Joint Institute for Computational Sciences

Introduction to Parallel Programming with MPI

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Main Menu

Outline

- Message Passing Interface (MPI)
- Point to Point Communications

Thursday, 30-Jan-14

- Collective Communications
- Derived Datatypes
- Communicators and Groups
- MPI Tips and Hints

Today, 4-Feb-14

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Collective Communications

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Overview

- Generally speaking, collective calls are substitutes for a more complex sequence of point-to-point calls
- Involve all the processes in a process group
- Called by all processes in a communicator
- All routines block until they are locally complete
  - With MPI-3, collective operations can be blocking or non-blocking.
- Restrictions
  - Receive buffers must be exactly the right size
  - No message tags are needed
  - Can only be used with MPI predefined datatypes

Three Types of Collective Operations

- Synchronization
  - processes wait until all members of the group have reached the synchronization point.
- Data movement
  - broadcast, scatter/gather, all to all
- Global computation (reduction)
  - one member of the group collects data from the other members and performs an operation (min, max, add, multiply, etc.) on that data

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Synchronization Routine – MPI_Barrier

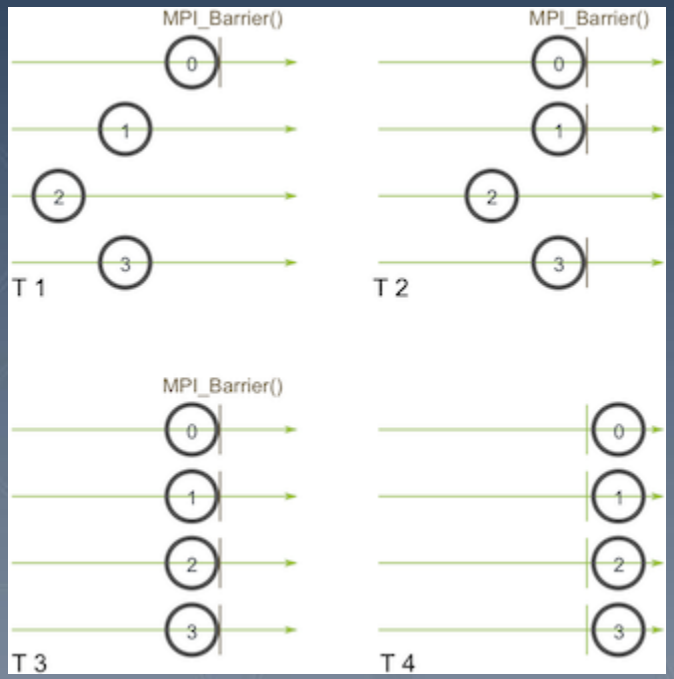
- To synchronize all processes within a communicator
- No processes in the communicator can pass the barrier until all of them call the function.

- C:

```
ierr = MPI_Barrier(comm)
```

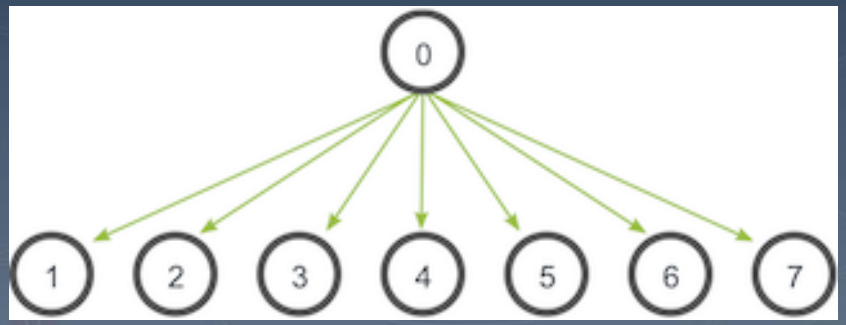
- Fortran:

```
call MPI_Barrier(comm, ierr)
```



Data Movement Routine: MPI Broadcast

- One process broadcasts (sends) a message to all other processes in the group
- The `MPI_Bcast` must be called by each node in a group, specifying the same communicator and root.



C:

```
ierr = MPI_Bcast(buffer,count,datatype,root,comm)
```

Fortran:

```
call MPI_Bcast(buffer,count,datatype,root,comm,ierr)
```

Data Movement Routine: MPI Scatter

- Distributes distinct messages from one process to all other processes in the group
- Data are distributed into n equal segments, where the i^{th} segment is sent to the i^{th} process in the group, which contains all n processes.

