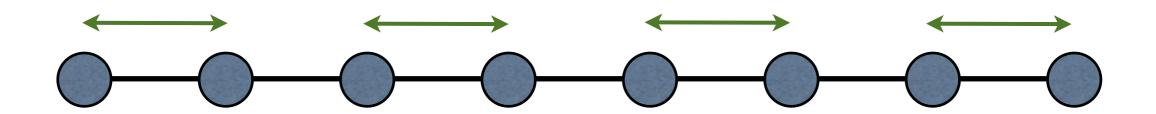
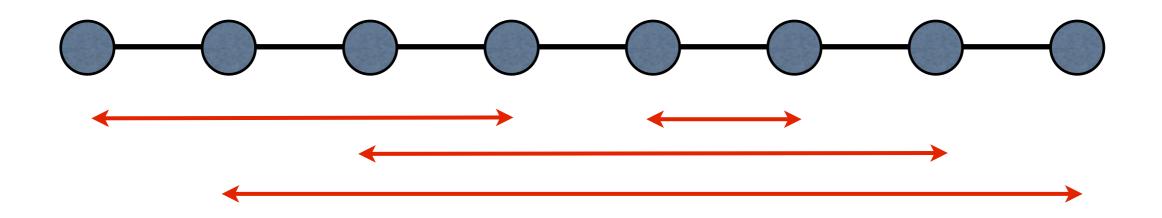


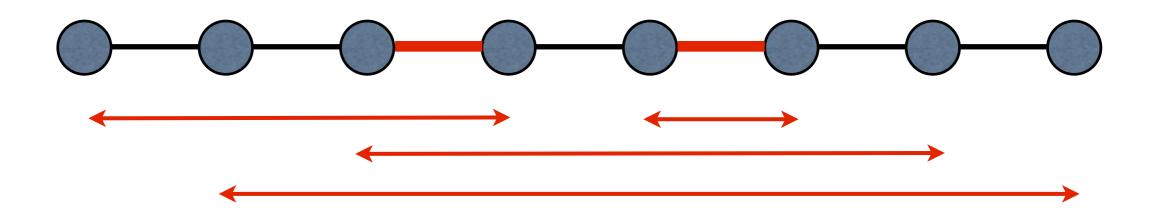
 Running a parallel application on a linear array of processors:



 Running a parallel application on a linear array of processors:

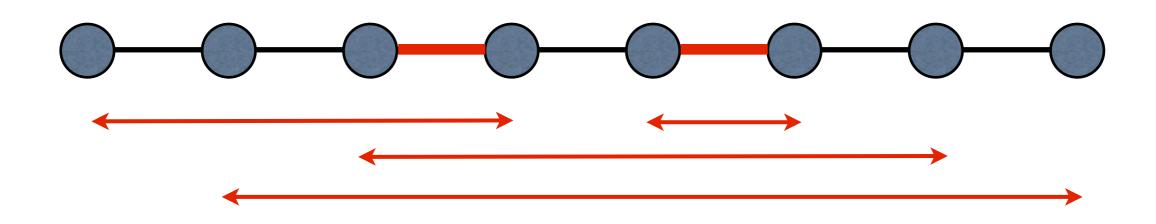


 Running a parallel application on a linear array of processors:





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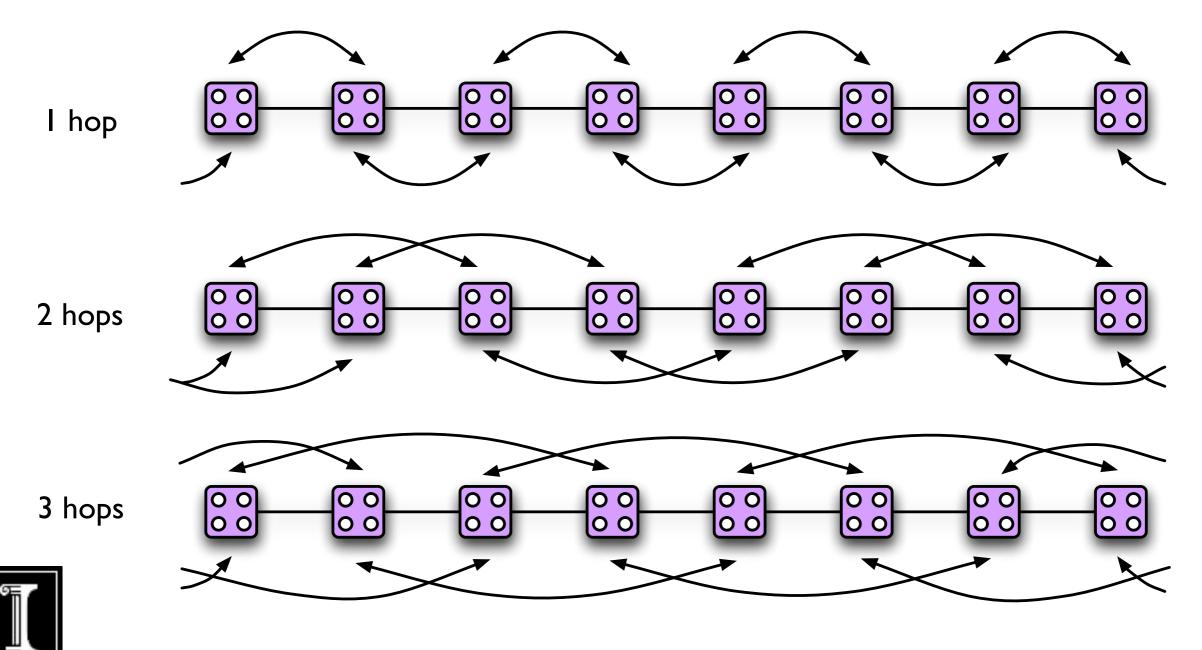


 Typical communication is between random pairs of processors simultaneously



## Benchmark Creating Artificial Contention

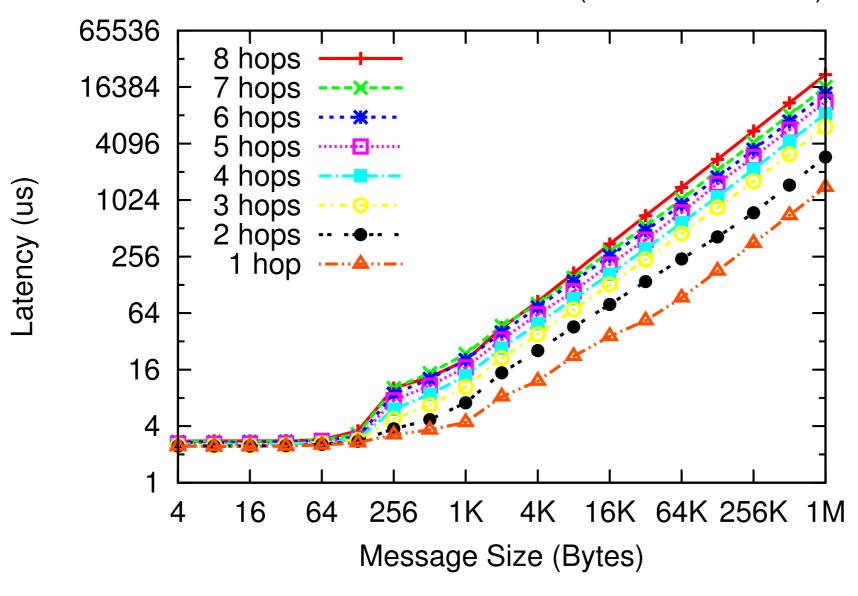
Pair each processor with a partner that is n hops away





## Results: Contention

Effect of distance on latencies (Torus - 8 x 8 x 16)



Blue Gene/P

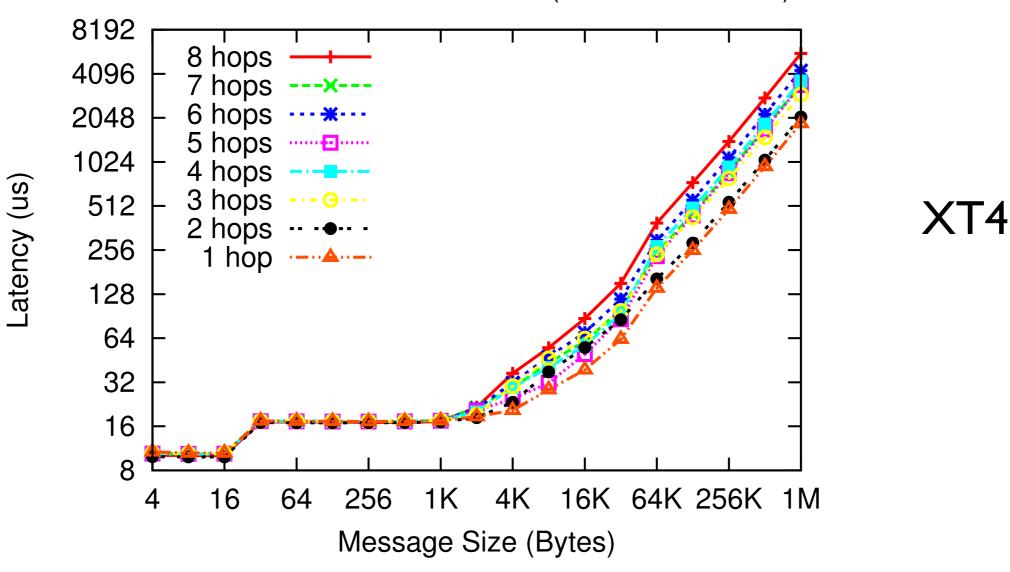


Bhatele A., Kale L.V., Quantifying Network Contention on Large Parallel Machines, *Parallel Processing Letters* (Special Issue on Large-Scale Parallel Processing), 2009. Best Poster Award, ACM Student Research Competition, Supercomputing 2008, Austin, TX.



## Results: Contention

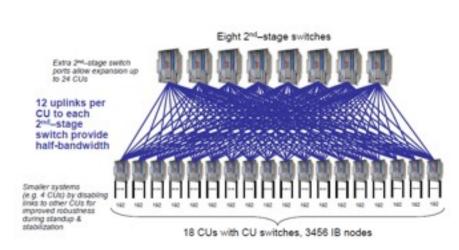
Effect of distance on latencies (Torus - 8 x 8 x 16)





# Interconnect Topologies

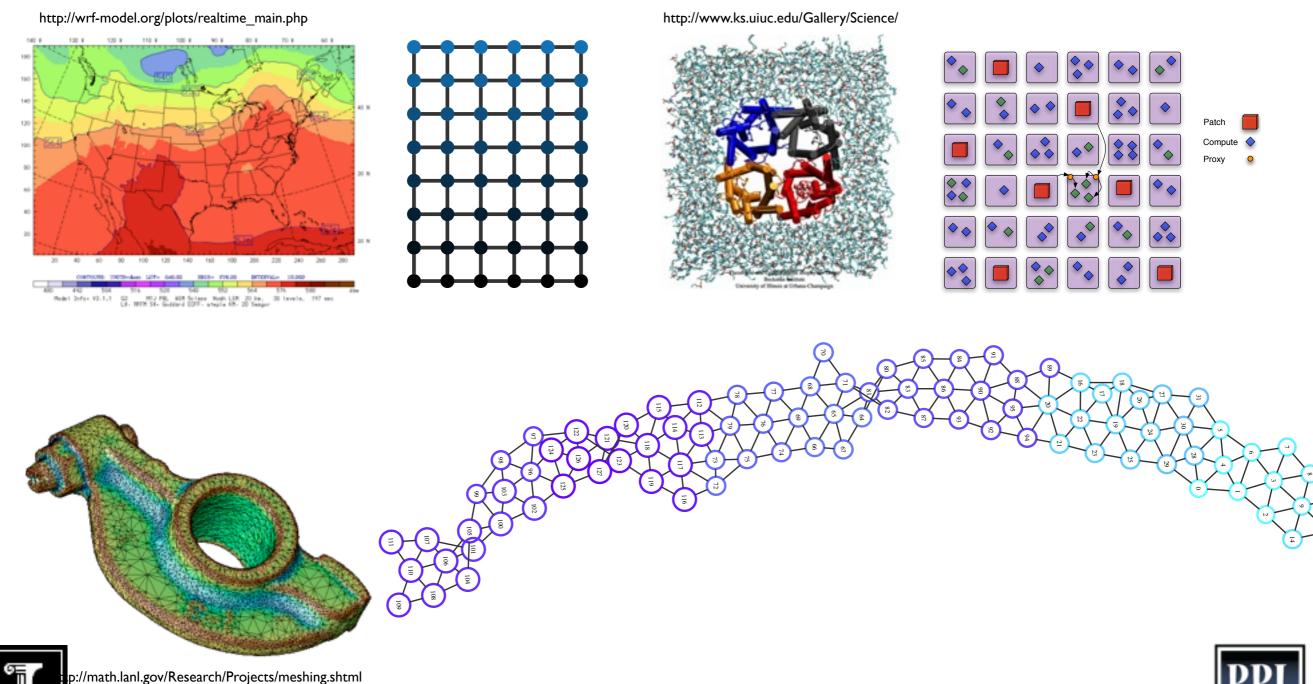
- Three dimensional meshes
  - 3D Torus: Blue Gene/L, Blue Gene/P, Cray XT4/5
- Trees
  - Fat-trees (Infiniband) and CLOS networks (Federation)
- Dense Graphs
  - Kautz Graph (SiCortex), Hypercubes
- Future Topologies?
  - Blue Waters, Blue Gene/Q



Roadrunner Technical Seminar Series, March 13th 2008, Ken Koch, LANL

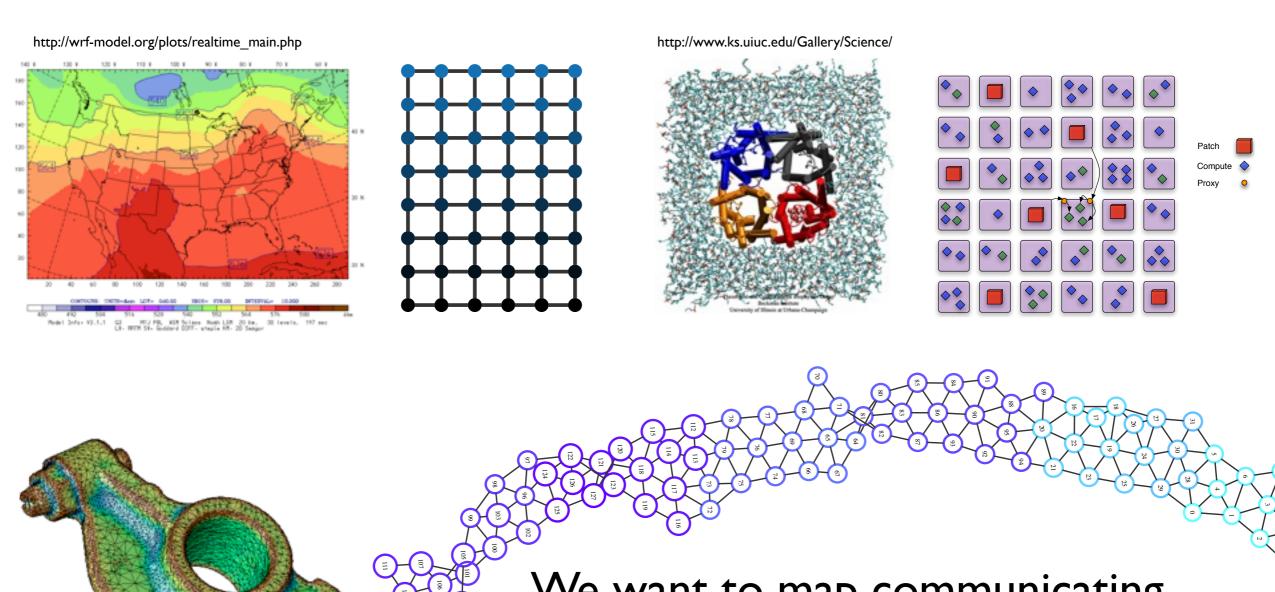


# Application Topologies



December 16th, 2010

# Application Topologies



We want to map communicating objects closer to one another



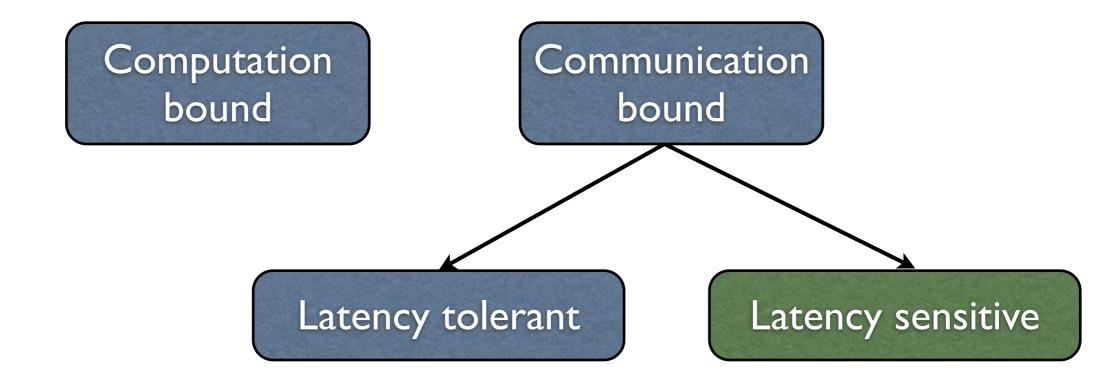
# The Mapping Problem

- Applications have a communication topology and processors have an interconnect topology
- Definition: Given a set of communicating parallel "entities", map them on to physical processors to optimize communication
- Goals:
  - Minimize communication traffic and hence contention
  - Balance computational load (when n > p)



