Lecture 28: Process Topology and MPI

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Virtual and Physical Topologies

- A *virtual topology* represents the way that MPI processes communicate
  - Nearest neighbor exchange in a mesh
  - Recursive doubling in an all-to-all exchange
- A *physical topology* represents that connections between the cores, chips, and nodes in the hardware

Virtual and Physical Topologies

- Issue is mapping of the virtual topology onto the physical topology
  - ♦ Hierarchical systems (e.g., nodes of chips of cores) makes this more complicated; no simple topology
- Questions to ask
  - ♦ Does it really matter what mapping is used?
  - ♦ How does one get a good mapping?
  - ♦ How bad can a bad mapping be?
  - ♦ What if the mapping is random?
- This lecture is about using MPI to work with virtual topologies and make it possible for the MPI implementation to provide a good mapping

MPI's Topology Routines

- MPI provides routines to create new communicators that order the process ranks in a way that *may* be a better match for the *physical topology*
- Two types of virtual topology supported:
  - Cartesian (regular mesh)
  - Graph (several ways to define in MPI)
- Additional routines provide access to the defined virtual topology
- (Virtual) topologies are properties of a communicator
  - Topology routines all create a *new* communicator with properties of the specified virtual topology

MPI Cartesian Topology

- Create a new virtual topology using
  - MPI_Cart_create
- Determine "good" sizes of mesh with
  - MPI_Dims_create

MPI_Cart_create

- MPI_Cart_create(MPI_Comm oldcomm,
  int ndim, int dims[], int qperiodic[],
  int qreorder,
  MPI_Comm *newcomm)
  - Creates a new communicator **newcomm** from **oldcomm**, that represents an **ndim** dimensional mesh with sizes **dims**. The mesh is periodic in coordinate direction i if **qperiodic[i]** is true. The ranks in the new communicator are reordered (to better match the physical topology) if **qreorder** is true

MPI_Dims_create

- MPI_Dims_create(int nnodes,
  int ndim, int dims[])
- Fill in the **dims** array such that the product of **dims[i]** for i=0 to **ndim**-1 equals **nnodes**.
- Any value of **dims[i]** that is 0 on input will be replaced; values that are > 0 will not be changed

MPI_Cart_create Example

- ```
  int periods[3] = {1,1,1};
  int dims[3] = {0,0,0}, wsize;
  MPI_Comm cartcomm;

  MPI_Comm_size(MPI_COMM_WORLD, &wsize);
  MPI_Dims_create(wsize, 3, dims);
  MPI_Cart_create(MPI_COMM_WORLD, 3, dims,
                  periods, 1, &cartcomm);
  ```

