MPI

https://github.com/ResearchComputing/Final_Tutorials/tree/master/MPI

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Overview

- Background
- MPI
- Interactive Session
- Communicator
- Data Types
- Communications
- Point to Point Communications
- Collective Communications

Overview

Background

MPI

Interactive Session

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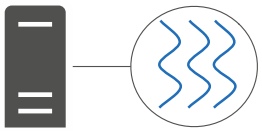
Parallelism

Parallelism can be achieved across many levels

- Nodes – MPI

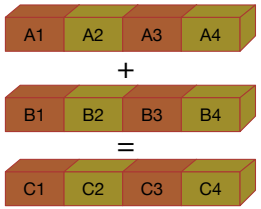
- Threads – OpenMP



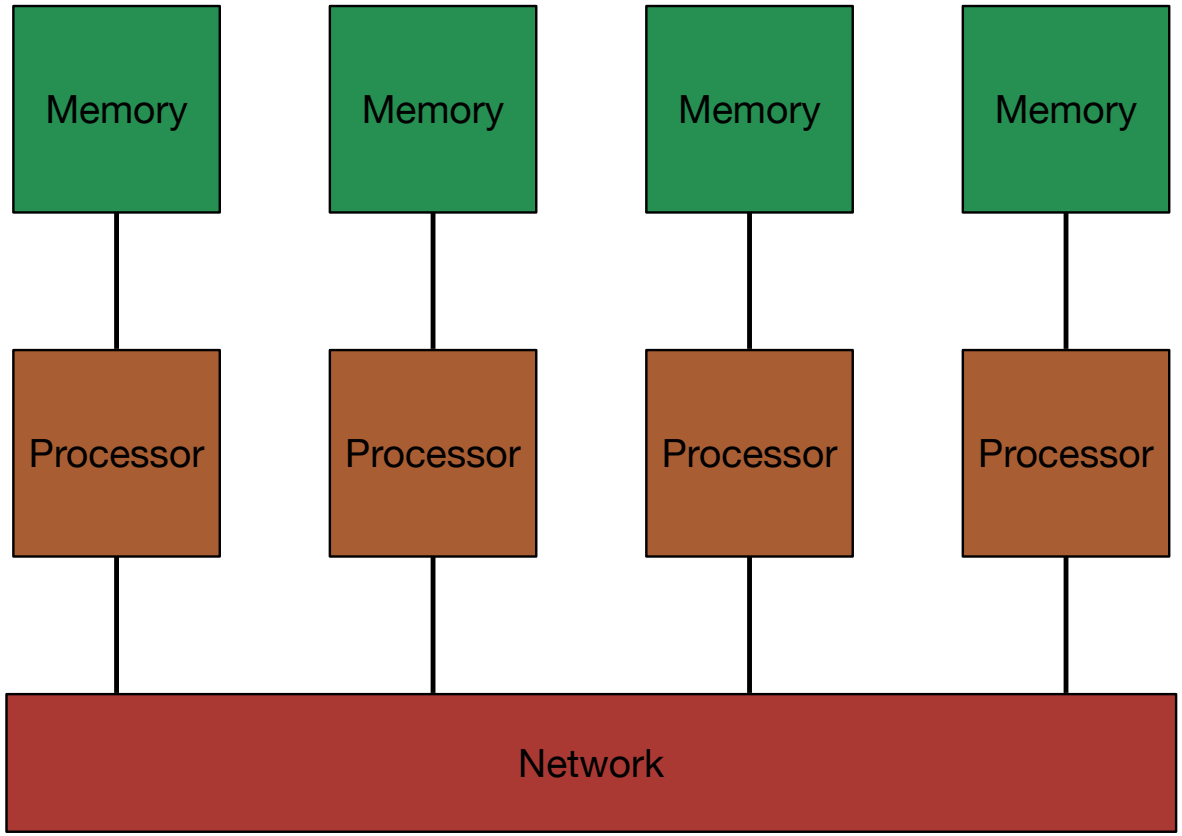
- Instructions – ILP

```
I1: add R1,   R2, R3
I2: sub R4,   R1, R5
I3: xor  R10, R2, R11
```

- Data – SIMD



Distributed Memory Model



- All processors see a different view of data.
- Processors interact and synchronize by passing messages.

Message Passing

- Most natural and efficient paradigm for distributed-memory systems.
- Two-sided, send and receive communication between processes.
- Efficiently portable to shared-memory or almost any other parallel architecture: “assembly language of parallel computing” due to universality and detailed, low-level control of parallelism.

