Introduction to MPI

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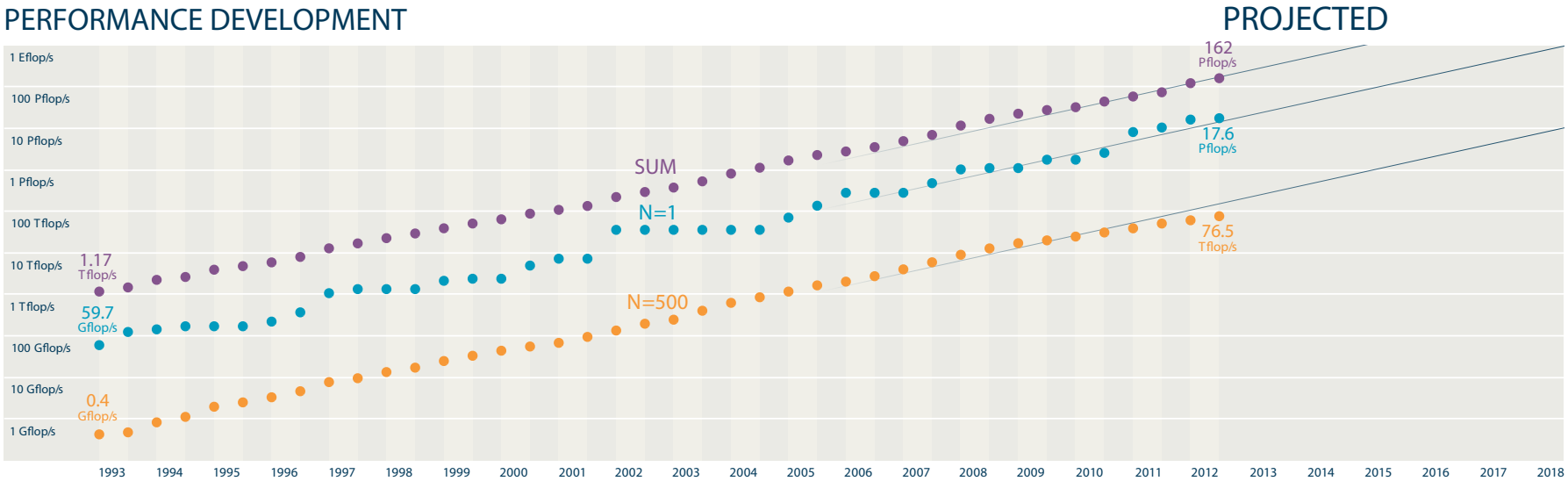
Top500.org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1 Gflop/s
SUM
N=1
N=500
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0.4 Gflop/s
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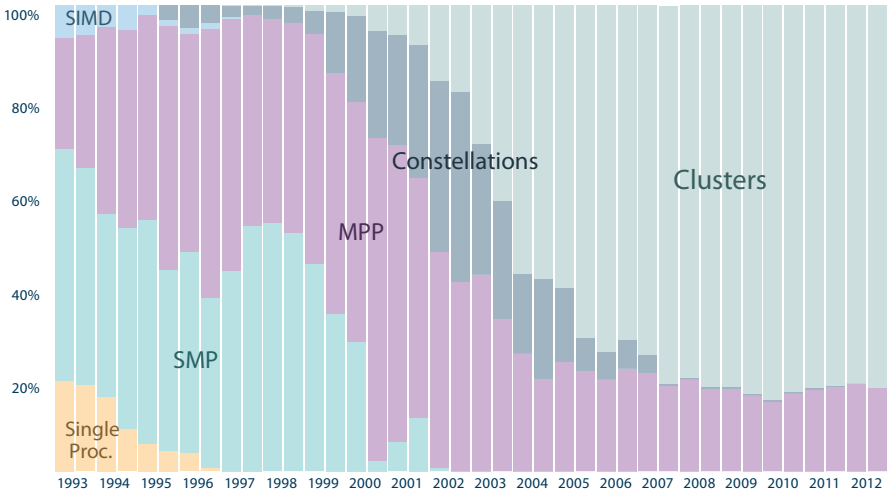
ARCHITECTURES
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Single Proc.
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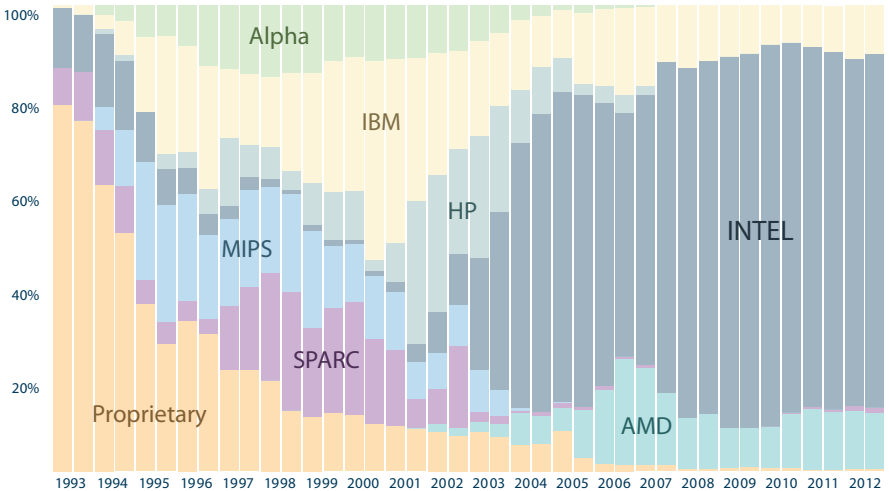
CHIP TECHNOLOGY
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Types of Parallelism