# Scope of this work

- Currently we are focused on 3D mesh/torus machines
- For certain classes of applications







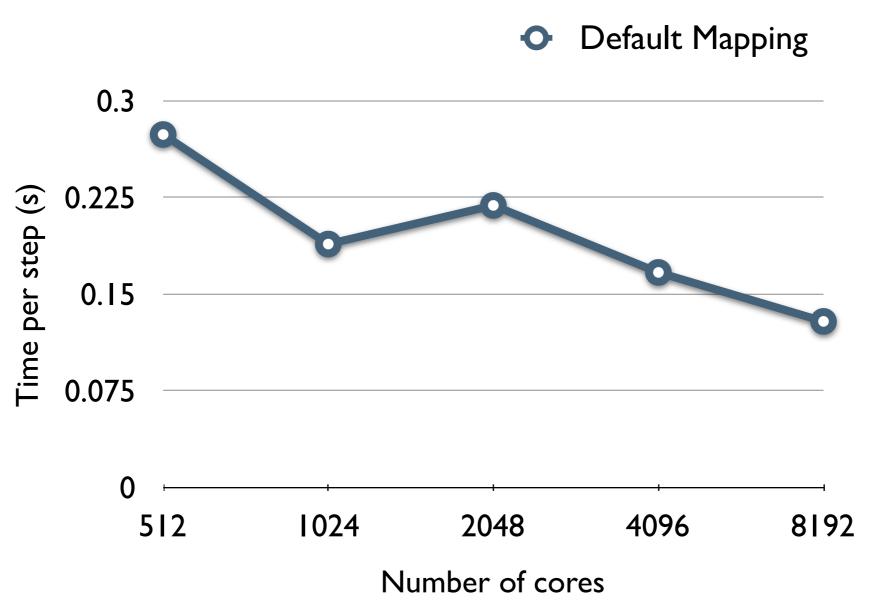
## Outline

- Case studies:
  - OpenAtom
  - NAMD
- Automatic Mapping Framework
  - Pattern matching
- Heuristics for Regular Graphs
- Heuristics for Irregular Graphs



# Case Study I: OpenAtom

#### Performance on Blue Gene/L







CNIC @ CAS © Abhinav Bhatele

# Diagnosis

8.48 secs

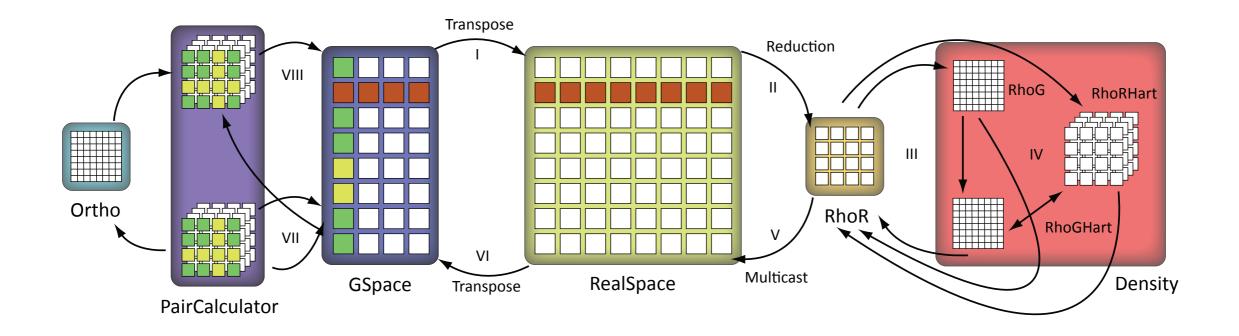




Timeline view (OpenAtom on 8,192 cores of BG/L) using the performance visualization tool, Projections



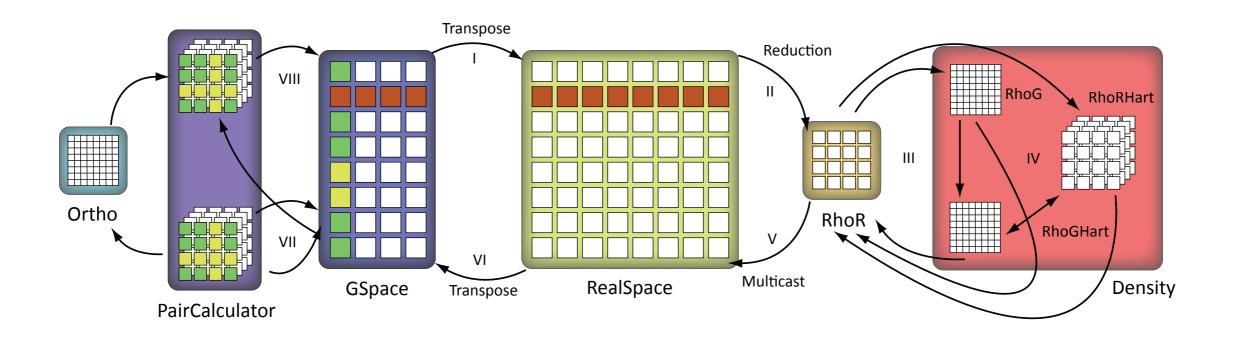
# Mapping of OpenAtom Arrays







# Mapping of OpenAtom Arrays



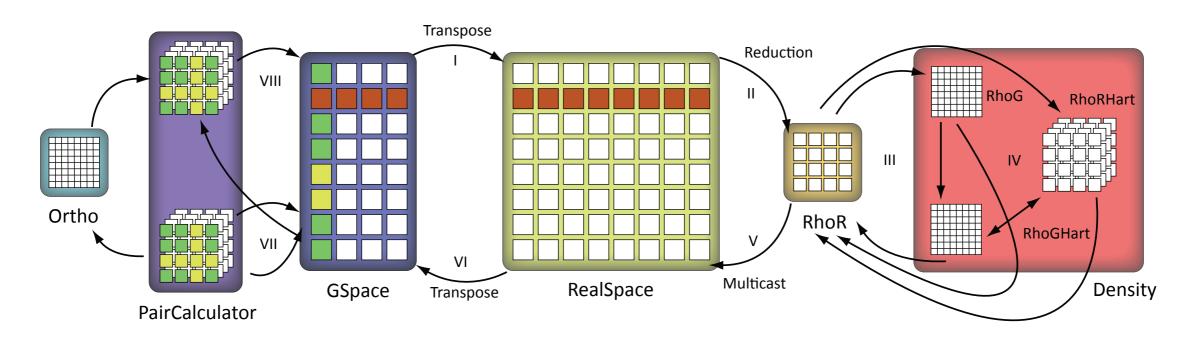
Paircalculator and GSpace have plane-wise communication

RealSpace and GSpace have state-wise communication

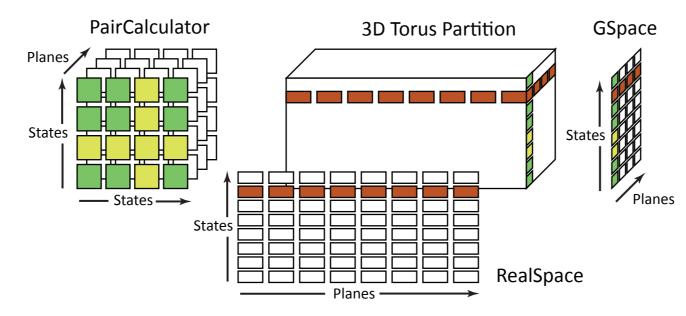




# Mapping of OpenAtom Arrays



Paircalculator and GSpace have plane-wise communication



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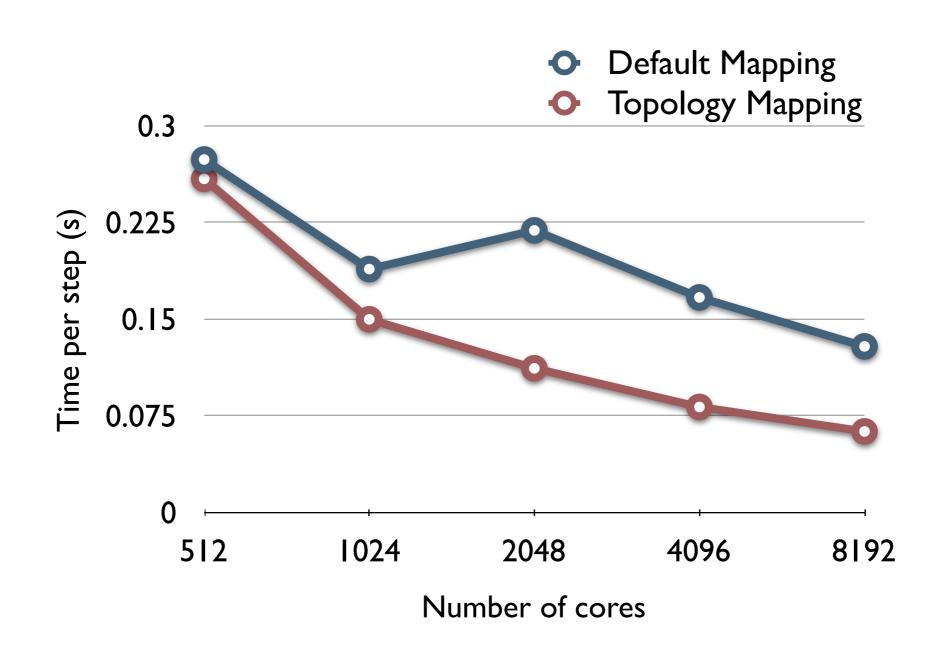


A. Bhatele, E. Bohm, and L.V. Kale. A Case Study of Communication Optimizations on 3D Mesh Interconnects. In Euro-Par, LNCS 5704, pages 1015–1028, 2009. Distinguished Paper Award, Feng Chen Memorial Best Paper Award



## Performance Benefits from Mapping

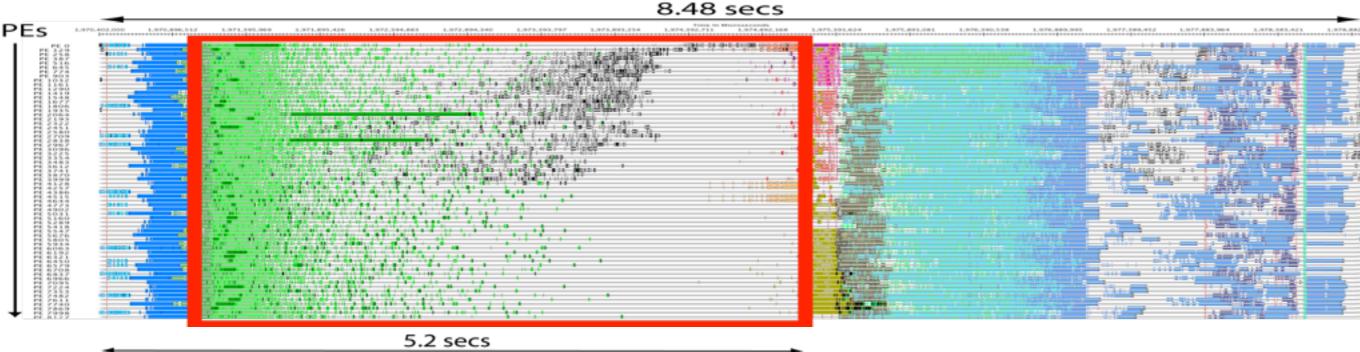
#### Performance on Blue Gene/L

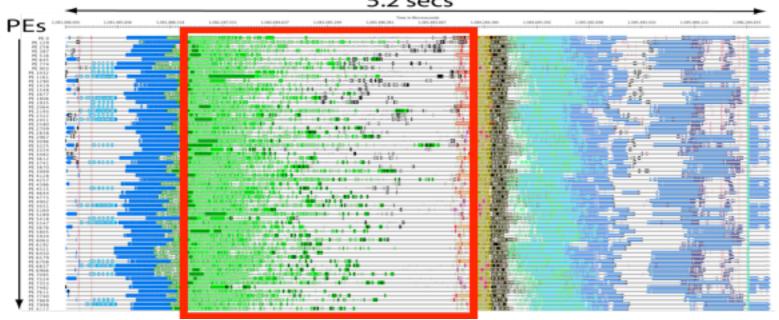






# Diagnosis of Improvement





Timeline of I iteration of OpenAtom running WATER\_256M\_70Ry on 8192 cores of BG/L

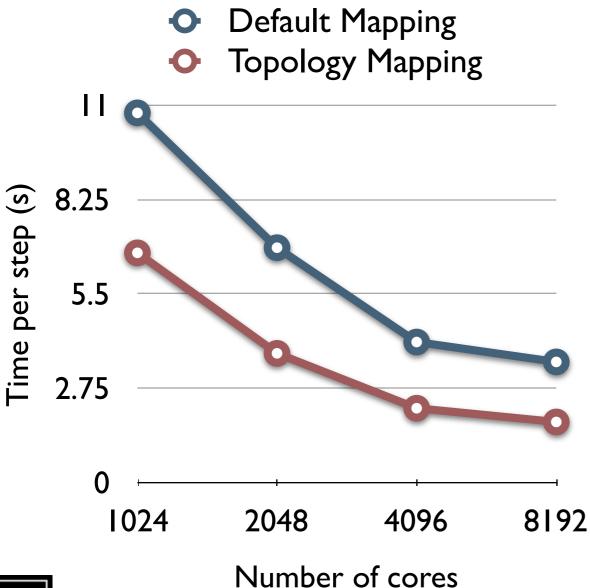


Timeline view using the performance visualization tool, Projections



## OpenAtom Performance on Blue Gene/P

### Application Performance



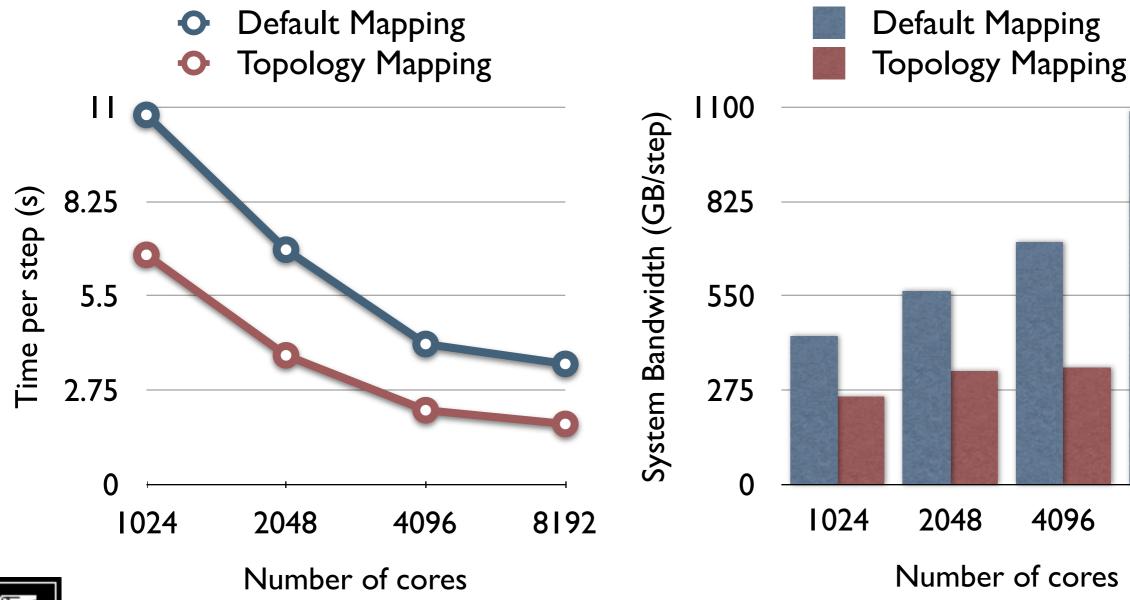




### OpenAtom Performance on Blue Gene/P

### Application Performance

#### Performance Counters



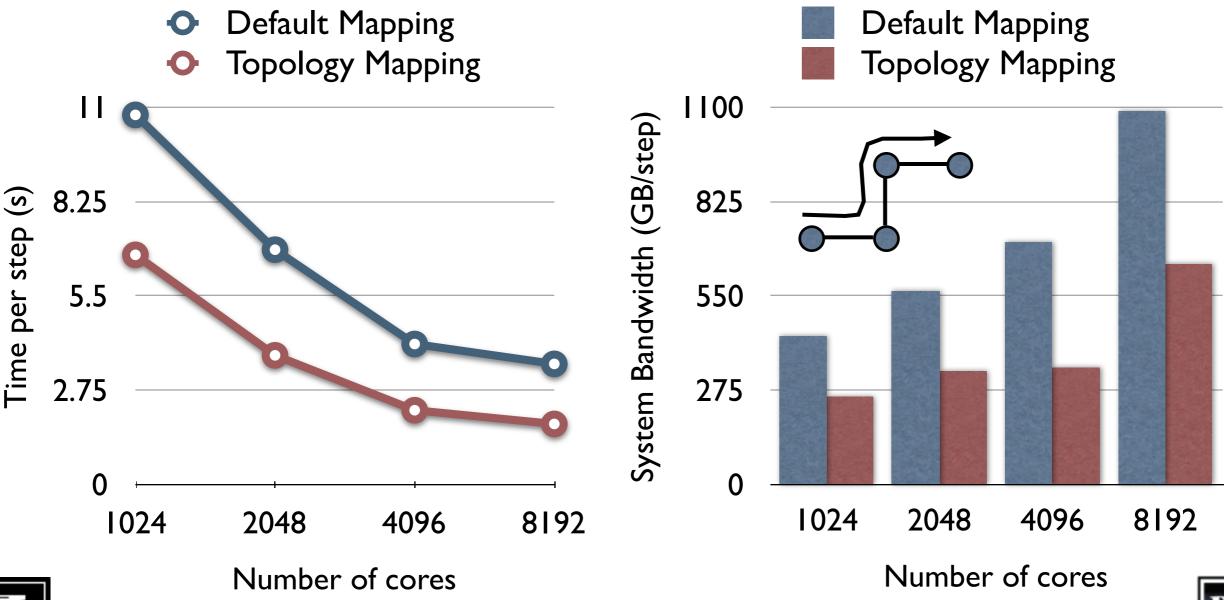


8192

### OpenAtom Performance on Blue Gene/P

### Application Performance

#### Performance Counters







### • Cray XT3:

- Link bandwidth 3.8 GB/s (XT3), 0.425 (BG/P), 0.175 (BG/L)
- Bytes per flop 8.77 (XT3),
   0.375 (BG/P and BG/L)