- Creates a new communicator **cartcomm** that *may* be efficiently mapped to the physical topology
  ```

Information About a Cartesian Topology

- MPI_Cartdim_get
  - Dimension of Cartesian mesh (**ndim**)
- MPI_Cart_get
  - Size of dimensions (**dims**), periodic dimensions (**qperiodic**), coordinates of calling process in mesh

Determine Neighbor Ranks

- Can be computed from rank (in the cartcomm), dims, and periods, since ordering defined in MPI
  - ♦ See Section 7.5 in MPI-3 Standard
- Easier to use either
  - ♦ MPI_Cart_coords, MPI_Cart_rank
  - ♦ MPI_Cart_shift

MPI_Cart_shift

- MPI_Cart_shift(MPI_Comm comm,
  int direction, int disp,
  int *rank_source, int *rank_dest)
- Returns the ranks of the processes that are a shift of **disp** steps in coordinate **direction**
- Useful for nearest neighbor communication in the coordinate directions
  - ♦ Use MPI_Cart_coords, MPI_Cart_rank for more general patterns

MPI Graph Topology

- MPI provides routines to specify a general graph virtual topology
  - Graph vertices represent MPI processes (usually one per process)
  - Graph edges indicate important connections (e.g., nontrivial communication between the connected processes)
  - Edge weights provide more information (e.g., amount of communication)

MPI_Dist_graph_create_adjacent

- MPI_Dist_graph_create_adjacent(MPI_Comm oldcomm,
  int indegree, int sources[], int sourceweights[],
  int outdegree, int dests[], int destweights[],
  MPI_Info info, int qreorder,
  MPI_Comm *newcomm)
- Describe *only* the graph vertex corresponding to the calling process
  - Hence "Dist_graph" – distributed description of graph
- Graph is directed – separate in and out edges
- **info** allows additional, implementation-specific information
- **qreorder** if true lets MPI implementation reorder ranks for a better mapping to physical topology
- **MPI_UNWEIGHTED** may be used for weights *arrays*

Other Graph Routines

- MPI_Dist_graph_create
  - More general, allows multiple graph vertices per process
- Information on graph
  - MPI_Dist_graph_neighbors_count, MPI_Dist_graph_neighbors

Some Results (Good and Bad)

- A common virtual topology is *nearest neighbor in a mesh*
  - Matrix computations
  - PDE Simulations on regular computational grids
- Many Large Scale Systems use a mesh as the physical topology
  - IBM Blue Gene series; Cray through XE6/XK7
- Performance can depend on how well the virtual topology is mapped onto the physical topology

Why Mesh Networks?

- Pros:
  - Scaling cost of adding a node is constant
  - Nearest neighbor bandwidth proportional to the number of nodes (thus scales perfectly as well)
  - Cabling relatively simple
- Cons:
  - Bisection bandwidth does *not* scale with network size
    - For 3D mesh, scales as $n^2/n^3 = n^{2/3}$ for nxnxn mesh
  - Non-nearest neighbor communication suffers from contention

Mesh Performance Limits

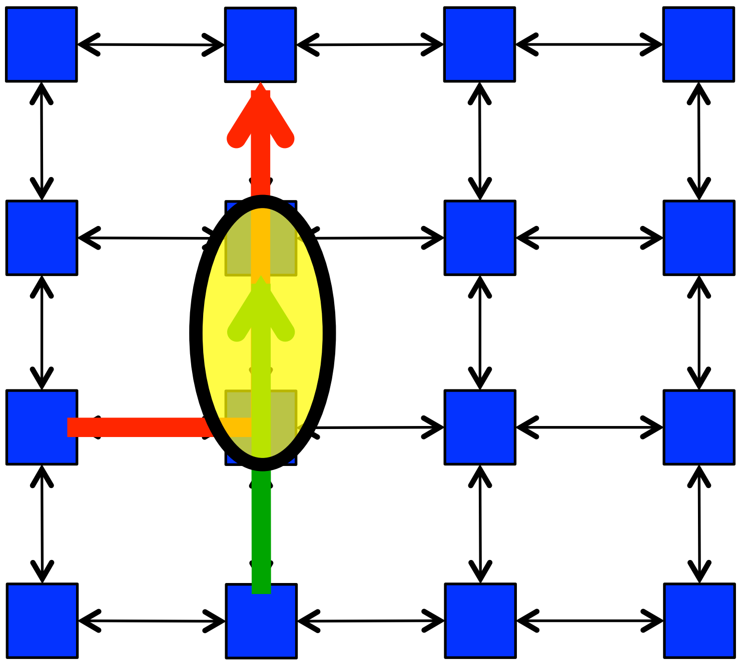
- What is the maximum aggregate bandwidth of an n x n x n mesh, assuming:
  - ♦ Each interior node sends at bandwidth L to each of its 6 neighbors (±x,±y,±z direction)
  - ♦ Edge nodes send to their immediate neighbors
- What is the bisection bandwidth of this network (simple cut along any coordinate plane)?

Mesh Performance

- Aggregate bandwidth
  - Simple, overestimate: n^3 nodes * 6 links/node * L bytes/sec/link = $6Ln^3$ bytes/sec
  - More accurate
    - $6L(n-2)^3 + 6(n-2)^2 5L + 12(n-2)4L + 8(1)3L$
    - i.e., Interior + 6 faces + 12 edges + 8 corners
- Bisection Bandwidth
  - Ln^2
- Note: Nearest neighbor bandwidth is more than n times bisection bandwidth
- For n=24, L = 2GB/sec
  - Neighbor = L*79488 = 159 TB/sec
  - Bisection = L*576 = 1.2TB/sec

Communication Cost Includes More than Latency and Bandwidth

- Communication does not happen in isolation
- Effective bandwidth on shared link is ½ point-to-point bandwidth
- Real patterns can involve many more (integer factors)
- Loosely synchronous algorithms ensure communication cost is worst case



Halo Exchange on BG/Q and Cray XE6