C :

```
ierr = MPI_Scatter(&sbuff, scount, sdatatype,
&rbuf, rcount, rdatatype, root, comm)
```

Fortran :

```
call MPI_Scatter(sbuff, scount, sdatatype, rbuf,
rcount, rdatatype, root , comm, ierr)
```

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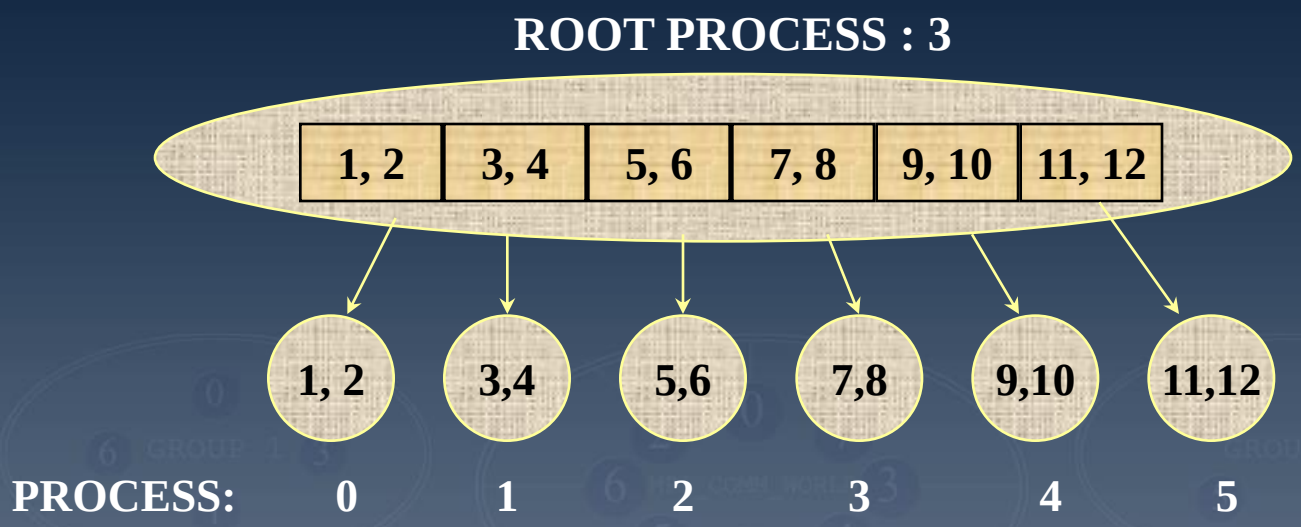
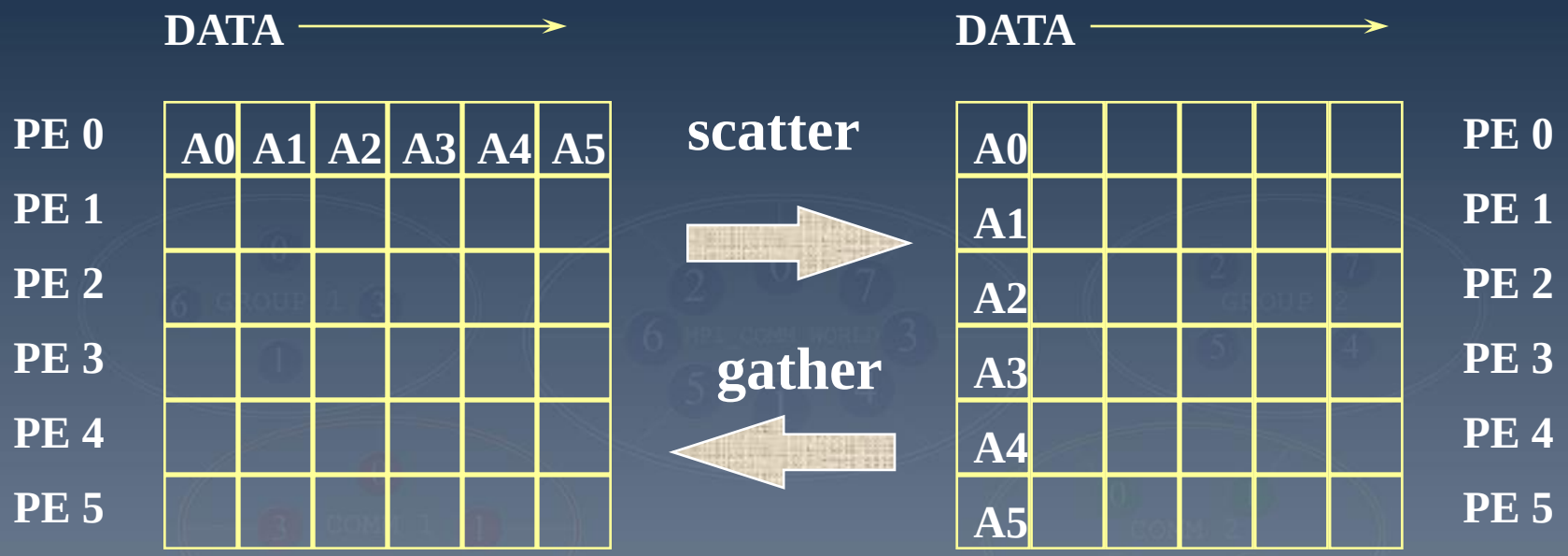
Example : MPI_Scatter




```
real sbuf(12), rbuf(2)
call MPI_Scatter(sbuf, 2, MPI_INT, rbuf, 2, MPI_INT, 3,
MPI_COMM_WORLD, ierr)
```

Scatter and Gather



Data Movement Routine: MPI Gather

- Gathers distinct messages from each processes in the group to a single process in the order of process ranks
- The reverse operation of MPI_Scatter

