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Distributed Computing - MPI

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Intro and motivation
Code Body
Communicators
Send and Receive
Other P2P Funcs
Global Funcs
Timing
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Topology

What You Should Know...

- Programming in FORTRAN/C/C++/Java
- Basics in hardware - CPU, RAM, Network

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Outline

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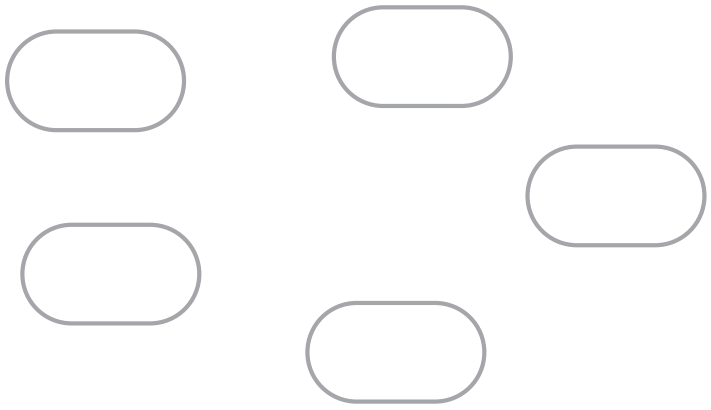

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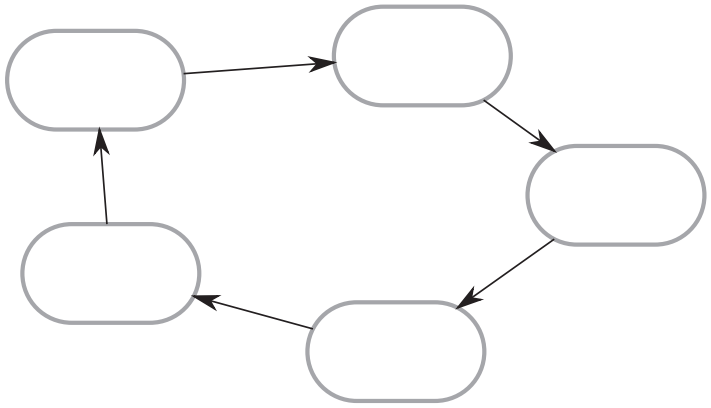
Distributed computing



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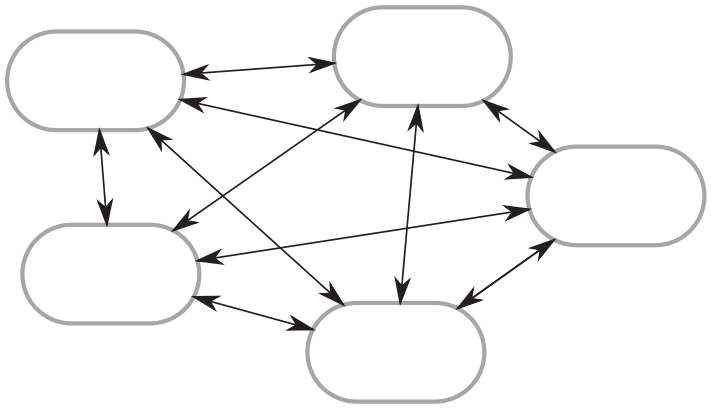

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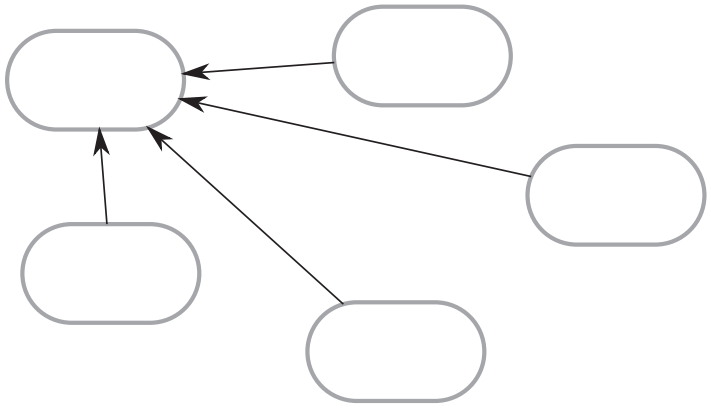
Distributed computing



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Distributed computing

How to communicate?