SISD	Single Instruction–Single Data	single core PCs
SIMD	Single Instruction–Multiple Data	GPUs
MISD	Multiple Instruction–Single Data	Esoteric
MIMD	Multiple Instruction–Multiple Data	multi-core PCs; most parallel computers

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$$\text{MIMD} \implies \text{Need to manage tasks and data}$$

$$\implies \text{MPI}$$

What is MPI?

MPI—Message Passing Interface

- Developed in early 1990s
- "...a portable, efficient, and flexible standard for message passing that will be widely used for writing message passing programs" [a]
- Describes a means to pass information between processes

[a] Blaise, `https://computing.llnl.gov/tutorials/mpi`

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MPI implementations

- Open source
  - MPICH (DOE's Argonne) `http://www.mpich.org`
  - MVAPICH (OSU) `http://mvapich.cse.ohio-state.edu/overview/mvapich2`
  - OpenMPI (community) `http://www.open-mpi.org`
- Vendor-specific (IBM, SGI, ...)

Why Use MPI?

1. Available: on nearly every parallel computer (including single CPU, multi-core systems)
2. Flexible: runs equally well on distributed memory, shared memory, and hybrid machines
3. Portable: same code runs on different machines without modification[1]
4. Fast: vendors *can* implement (parts of it) in hardware
5. Scalable: demonstrated to work well on 1,000,000+ processes
6. Stable: future exascale machines are expected to have MPI
7. Multi-lingual: MPI available in Fortran 77/90+, C, C++, Python, ...

[1] Usually, unless you and/or the implementation has a bug

MPI $\Longrightarrow$ Explicit Parallelism

Within MPI you, the programmer, must explicitly include all parallelism, including:

- Task decomposition (how the data is to be distributed)
- Task granularity (problem size per MPI process)
- Message organization & handling (send, receive)
- Development of parallel algorithms (*e.g.*, sparse mat-vec multiply)

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- Development of parallel algorithms (*e.g.*, sparse mat-vec multiply)

Other programming models, like OpenMP, can handle the parallelism at the compile stage (but usually at a loss of performance or scalability)

Using MPI & OpenMP together has some advantages on emerging computers (*e.g.*, $\sim$1,000 nodes with $\sim$100s cores each)

MPI Program Structure in Fortran

```
Program NULL
  Include 'mpif.h'
  Implicit None
  Integer :: rank, numprocs, ierr
  Call MPI_Init(ierr)
  Call MPI_Comm_rank( MPI_COMM_WORLD, rank, ierr )
  Call MPI_Comm_size( MPI_COMM_WORLD, numprocs, ierr )
  Write (*,'(2(A,I5),A)') 'Processor ', rank, ' of ', &
    numprocs, ' ready.'
  < do stuff >
  Call MPI_Finalize ( ierr )
End Program
```

MPI Program Structure in C

```
#include <stdio.h>
#include <stdlib.h>
#include "mpi.h"
int main (int argc, char *argv[])
{
  int ierr, rank, numprocs;
  ierr = MPI_Init();
  ierr = MPI_Comm_rank ( MPI_COMM_WORLD, &rank );
  ierr = MPI_Comm_size ( MPI_COMM_WORLD, &numprocs );
  printf("Processor %d of %d ready.\n"; rank, numprocs);
  < do stuff >
  ierr = MPI_Finalize();
  return EXIT_SUCCESS;
}
```