- Provides natural synchronization among processes (through blocking receives, for example), so explicit synchronization of memory access is unnecessary.
- Sometimes deemed tedious and low-level, but thinking about locality promotes:
  - good performance
  - scalability
  - portability

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Programming

- MPI (Message Passing Interface).
- Message passing standard, universally adopted library of communication routines callable from C, C++, Fortran, Java, (Python).
- 125+ functions—I will introduce a small subset of functions.

MPI

- MPI has been developed in three major stages, MPI 1, MPI 2 and MPI 3.
  - MPI 1 – 1994
  - MPI 2 – 1996
  - MPI 3 – 2012
- MPI Forum
  `http://www.mpi-forum.org/docs/docs.html`
- MPI Standard
  `http://www.mpi-forum.org/docs/mpi-3.0/mpi30-report.pdf`
- *Using MPI* and *Using Advanced MPI*
  `http://www.mcs.anl.gov/research/projects/mpi/usingmpi/`
- Online MPI tutorial
  `http://mpitutorial.com/beginner-mpi-tutorial/`

MPI 1

- Features of MPI-1 include:
  - Point-to-point communication.
  - Collective communication process.
  - Groups and communication domains.
  - Virtual process topologies.
  - Environmental management and inquiry.
  - Profiling interface bindings for Fortran and C.

MPI 2

- Additional features of MPI-2 include:
  - Dynamic process management input/output.
  - One-sided operations for remote memory access (update or interrogate).
  - Memory access bindings for C++.

MPI 3

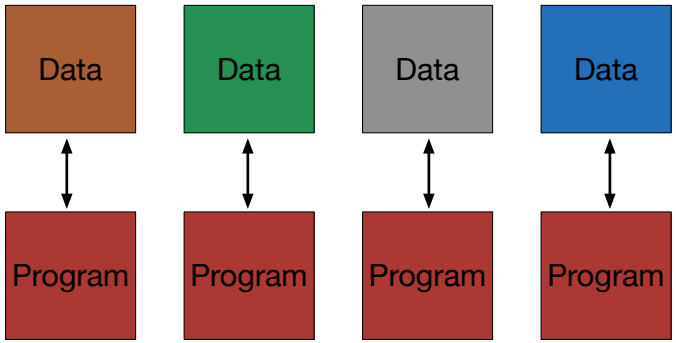
- Updates, corrections and clarifications of MPI-3 include:
  - Non-blocking collectives.
  - New one-sided communication operations.
  - Fortran 2008 bindings.

Implementations

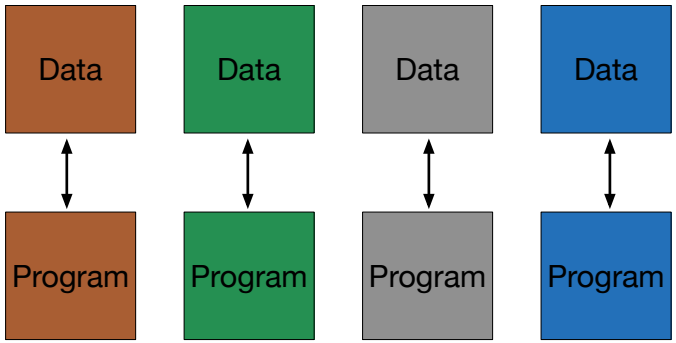
- MPICH `ftp://ftp.mcs.anl.gov/pub/mpi`
- OpenMPI `http://www.open-mpi.org/`
- Intel MPI
  `https://software.intel.com/en-us/intel-mpi-library`
- SGI
- Cray
- IBM

Programming Models

- Single Program Multiple Data (SPMD)
  - Same program runs on each process.



- Multiple Programs Multiple Data (MPMD)
  - Different programs runs on each process.



Compiling

Most MPI implementations have wrapper scripts for the compiler.

C

```
mpicc -o a.out a.c
```

Fortran

```
mpifc -o a.out a.f90
```

If not, you will need to specify the include path, library path and link to the library.

Execution

Once your program has compiled you can run it:

- Through a batch system (SLURM for example).

```
login01 ~$ srun -N 1 --ntasks-per-node=12 ./a.out
```

- Through `mpiexec`.

```
node0001 ~$ mpiexec -n 12 ./a.out
```

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Janus

1. Log in to Janus.

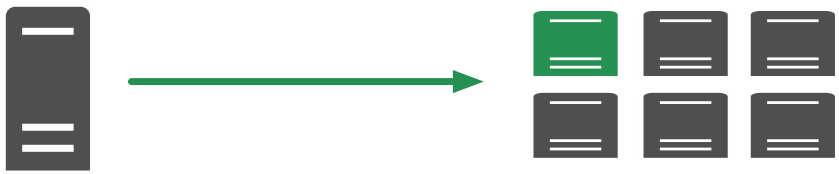
```
laptop ~$ ssh user0000@tutorial-login.rc.colorado.edu
```