- Sending data
- Receiving data
- Waiting for data
- Waiting for synchronization

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Message Passing Interface (MPI)

- MPI is a library for data and messages passing
- The communication is explicit (the user specify what/how needs to be sent)
- The number of processes is configured at start up

A MPI program:

- Communication functions (Send/Receive/etc)
- C, C++, FORTRAN (+ interface to others)
- To run the program you need a run-time agent (mpirun)
- Example *mpirun -np 2 ./program*

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Brief History

- 1992 - draft of the project
- 1994 - first version MPI 1.0
  - C, FORTRAN 77
  - Point-to-point
  - Global communication, groups
- 1997 - MPI 2.0
  - One-sided communication
  - C++, FORTRAN 90
  - Dynamic management
- 2008/09 - MPI 2.1 and 2.2
- 2012 - MPI-3.0
  - New one-sided communication

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The Body of Your Code / C, C++

The program should contain

- *#include <mpi.h>*
  - the include file for MPI
- MPI_Init(&agrc, &argv);
  - Initialize the MPI
  - Pass the arguments from the command line
- MPI_Finalize();
  - Finalize all communication

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Compile and Run Your Code / Linux

Compilation

- *mpicc -O3 -o program program.c*
- *mpiCC -O3 -o program program.cpp*

Execution

- *mpirun -np N ./program*
- where *N* is the number of process (integer number)

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Groups and Communicators

A group is an ordered set of processes.

- Each process is associate with ID number - called *rank*
- Processes can belong to different groups

Communicator object connect a group of processes in the MPI session.

- The standard (default) communicator for all MPI process is called *MPI_COMM_WORLD*

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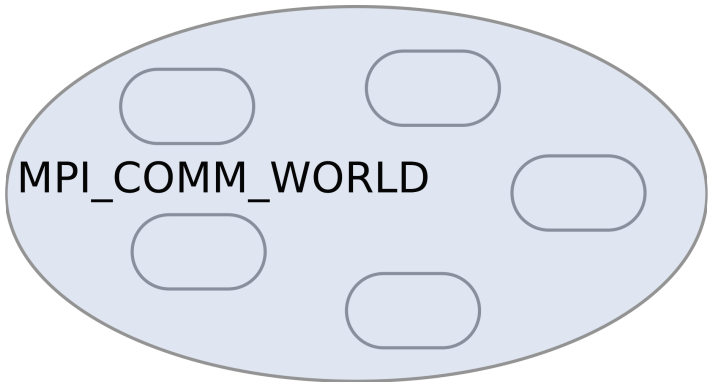
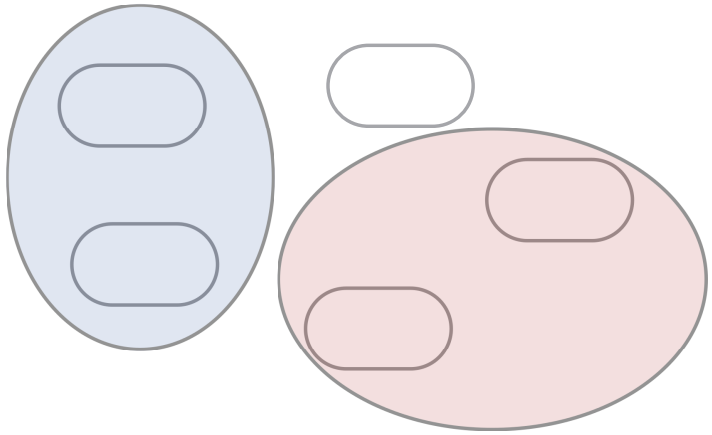
Communicators





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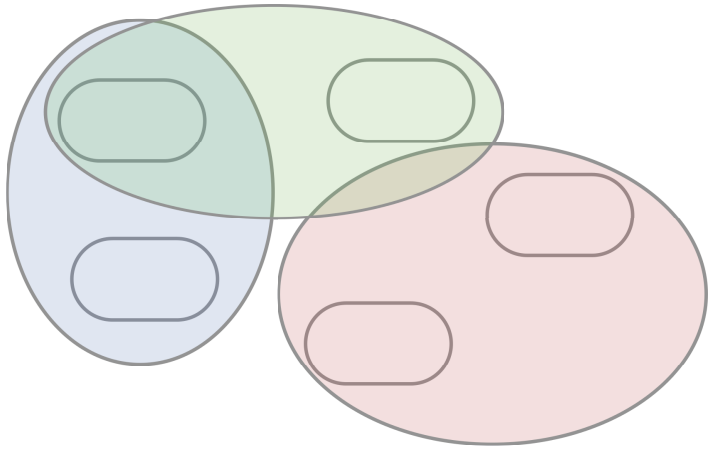
Communicators



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Communicators

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Communicator Functions

Get the current rank (ID)

- *MPI_Comm_rank()*

Get the size of the communicator

- *MPI_Comm_size()*

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Code Example

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

int main (int argc,
          char *argv[]) {
 int rank, size;

 MPI_Init (&argc, &argv);
 MPI_Comm_rank (MPI_COMM_WORLD, &rank);
 MPI_Comm_size (MPI_COMM_WORLD, &size);

 printf("Hello world from process %d of %d\n",
        rank, size );