- 2048 doubles to each neighbor
- Rate is MB/sec (for all tables)

BG/Q	**8 Neighbors**	
	Irecv/Send	Irecv/Isend
World	662	1167
Even/Odd	711	1452
1 sender		2873

Cray XE6	**8 Neighbors**	
	Irecv/Send	Irecv/Isend
World	352	348
Even/Odd	338	324
1 sender		5507

Discovering Performance Opportunities

- Lets look at a single process sending to its neighbors.
- Based on our performance model, we *expect* the rate to be roughly twice that for the halo (since this test is only sending, not sending and receiving)

System	4 neighbors		8 Neighbors	
		Periodic		Periodic
BG/L	488	490	389	389
BG/P	1139	1136	892	892
BG/Q			2873	
XT3	1005	1007	1053	1045
XT4	1634	1620	1773	1770
XE6			5507	

Discovering Performance Opportunities

- Ratios of a single sender to all processes sending (in rate)
- *Expect* a factor of roughly 2 (since processes must also receive)

System	4 neighbors		8 Neighbors	
		Periodic		Periodic
BG/L	2.24		2.01	
BG/P	3.8		2.2	
BG/Q			1.98	
XT3	7.5	8.1	9.08	9.41
XT4	10.7	10.7	13.0	13.7
XE6			15.6	15.9

- BG gives roughly double the halo rate. XTn and XE6 are much higher.
  - It should be possible to improve the halo exchange on the XT by scheduling the communication
  - Or improving the MPI implementation

Limitations of MPI Process Topology Routines: Cartesian

- Dims_create
  - Only for MPI_COMM_WORLD; if strictly implemented, nearly useless
  - Standard defines exact output, makes this a convenience routine for computing factors of an integer. This was the wrong definition
- Cart routines
  - Can be implemented, but can be nontrivial in non-mesh network

Limitations of MPI Process Topology Routines: Graph

- Graph routines
  - ♦ Complex to implement. No good implementations in general use; research work limited
    - E.g., minimize "bandwidth" in the numerical sparse matrix sense of the connection graph. Does not minimize contention
- One-level
  - ♦ Doesn't address cores/chips, though cart/graph_map *could*

MPI's Original Graph Routines

- MPI-1 and MPI-2 contained a different set of Graph topology routines
  - These required each process to provide the *entire* graph
  - Simplifies determination of virtual to physical topology mapping
  - Sensible when maximum number of processes was < 200 (when MPI-1 created)
  - These routines are MPI_Graph_xxx
  - Do not use these in new codes

Nonstandard Interfaces

- Many systems provide ways to
  - Control mapping of processes
  - Access the mapping
- Mapping on Job Startup
  - Sometimes called allocation mapping
  - Typically specified by environment variable or command line option

Example: Blue Waters Allocation Mapping

- Environment variable
  - MPICH_RANK_REORDER_METHOD
  - Values:
    - 0 = Round robin by *node*
    - 1 = Fill each node with processes before going to next node ("SMP ordering")
    - 2 = Folded by node (0,1,2,…,q,q,q-1,…,0)
    - 3 = Read from file named MPICH_RANK_ORDER
- Mapping to cores within node controlled by –cc and –d options to aprun
- https://bluewaters.ncsa.illinois.edu/topology-considerations

Example Blue Gene/Q Allocation Mapping

- Option to runjob:
  - --mapping ABCDET
  - where order of letters indicates which torus coordinate (A-E) or process on node (T) increments (starting from the *right*)
  - Mapping with a file also possible
- http://www.redbooks.ibm.com/redbooks/pdfs/sg247948.pdf

Mapping at Runtime

- Also known as Rank Reordering
- Create a new communicator that gives each MPI process a new rank to achieve a "better" mapping from virtual to physical topology
  - This is what the MPI Topology routines do
- Requires access to the physical topology
  - No standard method, but many systems provide an API
  - Clusters may provide hwloc http://www.open-mpi.org/projects/hwloc/

Access to Mesh Topology

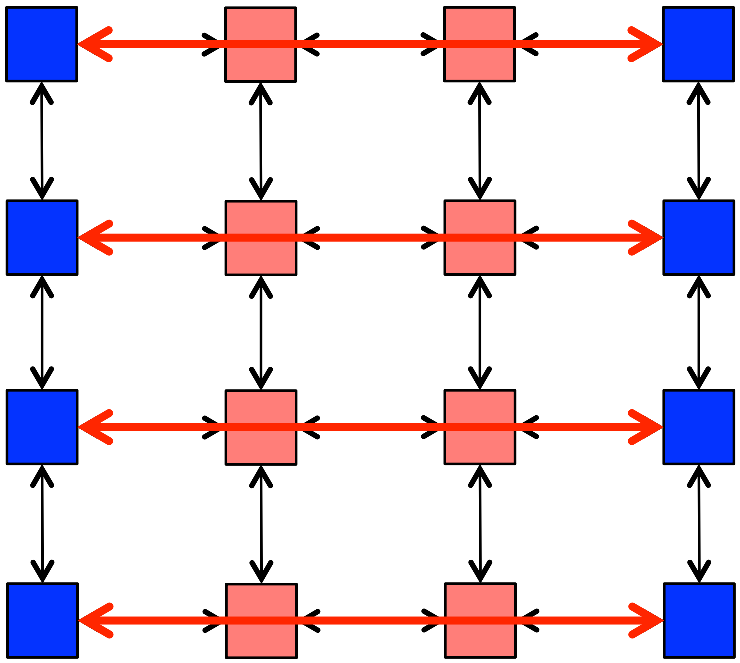
- Simple routines available for Blue Waters (Cray systems with Gemini interconnect) and IBM Blue Gene/Q
- Provides access to physical mesh coordinates as well as chip, core number within node
- Example of scalable access to regular network

Access to Mesh Topology