Dissecting The Program Structure

Structure of an MPI program (in any language):

1. Initialize code in *serial*
2. Initialize MPI
3. Do good work in parallel
4. Finalize MPI
5. Finalize code in *serial*

```
#include <stdio.h>
#include <stdlib.h>
#include "mpi.h"
int main (int argc, char *argv[])
{
  int ierr, rank, numprocs;
  ierr = MPI_Init();
  ierr = MPI_Comm_rank ( MPI_COMM_WORLD, &rank );
  ierr = MPI_Comm_size ( MPI_COMM_WORLD, &numprocs );
  printf("Processor %d of %d ready.\n"; rank, numprocs);
  < do stuff >
  ierr = MPI_Finalize();
  return EXIT_SUCCESS;
}
```

The MPI commands above define the Environment Management routines.

MPI_COMM_WORLD and Communicators

MPI Communicators

- Establish a group of MPI processes
- MPI_COMM_WORLD is the default and contains all processes
- Can be created, copied, split, destroyed
- Serve as an argument for most point-to-point and collective operations

Communicator datatypes

- Fortran: Integer (*e.g.*, `Integer :: mycomm`)
- C: MPI_Comm (*e.g.*, `MPI_Comm mycomm;`)
- C++: (*e.g.*, `MPI::Intercomm mycomm;`)

Communicator Examples :: MPI_COMM_WORLD

30	31	32	33	34	35
24	25	26	27	28	29
18	19	20	21	22	23
12	13	14	15	16	17
6	7	8	9	10	11
0	1	2	3	4	5

MPI_COMM_WORLD contains all 36 processors, ranks 0 through 35

Communicator Examples :: Other Possibilities

30	31	32	33	34	35
24	25	26	27	28	29
18	19	20	21	22	23
12	13	14	15	16	17
6	7	8	9	10	11
0	1	2	3	4	5

Each color could be a different communicator

Communicator Examples :: Other Possibilities

Each color (including white) could be a different communicator

Interlude #1—Parallel 'Hello, World!'

Write a MPI program that prints "Hello, World!" as below:

```
rank 0:  ‘‘Hello, World!’’
rank 1:  ‘‘Hello, World!’’
...
rank <numprocs-1>:  ‘‘Hello, World!’’
```

Do the processes write in ascending order?

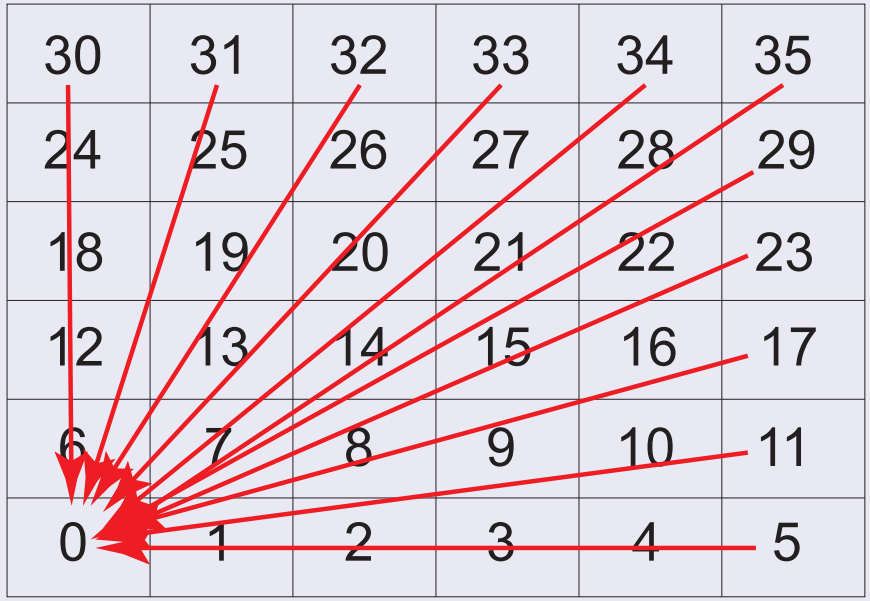
You have 30 minutes for this task.