 MPI_Finalize();
 return 0;
}
```

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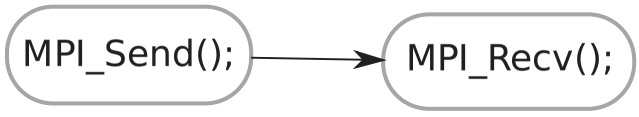
Send and Receive



- Point-to-point communication

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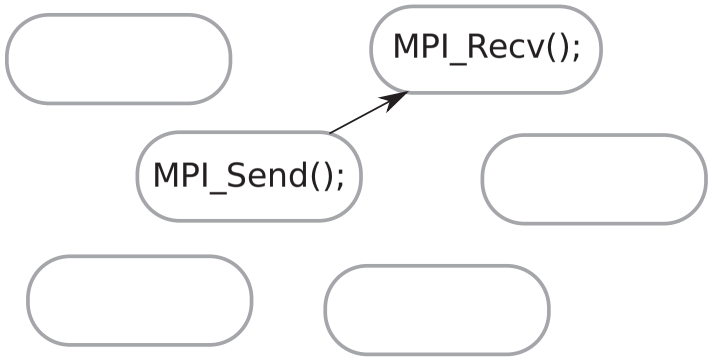
Send - Recv



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Send

```
MPI_Send(  buff,
           count,
           datatype,
           dest,
           tag,
           comm);
```

void*	buff	Address of the buffer
int	count	Number of elements in the buff
MPI_Datatype	datatype	Data type(MPI_INT,...)
int	dest	Destination (rank)
int	tag	Tag
MPI_Comm	comm	MPI-Communicator

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Recv

```
MPI_Recv(  buff,
           count,
           datatype,
           source,
           tag,
           comm
           status);
```

void*	buff	Address of the buffer
int	count	Number of elements in the buff
MPI_Datatype	datatype	Data type(MPI_INT,...)
int	src	Source (rank)
int	tag	Tag
MPI_Comm	comm	MPI-Communicator
MPI_status*	status	Status

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Code Example

The following code compute the following

- Proc 0 sends data to Proc 1
- Proc 1 sends data to Proc 2
- ...
- Proc N-1 sends data to Proc 0

The data is a double value, where each process adds its rank. Thus, at the end the data will contain the sum of all ranks (0+1+2+3+4+...+N-1).

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Code Example

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

int main(int argc, char *argv[]){
 int size, rank;
 MPI_Status status;
 double bot;

 MPI_Init(&argc, &argv);
 MPI_Comm_rank(MPI_COMM_WORLD, &rank);
 MPI_Comm_size(MPI_COMM_WORLD, &size);
 bot = 0.0;
```


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Code Example

```
if(rank==0){
 MPI_Send(&bot,1,MPI_DOUBLE,1,1,MPI_COMM_WORLD);
 MPI_Recv(&bot,1,MPI_DOUBLE,size-1,1,
              MPI_COMM_WORLD,&status);
 printf("result: %1f\n", bot);

}else {

 MPI_Recv(&bot,1,MPI_DOUBLE,rank-1,1,
 MPI_COMM_WORLD,&status);
 bot += rank;
 MPI_Send(&bot,1,MPI_DOUBLE,
        (rank+1)%size,1,MPI_COMM_WORLD);
}
MPI_Finalize();
return 0;
}
```

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(Non-)Blocking/(A-)Synchronous

Blocking mode

- The current process waits until the its part finished

Synchronous mode

- The process waits for the start of the other side

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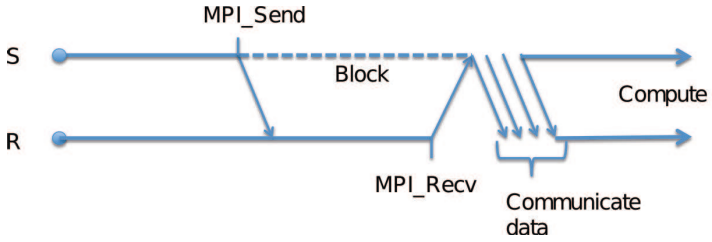
MPI_Send

Blocking Send (Same as MPI_Ssend)



- The processor is blocked until data has been sent
- Receive can be posted before the send
- Receiver waits for the ready-to-send-signal
- Deadlock will occur if no matching send/receive

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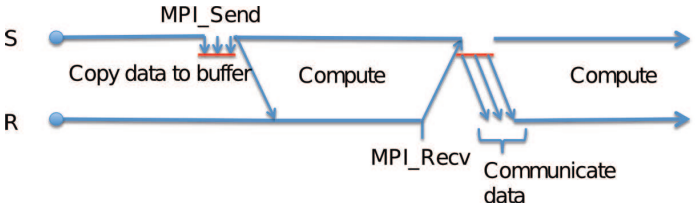
MPI_Send

When the data if very small (size<threshold)



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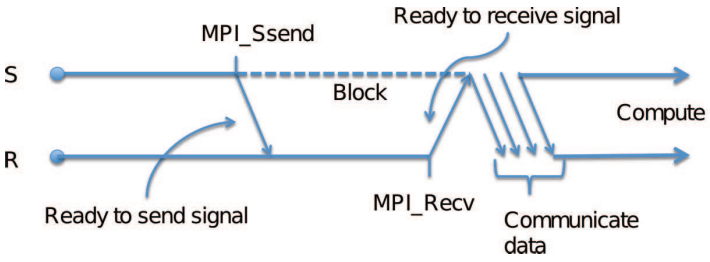
MPI_Ssend

Blocking MPI_Ssend



- It will always wait until the receive has been posted on the receiving end.