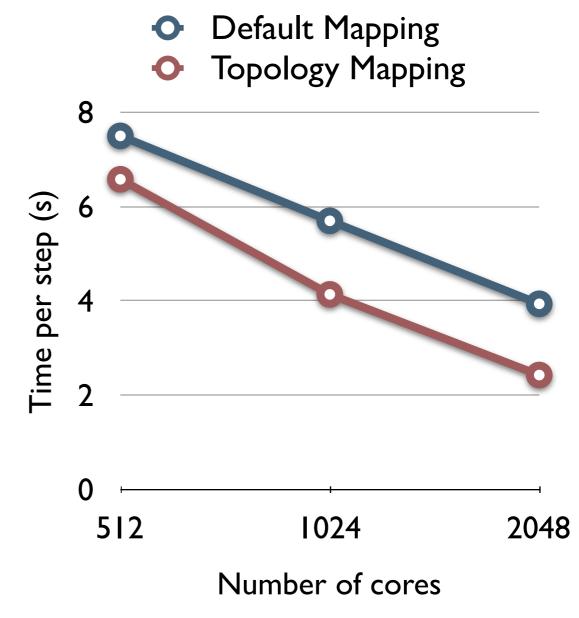


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- Job schedulers on Cray are not topology aware



### Cray XT3:

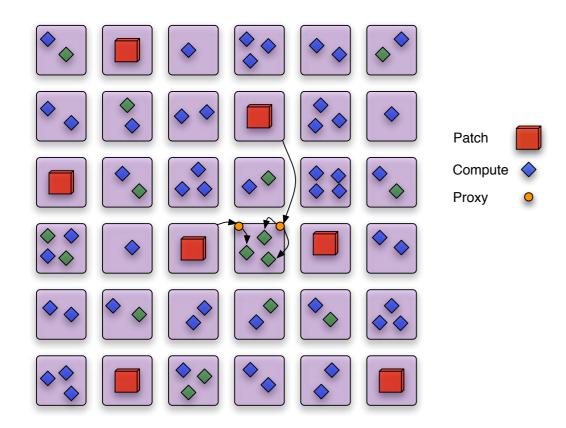
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- Bytes per flop 8.77 (XT3),
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- Job schedulers on Cray are not topology aware
- Performance Benefit at 2048 cores: 40% (XT3), 45% (BG/P), 41% (BG/L)

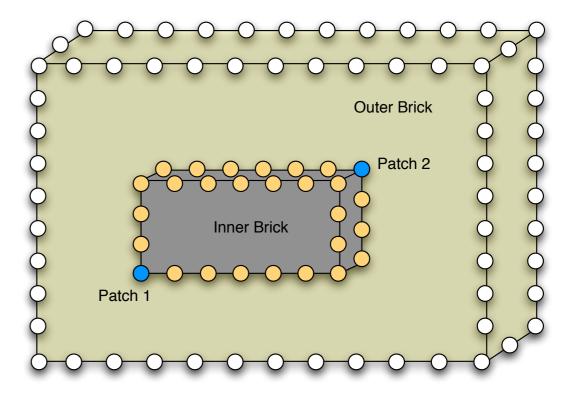






# Case Study II: NAMD





Communication between patches and computes

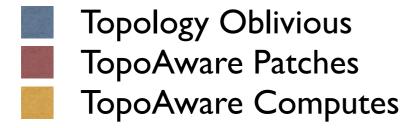
Topology aware placement of computes

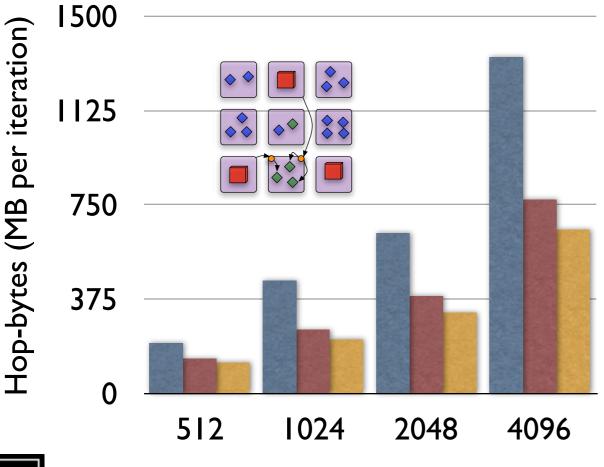


A. Bhatele, L.V. Kale and S. Kumar, Dynamic Topology Aware Load Balancing Algorithms for Molecular Dynamics Applications, In 23rd ACM International Conference on Supercomputing (ICS), 2009.



### Measured Hop-bytes





Number of cores

Evaluation Metric: Hop-bytes

$$HB = \sum_{i=1}^{n} d_i \times b_i$$
  $\mathbf{d_i} = \mathbf{distance}$   $\mathbf{b_i} = \mathbf{bytes}$   $\mathbf{n} = \mathbf{no.}$  of messages

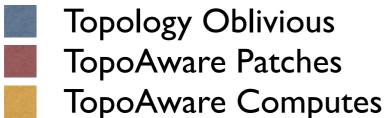
- Indicates amount of traffic and hence contention on the network
- Previously used metric: maximum dilation

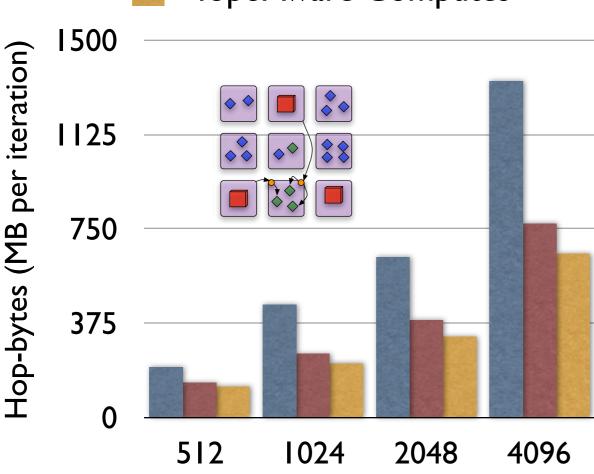
$$d(e) = \max\{d_i | e_i \in E\}$$





### Measured Hop-bytes

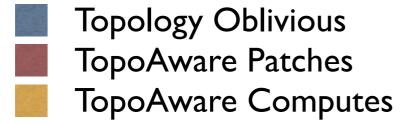


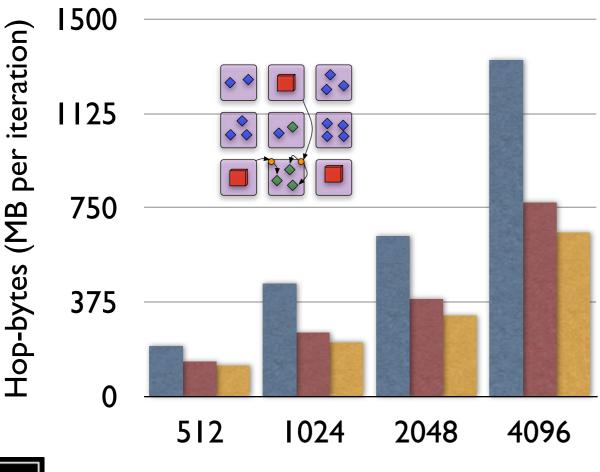




PPL

#### Measured Hop-bytes

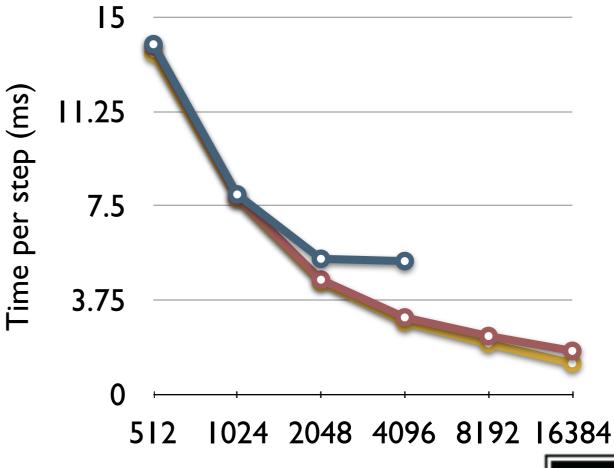




Number of cores

### Application Performance

- Topology Oblivious
- TopoAware Patches
- TopoAware Computes

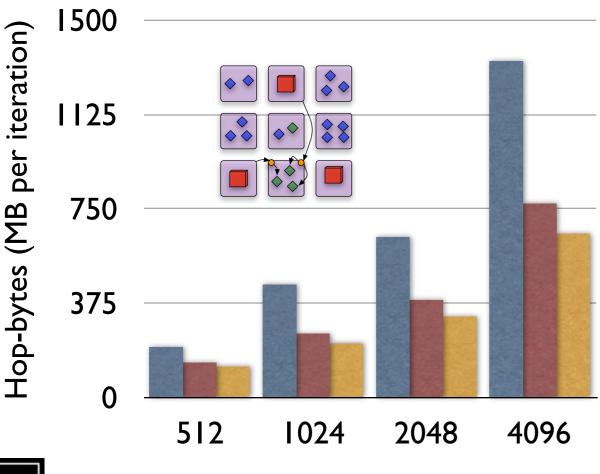




Number of cores

### Measured Hop-bytes

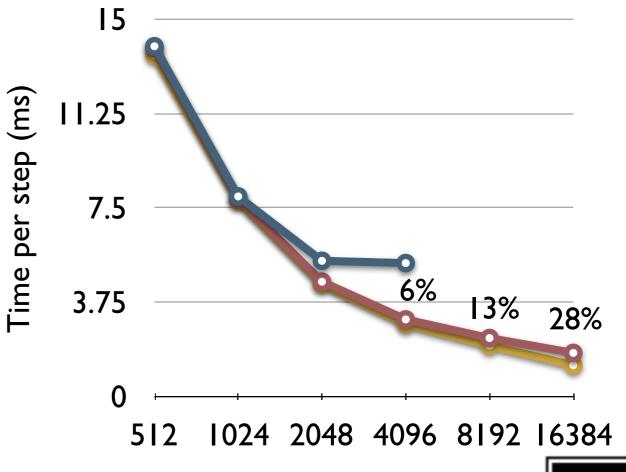




Number of cores

### Application Performance

- Topology Oblivious
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- TopoAware Computes





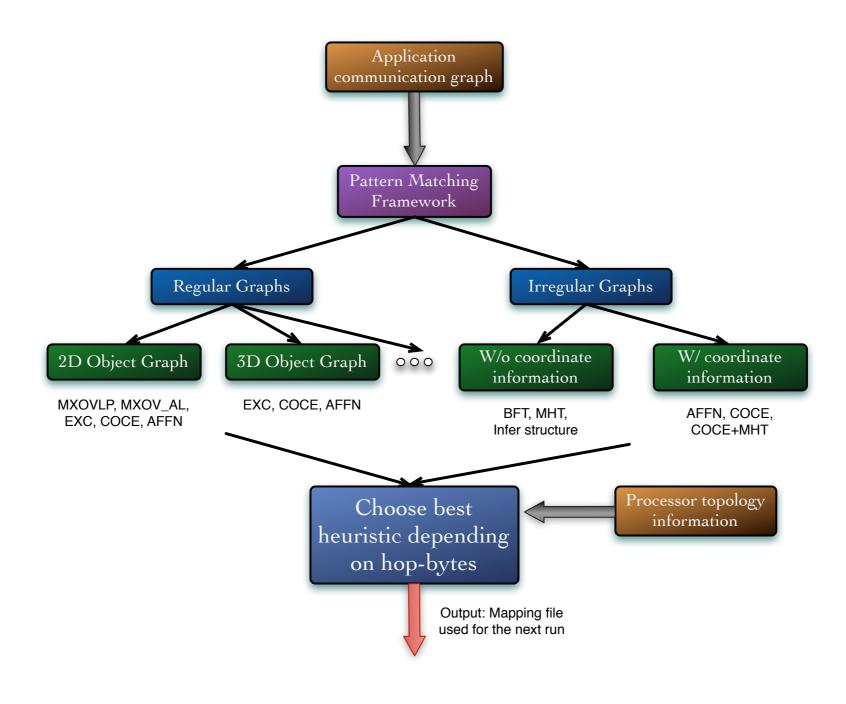


## Outline

- Case studies:
  - OpenAtom
  - NAMD
- Automatic Mapping Framework
  - Pattern matching
- Heuristics for Regular Graphs
- Heuristics for Irregular Graphs