Interprocess Communication in MPI

There are two primary types of communication

Point-to-point

Collective



Point-to-Point Send/Recv Communication in MPI

Process 13 'Send'

```
...
if (rank == 13) &
     Call MPI_Send (sbuf, count, type, dest, &
                    tag, comm, ierr)
...
```

variable	comment
sbuf	sending variable
count	sbuf element size
type	sbuf variable type
dest	process id in comm
tag	message tag
comm	communicator

Process 27 'Recv'

```
...
if (rank == 27) &
     Call MPI_Recv (rbuf, count, type, source, &
                    tag, comm, status, ierr)
...
```

variable	comment
rbuf	receiving variable
count	rbuf element size
type	rbuf variable type
source	process id in comm
tag	message tag
comm	communicator
status	message status

Point-to-Point Send/Recv Communication in MPI

```
Call MPI_Send (sbuf, count, type, dest, tag, comm, ierr)
```

Example:

```
Integer :: N, dest, tag, ierr
Real(KIND=8), Pointer :: sbuf(:)
...
N = 100
tag = 1
dest = 27
allocate(sbuf(N))
Call MPI_Send (sbuf, N, MPI_REAL8, dest, tag, &
               MPI_COMM_WORLD, ierr)
...
```

Point-to-Point Send/Recv Communication in MPI

```
Call MPI_Recv (rbuf, count, type, source, tag, comm, status, i
```

Example:

```
Integer :: N, dest, tag, ierr
Real(KIND=8), Pointer :: rbuf(:)
Integer :: status(MPI_STATUS_SIZE)
...
N = 100
tag = 1
source = 13
allocate(rbuf(N))
Call MPI_Recv (rbuf, N, MPI_REAL8, source, tag, &
               MPI_COMM_WORLD, status, ierr)
...
```

Note: `status` contains source id, tag, and count of the message received (useful for debugging when sending multiple messages)

MPI Predefined Datatypes[2]

Fortran	C	Comment
MPI_CHARACTER	MPI_CHAR	Character
MPI_INTEGER	MPI_INT	Integer
MPI_REAL	MPI_FLOAT	Single precision
MPI_REAL8	—	`Real(KIND=8)` in Fortran
MPI_DOUBLE_PRECISION	MPI_DOUBLE	Double precision
MPI_LOGICAL	MPI_C_BOOL	Logical
...		

[2] There exist many more!

Interlude #2a—Send/Recv Example

Write a MPI program that passes one integer from process 0 to process `numprocs-1` through each process (1, 2, ..., `numprocs-2`) and adds one to it after each `MPI_Recv`.

You have 30 minutes for this task.

MPI_Send and MPI_Recv Are Blocking

When `MPI_Send` or `MPI_Recv` are called, that process waits and is blocked from performing further communication and/or computation.

Advantage: buffers `sbuf` and `rbuf` are able to be reused once the call finishes.

Disadvantage: code waits for matching Send/Recv pair to complete.

MPI provides non-blocking communication routines `MPI_Isend` and `MPI_Irecv`.

```
Call MPI_Isend (sbuf, count, datatype, dest, tag, comm, &
                request, ierr)
Call MPI_Irecv (rbuf, count, datatype, src, tag, comm, &
                request, ierr)
Call MPI_Wait (request, status, ierr)
```

Must watch buffer use closely.

Non-Blocking Point-to-Point Communication

Communication and computation can overlap—the key to getting good scalability!

High-Level Example

```
...
Call MPI_Isend (sbuf, count, datatype, dest, tag(1), comm, &
                request(1), ierr)
Call MPI_Irecv (rbuf, count, datatype, src, tag(2), comm, &
                request(2), ierr)

< do work while the Send and Recv complete >

Call MPI_Waitall (2, request, status, ierr)
...
```