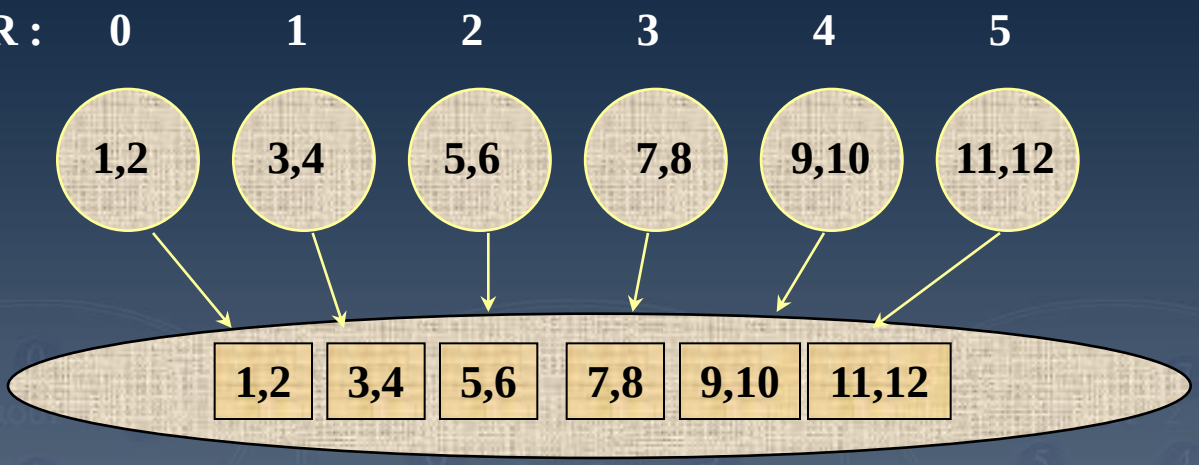
- C :

```
ierr = MPI_Gather(&sbuf, scount, sdatatype,
&rbuf, rcount, rdatatype, root, comm)
```

- Fortran :

```
call MPI_Gather(sbuff, scount, sdatatype,
rbuff, rcount, rdtatatype, root, comm, ierr)
```

Example : MPI_Gather




```
real sbuf(2),rbuf(12)
call MPI_Gather(sbuf,2,MPI_INT, rbuf, 2, MPI_INT, 3,
MPI_COMM_WORLD, ierr)
```

MPI_Scatterv and MPI_Gatherv

- Allows varying count of data and flexibility for data placement

- C :

```
ierr = MPI_Scatterv( &sbuf, &scount, &displace,
sdatatype, &rbuf, rcount, rdatatype, root, comm)
```

- Fortran :

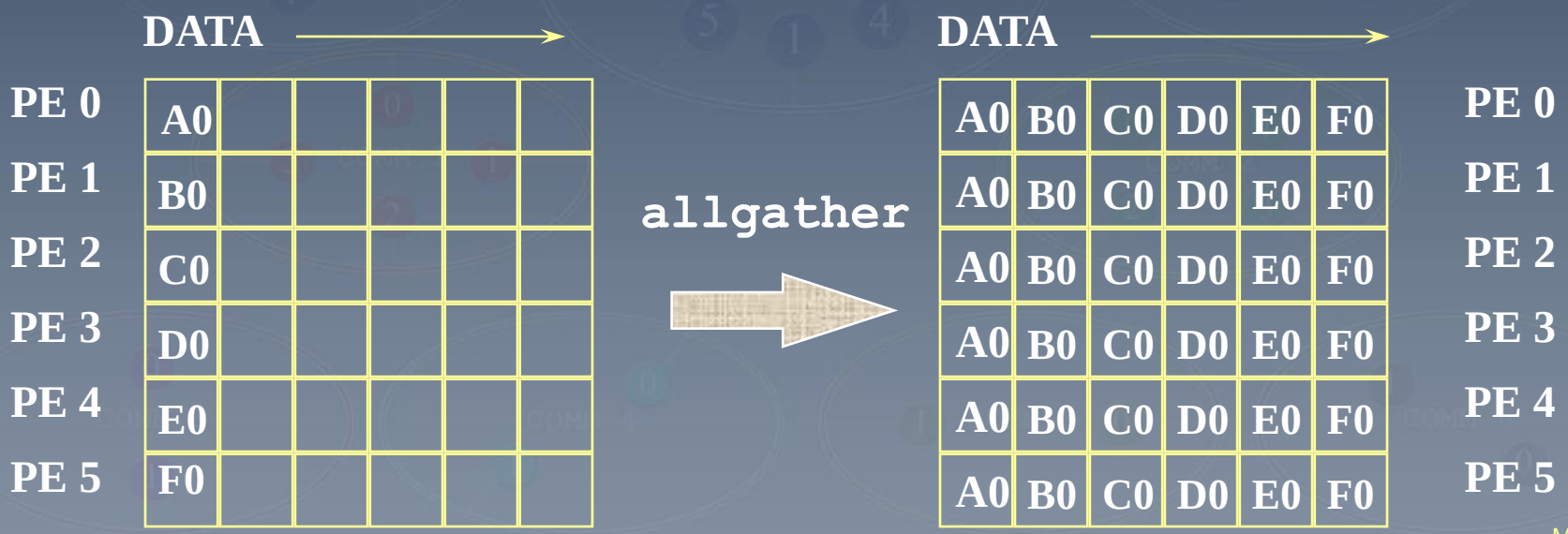
```
call MPI_Scatterv(sbuf,scount,displace,sdatatype, rbuf,
rcount, rdatatype, root, comm, ierr)
```

