Advanced MPI

M. D. Jones, Ph.D.

Center for Computational Research
University at Buffalo
State University of New York

High Performance Computing I, 2013

The Need For Derived Datatypes

- Optimal message construction for mixed data types (our examples thus far have been of a uniform type, contiguous in memory - not exactly real world conditions).
- It might be tempting to send messages of different type separately - but that incurs considerable overhead (especially for small messages) leading to inefficient message passing.
- Type casting or conversion is hazardous, and best avoided.

Derived Datatypes

A derived datatype consists of two things:

- A sequence of primitive types
- A sequence of integer (byte) displacements, **not** necessarily positive, distinct, or ordered.

The **type map** is this pair of sequences,

$$\text{typemap} = \{(\text{type}_0, \text{disp}_0), (\text{type}_1, \text{disp}_1), \ldots, (\text{type}_{N-1}, \text{disp}_{N-1})\}, \quad (1)$$

with the **type signature** being the sequence of primitive types

$$\text{typesig} = \{\text{type}_0, \text{type}_1, \ldots, \text{type}_{N-1}\}, \quad (2)$$

taken together with a base memory address, the type map specifies a communication buffer.

Datatype Constructors

This is a sampling of the most-commonly used routines that are available (there are many more ...) in rough order of increasing complexity:

MPI_TYPE_DUP

```
MPI_TYPE_DUP(oldtype,newtype)
```

oldtype (IN), datatype (handle)
newtype (OUT), copy of type (handle)

- Simple duplication (more useful for library writers)

MPI_TYPE_CONTIGUOUS

```
MPI_TYPE_CONTIGUOUS(count,oldtype,newtype)
```

- **count** (IN), replication count (int)
- **oldtype** (IN), old datatype (handle)
- **newtype** (OUT), new datatype (handle)

- duplication and replication (by concatenation) of datatypes.

MPI_TYPE_VECTOR

```
MPI_TYPE_VECTOR(count,blocklen,stride,oldtype,
                newtype)
```

- **count** (IN), number of blocks (int)
- **blocklen** (IN), number elements in each block (int)
- **stride** (IN), spacing (in elements) between start of each block (int)
- **oldtype** (IN), old datatype (handle)
- **newtype** (OUT), new datatype (handle)

- Replication of datatype into equally spaced (equal stride = extent of oldtype) blocks

MPI_TYPE_CREATE_HVECTOR

```
MPI_TYPE_CREATE_HVECTOR(count,blocklen,stride,
            oldtype,newtype)
```

- **count** (IN), number of blocks (int)
- **blocklen** (IN), number elements in each block (int)
- **stride** (IN), spacing (in bytes) between start of each block (int)
- **oldtype** (IN), old datatype (handle)
- **newtype** (OUT), new datatype (handle)

- replicate a datatype into equally spaced locations, separated by byte stride (bytes for HVECTOR, extents of the old datatype for VECTOR).

MPI_TYPE_INDEXED

```
MPI_TYPE_INDEXED(count,array_blocklen,
          array_disp,oldtype,newtype)
```

- **count** (IN), number of blocks (int)
- **array_blocklen** (IN), number of elements per block (int array)
- **array_disp** (IN), displacements (in elements) for each block (int array)
- **oldtype** (IN), old datatype (handle)
- **newtype** (OLD), new datatype (handle)

- Indexed allows the user to specify a noncontiguous data layout where separations between blocks is not the same (unequal strides).

MPI_TYPE_CREATE_STRUCT

```
MPI_TYPE_CREATE_STRUCT(count,array_blocklen,
      array_disp, array_type,newtype)
```

- **count** (IN), number of blocks (int)
- **array_blocklen** (IN), number of elements per block (int array)
- **array_disp** (IN), displacements (in elements) for each block (int array)
- **array_type** (IN), type of elements in each block (handle array)
- **newtype** (OUT), new datatype (handle)

- the most general type constructor, allowing each block to consist of replications of different datatypes

... and many more ... `MPI_TYPE_CREATE_INDEXED_BLOCK` (constant blocksize, arbitrary displacements), `MPI_TYPE_CREATE_HINDEXED`(block displacements specified in Bytes) ... ...

Datatype Accessors

Routines to determine information on derived datatypes (they will work on predefined datatypes as well, of course):

MPI_TYPE_GET_EXTENT

```
MPI_TYPE_GET_EXTENT(datatype, lb, extent)
```

- **datatype** (IN), datatype on which to return info (handle)
- **lb** (OUT), lower bound of datatype (int)
- **extent** (OUT), extent of datatype (int)

- “size” of the datatype, i.e. use `MPI_TYPE_GET_EXTENT` for MPI types, rather than C’s `sizeof(datatype)`

MPI_TYPE_SIZE

```
MPI_TYPE_SIZE(datatype, size)
```

- **datatype** (IN), datatype on which to return info (handle)
- **size** (OUT), datatype siz, in bytes (int)

- total size, in Bytes, of entries in datatype signature

Committed Datatypes

A derived datatype must be **committed** before use, once committed, a derived datatype can be used as input for further datatype construction.