Interlude #2b—Blocking vs. Nonblocking Send/Recv

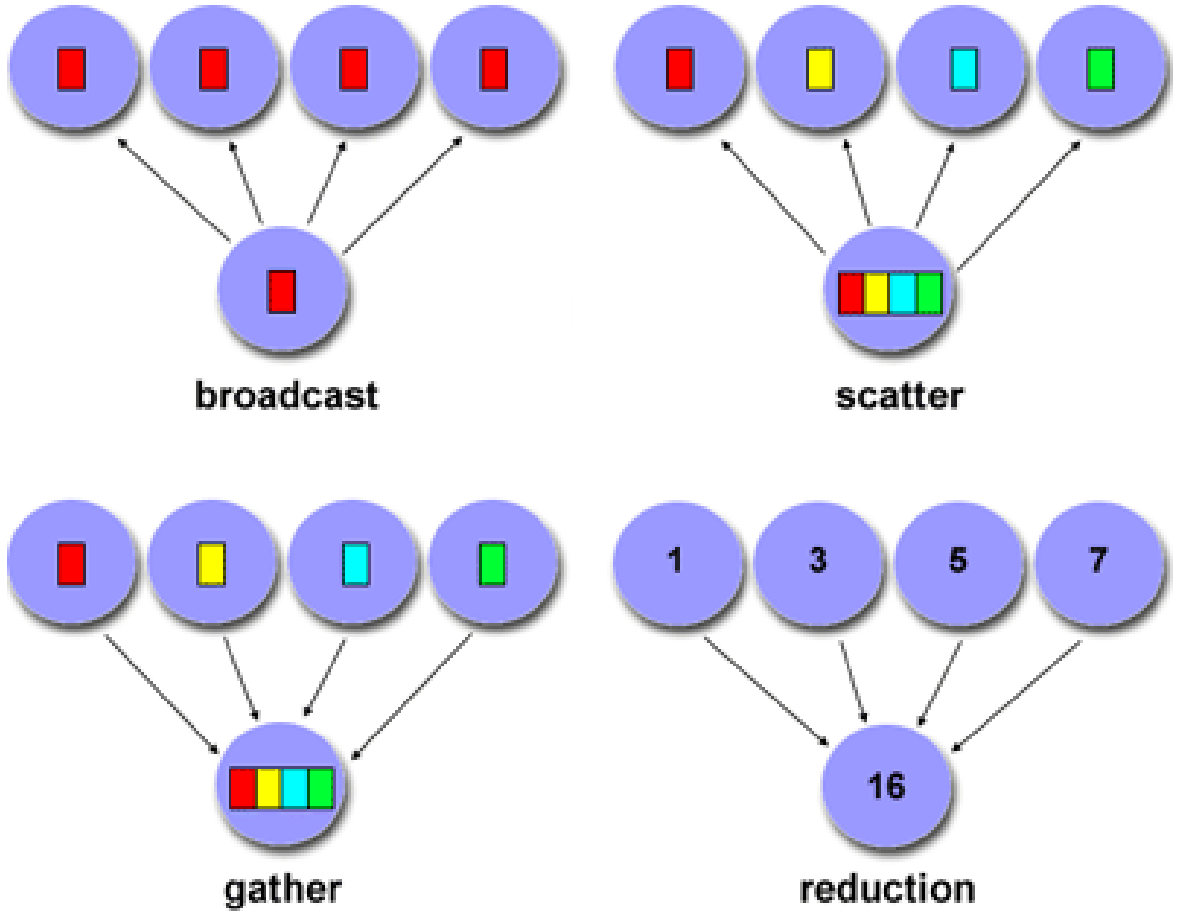
Compile and run Blaise Barney's `mpi_bandwidth.[c,f]` and `mpi_bandwidth_nonblock.[c,f]` to observe the differences between blocking and non-blocking communications.

file	url
mpi_bandwidth.c	`https://computing.llnl.gov/tutorials/mpi/samples/C/mpi_bandwidth.c`
mpi_bandwidth_nonblock.c	`https://computing.llnl.gov/tutorials/mpi/samples/C/mpi_bandwidth_nonblock.c`
mpi_bandwidth.f	`https://computing.llnl.gov/tutorials/mpi/samples/Fortran/mpi_bandwidth.f`
mpi_bandwidth_nonblock.f	`https://computing.llnl.gov/tutorials/mpi/samples/Fortran/mpi_bandwidth_nonblock.f`

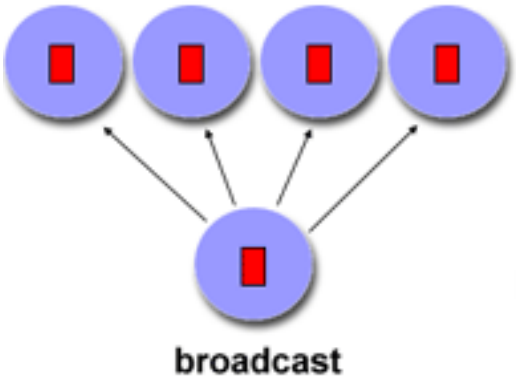
You have 15 minutes for this task.

Collective Communications

In many circumstances, all processes on a communicator must exchange data $\Longrightarrow$ collective communication.