Data Movement Routine: `MPI_Allgather`

- Concatenation of data to all tasks in a group.
- Each task in the group, in effect, performs a one-to-all broadcasting operation within the group

- C:

```
ierr = MPI_Allgather(&sbuf, &scount, stype, &rbuf,
rcount, rtype, comm)
```



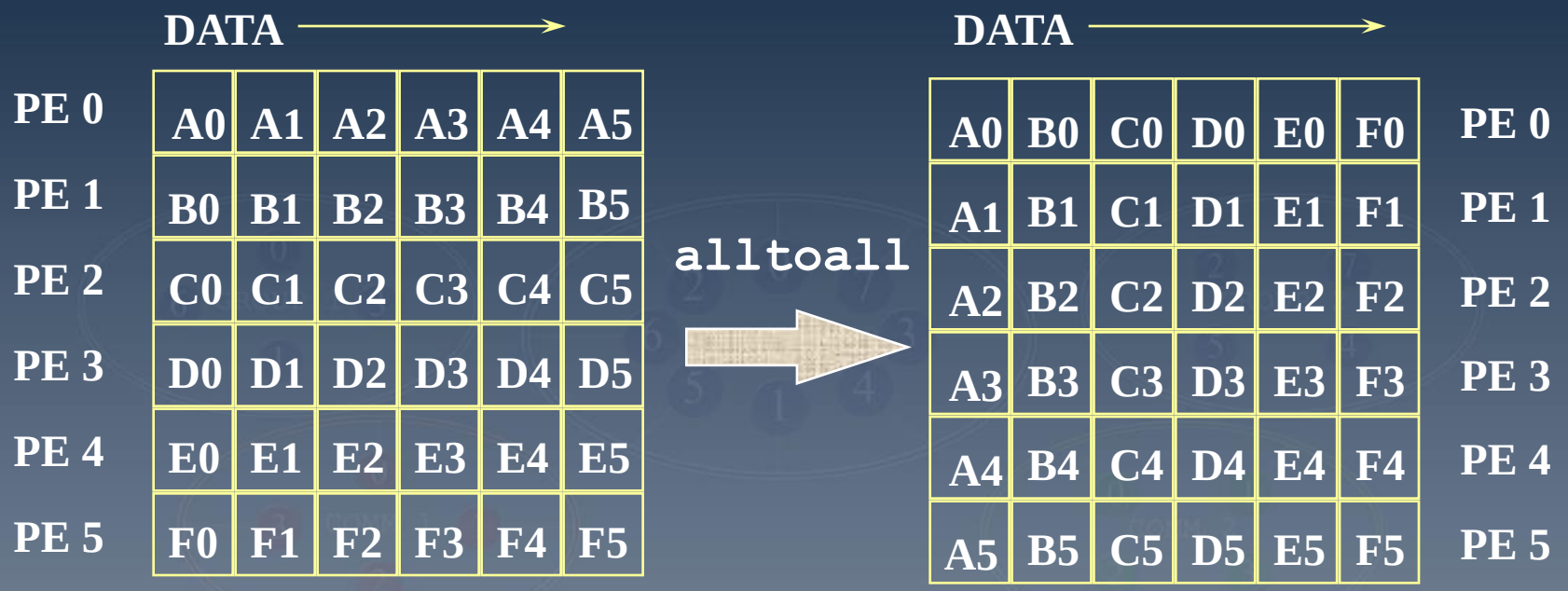
Data Movement Routine: `MPI_Alltoall`

- Sends data from all to all processes

```
MPI_Alltoall(sbuf,scount,stype,rbuf,rcount,rtype,comm)
```

`sbuf` :	starting address of send buffer (*)
`scount` :	number of elements sent to each process
`stype` :	data type of send buffer
`rbuff` :	address of receive buffer (*)
`rcount` :	number of elements received from any process
`rtype` :	data type of receive buffer elements
`comm` :	communicator

Example : MPI_Alltoall



Global Computation Routines

- One process of the group collects data from the other processes and performs an operation (min, max, etc.) on that data.
- Basic MPI reduction operations are predefined.
- Users can also define their own reduction functions by using the `MPI_Op_create` routine.
- Examples :
  - global sum or product
  - global maximum or minimum
  - global user-defined operation

Predefined Reduction Operations

MPI NAME	FUNCTION	MPI NAME	FUNCTION
MPI_MAX	Maximum	MPI_LOR	Logical OR
MPI_MIN	Minimum	MPI_BOR	Bitwise OR
MPI_SUM	Sum	MPI_LXOR	Logical exclusive OR
MPI_PROD	Product	MPI_BXOR	Bitwise exclusive OR
MPI_LAND	Logical AND	MPI_MAXLOC	Maximum and location
MPI_LOR	Bitwise AND	MPI_MINLOC	Minimum and location