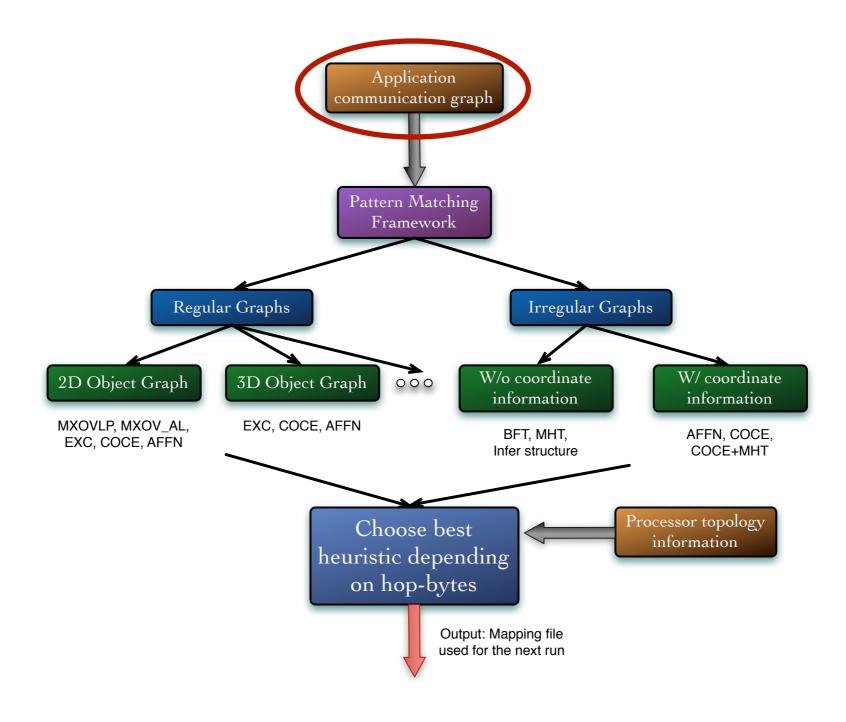
# Automatic Mapping Framework







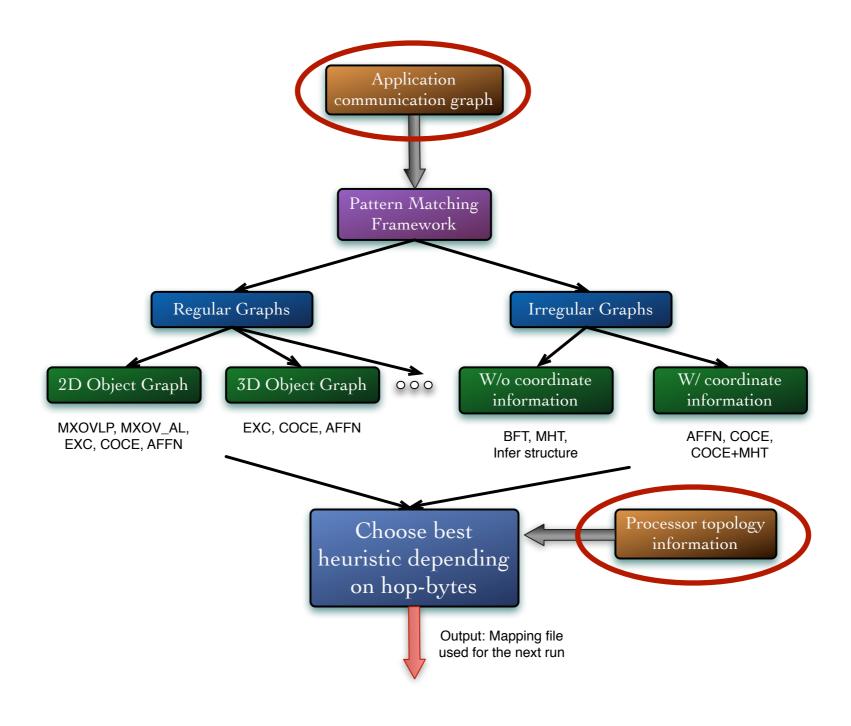
# Automatic Mapping Framework







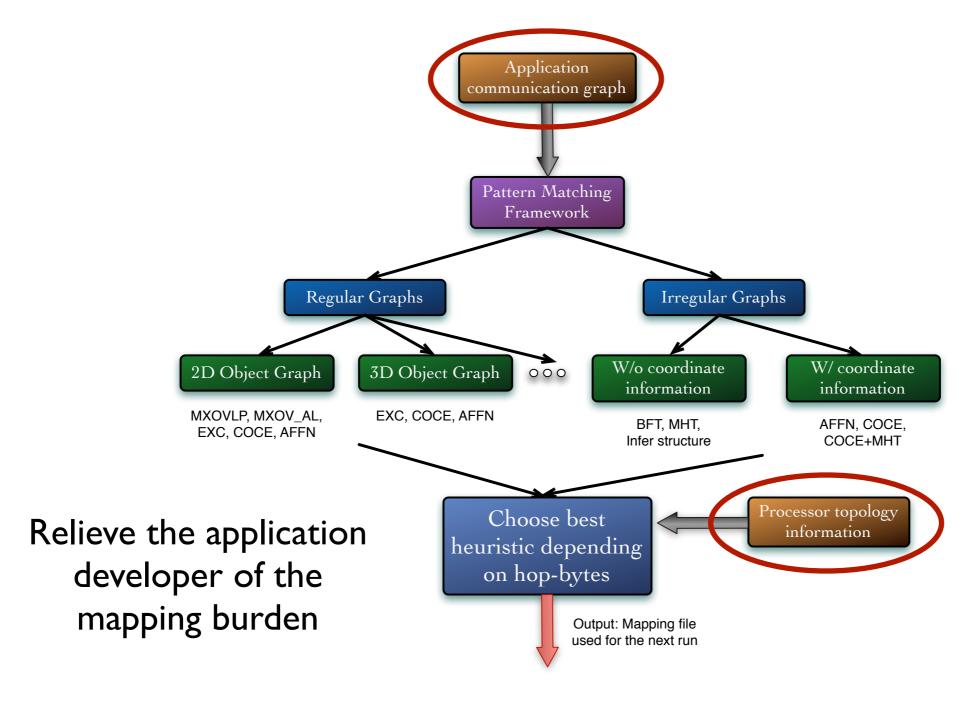
## Automatic Mapping Framework







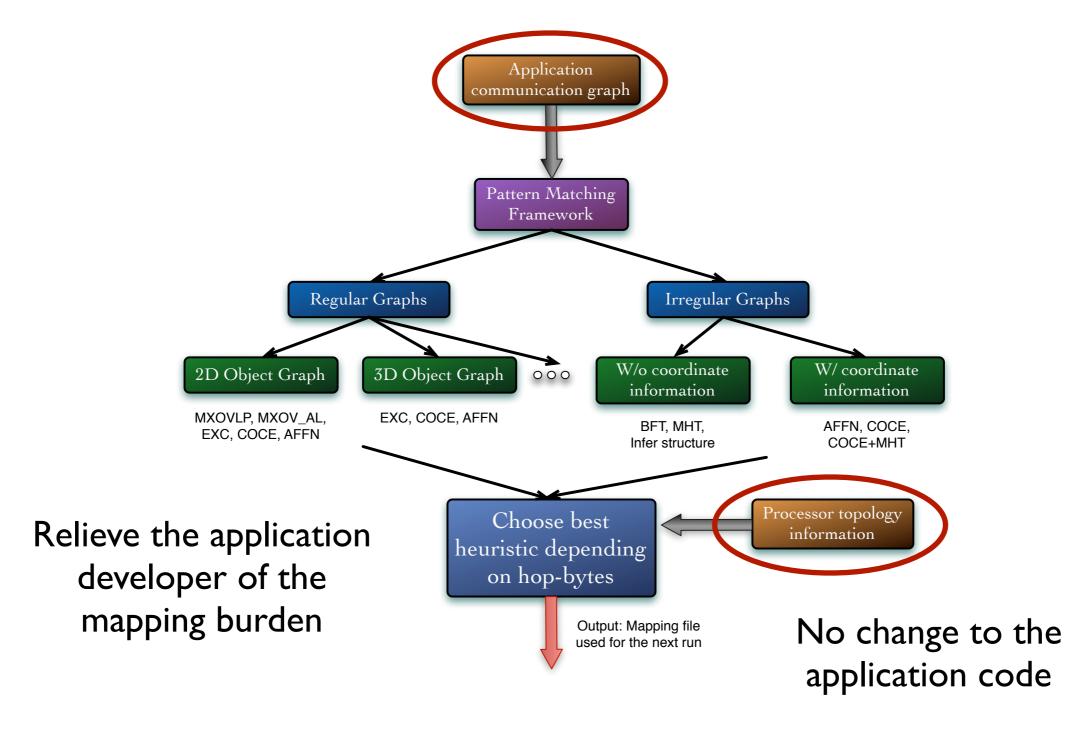
## Automatic Mapping Framework







## Automatic Mapping Framework







## Topology Discovery

- Topology Manager API: for 3D interconnects (Blue Gene, XT)
- Information required for mapping:
  - Physical dimensions of the allocated job partition
  - Mapping of ranks to physical coordinates and vice versa
- On Blue Gene machines such information is available and the API is a wrapper
- On Cray XT machines, jump several hoops to get this information and make it available through the same API





## Application communication graph

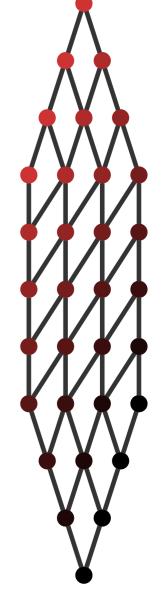
- Several ways to obtain the graph
- MPI applications:
  - Profiling tools (IBM's HPCT tools)
  - Collect information using the PMPI interface
  - Manually provided by the application end user
- Charm++ applications:
  - Instrumentation at runtime
  - Profiling tools (HPCT): when n = p



### Pattern Matching

We want to identify regular 2D/3D communication patterns

```
Input: CM_{n,n} (communication matrix)
Output: isRegular (boolean, true if communication is regular)
         dims[] (dimensions of the regular communication graph)
for i = 1 to n do
   find the maximum number of neighbors for any rank in CM_{i,n}
end for
if max neighbors \leq 5 then
   // this might be a case of regular 2D communication
   select an arbitrary rank start_{pe} find its distance from its neighbors
   dist = difference between ranks of start_{pe} and its top or bottom neighbor
   for i := 1 to n do
      if distance of all ranks from their neighbors == 1 or dist then
          isRegular = true
          \dim[0] = dist
          \dim[1] = n/dist
      end if
   end for
end if
```

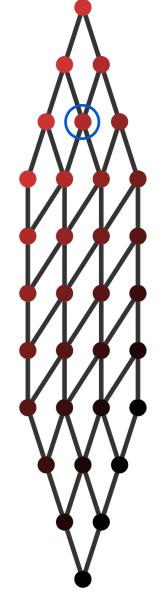




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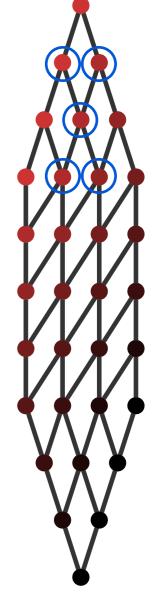




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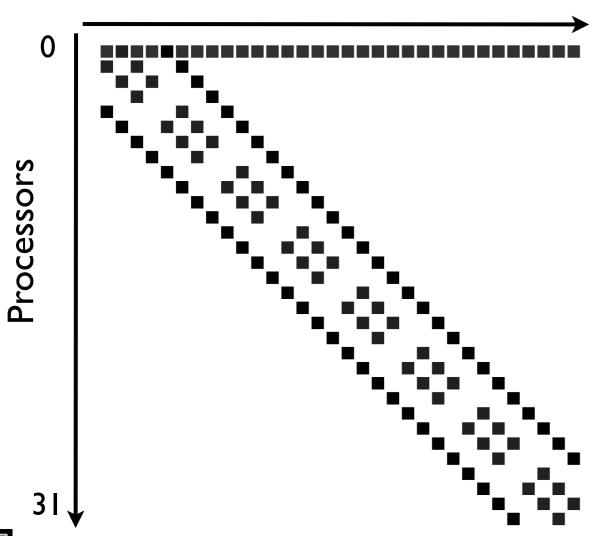
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## Example

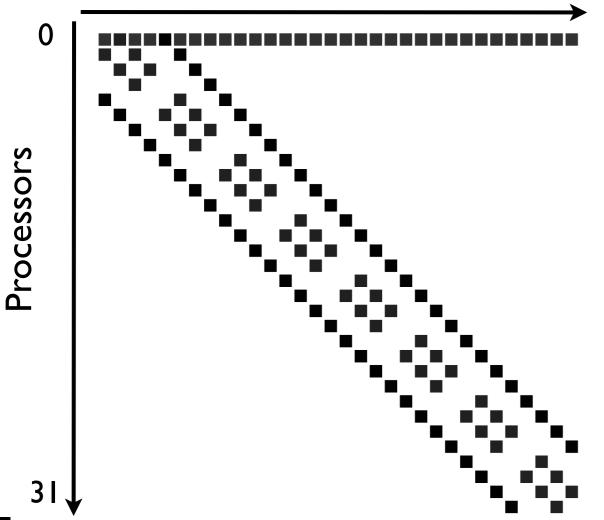
WRF running on 32 cores of Blue Gene/P





## Example

WRF running on 32 cores of Blue Gene/P



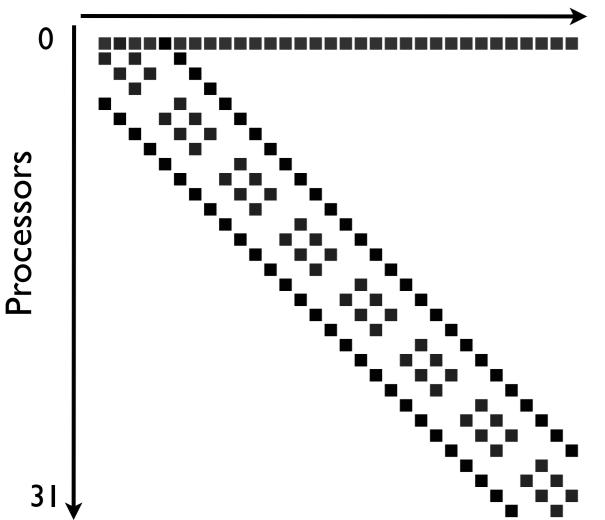
Pattern matching to identify regular communication patterns such as 2D/3D near-neighbor graphs

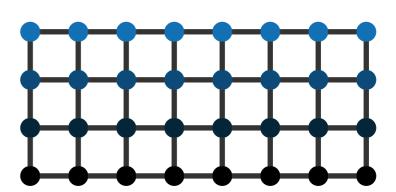




### Example

WRF running on 32 cores of Blue Gene/P





Pattern matching to identify regular communication patterns such as 2D/3D near-neighbor graphs





### Communication Graphs

- Regular communication:
  - POP (Parallel Ocean Program): 2D Stencil like computation
  - WRF (Weather Research and Forecasting model): 2D Stencil
  - MILC (MIMD Lattice Computation): 4D near-neighbor
- Irregular communication:
  - Unstructured mesh computations: FLASH, CPSD code
  - Many other classes of applications



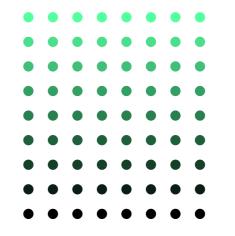
#### Outline

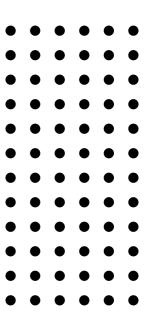
- Case studies:
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Maximum Overlap (MXOVLP)

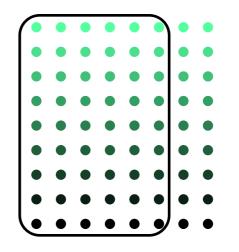
Object Graph: 9 x 8

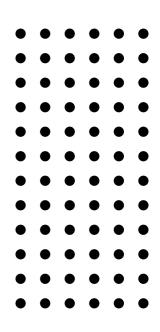




Maximum Overlap (MXOVLP)

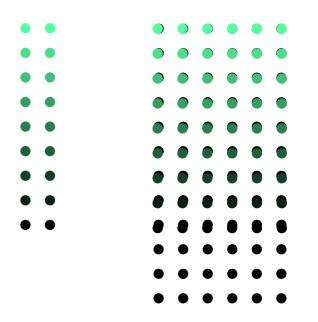
Object Graph: 9 x 8





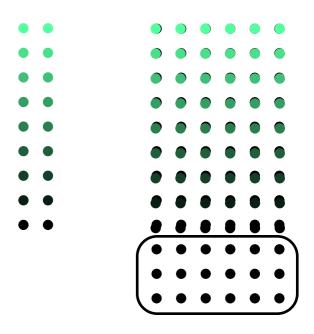
Maximum Overlap (MXOVLP)

Object Graph: 9 x 8



Maximum Overlap (MXOVLP)

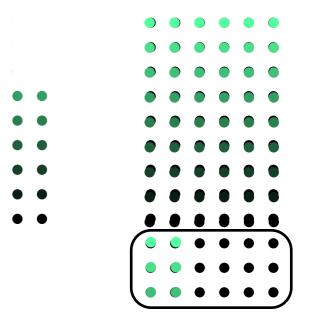
Object Graph: 9 x 8





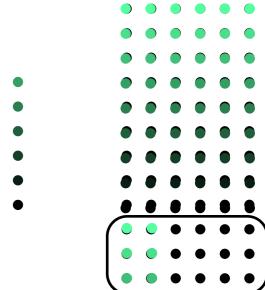
Maximum Overlap (MXOVLP)

Object Graph: 9 x 8



Maximum Overlap (MXOVLP)

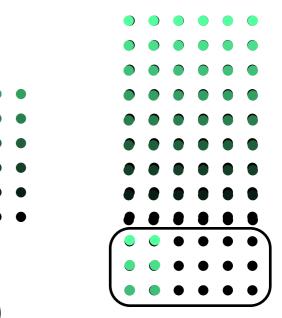
Object Graph: 9 x 8



- Maximum Overlap with Alignment (MXOV+AL)
  - Alignment at each recursive call

Maximum Overlap (MXOVLP)

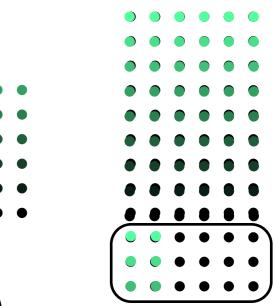
Object Graph: 9 x 8



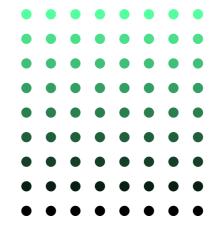
- Maximum Overlap with Alignment (MXOV+AL)
  - Alignment at each recursive call
- Expand from Corner (EXCO)

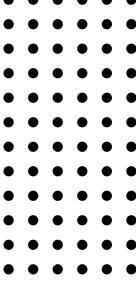
Maximum Overlap (MXOVLP)

Object Graph: 9 x 8



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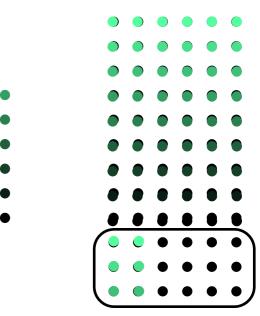




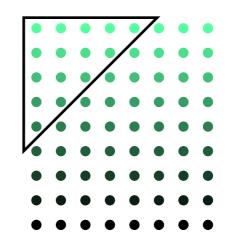


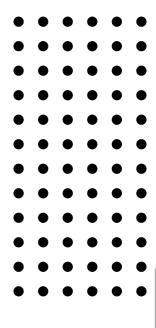
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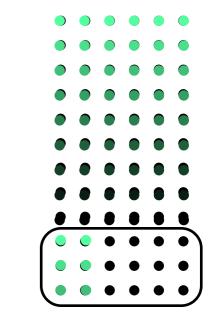