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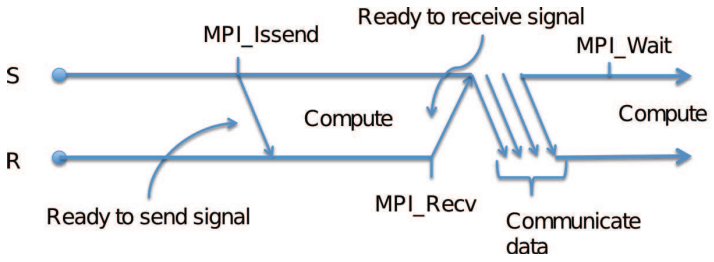
MPI_Issend

Non-blocking MPI_Issend



- The sender is not blocked but we need to do an explicit wait to ensure that the data buffer is safe to use (data has been transmitted) with MPI_Wait! Can also do a non-blocking MPI_Test.

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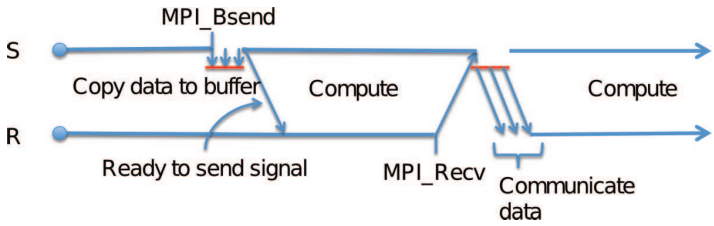
MPI_Bsend

Buffered MPI_Bsend



- It copies data to a user-supplied communication buffer and then returns (no blocking of processor). It is safe to modify the original data and no need to wait for the communication to complete.

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MPI_Bsend

Need to allocate the buffer first (enough space for all pending mess):

- int buflen=totlen*sizeof(double) + MPI_BSEND_OVERHEAD;
- double *buffer=malloc(buflen);
- MPI_Buffer_attach(buffer,buflen);
- MPI_Bsend(data,count,type,dest,tag,comm);

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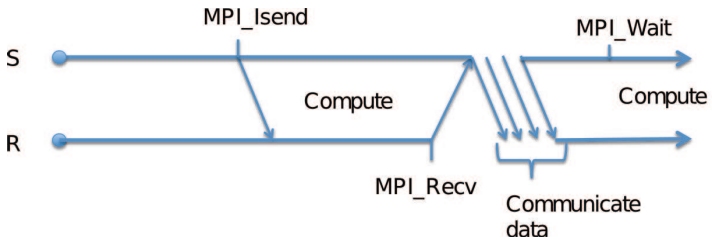
MPI_Isend

Non-blocking MPI_Isend



- Same behavior as for non-blocking synchronous send MPI_Issend, need to do an explicit wait/test to ensure that the communication has completed and it is safe to modify the data.

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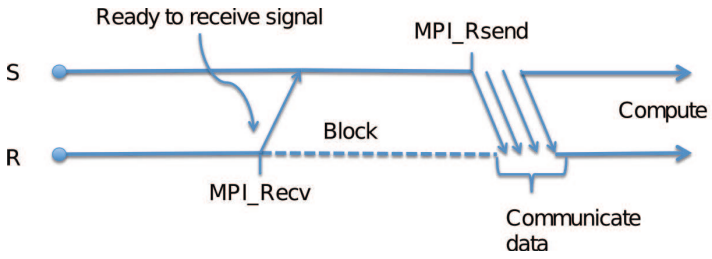
MPI_Rsend

Ready send MPI_Rsend



- It sends the message, there must be a receive waiting (if not, the message is lost).

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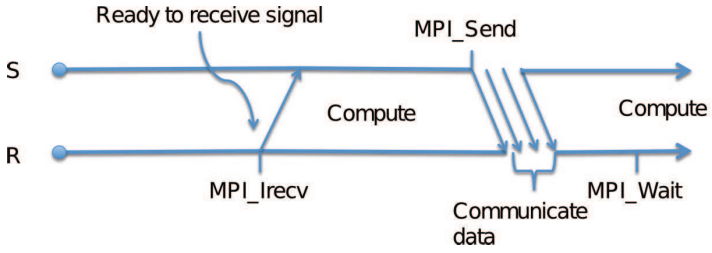
MPI_Irecv

Non-blocking MPI_Irecv



- The non-blocking receive does not block the processors but then we need to do an explicit wait or test to check if data has arrived.