Global Computation Routine: MPI_Reduce and MPI_Allreduce

MPI_Reduce(sbuf, rbuf, count, stype, op, root, comm)

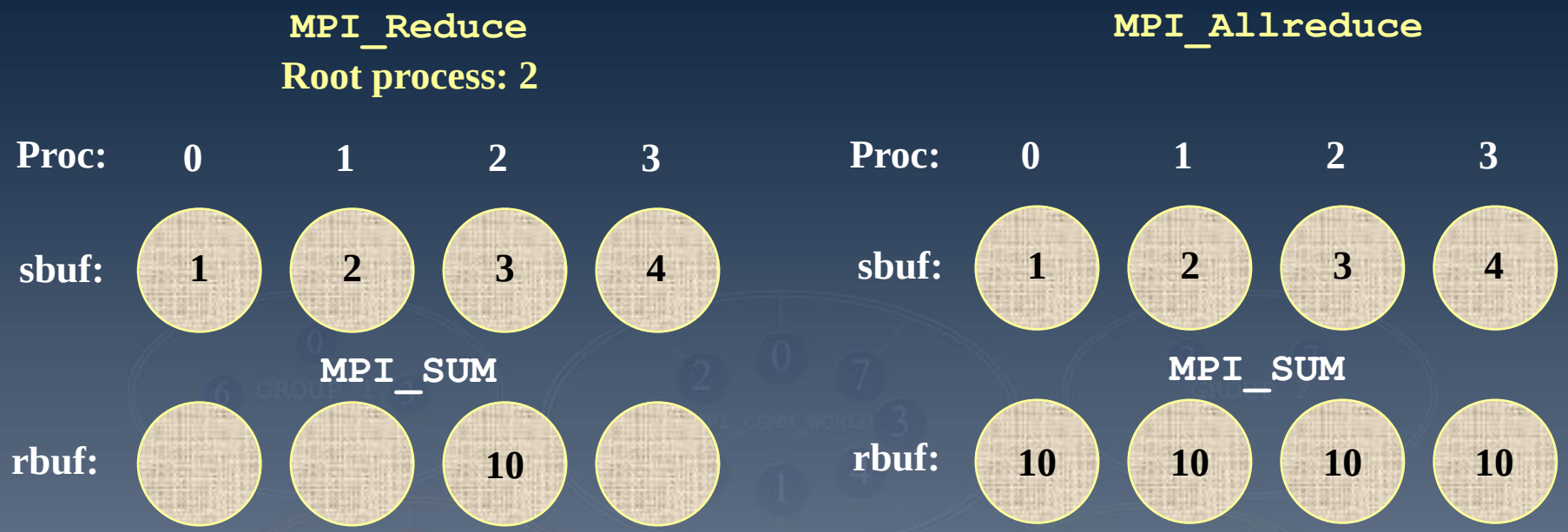
- Applies a reduction operation on all tasks in the group and returns the result to one task

MPI_Allreduce(sbuf, rbuf, count, stype, op, comm)

- Applies a reduction operation on all tasks in the group and returns the result to all tasks

sbuf:	address of send buffer
rbuf:	address of receive buffer
count:	the number of elements in the send buffer
stype:	the datatype of elements of send buffer
op:	the reduce operation function, predefined or user-defined
root:	the rank of the root process
comm:	communicator

Example : MPI_Reduce




```
MPI_Reduce(sbuf, rbuf, 1, MPI_INT, MPI_SUM, 2, MPI_COMM_WORLD)

MPI_Allreduce(sbuf, rbuf, 1, MPI_INT, MPI_SUM, MPI_COMM_WORLD)
```

Derived Datatypes

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Predefined (Basic) MPI Datatypes for C

MPI Datatypes	C Datatypes
MPI_CHAR	signed char
MPI_INT	signed int
MPI_LONG	signed long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	--------
MPI_SHORT	signed short int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED_LONG	unsigned long int
MPI_UNSIGNED	unsigned int
MPI_PACKED	--------

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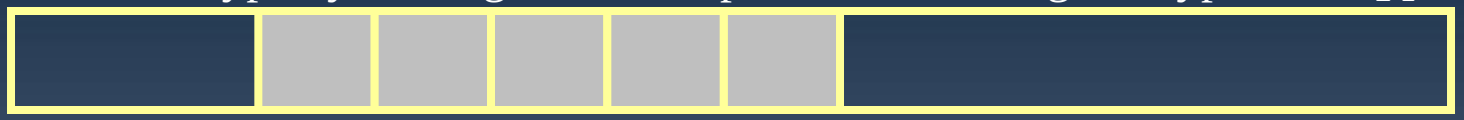
MPI Derived Datatypes: Overview

- MPI allows you to define (derive) your own data structures based upon sequences of the MPI basic datatypes.
- Derived datatypes provide an efficient way of communicating mixed types or non-contiguous types in a single message
  - MPI-IO uses derived datatypes extensively
- MPI datatypes are created at run-time through calls to MPI library
- MPI provides several methods for constructing derived datatypes:
  - Contiguous
  - Vector
  - Indexed
  - Struct