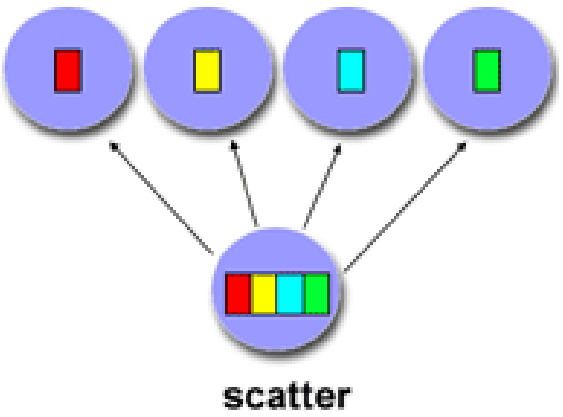
MPI_Bcast




```
Call MPI_BCAST (buffer, count, datatype, &
                root, comm, ierr)

MPI_Bcast (&buffer, count, datatype,
           root, comm);
```

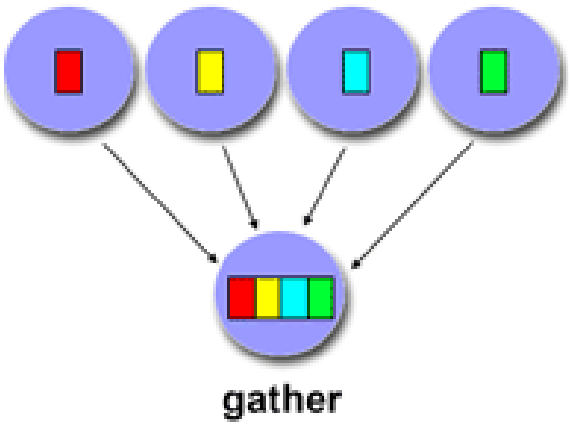
MPI_Scatter




```
Call MPI_SCATTER (sbuf, scount, stype, &
                  rbuf, rcount, rtype, &
                  root, comm, ierr)

MPI_Scatter (&sbuf, scount, stype,
             &rbuf, rcount, rtype,
             root, comm);
```

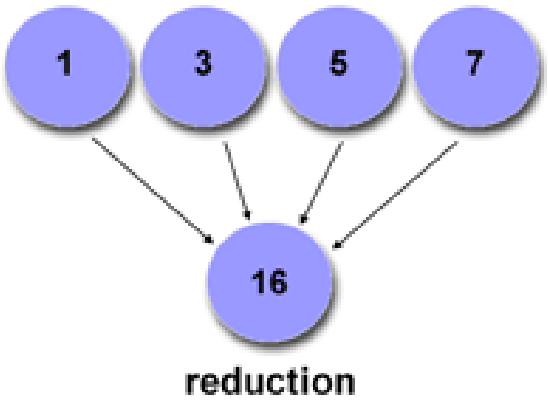
MPI_Gather




```
Call MPI_GATHER (sbuf, scount, stype, &
                 rbuf, rcount, rtype, &
                 root, comm, ierr)
```

```
MPI_Gather (&sbuf, scount, stype,
            &rbuf, rcount, rtype,
            root, comm);
```

MPI_Reduce




```
Call MPI_REDUCE (sbuf, rbuf, rcount, &
                 rtype, op, root, &
                 comm, ierr)

MPI_Reduce (&sbuf, &rbuf, rcount, &
            rtype, op, root, &
            comm);
```