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Send/Recv

We have four basic communication modes:

- MPI_Send, MPI_Isend – Standard mode
- MPI_Ssend, MPI_Issend – Synchronous mode
- MPI_Rsend, (MPI_Irsend) – Ready mode
- MPI_Bsend, (MPI_Ibsend) – Buffered mode

All modes can be blocked -or- non-blocked Blocking suspends the execution until the message (data) buffer is safe to use (message has been sent/ received/copied). Non-blocking calls returns immediately after initiating the communication.

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Note - Send/Recv

All send calls need to be matched with a receive call!
and
Deadlock will occur if no matching send/receive!

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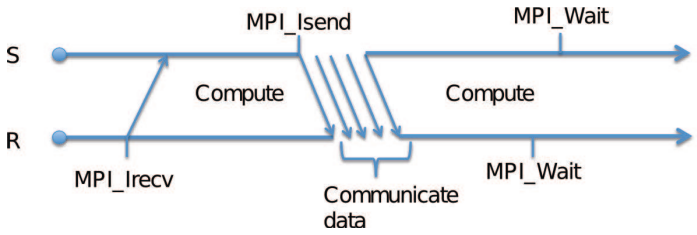
Tips



- Post a non-blocking send and a non-blocking receive as early as possible and overlap the communication with other computations.
- Using standard non-blocking send and receive is in most cases sufficient and gives good performance.

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Other Point-to-Point Functions

MPI_Wait

- Wait for request to complete
- Example: MPI_Irecv

MPI_Waitall

- Wait for all requests to complete
- Example: Multiple MPI_Irecv (different tags, senders, etc)

MPI_Waitany

- Wait for any(≥ 1) specififed requests to complete

MPI_Waitsome

- Wait for some (1) specififed requests to complete

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Other Point-to-Point Functions

MPI_Test, MPI_Testall, MPI_Testany, MPI_Testsome

- Same as Wait but
- it only test and returns immedietly

MPI_Probe, MPI_Iprobe

- Check for receiving messages
- Example: getting a receiving status without actually receiving the data

MPI_Cancel

- Abort the operation

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Global Functions

Barrier
- All processes wait on it

Broadcast
- Send to all processes

Reduce
- Collect data with an operation

Scatter/Gatter
- Send/Receive to/from all

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Barrier

- A global barrier

int MPI_Barrier(MPI_Comm comm);

```
...
// parallel computing
...
MPI_Barrier(MPI_COMM_WORLD);
...
/// parallel computing
...
```


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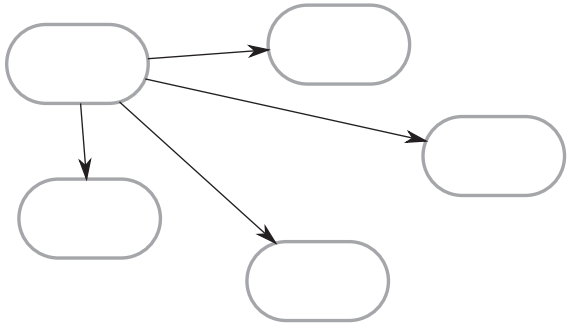
Broadcast

- A processor sends data to all others



int MPI_Bcast(void *buffer, int count, MPI_Datatype datatype, int root, MPI_Comm comm);

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Broadcast

```
...

int global_var;

if (rank == 0)
 global_var = read_file("var.dat");

MPI_Bcast(global_var, 1, MPI_INT, 0,
          MPI_COMM_WORLD);

...
```


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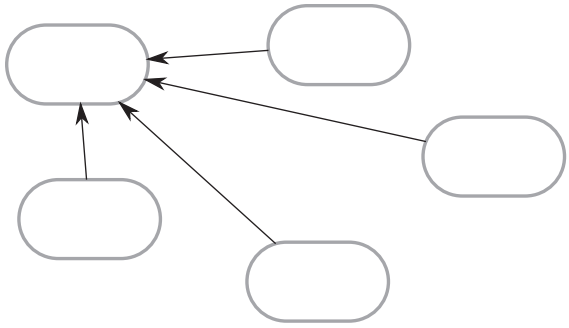
Reduce

- Reduces values on all processes to a single value



int MPI_Reduce(void *sendbuf, void *recvbuf, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm);

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Reduce

```
...
// declare and compute a[]
...
double local_sum = 0.0;

for( int i = 0; i < n; i++)
 local_sum += a[i];

double total;
MPI_Reduce(sum, total, 1, MPI_DOUBLE, MPI_SUM,
           0, MPI_COMM_WORLD);

...
```