Four MPI Datatype Constructors

`MPI_Type_contiguous``(count, oldtype, &newtype)`

Produces a new data type by making `count` copies of an existing datatype `oldtype`



`MPI_Type_vector``(count, blen, stride, oldtype, &newtype)`

Similar to contiguous, but allows for regular gaps. '`count`' blocks with '`blen`' elements of '`oldtype`' spaced by '`stride`'

`MPI_Type_indexed``(count, blens[], strides[], oldtype, &newtype)`

Extension of vector with varying '`blens`' and '`strides`'

`MPI_Type_struct``(count, blens[], strides[], oldtypes, &newtype)`

Extension of indexed with varying `oldtypes`

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Example: MPI_Type_vector

- Replicates basic datatypes by placing blocks at fixed offsets.
  `MPI_Type_vector(count,blocklen,stride,oldtype,&newtype)`
- The new datatype consists of…
  - `count` number of blocks (nonnegative integer)
  - `blocklen` number of elements in each block (nonnegative integer)
  - `stride` number of elements between start of each block (integer)
  - `oldtype` old datatype (handle)
- Example
  - `count` = 4, `blocklen` = 1, `stride` = 4, `oldtype` = {MPI_FLOAT}

```
float           A[4][4];
int             dest, tag;
MPI_Datatype    newtype;

MPI_Type_vector( 4,          /* number column elements */
                 1,          /* 1 column only */
                 4,          /* skip 4 elements */
                 MPI_FLOAT, /* elements are float */
                 &newtype); /* new MPI derived datatype */

MPI_Type_commit(&newtype);

MPI_Send(&A[0][1], 1, newtype, dest, tag, MPI_COMM_WORLD);
```

A[4][4]

1.0	2.0	3.0	4.0
5.0	6.0	6.0	8.0
9.0	10.0	11.0	12.0
13.0	14.0	15.0	16.0

1 element of newtype

2.0	6.0	10.0	14.0

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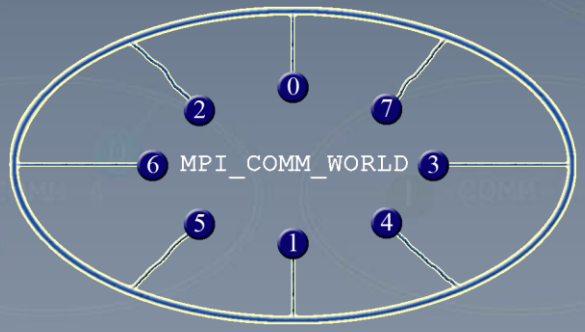
Communicators and Groups

Main Menu

MPI Communicators and Groups: MPI_COMM_WORLD

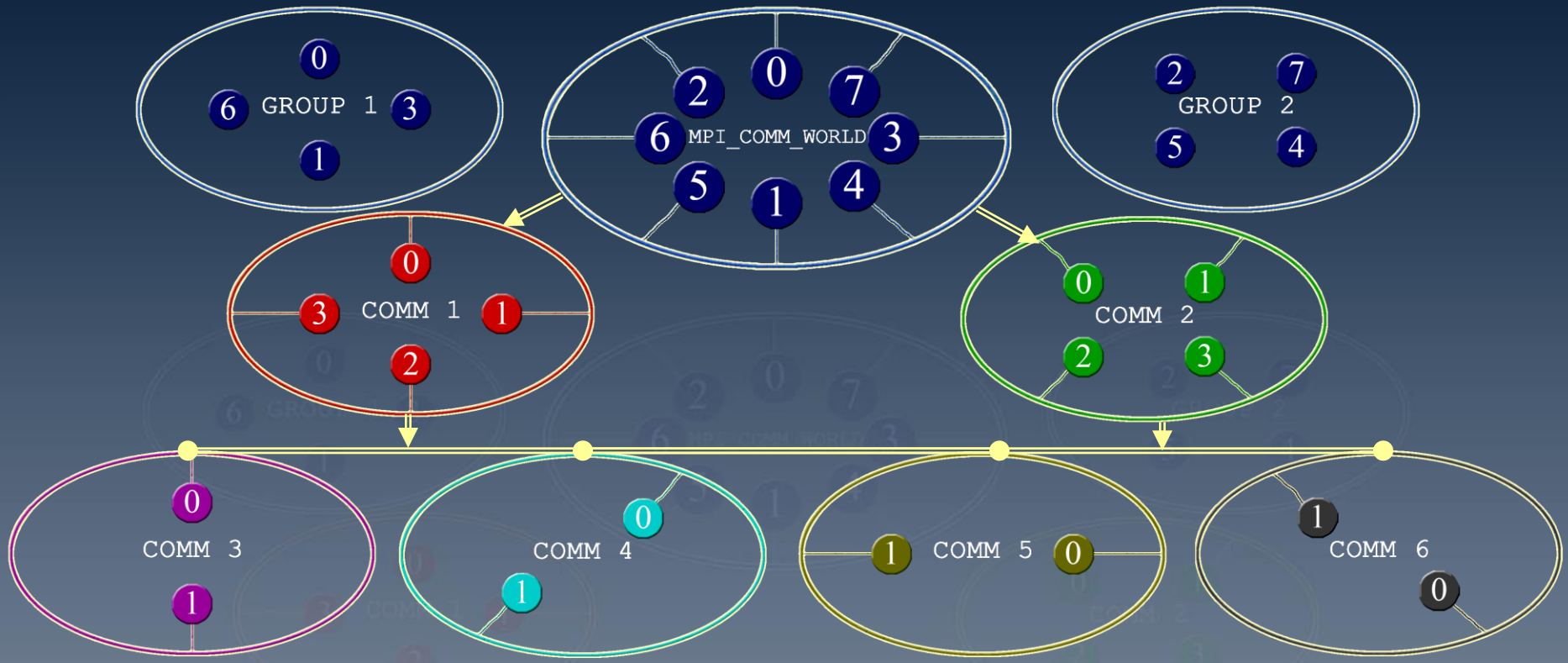
- MPI uses objects called *communicators* and *groups* to define which collection of processes may communicate with each other.
- All MPI communication calls require a *communicator argument* and MPI processes can only communicate if they share a communicator.
- MPI_Init() initializes a default communicator: MPI_COMM_WORLD
- The *base group* of MPI_COMM_WORLD contains all processes
- Process grouping capability allows the programmer to:
  - Organize tasks based upon application nature into task groups.
  - Enable Collective Communications operations across a subset of related tasks.
  - Provide basis for implementing virtual communication topologies.