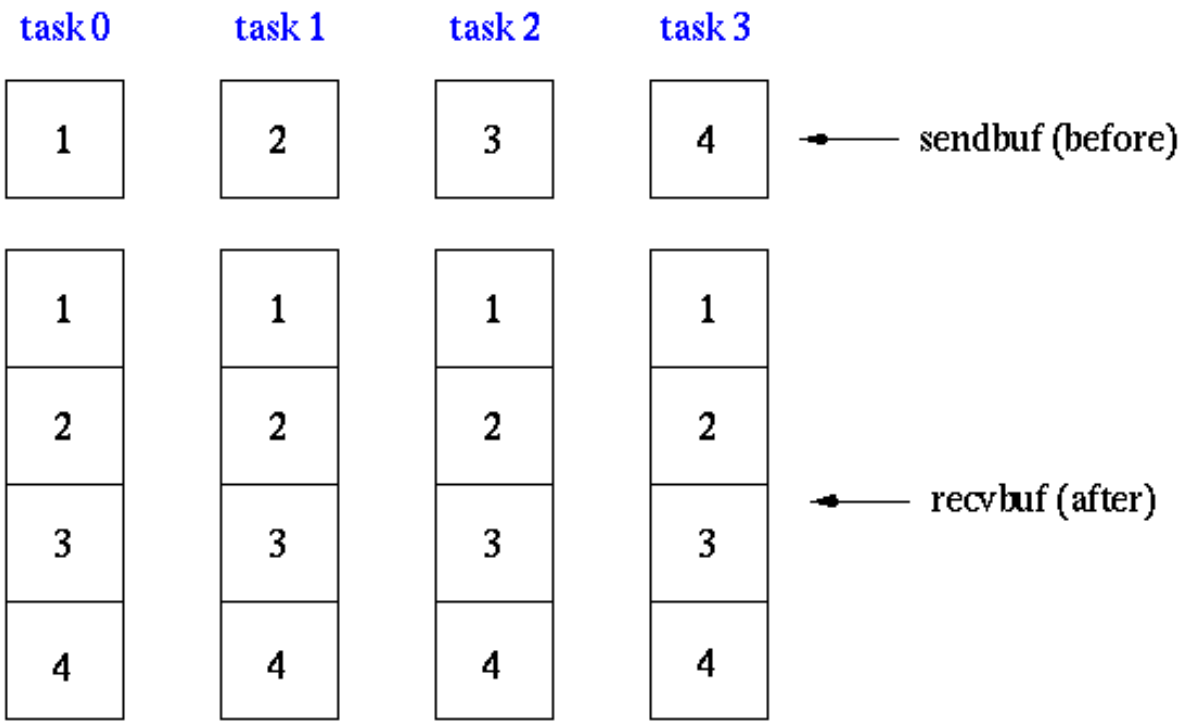
op	description
MPI_MAX	maximum
MPI_MIN	minimum
MPI_SUM	sum
MPI_PROD	product
⋮	

'All' Variants of MPI Collective Routines

MPI_Allgather

Gathers together values from a group of processes and distributes to all

```
sendcnt = 1;
recvcnt = 1;
MPI_Allgather(sendbuf, sendcnt, MPI_INT,
              recvbuf, recvcnt, MPI_INT,
              MPI_COMM_WORLD);
```

