Advanced MPI

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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

```
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

```c
 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

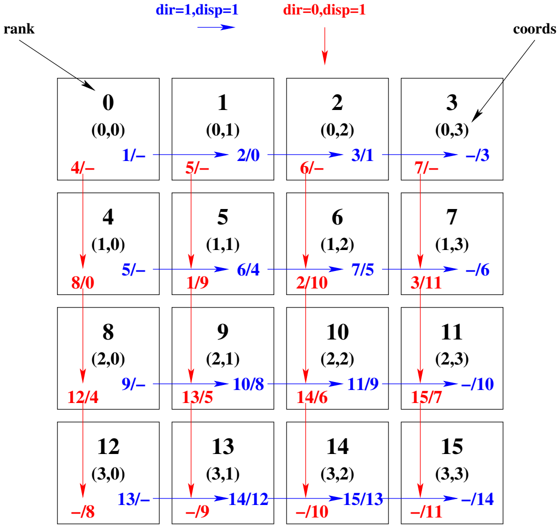
Simple example to illustrate Cartesian topology:

- 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 */
```

```
    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

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

```
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=  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=  14                  inbuf(u,d,l,r)=     10  -1  13  15
```

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

```
#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);
```

```
  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`. 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:

```
#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;
}
```

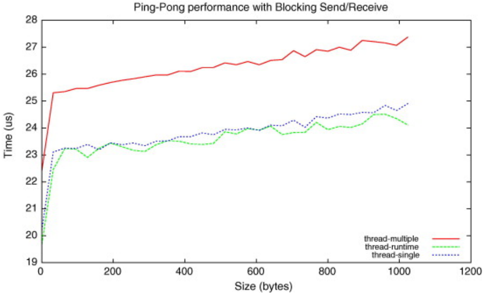
U2 Example

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

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