MPI Communicators and Groups: Overview

- MPI Groups
  - A group is an ordered set of processes.
  - Each process in a group is associated with a unique integer rank
  - Rank values start at zero and go to N-1, where N is the number of processes in the group.
  - One process can belong to two or more groups.
- MPI Communicators
  - The communicator determines the scope and the "communication universe“
  - Each communicator contains a group of valid participants.
- Groups and communicators are dynamic objects in MPI and can be created and destroyed during program execution.

MPI Communicators and Groups: Illustration



WORLD, rank0	WORLD, rank3	WORLD, rank1	WORLD, rank6
COMM 1, rank0	COMM 1, rank1	COMM 1, rank2	COMM 1, rank3
COMM 3, rank0	COMM 5, rank0	COMM 3, rank1	COMM 5, rank1
WORLD, rank2	WORLD, rank7	WORLD, rank5	WORLD, rank4
COMM 2, rank0	COMM 2, rank1	COMM 2, rank2	COMM 2, rank3
COMM 6, rank1	COMM 4, rank0	COMM 4, rank1	COMM 6, rank0

Every process has three communicating groups and a distinct rank associated to it

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MPI Communicators and Groups: Usage

- MPI provides over 40 routines related to groups, communicators, and virtual topologies.

- Typical usage:
  - Extract handle of global group from MPI_COMM_WORLD using MPI_Comm_group
  - Form new group as a subset of global group using MPI_Group_incl
  - Create new communicator for new group using MPI_Comm_create
  - Determine new rank in new communicator using MPI_Comm_rank
  - Conduct communications using any MPI message passing routine
  - When finished, free up new communicator and group (optional) using MPI_Comm_free and MPI_Group_free

- A Note on Virtual Topologies
  - Describes a mapping of MPI processes into a geometric "shape“
  - The two main types of topologies are Cartesian (grid) and Graph
  - Virtual topologies are built upon MPI communicators and groups.

0 (0,0)	1 (0,1)	2 (0,2)	3 (0,3)
4 (1,0)	5 (1,1)	6 (1,2)	7 (1,3)
8 (2,0)	9 (2,1)	10 (2,2)	11 (2,3)
12 (3,0)	13 (3,1)	14 (3,2)	15 (3,3)

Main Menu

Cray MPI Environment Variables

- Why use MPI environment variables?
  - Allow users to tweak optimizations for specific application behavior
  - Flexibility to choose cutoff values for collective optimizations
  - Determine maximum size of internal MPI resources - buffers/queues, etc.

- MPI Display Variables
  - **`export MPICH_VERSION_DISPLAY=1`**
    - Displays version of Cray MPI being used
  - **`export MPICH_ENV_DISPLAY=1`**
    - Displays all MPI environment variables and their current values
    - Helpful to determine what defaults are set to