MPI_COMMIT

`MPI_COMMIT(datatype)`

datatype (INOUT), datatype to be committed (handle)

and a routine to free up a datatype object:

MPI_TYPE_FREE

`MPI_TYPE_FREE(datatype)`

datatype (INOUT), datatype to be freed (handle)

and there are routines for greater control (and more complexity) ...
`MPI_GET_ADDRESS` (find the address of a location in memory),
`MPI_GET_ELEMENTS` (number of primitive elements received),
`MPI_TYPE_CREATE_RESIZED` (the ability to resize an existing user defined datatype),
`MPI_TYPE_GET_TRUE_EXTENT` (overlook “artificial” extents)...

A Derived Datatype Example

```c
double a[100][100]; /* matrix, order 100 */
int disp[100],blocklen[100],i,dest,tag;
MPI_Datatype upperTri; /* upper triangular part of the matrix */
...
for (i=0,i<=99;i++) {
  disp[i] = 100*i+i;
  blocklen[i] = 100-i;
}
MPI_Type_indexed(100,blocklen,disp,MPI_DOUBLE,&upperTri); /* create datatype */
MPI_Type_commit(&upperTri);
MPI_Send(a,1,upperTri,dest,tag,MPI_COMM_WORLD);
```

- A handle to a derived datatype can appear in sends/receives (including collective ops).
- Note that the predefined MPI datatypes are just special cases of a derived datatype. For example, `MPI_FLOAT` is a predefined handle to a datatype with type map $\{(\text{float}, 0)\}$.

Packing it In

MPI_PACK

```
MPI_PACK(in_buffer,in_count,datatype,
         out_buffer,out_size,pos,comm)
```

in_buffer (IN), input buffer (choice)
in_count (IN), number of input components (int)
datatype (IN), datatype of each input component (handle)
out_buffer (OUT), output buffer (choice)
out_size (IN), output buffer size, in bytes (int)
pos (INOUT), current positionin buffer, in bytes (int)
comm (IN), communicator for packed messages (handle)

MPI_UNPACK

`MPI_UNPACK(in_buffer,in_size,pos,out_buffer, out_count,datatype,comm)`

- in_buffer (IN), input buffer (choice)
- in_size (IN), input buffer size, in bytes (int)
- pos (INOUT), current position in buffer, in bytes (int)
- out_buffer (OUT), output buffer (choice)
- out_count (IN), number of components to unpack (int)
- datatype (IN), datatype of each input component (handle)
- comm (IN), communicator for packed messages (handle)

These routines (`MPI_PACK, MPI_UNPACK`) allow you to fill a buffer with non-contiguous data in a streamlined fashion - the following routine will tell you how much space the message will occupy, if you want to manage your buffers:

MPI_PACK_SIZE

`MPI_PACK_SIZE(in_count, datatype, comm, size)`

- in_count (IN), count argument to packing call (int)
- datatype (IN), datatype argument to packing call (handle)
- comm (IN), communicator argument to packing call (handle)
- size (OUT), upper bound on size of packed message, in bytes (int)

The data format used for packed data is implementation dependent.

An Example of Message Packing

```
int my_i,pos=0;
char a[100],buff[110];
MPI_Status status;
...
if (myrank == 0) {
  MPI_Pack(&my_i,1,MPI_INT,buff,110,&pos,MPI_COMM_WORLD);
  MPI_Pack(a,100,MPI_CHAR,buff,110,&pos,MPI_COMM_WORLD);
  MPI_Send(buff,pos,MPI_PACKED,1,0,MPI_COMM_WORLD);
}
else {
  MPI_Recv(buff,110,MPI_PACKED,1,0,MPI_COMM_WORLD,&status);
  MPI_Unpack(buff,110,&pos,&my_i,1,MPI_INT,MPI_COMM_WORLD);
  MPI_Unpack(buff,110,&pos,a,100,MPI_CHAR,MPI_COMM_WORLD);
}
...
```


Derived Datatypes vs. Pack/Unpack

- The data format used for packed data is implementation dependent.
- Messages are the same size
- May take longer to access non-contiguous memory of derived types
- Packing executes a function call for each packed item, and possibly additional memory-to-memory copies (packing has to copy the data, derived types need to store the layout). Most implementations can expect better performance from derived types.

MPI Communicators

- Provides a separate communication space, especially useful for libraries and modules (can use their own numbering scheme).
- If you are uncomfortable dealing with multiple spaces for communications, just use a single one - the pre-defined `MPI_COMM_WORLD`.

- Two types of communicators:
  1. **intra-communicator** - for comms within a group of processes. Can also have a topology describing the process layout.
  2. **inter-communicator** - for comms between two disjoint groups of processes. No topology.

Functionality	Intra-	Inter-
Number of groups involved	1	2
Communication Safety	Y	Y
Collective Ops	Y	Y(MPI-2)
Topologies	Y	N
Caching	Y	Y

More Communication Domains

- You can think of a communicator as an array of links to other communicators.
- Each intra-group communication domain consists of a set of communicators such that:
  - the links form a complete graph in which each communicator is linked to all communicators in the set (including itself)
  - the links have consistent indices, for each communicator the i-th link points to the communicator for process i.
- Each process holds a complete list of group members - not necessarily a scalable design.