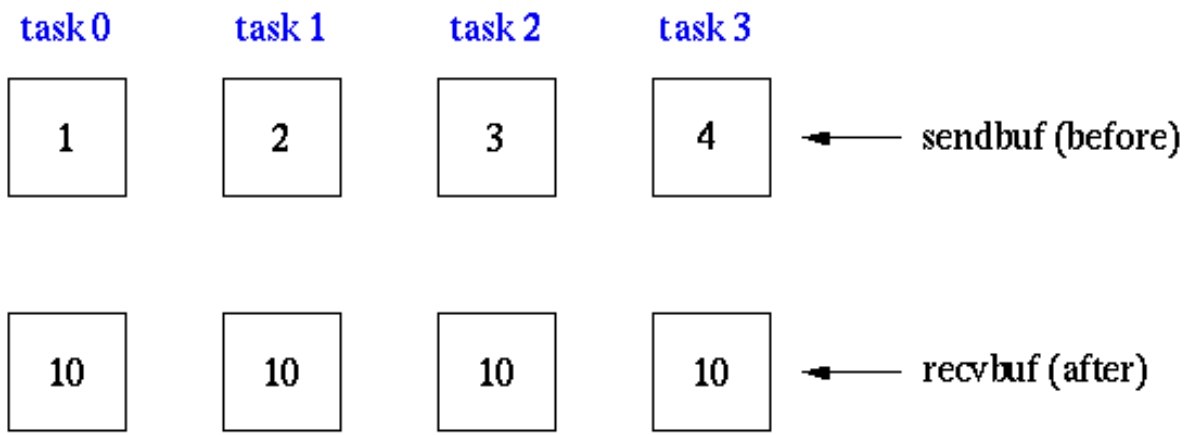


'All' Variants of MPI Collective Routines

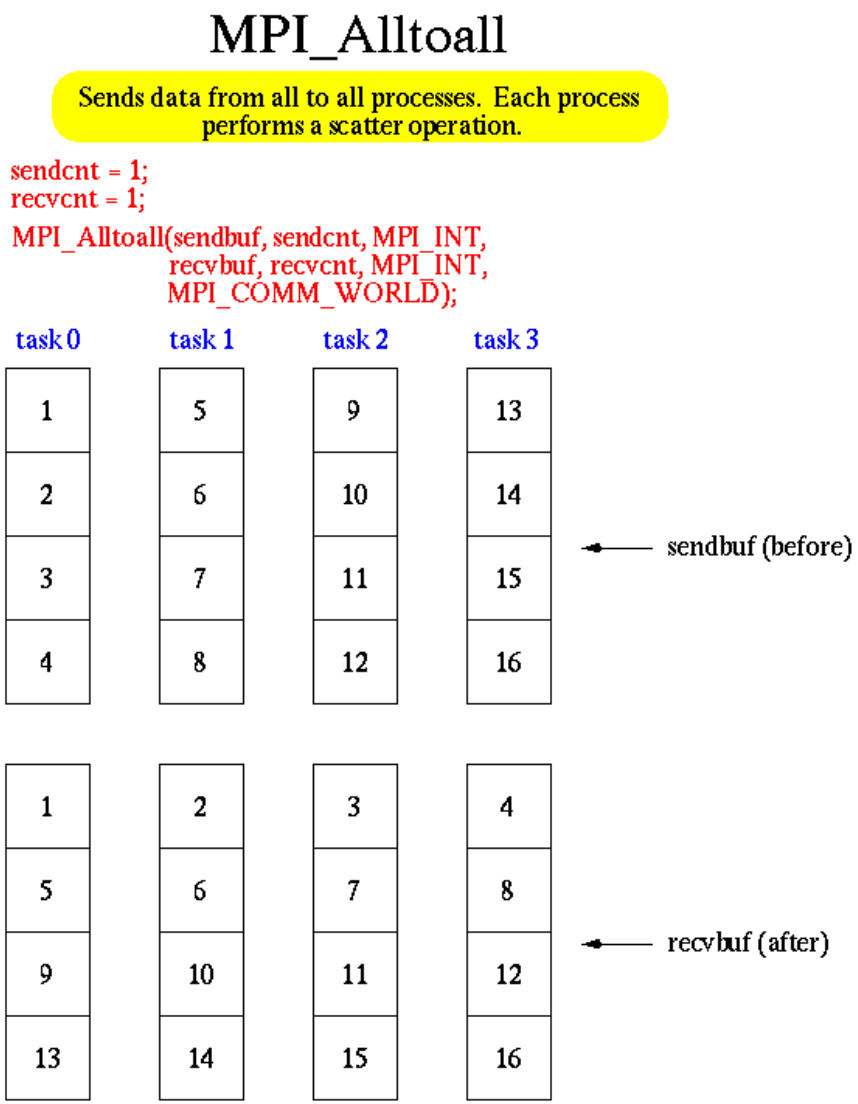
MPI_Allreduce

Perform and associate reduction operation across all tasks in the group and place the result in all tasks

```
count = 1;
MPI_Allreduce(sendbuf, recvbuf, count, MPI_INT, MPI_SUM,
              MPI_COMM_WORLD);
```



‘All’ Variants of MPI Collective Routines



Useful for matrix transpose and FFTs. (NOTE: It’s future on exascale machines is not clear.)

Interlude #3—Parallel Inner Product

Develop a parallel code to take the scalar product of two $N \times 1$ vectors $\vec{x}$ and $\vec{y}$, *i.e.*, $\vec{x}^T \vec{y}$. Choose $N > 5N_p$, where N_p is the number of MPI processes. Have the scalar answer stored on all processors.

You have 30 minutes for this task.

Interlude #4—Parallel Matrix Transpose

Use `MPI_Alltoall` to take the transpose of a $10N_p \times 10N_p$ matrix, where N_p is the number of MPI processes used.

You have 30 minutes for this task.

Summary

What MPI commands did we learn?

- MPI_Init
- MPI_Comm_rank, MPI_Comm_size
- MPI_Finalize
- MPI_Send, MPI_Recv
- MPI_Isend, MPI_Irecv
- MPI_Waitall
- MPI_Scatter, MPI_Bcast
- MPI_Gather, MPI_Reduce
- MPI_Allreduce, MPI_Allscatter
- MPI_Alltoall
- MPI_Barrier

These commands will get you very far in your parallel program development.

Additional Resources

1. http://www.mcs.anl.gov/research/projects/mpi/tutorial/index.html
2. https://computing.llnl.gov/tutorials/parallel_comp/
3. https://computing.llnl.gov/tutorials/mpi/
4. http://www.mpi-forum.org/