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Reduce Operations

MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_SUM	Sum
MPI_PROD	Product
MPI_LAND	Logical AND
MPI_BAND	Bitwise AND
MPI_LOR	Logical OR
MPI_BOR	Bitwise OR
MPI_LXOR	Logical XOR
MPI_BXOR	Bitwise XOR
MPI_MAXLOC	Max value and location
MPI_MINLOC	Min value and location

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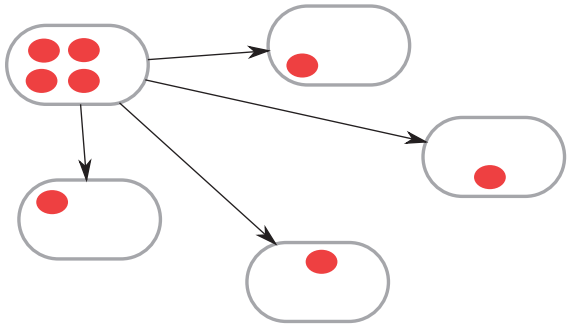
Scatter

- A processor sends data to all others



int MPI_Scatter(void *sendbuf, int sendcount,
MPI_Datatype sendtype, void *recvbuf, int rcount,
MPI_Datatype recvtype, int root, MPI_Comm comm);

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Scatter

```
...
MPI_Comm comm;
int gsize,*sendbuf;
int root, rbuf[100];
...
MPI_Comm_rank( comm, myrank);
if ( myrank == root) {
 MPI_Comm_size( comm, &gsize);
 sendbuf = (int *)malloc(gsize*100*sizeof(int));
}
...
MPI_Scatter(sendbuf, 100, MPI_INT, rbuf, 100,
            MPI_INT, root, comm);
...
```

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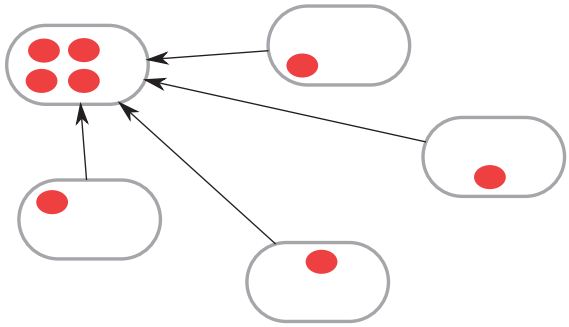
Gather

- A processor sends data to all others



int MPI_Gather(void *sendbuf, int sendcount,
MPI_Datatype sendtype, void *recvbuf, int rcount,
MPI_Datatype recvtype, int root, MPI_Comm comm);

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Gather

```
...
MPI_Comm comm;
int gsize,sendarray[100];
int root, myrank, *rbuf;
...
MPI_Comm_rank( comm, myrank);
if ( myrank == root) {
   MPI_Comm_size( comm, &gsize);
   rbuf = (int *)malloc(gsize*100*sizeof(int));
}

MPI_Gather(sendarray, 100, MPI_INT, rbuf, 100,
           MPI_INT, root, comm);
...
```

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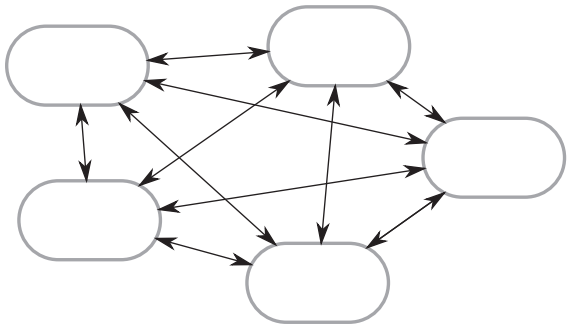
MPI_All*

- MPI_Allreduce
- MPI_Allgather
- MPI_Alltoall



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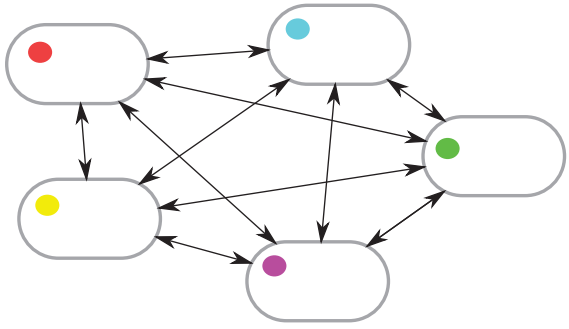
MPI_Allreduce