Key Group Routines

MPI_COMM_GROUP

`MPI_COMM_GROUP(comm,group)`

comm (IN), communicator (handle)

group (OUT), group corresponding to comm (handle)

- obtain the group handle for a given communicator - new groups have to be built from old ones (they can not be built from scratch)
- returned handle can then be used as input to `MPI_GROUP_INCL`, `MPI_COMM_CREATE`, `MPI_GROUP_RANK`.

MPI_GROUP_INCL

`MPI_GROUP_INCL(group, n, ranks, newgroup)`

- **group** (IN), group (handle)
- **n** (IN), number of elements in array ranks (and size of newgroup) (int)
- **ranks** (IN), ranks of processes in group to appear in newgroup (int array)
- **newgroup** (OUT), new group derived from input, in order defined by ranks (handle)

- creates a new group whose i-th process had ranks[i] in the old group
- n=0 results in newgroup having the value `MPI_GROUP_EMPTY`.

MPI_GROUP_EXCL

`MPI_GROUP_EXCL(group, n, ranks, newgroup)`

- **group** (IN), group (handle)
- **n** (IN), number of elements in array ranks (and size of newgroup) (int)
- **ranks** (IN), ranks of processes in group to appear in newgroup (int array)
- **newgroup** (OUT), new group derived from input, in order defined by ranks (handle)

- newgroup created from group by deleting processes with ranks ranks[0]...ranks[n-1]
- n=0 newgroup is identical to group

MPI_GROUP_RANK

`MPI_GROUP_RANK(group,rank)`

- **group** IN, group (handle)
- **rank** OUT, rank of the calling process in group (int)

- returns the rank of the calling process in group
- if calling process is not a member of group, `MPI_UNDEFINED` is returned.

MPI_GROUP_SIZE

`MPI_GROUP_SIZE(group,size)`

- **group** (IN), group (handle)
- **size** (OUT), number of processes in group (int)

MPI_GROUP_FREE

`MPI_GROUP_FREE(group)`

- **group** (INOUT), group (handle)

- mark group fro deallocation
- handle group is set to `MPI_GROUP_NULL`

Key Communicator Routines

MPI_COMM_CREATE

`MPI_COMM_CREATE(comm,group,newcomm)`

- **comm** (IN), communicator (handle)
- **group** (IN), group, a subset of the group of comm
- **newcomm** (OUT), new communicator (handle)

- must be executed by all processes in comm
- returns `MPI_COMM_NULL` to processes not in group

Our old friend, but in a new context ...

MPI_COMM_RANK

`MPI_COMM_RANK(comm, rank)`

- **comm** (IN), communicator (handle)
- **rank** (OUT), rank of the calling process in group of comm (int)

- if comm is an intra-communicator, rank is the rank of the calling process
- rank is relative to the group associated with comm

Primary API call for forming new communicators:

MPI_COMM_SPLIT

`MPI_COMM_SPLIT(comm, color, key, newcomm)`

- **comm** (IN), communicator (handle)
- **color** (IN), control of subset assignment (int)
- **key** (IN), control of rank assignment (int)
- **newcomm** (OUT), new communicator (handle)

`MPI_COMM_SPLIT(comm, color, key, newcomm):`

- partitions group associated with comm into disjoint subgroups, one for each value of color.
- a collective call, but each process can provide its own color and key
- a color of `MPI_UNDEFINED` results in a newcomm of `MPI_COMM_NULL`
- for same key values, rank in new communicator is relative to ranks in the old communicator
- a very useful call for breaking a single communicator group into a user controlled number of subgroups. Multigrid, linear algebra, etc.

Master/Worker Example Using Group/Communicator Routines

We can use the communicator and group routines to lay out a simple code for performing master/worker tasks:

- Master is process zero, rest are workers
- Create a group of workers by eliminating server process
- Create communicator for workers
- Master/worker task code


```c
int ServerTask, myRank, myWorkerRank;
MPI_Comm comm_workers;
MPI_Group group_world, group_workers;

MPI_Comm_rank(MPI_COMM_WORLD, &myRank);

ServerTask = 0;
MPI_Comm_group(MPI_COMM_WORLD, &group_world);
MPI_Group_excl(group_world, 1, ServerTask, &group_workers);
MPI_Comm_create(MPI_COMM_WORLD, &group_workers, &comm_workers);
MPI_Group_free(&group_workers);    /* if no longer needed */

if (myRank == ServerTask) {
    RunServer();
} else {
    MPI_Comm_rank(comm_workers, &myWorkerRank);
    WorkerBees();
}
...
```


Virtual Topologies

- An extra, optional attribute for an intra-communicator
- Convenient naming mechanism for processes in a group
- Many applications can benefit from a 2d or 3d topological communication pattern
- Possible mapping of runtime processes to available hardware
- “Virtual” topology is all that we will discuss - machine independent
- Two main topology types in MPI - Cartesian (grid) and graphs - while graphs are the more general case, majority of applications use regular grids

Topology Benefits

Key benefits of MPI topologies:

- Applications have specific communication patterns (e.g. a 2D Cartesian topology suits 4-way nearest neighbor communications)
- Topologies are advisory to the implementation - topological aspects of the underlying hardware may offer performance advantages to various communication topologies

Key Topology Routines

MPI_CART_CREATE

`MPI_CART_CREATE(comm_old,ndims,dims,periods,`
`                reorder,comm_cart)`

- **comm_old** (IN), input communicator (handle)
- **ndims** (IN), dimensions in Cartesian grid (int)
- **dims** (IN), processes in each dimension (int array)
- **periods** (IN), periodic (true) in each dim (logical array)
- **reorder** (IN), ranks may be reordered (true) or not (logical)
- **comm_cart** (OUT), comm. with new topology (handle)

- Must be called by all processes in the group, extras will end up with `MPI_COMM_NULL`.