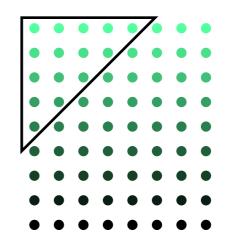


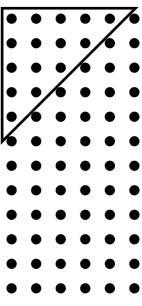
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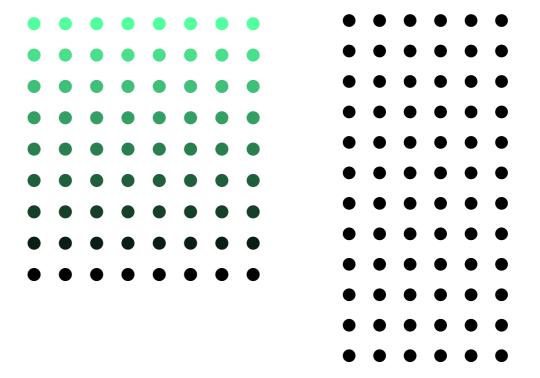
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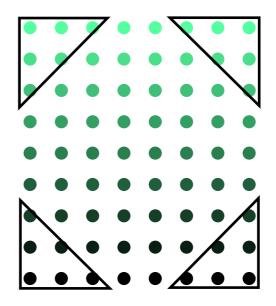
- Corners to Center (COCE)
  - Start simultaneously from all corners

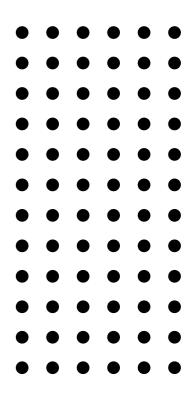






- Corners to Center (COCE)
  - Start simultaneously from all corners

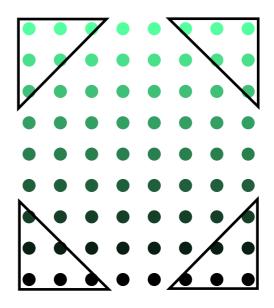


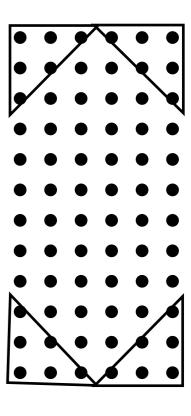






- Corners to Center (COCE)
  - Start simultaneously from all corners

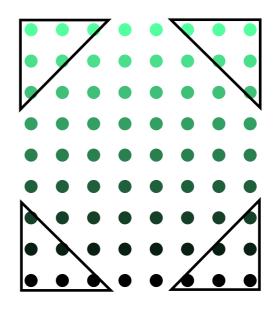


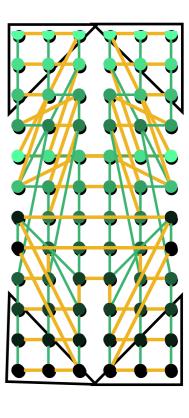






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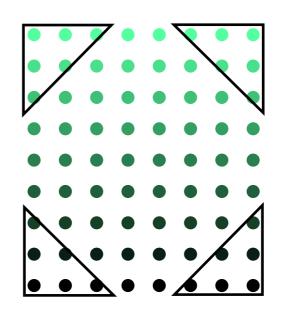


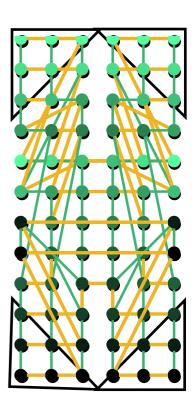






- Corners to Center (COCE)
  - Start simultaneously from all corners





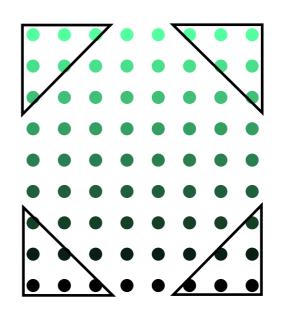
Affine Mapping (AFFN)

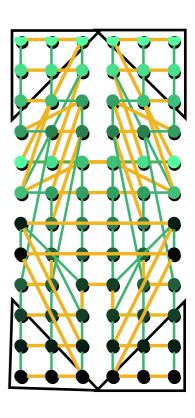




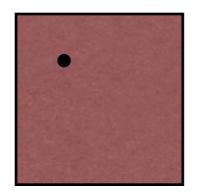


- Corners to Center (COCE)
  - Start simultaneously from all corners





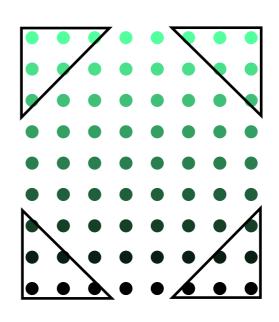
Affine Mapping (AFFN)

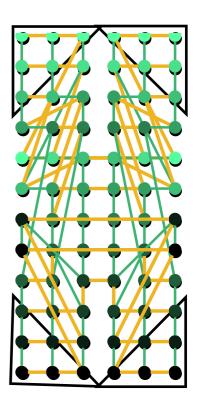






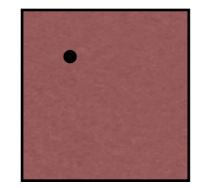
- Corners to Center (COCE)
  - Start simultaneously from all corners





Affine Mapping (AFFN)

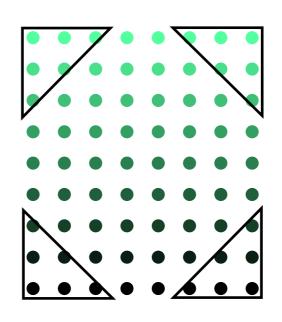
$$(x,y) \to (\lfloor P_x * \frac{x}{O_x} \rfloor, \lfloor P_y * \frac{y}{O_y} \rfloor)$$

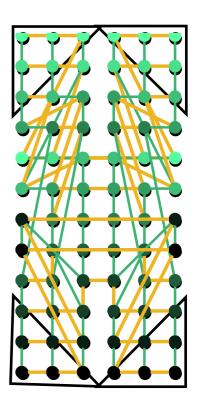






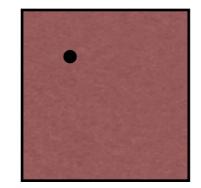
- Corners to Center (COCE)
  - Start simultaneously from all corners

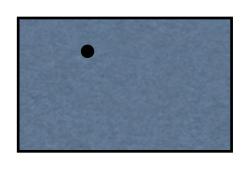




Affine Mapping (AFFN)

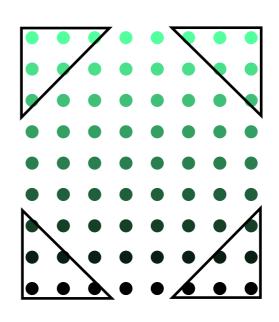
$$(x,y) \to (\lfloor P_x * \frac{x}{O_x} \rfloor, \lfloor P_y * \frac{y}{O_y} \rfloor)$$

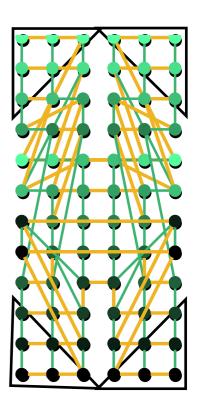






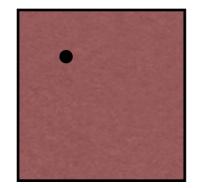
- Corners to Center (COCE)
  - Start simultaneously from all corners

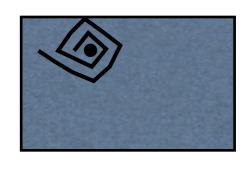




Affine Mapping (AFFN)

$$(x,y) \to (\lfloor P_x * \frac{x}{O_x} \rfloor, \lfloor P_y * \frac{y}{O_y} \rfloor)$$

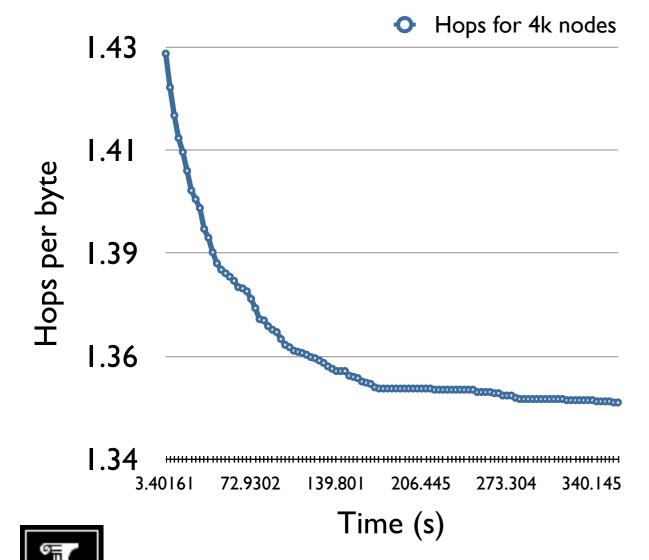






## Running Time

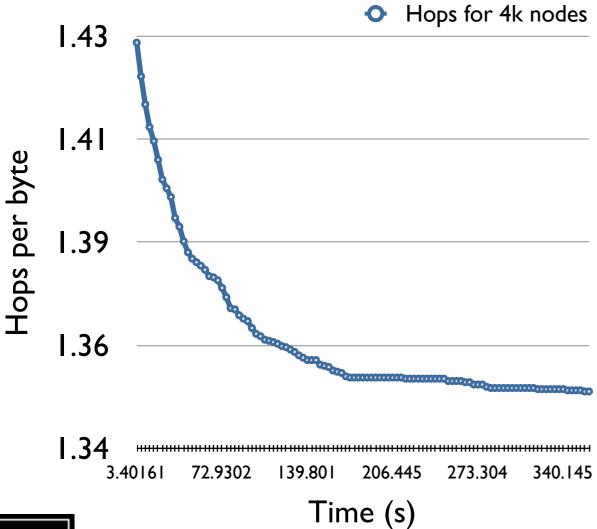
- Pairwise Exchanges (PAIRS)
  - Bokhari, Lee et al.

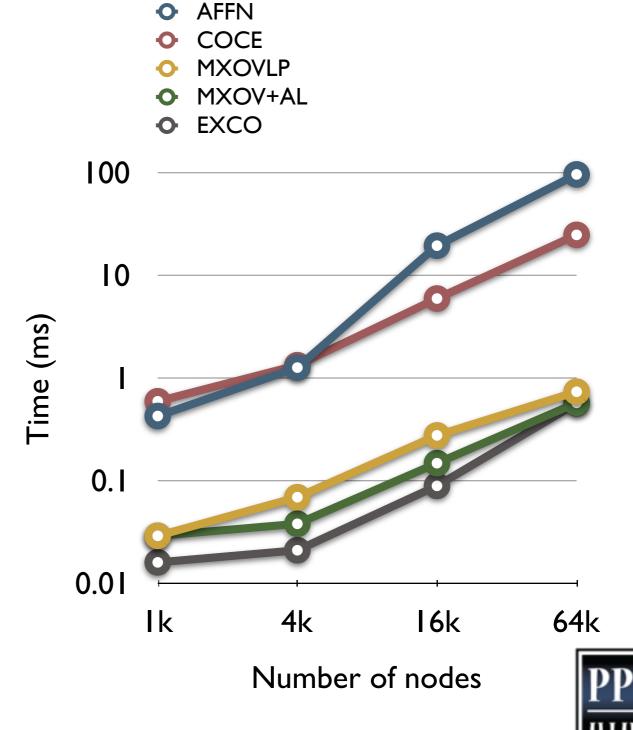




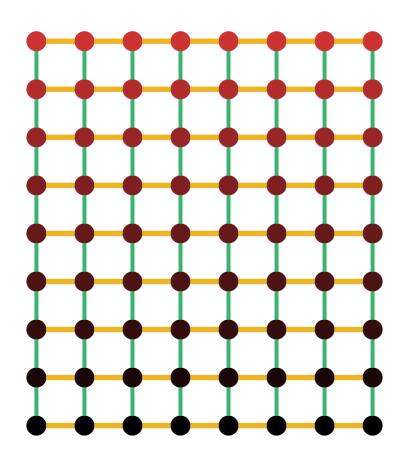
### Running Time

- Pairwise Exchanges (PAIRS)
  - Bokhari, Lee et al.



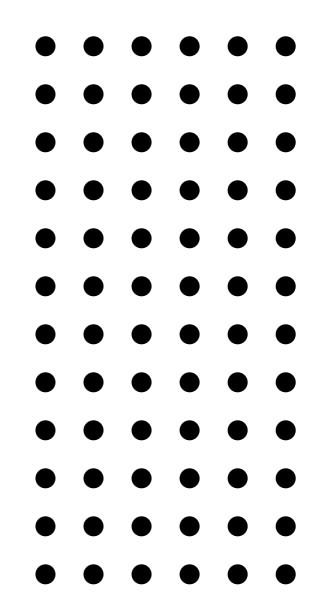


## Example Mapping



Object Graph: 9 x 8

Processor Graph: 12 x 6

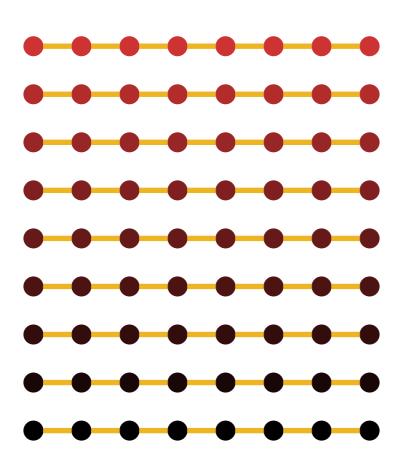




Aleliunas, R. and Rosenberg, A. L. On Embedding Rectangular Grids in Square Grids. IEEE Trans. Comput., 31(9):907–913, 1982

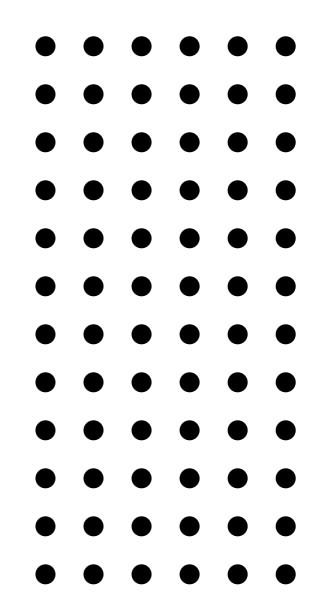


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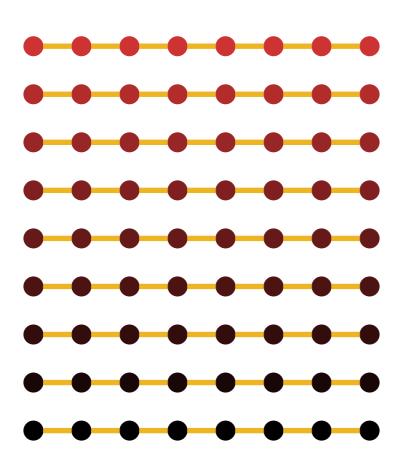
Processor Graph: 12 x 6





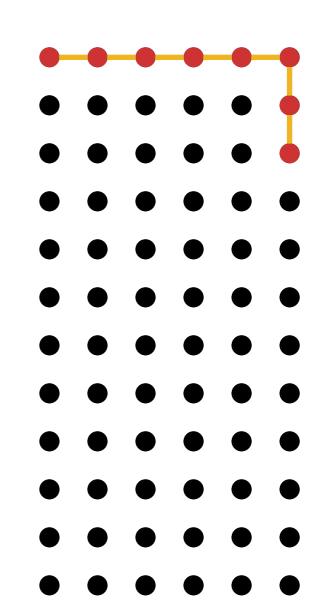
Aleliunas, R. and Rosenberg, A. L. On Embedding Rectangular Grids in Square Grids. IEEE Trans. Comput., 31(9):907–913, 1982