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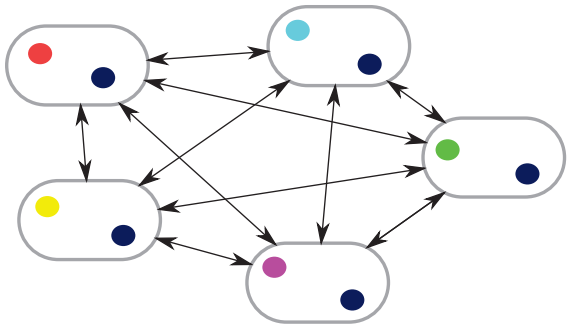
MPI_Allreduce



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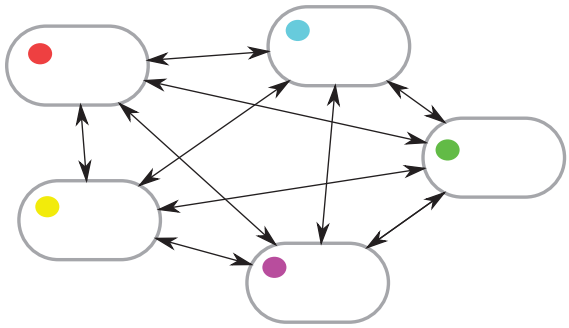

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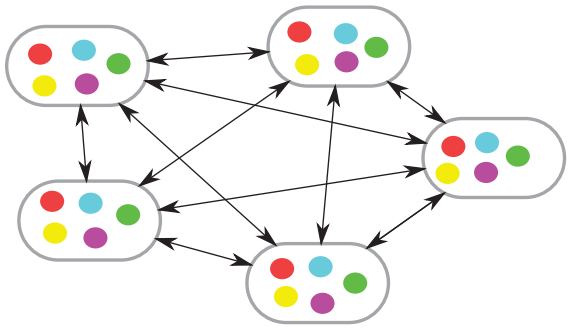
MPI_Allgather



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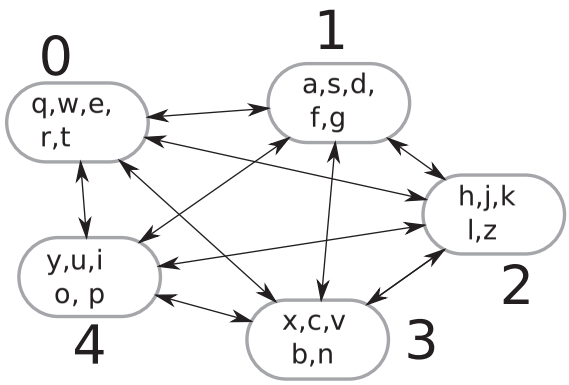
MPI_Alltoall



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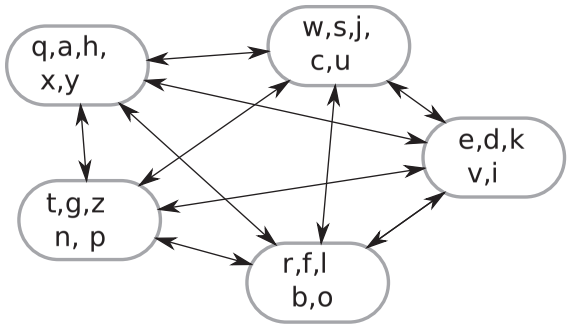
MPI_Alltoall



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Timing in MPI

```
double start_time;
start_time = MPI_Wtime();
...
// Compute
...
double finish_time;
finish_time = MPI_Wtime();

// Elapsed time
double elapsed_time;
elapsed_time = finish_time - start_time;
```


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MPI Datatype

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

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Derived Datatype

- Send non-contiguous data
- Reduce the number of communication calls

- MPI_Type_vector() – regular distribution
- MPI_Type_indexed() – irregular distribution
- MPI_Type_struct() – different datatypes

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MPI_TYPE_VECTOR

- MPI_Type_vector(rows,cols,stride,old_type,newtype);
- Makes a row x cols vector
- Cols is number of contiguous elements for each row
- Contents of the new array will be columns of original array

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MPI_TYPE_VECTOR

$A = [1, 2, 3, 4; 5, 6, 7, 8; 9, 10, 11, 12];$

- MPI_Datatype newtype;
- MPI_Type_vector(2,1,4,MPI_INT,&newtype);
- MPI_Commit(&newtype);
- MPI_Send(&A[0] [1],1,newtype,1,0,comm);
- Sends new array [2 6] to process 1
- MPI_Send(&A[1][3],1,newtype,1,0,comm);
- Sends new array [8 12] to process 1

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MPI_TYPE_VECTOR

$A = [1, 2, 3, 4; 5, 6, 7, 8; 9, 10, 11, 12]$;

- MPI_Datatype newtype;
- MPI_Type_vector(3,2,4,MPI_INT,&newtype);
- MPI_Commit(&newtype);
- MPI_Send(&A[0][1],1,newtype,1,0,comm);
- Sends new array [2 3 6 7 10 11] to process 1
- Could be interpreted as matrix with 3 rows, 2 cols