MPI_CART_COORDS

`MPI_CART_COORDS(comm,rank,maxdims,coords)`

- **comm** (IN), communicator with Cartesian structure (handle)
- **rank** (IN), rank of a process within group comm (int)
- **maxdims** (IN), length of vector coord in the calling program (int)
- **coords** (OUT), array containing Cartesian coordinates of specified process (int array)

- rank to coordinates translator (the inverse of `MPI_CART_RANK`)

MPI_CART_RANK

`MPI_CART_RANK(comm,coords,rank)`

- **comm** (IN), communicator with Cartesian structure (handle)
- **coords** (IN), specifies the Cartesian coordinates of a process (int array)
- **rank** (OUT), rank of specified process (int)

- coordinates to rank translator (the inverse of `MPI_CART_COORDS`).

MPI_CART_SUB

`MPI_CART_SUB(comm,remain_dims,newcomm)`

- **comm** (IN), communicator with Cartesian structure (handle)
- **remain_dims** (IN), i-th entry = true, then i-th dimension is kept in the subgrid (array of logicals)
- **newcomm** (OUT), communicator containing subgrid that includes calling process (handle)

- A collective routine to be called by all processes in comm
- Partitions communicator group into subgroups that form lower dimensional Cartesian subgrids

MPI_CARTDIM_GET

`MPI_CARTDIM_GET(comm,ndims)`

- **comm** (IN), communicator with Cartesian structure (handle)
- **ndims** (OUT), number of dimensions of the structure (int)

MPI_CART_GET

`MPI_CART_GET(comm,maxdims,dims,periods,coords)`

- **comm** (IN), communicator with Cartesian structure (handle)
- **maxdims** (IN), length of vector dims, periods, coords in calling program (int)
- **dims** (OUT), number processes in each Cartesian dim (int array)
- **periods** (OUT), periodicity in each dim (logical array)
- **coords** (OUT), coordinates of calling process in structure (int array)

MPI_CART_SHIFT

```
MPI_CART_SHIFT(comm,direction,displ,
          rank_source,rank_dest)
```

- **comm** (IN), communicator with Cartesian structure (handle)
- **direction** (IN), coordinate dimensions of shift (int)
- **displ** (IN), displacement (>0 for up, <0 down) (int)
- **rank_source** (OUT), rank of source process (int)
- **rank_dest** (OUT), rank of destination process (int)

- direction has range [0,..,ndim-1] (e.g. for 3D from 0 to 2)
- if destination is out of bound, a negative value is returned (`MPI_UNDEFINED`), which implies no periodicity in that direction.

Cartesian Topology Example

Simple example to illustrate Cartesian topology:

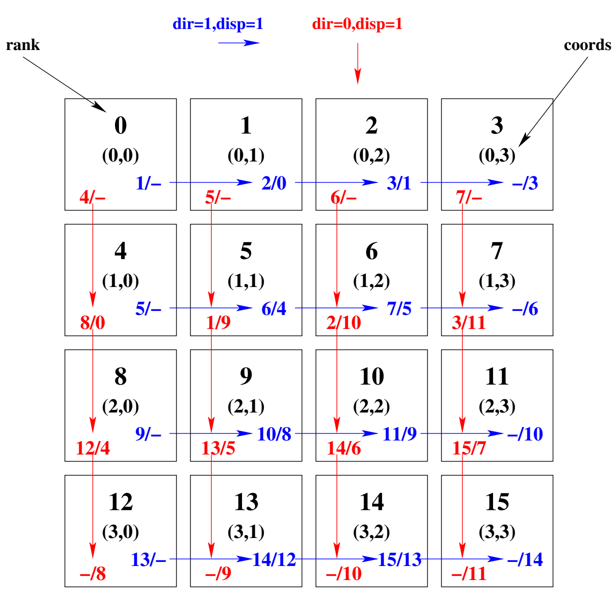
- Construct a 2D, 4x4 grid
- Treat without periodic boundaries (e.g. as a domain decomposition with fixed boundaries)
- Construct list of `SENDRECV` pairs for each process in the grid

```c
#include "mpi.h"
#include <stdio.h>
#define SIZE 16
#define UP     0
#define DOWN   1
#define LEFT   2
#define RIGHT  3

int main(int argc,char **argv)
{
   int numtasks, rank, source, dest, outbuf, i, tag=1,
      inbuf[4]={MPI_PROC_NULL,MPI_PROC_NULL,MPI_PROC_NULL,MPI_PROC_NULL,},
      nbrs[4], dims[2]={4,4},
      periods[2]={0,0}, reorder=0, coords[2];    /* not periodic, no reordering */

   MPI_Request reqs[8];
   MPI_Status stats[8];
   MPI_Comm cartcomm;

   MPI_Init(&argc,&argv);
   MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

   if (numtasks == SIZE) {
      MPI_Cart_create(MPI_COMM_WORLD, 2, dims, periods, reorder, &cartcomm);
      MPI_Comm_rank(cartcomm, &rank);
      MPI_Cart_coords(cartcomm, rank, 2, coords);
      MPI_Cart_shift(cartcomm, 0, 1, &nbrs[UP], &nbrs[DOWN]);     /* s/r +1 shift in rows */
      MPI_Cart_shift(cartcomm, 1, 1, &nbrs[LEFT], &nbrs[RIGHT]); /* s/r +1 shift in cols */
```



```c
      outbuf = rank;

      for (i=0; i<4; i++) {
        dest = nbrs[i];
        source = nbrs[i];
        MPI_Isend(&outbuf, 1, MPI_INT, dest, tag,
                  MPI_COMM_WORLD, &reqs[i]);
        MPI_Irecv(&inbuf[i], 1, MPI_INT, source, tag,
                  MPI_COMM_WORLD, &reqs[i+4]);
      }

      MPI_Waitall(8, reqs, stats);

      printf("rank= %3d coords= %3d %3d  neighbors(u,d,l,r)= %3d %3d %3d %3d\n",
             rank,coords[0],coords[1],nbrs[UP],nbrs[DOWN],nbrs[LEFT],
             nbrs[RIGHT]);
      printf("rank= %3d                   inbuf(u,d,l,r)=     %3d %3d %3d %3d\n",
             rank,inbuf[UP],inbuf[DOWN],inbuf[LEFT],inbuf[RIGHT]);
   }
   else
      printf("Must specify %d processors. Terminating.\n",SIZE);

   MPI_Finalize();
}
```