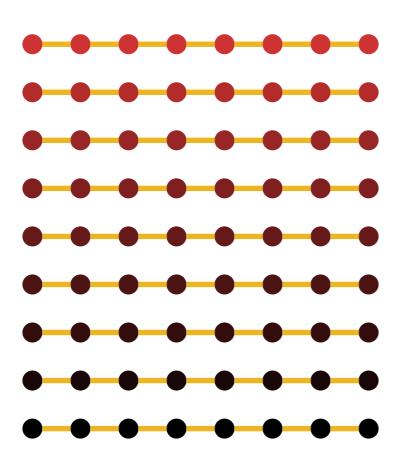
Object Graph: 9 x 8

Processor Graph: 12 x 6



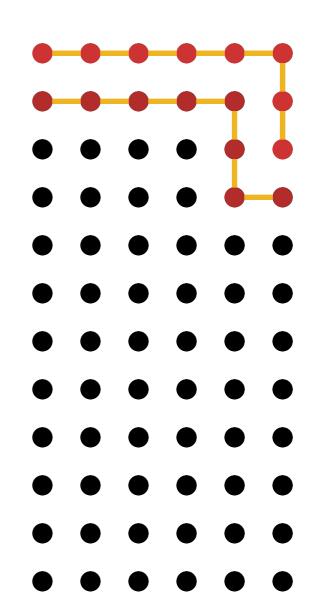






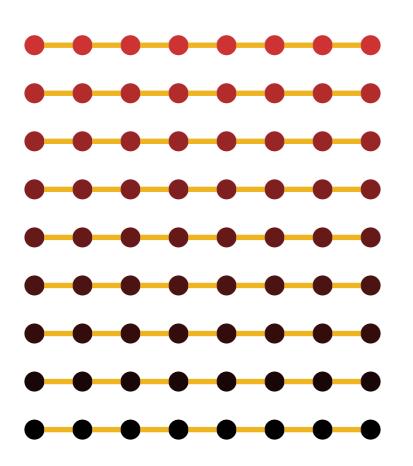
Object Graph: 9 x 8

Processor Graph: 12 x 6



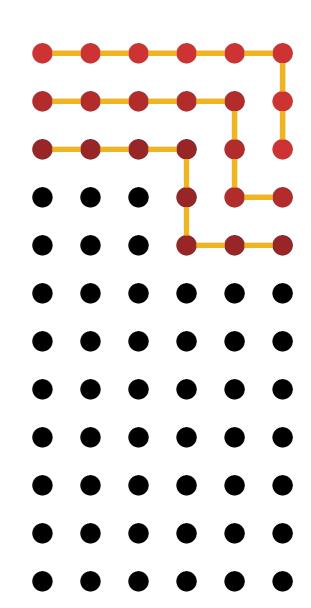






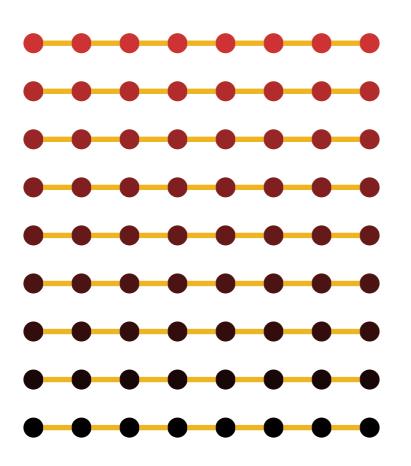
Object Graph: 9 x 8

Processor Graph: 12 x 6



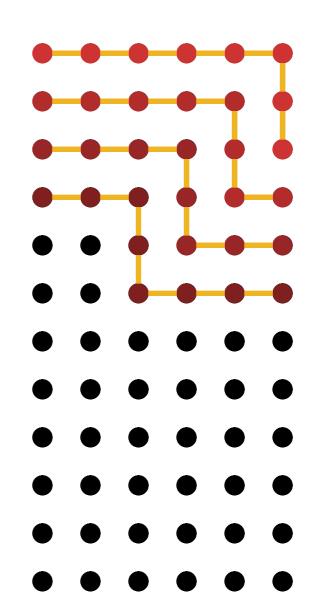






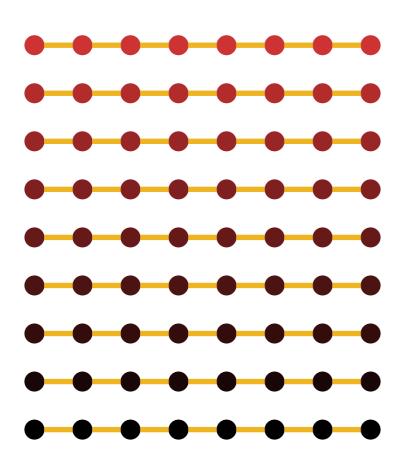
Object Graph: 9 x 8

Processor Graph: 12 x 6



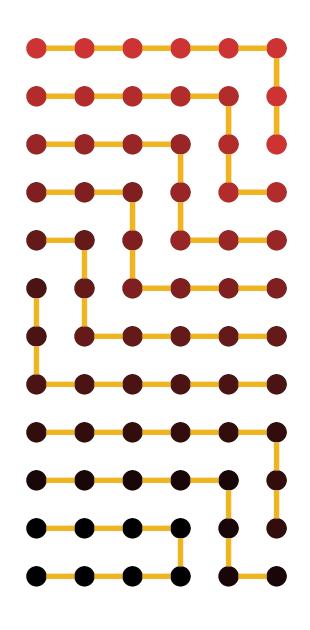






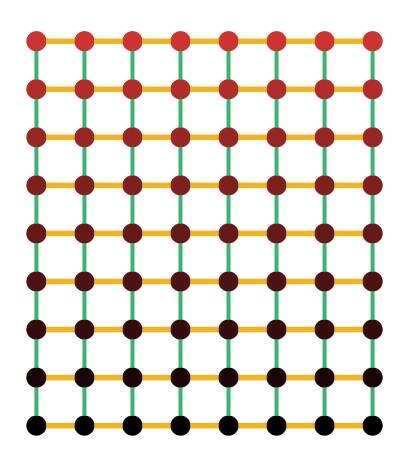
Object Graph: 9 x 8

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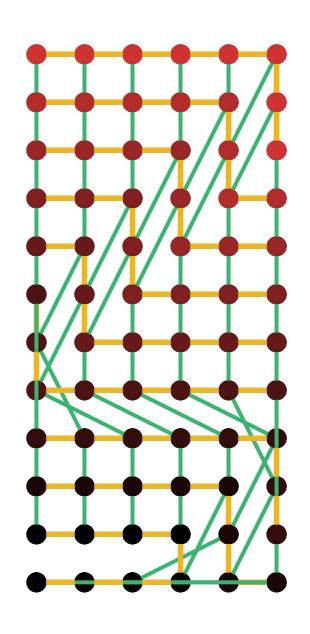






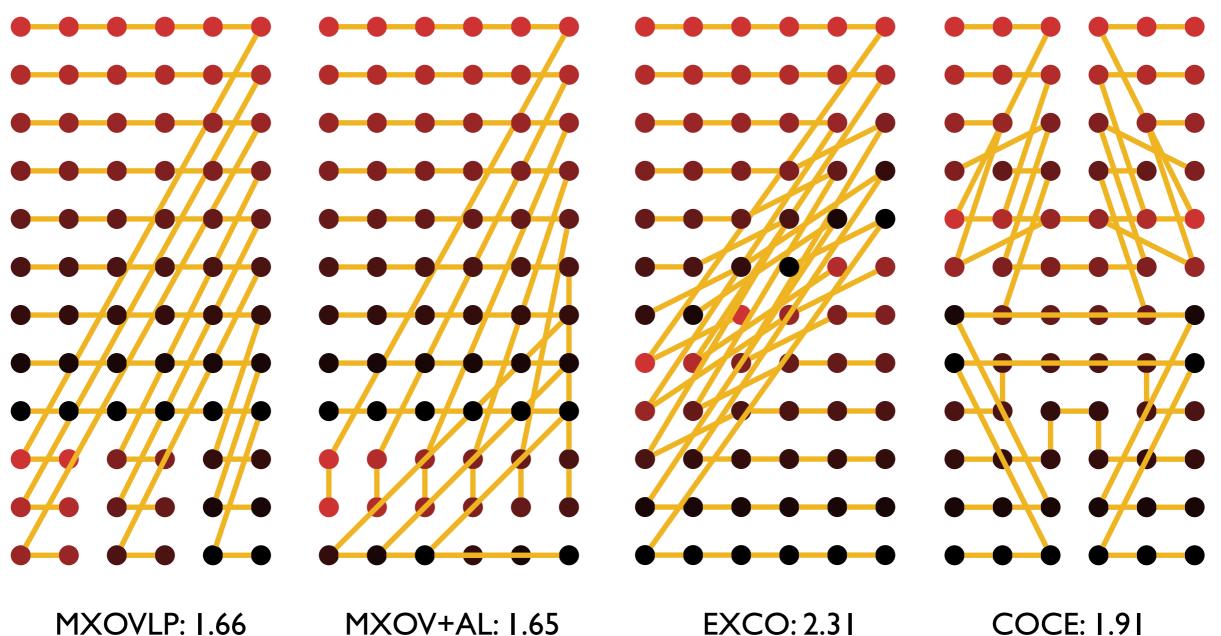
Object Graph: 9 x 8

Processor Graph: 12 x 6



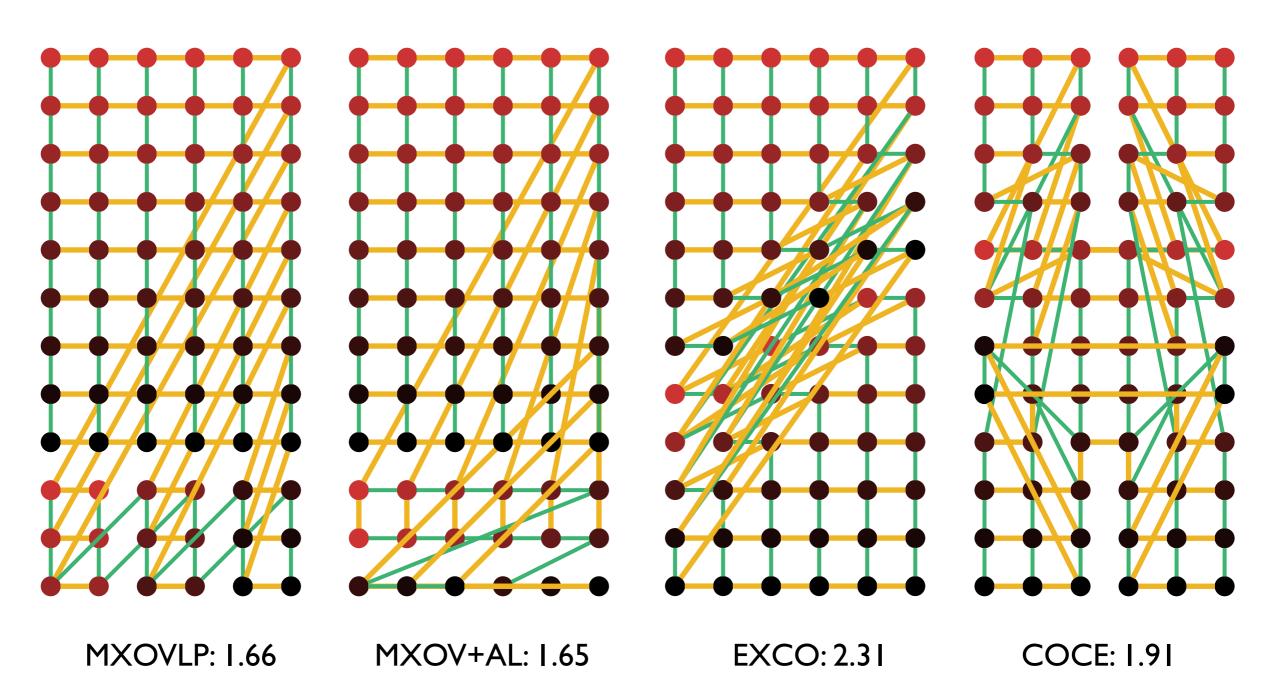






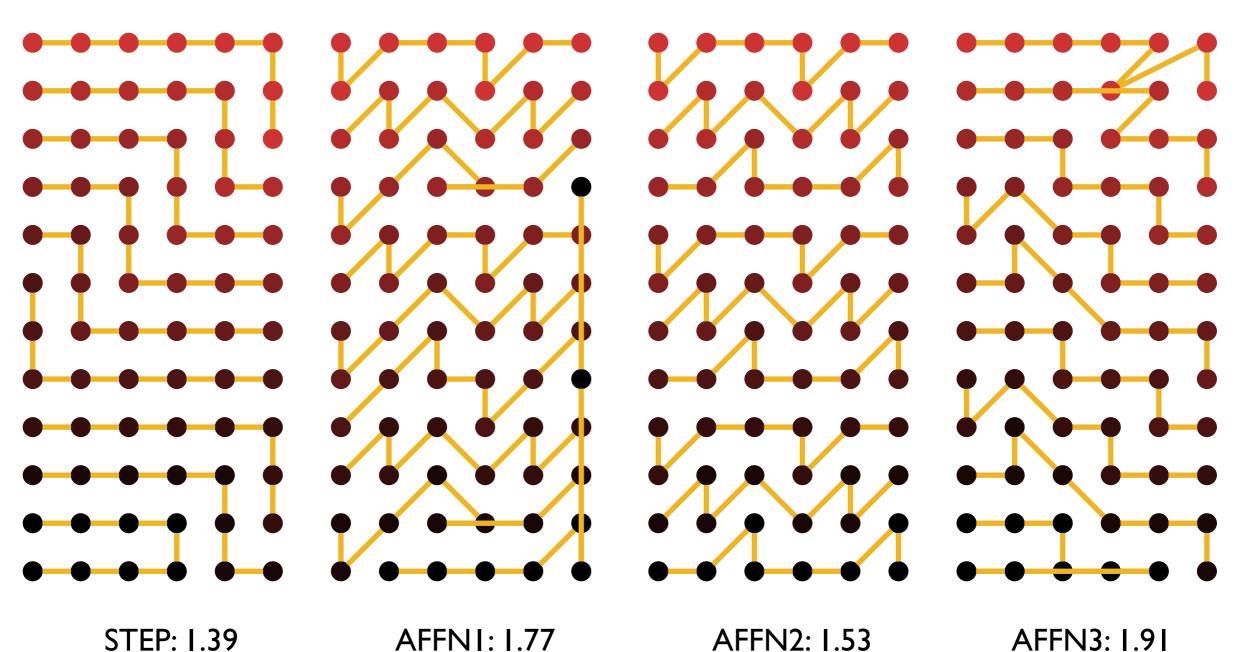


COCE: 1.91 **EXCO: 2.31** 



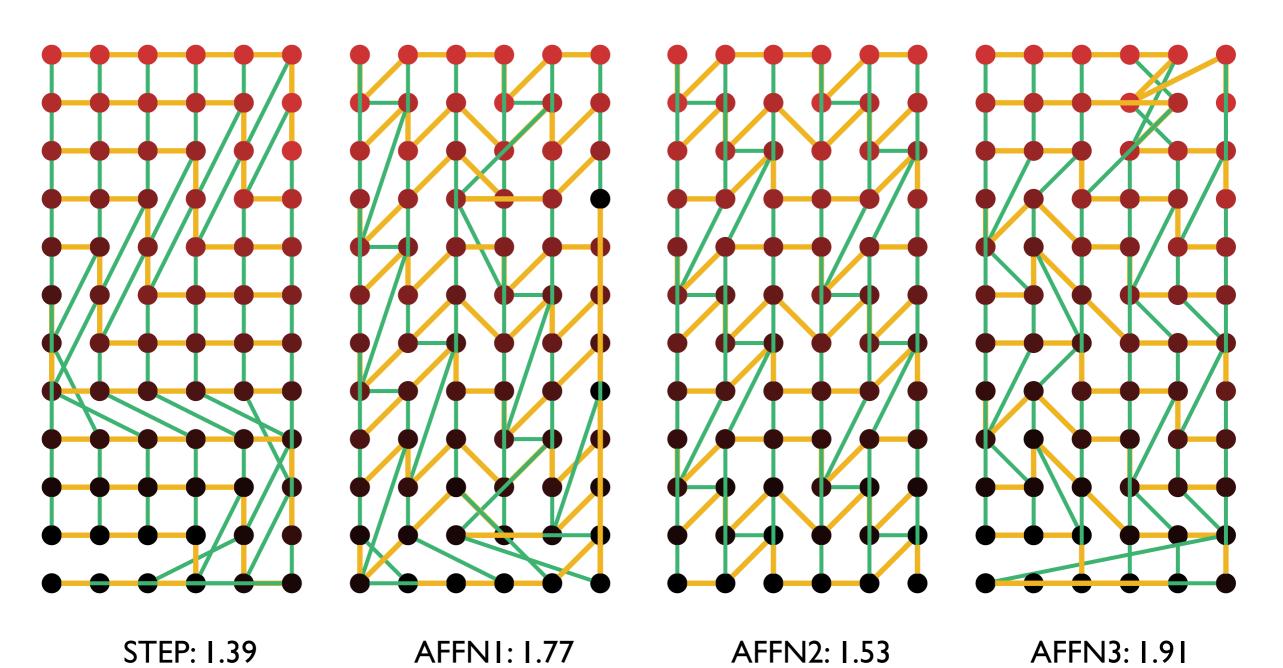








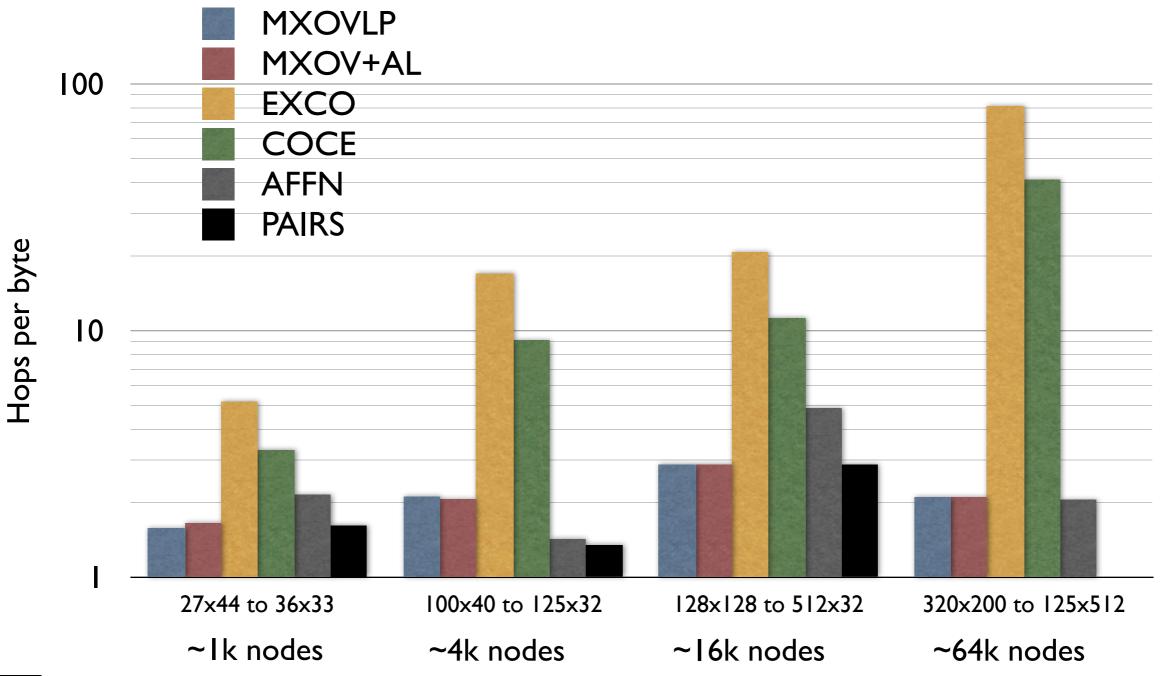
AFFN3: 1.91







### Evaluation

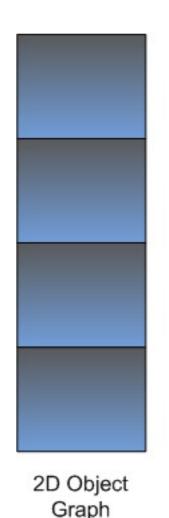


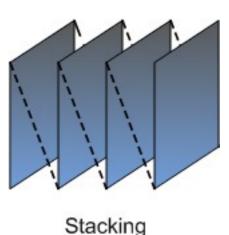


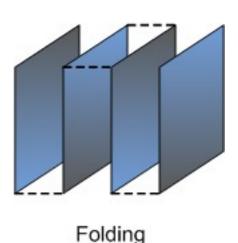


## Mapping 2D Graphs to 3D

- Map a two-dimensional object graph to a threedimensional processor graph
- Divide object graph into subgraphs once each for the number of planes
  - Stacking
  - Folding
- Best 2D to 2D heuristic chosen based on hop-bytes