MPI Environment Variables: Default Values

The default values of MPI environment variables:

```
MPI VERSION : CRAY MPICH2 XT version 3.1.2-
pre (ANL base 1.0.6)
BUILD INFO  : Built Thu Feb 26  3:58:36 2009
(svn rev 7308)
PE 0: MPICH environment settings:
PE 0:    MPICH_ENV_DISPLAY            = 1
PE 0:    MPICH_VERSION_DISPLAY        = 1
PE 0:    MPICH_ABORT_ON_ERROR         = 0
PE 0:    MPICH_CPU_YIELD              = 0
PE 0:    MPICH_RANK_REORDER_METHOD    = 1
PE 0:    MPICH_RANK_REORDER_DISPLAY   = 0
PE 0:    MPICH_MAX_THREAD_SAFETY      = single
PE 0:    MPICH_MSGS_PER_PROC          = 16384
PE 0: MPICH/SMP environment settings:
PE 0:    MPICH_SMP_OFF                = 0
PE 0:    MPICH_SMPDEV_BUFS_PER_PROC   = 32
PE 0:    MPICH_SMP_SINGLE_COPY_SIZE   = 131072
PE 0:    MPICH_SMP_SINGLE_COPY_OFF    = 0
PE 0: MPICH/PORTALS environment settings:
PE 0:    MPICH_MAX_SHORT_MSG_SIZE     = 128000
PE 0:    MPICH_UNEX_BUFFER_SIZE       = 62914560
PE 0:    MPICH_PTL_UNEX_EVENTS        = 20480
PE 0:    MPICH_PTL_OTHER_EVENTS       = 2048
PE 0:    MPICH_VSHORT_OFF             = 0
PE 0:    MPICH_MAX_VSHORT_MSG_SIZE    = 1024
PE 0:    MPICH_VSHORT_BUFFERS         = 32
PE 0:    MPICH_PTL_EAGER_LONG         = 0
PE 0:    MPICH_PTL_MATCH_OFF          = 0
PE 0:    MPICH_PTL_SEND_CREDITS       = 0
PE 0: MPICH/COLLECTIVE environment settings:
PE 0:    MPICH_FAST_MEMCPY            = 0
PE 0:    MPICH_COLL_OPT_OFF           = 0
PE 0:    MPICH_COLL_SYNC              = 0
PE 0:    MPICH_BCAST_ONLY_TREE        = 1
PE 0:    MPICH_ALLTOALL_SHORT_MSG     = 1024
PE 0:    MPICH_REDUCE_SHORT_MSG       = 65536
PE 0:    MPICH_REDUCE_LARGE_MSG       = 131072
PE 0:    MPICH_ALLREDUCE_LARGE_MSG    = 262144
PE 0:    MPICH_ALLGATHER_VSHORT_MSG   = 2048
PE 0:    MPICH_ALLTOALLVW_FCSIZE      = 32
PE 0:    MPICH_ALLTOALLVW_SENDWIN     = 20
PE 0:    MPICH_ALLTOALLVW_RECVWIN     = 20
PE 0: MPICH/MPIIO environment settings:
PE 0:    MPICH_MPIIO_HINTS_DISPLAY    = 0
PE 0:    MPICH_MPIIO_CB_ALIGN         = 0
PE 0:    MPICH_MPIIO_HINTS            = NULL
```

Dealing with errors

- If you see this error message:

  internal ABORT - process 0: Other MPI error, error stack:

  MPIDI_PortalsU_Request_PUPE(317): exhausted unexpected receive queue buffering increase via env. var. MPICH_UNEX_BUFFER_SIZE

- It means:

  The application is sending too many short, unexpected messages to a particular receiver.

- Try doing this to work around the problem:

  Increase the amount of memory for MPI buffering using the MPICH_UNEX_BUFFER_SIZE variable(default is 60 MB) and/or decrease the short message threshold using the MPICH_MAX_SHORT_MSG_SIZE (default is 128000 bytes) variable.

Pre-posting receives

- If possible, pre-post receives before sender posts the matching send
  - typically useful technique for all MPICH installations
- But be careful with excessive pre-posting of the receives though, as it will hit Portals internal resource limitations eventually

Error message

[0] MPIDI_Portals_Progress: dropped event on "other" queue, increase
[0] queue size by setting the environment variable MPICH_PTL_OTHER_EVENTS
aborting job: Dropped Portals event

Try doing this to work around the problem:

You can increase the size of this queue by setting the environment variable MPICH_PTL_OTHER_EVENTS to some value higher than the 2048 default.

Aggregating data

- For very small buffers, aggregate data into fewer MPI calls (especially for collectives)
  - Example: alltoall with an array of 3 reals is clearly better than 3 alltoalls with 1 real
  - Do not aggregate too much. The MPI protocol switches from an short (eager) protocol to a long message protocol using a receiver pull method once the message is larger than the eager limit. This limit can be changed with the MPICH_MAX_SHORT_MSG_SIZE environment variable.

MPI Tips on Cray XT5

http://www.nics.tennessee.edu/computing-resources/kraken/mpi-tips-for-cray-xt5

Resources for Users: `man` pages and MPI web-sites

- There are man pages available for MPI which should be installed in your MANPATH. The following man pages have some introductory information about MPI.

```
% man MPI
% man cc
% man ftn
% man qsub
% man MPI_Init
% man MPI_Finalize
```

- MPI man pages are also available online.
  http://www.mcs.anl.gov/mpi/www/
- Main MPI web page at Argonne National Laboratory
  http://www-unix.mcs.anl.gov/mpi
- Set of guided exercises
  http://www-unix.mcs.anl.gov/mpi/tutorial/mpiexmpl
- MPI tutorial at Lawrence Livermore National Laboratory
  https://computing.llnl.gov/tutorials/mpi/
- MPI Forum home page contains the official copies of the MPI standard.
  http://www.mpi-forum.org/