Cartesian Topology Example Illustrated



Running The Topology Example

```
[bono:~/d_mpi-samples]$ qsub -q debug -lnodes=8:ppn=2,walltime=00:15:00 -I
qsub: waiting for job 566107.bono.ccr.buffalo.edu to start
qsub: job 566107.bono.ccr.buffalo.edu ready

############################PBS Prologue############################
PBS prologue script run on host c15n28 at Tue Sep 18 13:50:40 EDT 2007
PBSTMPDIR is /scratch/566107.bono.ccr.buffalo.edu
[c15n28:~]$ cd $PBS_O_WORKDIR
[c15n28:~/d_mpi-samples]$ module load mpich/gcc-3.4.6/ch_p4/1.2.7p1
[c15n28:~/d_mpi-samples]$ mpiexec ./mpi-cart-ex
rank=  2 coords=  0  2  neighbors(u,d,l,r)=  -1   6   1   3
rank=  2                inbuf(u,d,l,r)=      -1   6   1   3
rank=  8 coords=  2  0  neighbors(u,d,l,r)=   4  12  -1   9
rank=  8                inbuf(u,d,l,r)=       4  12  -1   9
rank= 14 coords=  3  2  neighbors(u,d,l,r)=  10  -1  13  15
rank= 14                inbuf(u,d,l,r)=      10  -1  13  15
rank=  3 coords=  0  3  neighbors(u,d,l,r)=  -1   7   2  -1
rank=  3                inbuf(u,d,l,r)=      -1   7   2  -1
rank=  5 coords=  1  1  neighbors(u,d,l,r)=   1   9   4   6
rank=  5                inbuf(u,d,l,r)=       1   9   4   6
rank=  7 coords=  1  3  neighbors(u,d,l,r)=   3  11   6  -1
rank=  7                inbuf(u,d,l,r)=       3  11   6  -1
rank= 15 coords=  3  3  neighbors(u,d,l,r)=  11  -1  14  -1
rank= 15                inbuf(u,d,l,r)=      11  -1  14  -1
rank=  6 coords=  1  2  neighbors(u,d,l,r)=   2  10   5   7
rank=  6                inbuf(u,d,l,r)=       2  10   5   7
rank= 10 coords=  2  2  neighbors(u,d,l,r)=   6  14   9  11
rank= 10                inbuf(u,d,l,r)=       6  14   9  11
```

```
rank=  12  coords=   3    0   neighbors(u,d,l,r)=   8  −1   −1   13
rank=  12                     inbuf(u,d,l,r)=       8  −1   −1   13
rank=  11  coords=   2    3   neighbors(u,d,l,r)=   7  15   10   −1
rank=  11                     inbuf(u,d,l,r)=       7  15   10   −1
rank=   0  coords=   0    0   neighbors(u,d,l,r)=  −1   4   −1    1
rank=   0                     inbuf(u,d,l,r)=      −1   4   −1    1
rank=   1  coords=   0    1   neighbors(u,d,l,r)=  −1   5    0    2
rank=   1                     inbuf(u,d,l,r)=      −1   5    0    2
rank=   4  coords=   1    0   neighbors(u,d,l,r)=   0   8   −1    5
rank=   4                     inbuf(u,d,l,r)=       0   8   −1    5
rank=   9  coords=   2    1   neighbors(u,d,l,r)=   5  13    8   10
rank=   9                     inbuf(u,d,l,r)=       5  13    8   10
rank=  13  coords=   3    1   neighbors(u,d,l,r)=   9  −1   12   14
rank=  13                     inbuf(u,d,l,r)=       9  −1   12   14
```