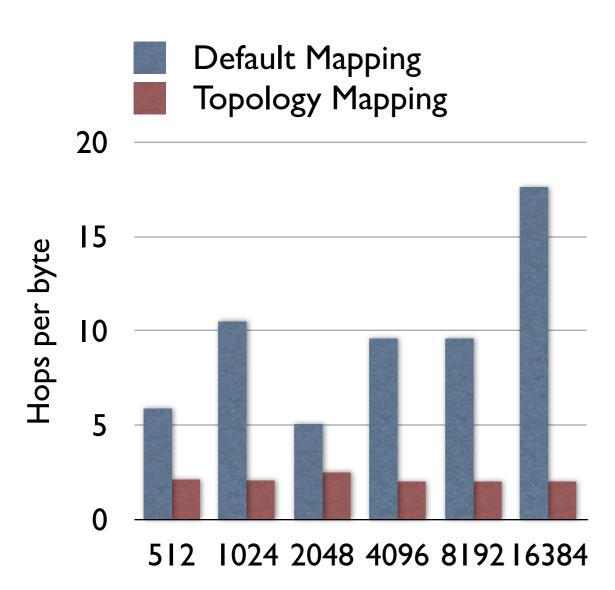






#### Results: 2D Stencil on Blue Gene/P

#### Hop-bytes

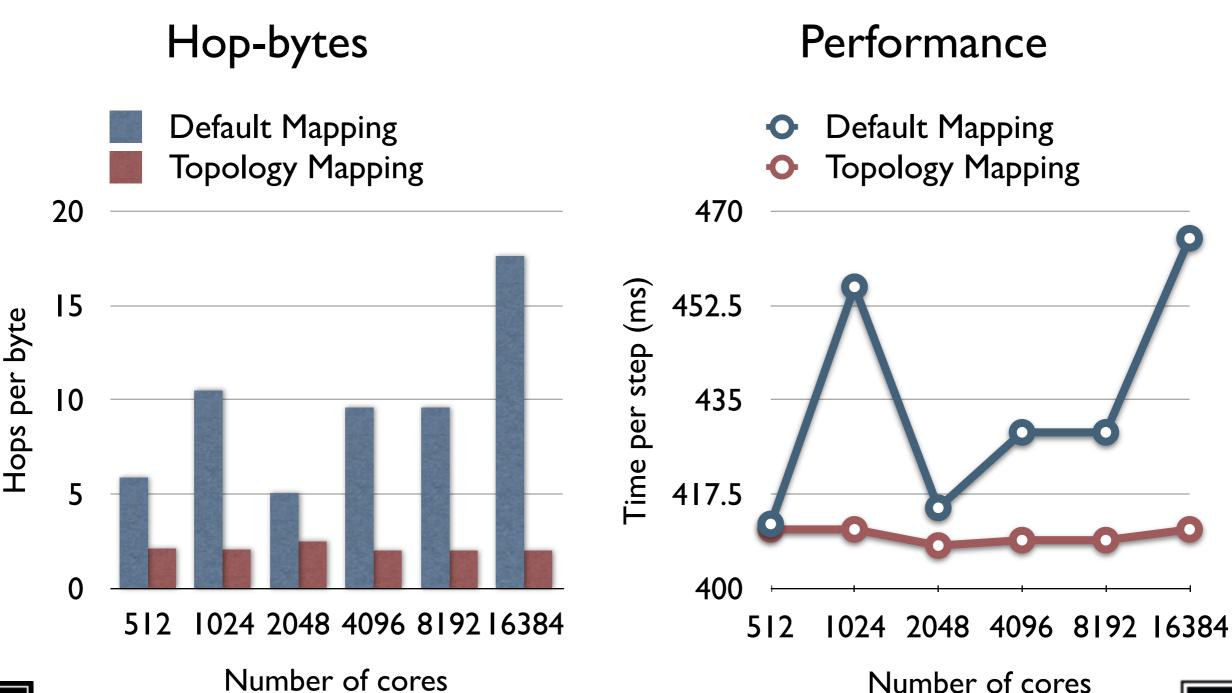




Number of cores



#### Results: 2D Stencil on Blue Gene/P



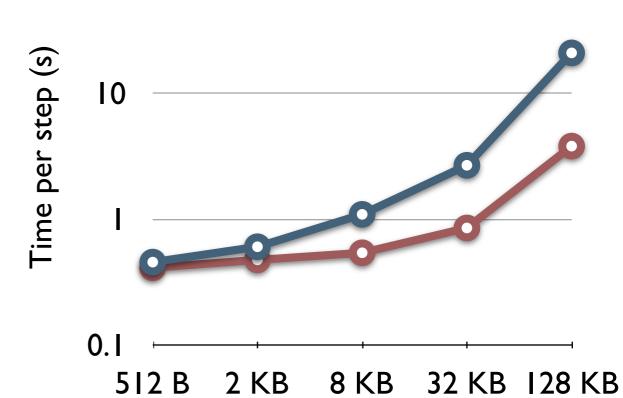


### Increasing communication

- With faster processors and constant link bandwidths
  - computation is becoming cheap
  - communication is a bottleneck
- Trend for bytes per flop
  - XT3: 8.77
  - XT4: 1.357
  - XT5: 0.23

#### 2D Stencil on BG/P

- Default Mapping
- Topology Mapping

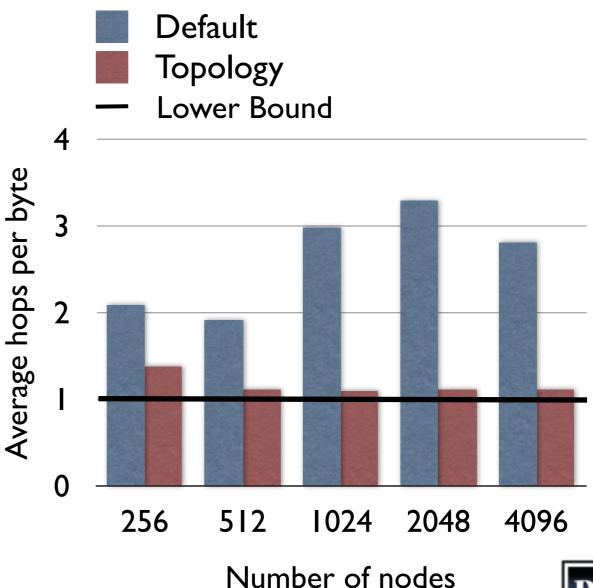


Message size



100

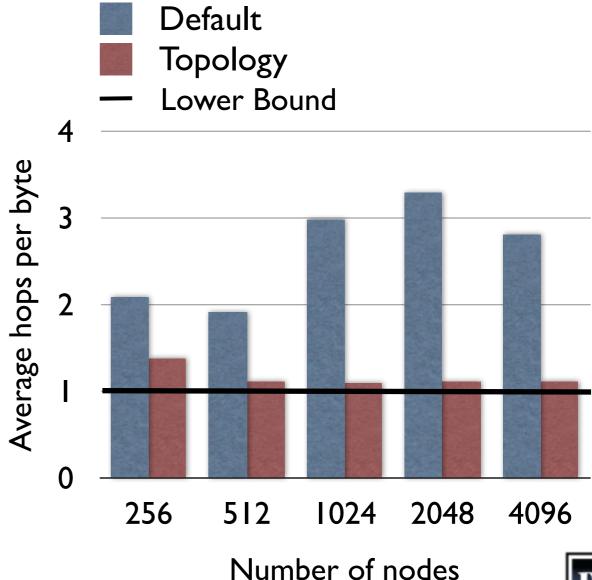
#### Hops from IBM HPCT





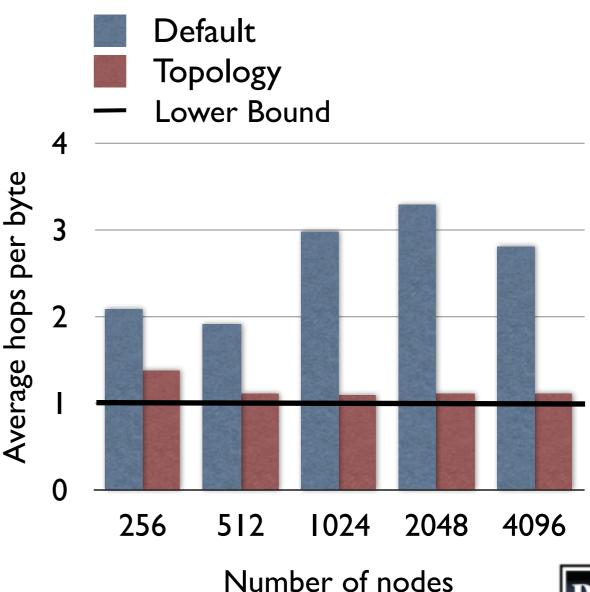
PPL UIUC

 Performance improvement negligible on 256 and 512 cores



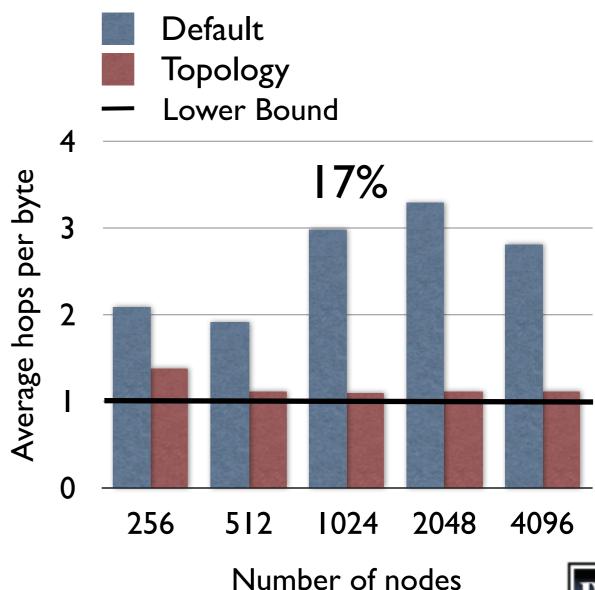


- Performance improvement negligible on 256 and 512 cores
- On 1024 nodes:
  - Hops reduce by: 63%
  - Time for communication reduces by 11%
  - Performance improves by 17%



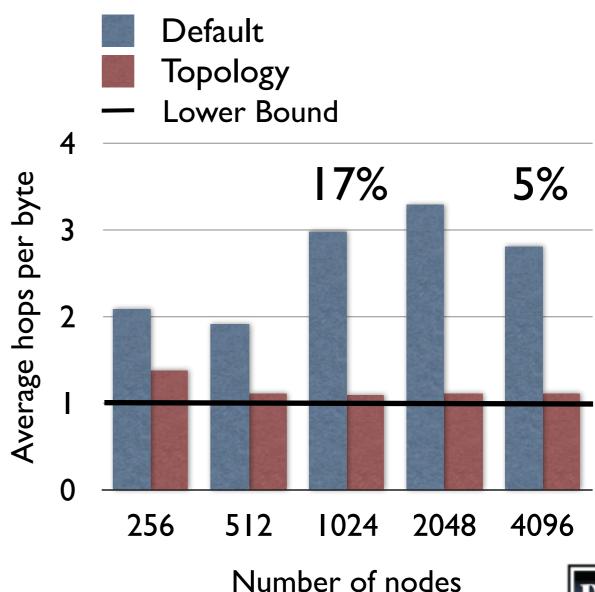


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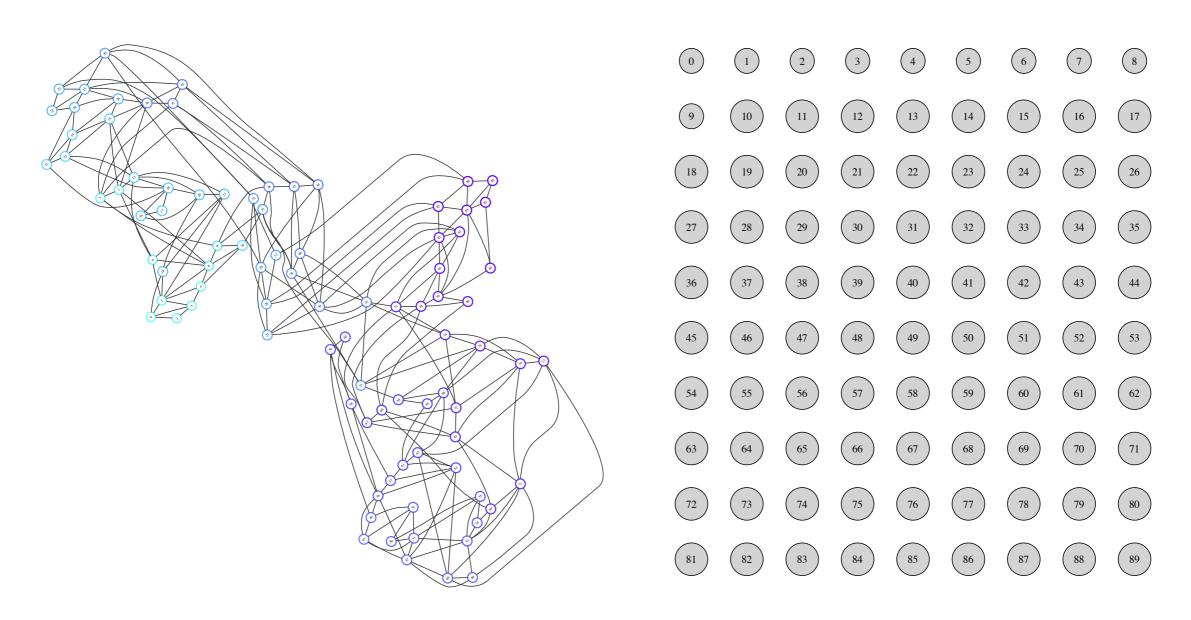


#### Outline

- Case studies:
  - OpenAtom
  - NAMD
- Automatic Mapping Framework
  - Pattern matching
- Heuristics for Regular Graphs
- Heuristics for Irregular Graphs



## Mapping Irregular Graphs





Processor Mesh: 10 x 9



Object graph: 90 nodes

### Two different scenarios

- There is no spatial information associated with the node
  - Option I:Work without it
  - Option 2: If we know that the simulation has a geometric configuration, try to infer the structure of the graph
- We have geometric coordinate information for each node
  - Use coordinate information to avoid crossing of edges and for other optimizations



### No coordinate information



#### No coordinate information

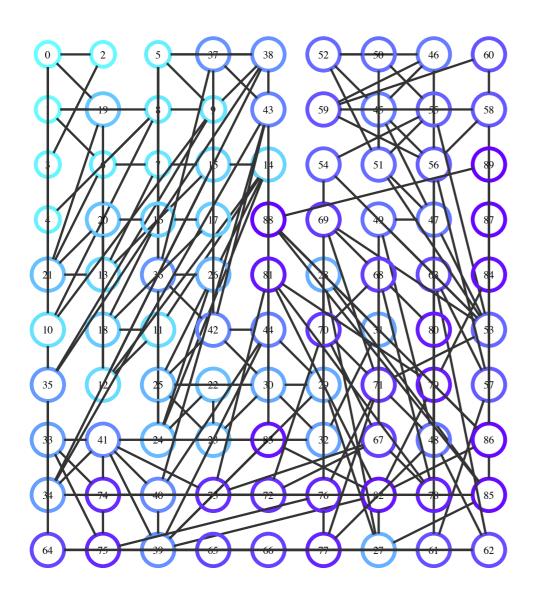
- Breadth first traversal (BFT)
  - Start with a random node and one end of the processor mesh
  - Map nodes as you encounter them close to their parent