```
#include <stdio.h>
#include <string.h>
#include "mpi.h”
#include "topoinfo.h”
int main(int argc, char **argv)
{
topoinfo_t *topoinfo;
int  wrank, verbose=0;
char leader[10];
MPI_Init(&argc,&argv);
if (argv[1] && strcmp(argv[1],"-v") == 0) verbose = 1;
MPI_Comm_rank(MPI_COMM_WORLD,&wrank);
snprintf(leader,sizeof(leader),"%d:",wrank);
topoInit(verbose,&topoinfo);
topoPrint(stdout,leader,topoinfo);
topoFinalize(&topoinfo);
MPI_Finalize();
return 0;
}
```

Impact of Other Jobs

- Even with a perfect mapping, programs can suffer from *interference* with other jobs
- Can be reduced by *topology-aware* scheduling
- Layout of I/O nodes, adaptive routing can create contention even with topology-aware scheduling
- In this example, either the blue job or the pink job can communicate without contention, but together they share all of the “x” links in the pink job



Readings

- Generic Topology Mapping Strategies for Large-scale Parallel Architectures, Hoefler and Snir http://dx.doi.org/10.1145/1995896.1995909
- Implementing the MPI Process Topology Mechanism, Traeff http://www.computer.org/csdl/proceedings/sc/2002/1524/00/15240028-abs.html
- Avoiding Hot Spots on Two-Level Direct Networks, Bhatele, Jain, Gropp, Kale http://dl.acm.org/citation.cfm?doid=2063384.2063486