MPI-2 Features

I will not attempt to fully cover MPI-2 extensions - in the slides that follow I will just give a broad outline of the new features:

- Dynamic process management (routines to create new processes)
- One-sided communications (put/get)
- Parallel I/O
- Additional language bindings (C++)
- Extended collective operations (non-blocking, inter-communicator)

Dynamic Process Management

- An MPI-1 application is static - no processes can be added (or removed) after it has started.
- MPI-2 introduces a spawning call for dynamic execution (can be true MPMD):

MPI_COMM_SPAWN

```
MPI_COMM_SPAWN(command,argv,maxprocs,info,root,
               comm,intercomm,array_err)
```

command	(IN), name of spawned program (string at root)
argv	(IN), arguments to command (string array)
maxprocs	(IN), maximum number processes to start (int)
info	(IN), key-value pairs where and how to start processes (handle)
root	(IN), rank of process in which previous arguments are examined (int)
comm	(IN), intra-communicator for group of spawning process (handle)
intercomm	(OUT), inter-communicator between original and new group
array_err	(OUT), one error code per process (int array)

Some Notes on MPI_COMM_SPAWN

Things to watch out for when using dynamic task management in MPI:

- Not supported in all implementations
- The attribute MPI_UNIVERSE_SIZE of MPI_COMM_WORLD gives a useful upper limit on the number of tasks (query using MPI_Comm_get_attr)
- Interaction with runtime system generally not visible to application, and not specified by MPI standard
- Static view in which all processes are started at once is still preferred method (for performance if not simplicity) - of course that obviates the dynamical picture completely!
- "Supported" by a lot of MPI implementations, but in practice has always been more than a little disappointing

One-sided Communication

- extends communication mechanisms of MPI through **RMA** (Remote Memory Access).
- three communication calls:
  - MPI_PUT remote write
  - MPI_GET remote read
  - MPI_ACCUMULATE remote update
- does **not** provide a shared memory programming model or support for direct shared-memory programming.
- Uses memory *windows* and all RMA communications are non-blocking.

One-sided Communication Semantics

RMA (remote memory access) in MPI uses a fundamental model:

1. Globally initialize an RMA window (MPI_Win_create)
2. Start an RMA synchronization (several options)
3. Perform communications
4. Stop RMA synchronization
5. Free window and anything associated (MPI_Win_free)

MPI One-sided Synchronization

Three methods in MPI for one-sided synchronization:

1. **Fence**, simplest method, start and end use MPI_Win_fence to bracket the RMA (somewhat similar to blocking calls in point-to-point)
2. **Post-Start-Complete-Wait**, target process uses MPI_Win_post and MPI_Win_wait, calling process uses MPI_Win_start and MPI_Win_complete to bracket the RMA calls (very similar to non-blocking in point-to-point, lots of calls can share the *exposed* chunk of memory). Takes an extra argument of type MPI_Group to specify the group of participating processes.
3. **Lock-Unlock**, similar to mutex in thread-based methods, uses MPI_Win_lock and MPI_Win_unlock, and MPI_LOCK_SHARED and MPI_LOCK_EXCLUSIVE to control whether other processes may access the target RMA window

One-sided Example

```c
#include <mpi.h>
#include <math.h>
#include <stdio.h>

/* Use MPI_get to copy data from an originating process to the
   current one.  Array B is copied from process Np-myid-1 to
   array A on process myid */

int main(int argc, char* argv[])
{
  int np, ierr, myid, idtarget, j, ne=2;
  int sizeofint;
  MPI_Win win;
  MPI_Comm comm;
  int B[ne], A[ne];

  /* Starts MPI processes ... */

  comm = MPI_COMM_WORLD;
  MPI_Init(&argc,&argv);        /* start MPI */
  MPI_Comm_rank(comm, &myid);   /* get current process id */
  MPI_Comm_size(comm, &np);     /* get number of processes */

  if (myid == 0 ) {
    printf(" myid   jid      B         A\n");
  }
  MPI_Barrier(comm);
```



```c
  MPI_Type_size(MPI_INT, &sizeofint);  /* create RMA window, win */
  MPI_Win_create(B, ne*sizeofint, sizeofint,MPI_INFO_NULL, comm, &win);

  MPI_Win_fence(0, win); /* sync on win */

  for (j=0; j<ne; j++) { /* Initialize B */
    B[j] = 10*(myid+1) + j + 1;
  }

  MPI_Barrier(comm);
  idtarget = np - myid -1;
  MPI_Get(A, ne, MPI_INT, idtarget, 0, ne, MPI_INT, win);

  MPI_Win_fence(0, win); /* sync on win */

  printf("%5d %5d", myid, idtarget);
  for (j=0; j<ne; j++) {
    printf("%5d", B[j]);
  }
  for (j=0; j<ne; j++) { /* Spit out A */
    printf("%5d", A[j]);
  }
  printf("\n");

  MPI_Win_free( &win);    /* Free RMA window */
  MPI_Finalize();
}
```


MPI I/O

- a programming interface for I/O
- parallel in the sense of I/O performed by a parallel application, but *cooperative* also, in the sense that many processes concurrently access a single file.
- does **not** specify a filesystem, should be able to interact with a variety of filesystems.
- provides support for asynchronous I/O, strided access, and control over physical file layout on storage devices.
- parallel I/O is a rich topic in its own right, so we will come back to talk about MPI-I/O later in a larger context.