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MPI_TYPE_INDEX

- MPI_Type_indexed (count, blocklens[], offsets[], old_type,newtype)
- Make blocks at different offsets
- Displacements between successive blocks need not be equal

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MPI_TYPE_INDEX

```
int numtasks, rank, source=0, dest, tag=1;
int blocklengths[2], displacements[2];
float a[16] =
 {1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0,
  9.0, 10.0, 11.0, 12.0, 13.0, 14.0, 15.0, 16.0};
float b[NELEMENTS];
MPI_Status stat;
MPI_Datatype indextype;

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

blocklengths[0] = 4;
blocklengths[1] = 2;
```


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MPI_TYPE_INDEX

```
displacements[0] = 5;
displacements[1] = 12;

MPI_Type_indexed(2, blocklengths, displacements,
                 MPI_FLOAT, &indextype);
MPI_Type_commit(&indextype);
if (rank == 0) {
 for (int i=0; i < numtasks; i++)
 MPI_Send(a, 1, indextype, i, tag, MPI_COMM_WORLI
}

MPI_Recv(b, NELEMENTS, MPI_FLOAT, source, tag,
         MPI_COMM_WORLD, &stat);
```

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MPI_TYPE_INDEX

```
Output:
rank= 0  b= 6.0 7.0 8.0 9.0 13.0 14.0
rank= 1  b= 6.0 7.0 8.0 9.0 13.0 14.0
rank= 2  b= 6.0 7.0 8.0 9.0 13.0 14.0
rank= 3  b= 6.0 7.0 8.0 9.0 13.0 14.0
```


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Topology

Communicator with structure. Makes a mapping to physical topology optimizing (localizing) the communication. Helps in algorithm construction.

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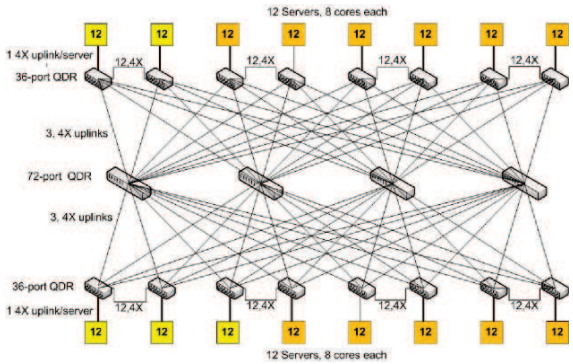
Network Topology



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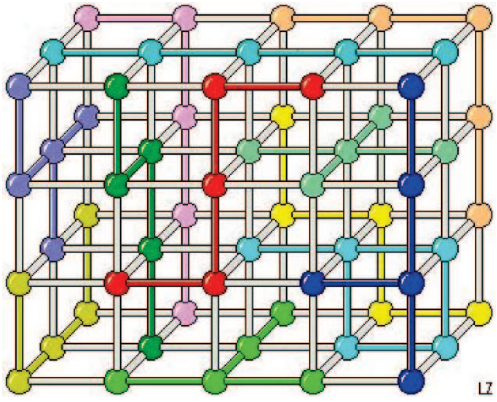
Virtual Topology



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Cartesian Topology

MPI_Cart_create(MPI_Comm old_comm, int ndims, int *dim_size, int *periods, int reorder, MPI_Comm *newcomm);

- Create a cartesian communicator
- with ndim (dimension) and dim_size (size)
- periods - 1 if some of the sides are periodic
- reorder - just ignor it

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MPI_Cart_create

```
MPI_Comm  old_comm, new_comm;
int ndims, reorder, ierr;
int dim_size[2], periods[2];

old_comm = MPI_COMM_WORLD;
ndims = 2;
dim_size[0] = 3;
dim_size[1] = 2;
periods[0] = 1;
periods[1] = 0;
reorder = 1;

MPI_Cart_create(old_comm, ndims, dim_size,
            periods, reorder, &new_comm);
```


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Cartesian Topology

Map rank to coordinate

- MPI_Cart_coords();
- Input rank
- Output coordinate

Map coordinate to rank

- MPI_Cart_rank();
- Input coordinate
- Output rank

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MPI_Cart_rank

```
MPI_Cart_create(old_comm, ndims, dim_size,
           periods, reorder, &new_comm);

for (i=0; i<nv; i++)
 for (j=0; j<mv; j++)  {
   coords[0] = i;
   coords[1] = j;
   MPI_Cart_rank(new_comm, coords, &rank);

   printf("%d, %d, %d\n",coords[0],coords[1],
          rank);
  }
```


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MPI_Cart_coords

```
MPI_Cart_create(old_comm, ndims, dim_size,
                periods, reorder, &new_comm);

 for (rank=0; rank<p; rank++) {
   MPI_Cart_coords(new_comm, rank, coords);
   printf("%d, %d\n ",rank, coords);
  }
```