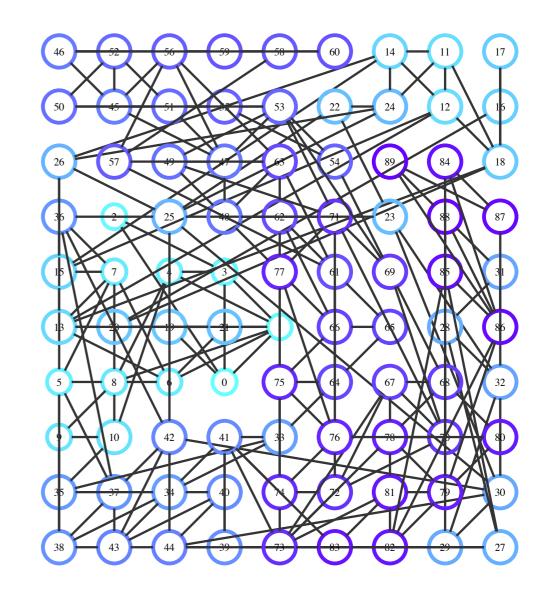
### No coordinate information

- Breadth first traversal (BFT)
  - Start with a random node and one end of the processor mesh
  - Map nodes as you encounter them close to their parent
- Max heap traversal (MHT)
  - Start with a random node and one end/center of the mesh
  - Put neighbors of a mapped node into the heap (node at the top is the one with maximum number of mapped neighbors)
  - Map elements in the heap one by one around the centroid of their mapped neighbors



## Mapping visualization





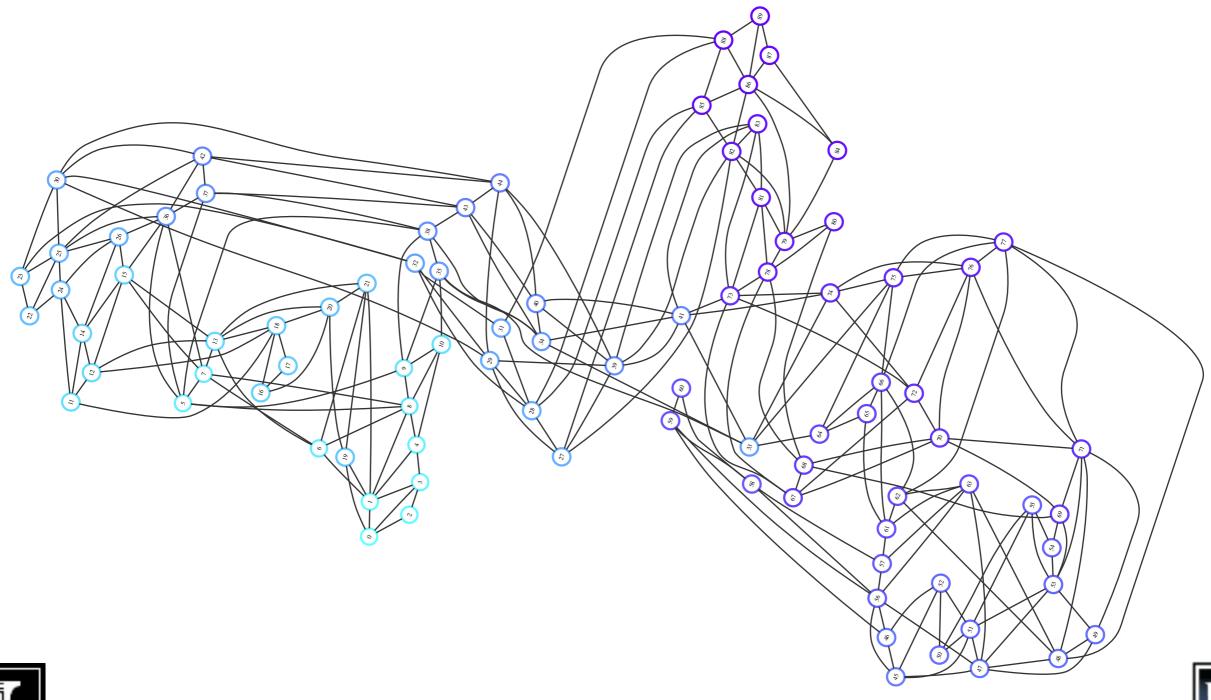


BFT: 2.89

MHT: 2.69



## Inferring the spatial placement



# Inferring the spatial placement

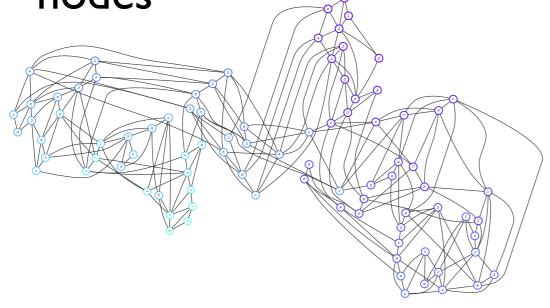
- Graph layout algorithms
  - Force-based layout to reduce the total energy in the system
- Use the graphviz library to obtain coordinates of the nodes

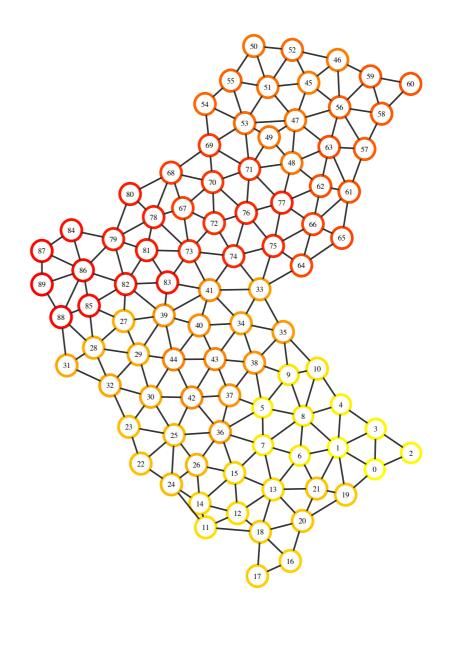




# Inferring the spatial placement

- Graph layout algorithms
  - Force-based layout to reduce the total energy in the system
- Use the graphviz library to obtain coordinates of the nodes









### With coordinate information

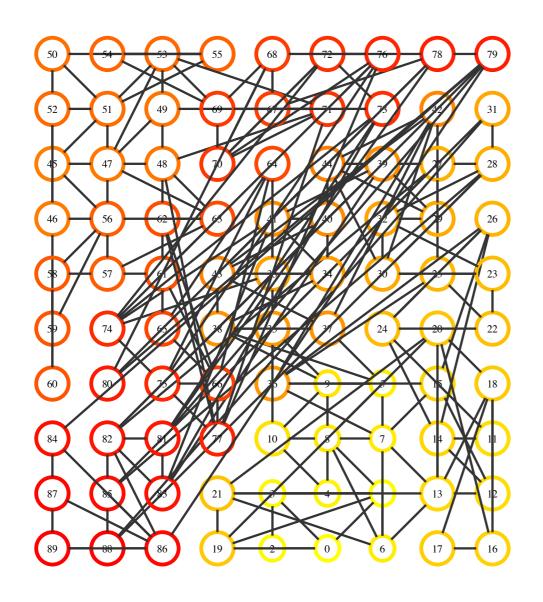
#### Affine Mapping (AFFN)

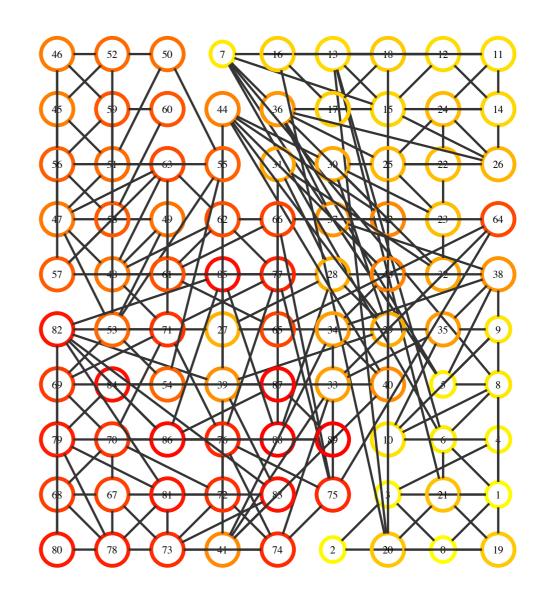
- Stretch/shrink the object graph (based on coordinates of nodes) to map it on to the processor grid
- In case of conflicts for the same processor, spiral around that processor
- Corners to Center (COCE)
  - Use four corners of the object graph based on coordinates
  - Start mapping simultaneously from all sides
    - Place nodes encountered during a BFT close to their parents





## Mapping visualization





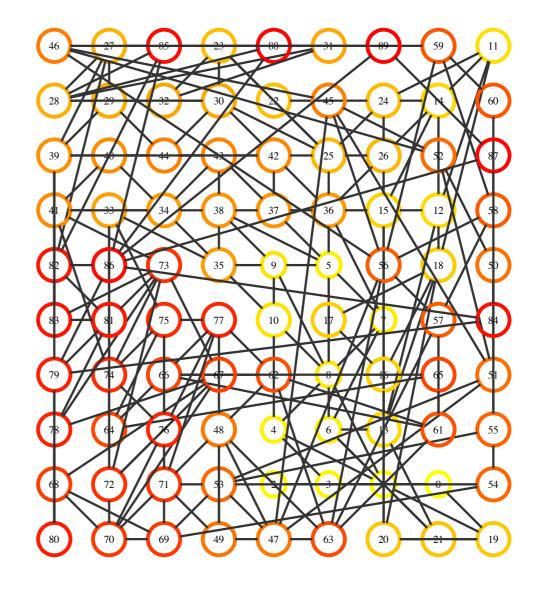


**COCE: 2.88** 



#### • COCE+MHT Hybrid:

- We fix four nodes at geometric corners of the mesh to four processors in 2D
- Put neighbors of these nodes into a max heap
- Map from all sides inwards
  - Starting from centroid of mapped neighbors



**COCE: 2.78** 





# Time Complexity



### Time Complexity

- All algorithms discussed above choose a desired processor and spiral around it to find the nearest available processor
  - Heuristics generally applicable to any topology

## Time Complexity

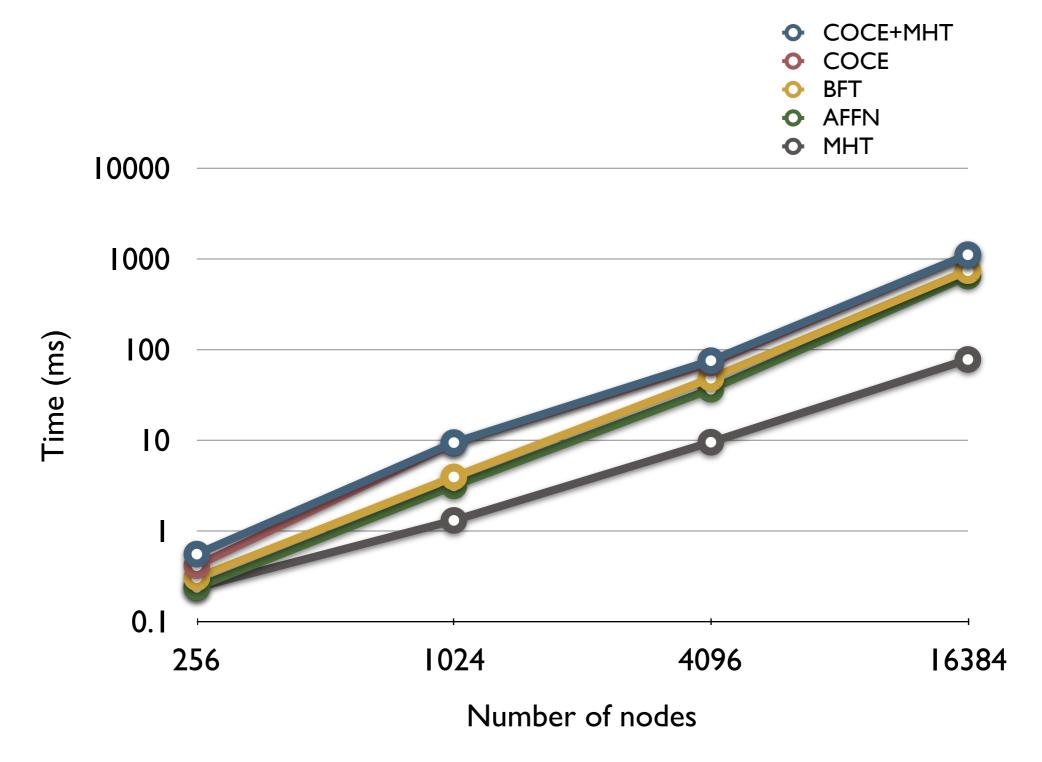
- All algorithms discussed above choose a desired processor and spiral around it to find the nearest available processor
  - Heuristics generally applicable to any topology
- Depending on the running time of findNext:

BFT	COCE	AFFN	MHT	COCE+MHT
O(n)	O(n)	O(n)	O(n logn)	O(n logn)
O(n (logn) <sup>2</sup> )				





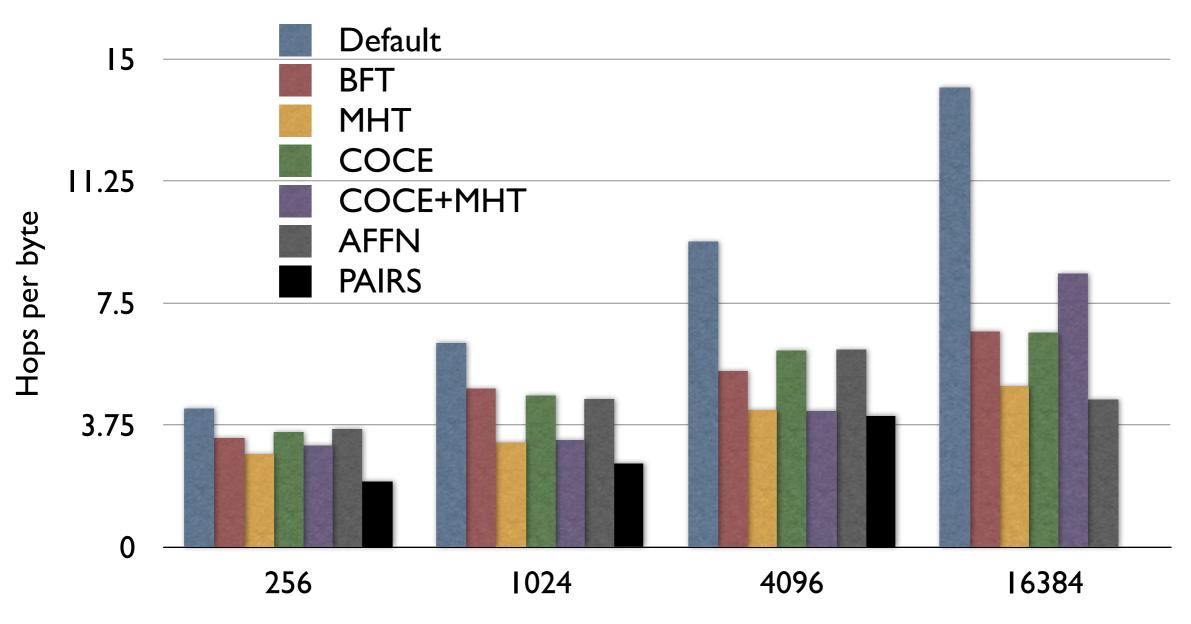
# Running Time







### Results: simple2D







### Summary

- Contention in modern day supercomputers can impact performance: makes mapping important
- Certain classes of applications (latency sensitive, communication bound) benefit most
  - OpenAtom shows performance improvements of up to 50%
  - NAMD improvements for > 4k cores
- Developing an automatic mapping framework
  - Relieve the application developer of the mapping burden



### Summary

- Topology discovery: Topology Manager API
- Object Communication Graph: Profiling, Instrumentation
- Pattern matching
  - Regular graphs
  - Irregular graphs
- Suite of heuristics for mapping
- Distributed strategies with global view



#### Future Work

- More sophisticated algorithms for pattern matching and mapping
  - Multicast and many-to-many patterns
- Handling multiple communication graphs
  - Simultaneous or occurring in different phases
- Extension of the work on distributed load balancing



### Thanks

Abhinav Bhatele. Automating Topology Aware Mapping for Supercomputers, PhD Thesis, Department of Computer Science, University of Illinois. <a href="http://hdl.handle.net/2142/16578">http://hdl.handle.net/2142/16578</a>

Charm++ Tutorial
Computer Network Information Center,
Chinese Academy of Sciences