MPI I/O Example

```c
#include "mpi.h"
#include <stdio.h>
#include <string.h>
#include <stdlib.h>

/* A simple performance test. The file name is taken as a
   command-line argument. */

#define SIZE (1048576*4)       /* read/write size per node in bytes */

int main(int argc, char **argv)
{
    int *buf, i, j, mynod, nprocs, ntimes=5, len, err, flag;
    double stim, read_tim, write_tim, new_read_tim, new_write_tim;
    double min_read_tim=10000000.0, min_write_tim=10000000.0, read_bw, write_bw;
    MPI_File fh;
    MPI_Status status;
    char *filename;

    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
    MPI_Comm_rank(MPI_COMM_WORLD, &mynod);
```

```
/* process 0 takes the file name as a command-line argument and
   broadcasts it to other processes */
   if (!mynod) {
        i = 1;
        while ((i < argc) && strcmp("-fname", *argv)) {
            i++;
            argv++;
        }
        if (i >= argc) {
            fprintf(stderr, "\n*#  Usage: perf -fname filename\n\n");
            MPI_Abort(MPI_COMM_WORLD, 1);
        }
        argv++;
        len = strlen(*argv);
        filename = (char *) malloc(len+1);
        strcpy(filename, *argv);
        MPI_Bcast(&len, 1, MPI_INT, 0, MPI_COMM_WORLD);
        MPI_Bcast(filename, len+1, MPI_CHAR, 0, MPI_COMM_WORLD);
        fprintf(stderr, "Access size per process = %d bytes, ntimes = %d\n", SIZE, ntimes);
   }
   else {
        MPI_Bcast(&len, 1, MPI_INT, 0, MPI_COMM_WORLD);
        filename = (char *) malloc(len+1);
        MPI_Bcast(filename, len+1, MPI_CHAR, 0, MPI_COMM_WORLD);
   }


   buf = (int *) malloc(SIZE);
```



```
    for (j=0; j<ntimes; j++) {
        MPI_File_open(MPI_COMM_WORLD, filename, MPI_MODE_CREATE |
            MPI_MODE_RDWR, MPI_INFO_NULL, &fh);
        MPI_File_seek(fh, mynod*SIZE, MPI_SEEK_SET);

        MPI_Barrier(MPI_COMM_WORLD);
        stim = MPI_Wtime();
        MPI_File_write(fh, buf, SIZE, MPI_BYTE, &status);
        write_tim = MPI_Wtime() - stim;
        MPI_File_close(&fh);

        MPI_Barrier(MPI_COMM_WORLD);

        MPI_File_open(MPI_COMM_WORLD, filename, MPI_MODE_CREATE |
            MPI_MODE_RDWR, MPI_INFO_NULL, &fh);
        MPI_File_seek(fh, mynod*SIZE, MPI_SEEK_SET);
        MPI_Barrier(MPI_COMM_WORLD);
        stim = MPI_Wtime();
        MPI_File_read(fh, buf, SIZE, MPI_BYTE, &status);
        read_tim = MPI_Wtime() - stim;
        MPI_File_close(&fh);

        MPI_Allreduce(&write_tim, &new_write_tim, 1, MPI_DOUBLE, MPI_MAX,
                      MPI_COMM_WORLD);
        MPI_Allreduce(&read_tim, &new_read_tim, 1, MPI_DOUBLE, MPI_MAX,
                      MPI_COMM_WORLD);
        min_read_tim = (new_read_tim < min_read_tim) ?
            new_read_tim : min_read_tim;
        min_write_tim = (new_write_tim < min_write_tim) ?
            new_write_tim : min_write_tim;
    }
```


MPI C++ Bindings

The C++ interface for MPI consists mainly of a small set of classes with a lightweight functional interface to MPI:

- Most C++ bindings for MPI functions are member functions of MPI classes
- All MPI classes, constants, and functions are declared as part of an MPI **namespace**
- Rather than `MPI_` prefix (as for C and Fortran), MPI functions in C++ have an `MPI::` prefix

MPI namespace

An abbreviated definition of the MPI namespace:

```
namespace MPI { // MPI-1
  class Comm {...};
  class Intracomm : public Comm {...};
  class Graphcomm : public Intracomm     {...};
  class Cartcomm  : public Intracomm     {...};
  class Intercomm : public Comm          {...};
  class Datatype                         {...};
  class Errhandler                       {...};
  class Exception                        {...};
  class Group                            {...};
  class Op                               {...};
  class Request                          {...};
  class Prequest  : public Request       {...};
  class Status                           {...};
  // MPI-2
  class File                             {...};
  class Grequest  : public Request       {...};
  class Info                             {...};
  class Win                              {...};
};
```

C++ MPI Semantics

Construction/Destruction:

```
MPI::<CLASS>()
~MPI::<CLASS>()
```

Copy/Assignment

```
MPI::<CLASS>(const MPI::<CLASS>& data)
MPI::<CLASS>& MPI::<CLASS>::operator=(const MPI::<CLASS>& data)
```


C++ Data Types

MPI datatype	C++ datatype
MPI::CHAR	char
MPI::SHORT	signed short
MPI::INT	signed int
MPI::LONG	signed long
MPI::SIGNED_CHAR	signed char
MPI::UNSIGNED_CHAR	unsigned char
MPI::UNSIGNED_SHORT	unsigned short
MPI::UNSIGNED	unsigned int
MPI::UNSIGNED_LONG	unsigned long int
MPI::FLOAT	float
MPI::DOUBLE	double
MPI::LONG_DOUBLE	long double
MPI::BOOL	bool
MPI::COMPLEX	Complex<float>
MPI::DOUBLE_COMPLEX	Complex<double>
MPI::LONG_DOUBLE_COMPLEX	Complex<long double>
MPI::BYTE	
MPI::PACKED	

Considerations for C++

The C++ bindings are really just translations of the C equivalents - so why use them at all?
Answer: Do not bother using them - use the C bindings instead, or something like `boost.MPI`. It has been reported that the C++ bindings will be deprecated as of MPI-3 ...

MPI and Thread-safety

MPI implementations are by no means guaranteed to be thread-safe - the MPI standard outlines means by which implementations can be made thread-safe, but it is still left to implementors to design and build efficient thread-safe MPI libraries.

MPI-2 Thread-safety

In MPI-2 the user selects the desired level of thread-safety:

- `MPI_THREAD_SINGLE`: Each process has only a single execution thread. Non-thread-safe MPI implementations follow this model.
- `MPI_THREAD_FUNNELED`: Each process can have multiple threads, but only the thread that called `MPI_INIT` can subsequently make MPI calls.
- `MPI_THREAD_SERIALIZED`: Each process can be multithreaded, but only one thread at a time can make MPI calls.
- `MPI_THREAD_MULTIPLE`: Processes multithreaded, and multiple threads allowed to make MPI calls. An MPI implementation is fully thread-safe if it supports this mode.

The user program uses `MPI_Init_thread` to explicitly initialize and check the level of thread-safety, as we will see in the following example.

Checking Thread-safety

A short code to check MPI support for multiple threads:

```c
#include <stdio.h>
#include <mpi.h>

int main(int argc, char **argv) {
  int provided;

  /* start MPI, asking for support for multiple threads */
  MPI_Init_thread(&argc,&argv,MPI_THREAD_MULTIPLE,&provided);

  /* report what level of support is actually provided */
  if ( MPI_THREAD_SINGLE     == provided ) printf(" MPI_THREAD_SINGLE\n");
  if ( MPI_THREAD_FUNNELED   == provided ) printf(" MPI_THREAD_FUNNELED\n");
  if ( MPI_THREAD_SERIALIZED == provided ) printf(" MPI_THREAD_SERIALIZED\n");
  if ( MPI_THREAD_MULTIPLE   == provided ) printf(" MPI_THREAD_MULTIPLE\n");

  MPI_Finalize();

  return 0;
}
```

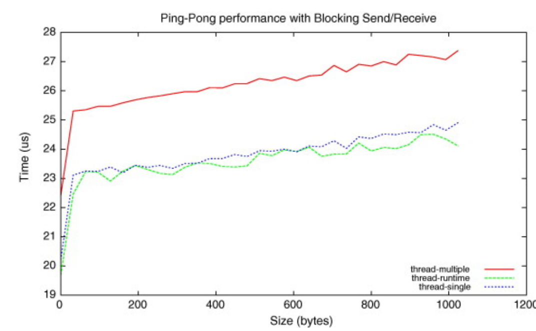

U2 Example

Note that actually using thread-safe libraries may require jumping through extra hoops:

```
[bono:~/d_mpi-samples]$ module load intel-mpi
[bono:~/d_mpi-samples]$ mpd --daemon
[bono:~/d_mpi-samples]$ mpiicc -o mpi_thread_check mpi_thread_check.c
[bono:~/d_mpi-samples]$ mpirun -np 1 ./mpi_thread_check
 MPI_THREAD_SINGLE
[bono:~/d_mpi-samples]$ mpicc -mt_mpi -o mpi_thread_check mpi_thread_check.c
[bono:~/d_mpi-samples]$ mpirun -np 1 ./mpi_thread_check
 MPI_THREAD_MULTIPLE
[bono:~/d_mpi-samples]$ mpdallexit
[bono:~/d_mpi-samples]$ module load mpich
[bono:~/d_mpi-samples]$ mpicc -o mpi_thread_check mpi_thread_check.c
[bono:~/d_mpi-samples]$ mpirun -np 1 ./mpi_thread_check
 MPI_THREAD_FUNNELED
```


MPI Thread Considerations

The following figure shows the effect of overhead for `MPI_THREAD_MULTIPLE` - tests were performed for `MPICH2` where the runtime used a full thread-safe version, and `MPI_THREAD_FUNNELED` selected during `MPI_Thread_init`:



(W. Gropp and R. Thakur, "Thread-safety in an MPI implementation: Requirements and analysis," Parallel Comp. **33**, 595-604 (2007).)

MPI-3 (upcoming) Highlights

The MPI-3 standard is out (late 2012), here are a few highlights (note that these features are not yet available in most MPI implementations):

- (deprecated) C++ bindings to be removed
- Extended nonblocking collective operations
- Extensions to one-sided operations
- Fortran 2008 bindings