2. Load the slurm module.

```
[user0000@tutorial-login ~]$ ml slurm
```

3. Start a compute job.

```
[user0000@tutorial-login ~]$ sinteractive  \
                             -t 01:00:00 -N 1    \
                             --reservation=meetup
```



4. Load the Intel compiler and MPI library.

```
[user0000@node1234 ~]$ ml intel
[user0000@node1234 ~]$ ml impi
```

Program Structure

C

```c
#incude <mpi.h>

int ierr = 0;
ierr = MPI_Init(&argc,
                &argv);
...
ierr = MPI_Finalize();
```

Fortran

```fortran
use mpi

integer :: ierr
ierr = 0
call MPI_Init(ierr)
...
call MPI_Finalize(ierr)
```

- C returns error codes as function values.
- Fortran uses the last argument (ierr).

Note: All MPI calls *should* have man-pages.

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Communicator

- A collection of processors working on some part of a parallel job.
- Used as a parameter for most MPI calls.
- Processors within a communicator are assigned ranks 0 to $n-1$.
- `MPI_COMM_WORLD` includes all of the processors in your job.
- Can create subsets of `MPI_COMM_WORLD`

Fortran

```fortran
program hello
  use mpi
  implicit none

  integer :: ierr
  integer :: id, nprocs
  ierr = 0
  call MPI_Init(ierr)
  call MPI_Comm_rank(MPI_COMM_WORLD, id, ierr)
  call MPI_Comm_size(MPI_COMM_WORLD, nprocs, ierr)
  call MPI_Finalize(ierr)

end program hello
```

- Determine the process rank (`id`).
- Total number of processes (`nprocs`).

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Data Types

Fortran	Optional	C
MPI_CHARACTER		MPI_CHAR
MPI_COMPLEX	8, 16, 32	MPI_DOUBLE
MPI_DOUBLE_COMPLEX		MPI_FLOAT
MPI_DOUBLE_PRECISION		MPI_INT
MPI_INTEGER	1, 2, 4, 8	MPI_LONG_DOUBLE
MPI_LOGICAL	1, 2, 4, 8	MPI_LONG_LONG
MPI_REAL	2, 4, 8, 16	MPI_LONG_LONG_INT
		MPI_SHORT
		MPI_SIGNED_CHAR
		MPI_UNSIGNED
		MPI_UNSIGNED_CHAR
		MPI_UNSIGNED_LONG
		MPI_UNSIGNED_LONG_LONG
		MPI_UNSIGNED_SHORT
		MPI_WCHAR

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Communications

- Bytes transferred from one processor to another.
- Specify destination, data buffer, and message ID (called a tag).
- Synchronous send: send call does not return until the message is sent.
- Asynchronous send: send call returns immediately, send occurs during other calculation ideally.
- Synchronous receive: receive call does not return until the message has been received (may involve a significant wait).
- Asynchronous receive: receive call returns immediately. When received data is needed, call a wait subroutine.
- Asynchronous communication used in attempt to overlap communication with computation.

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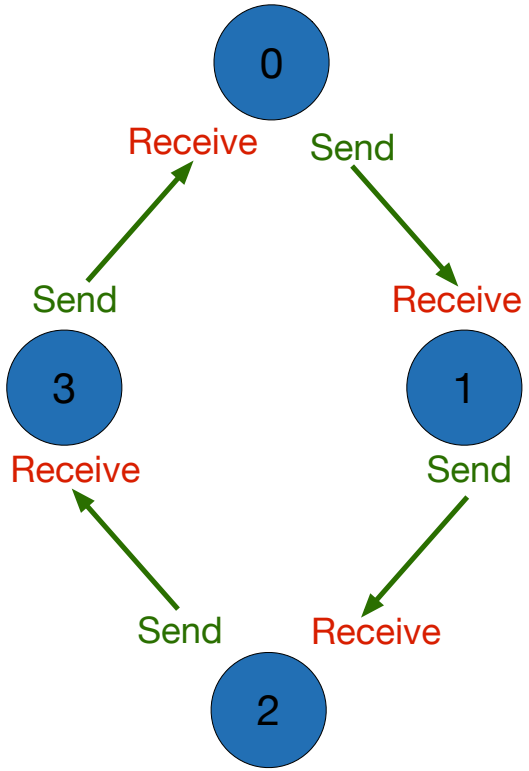
Point to Point Communications

- `MPI_Send()`
  - Does not return until the message data and envelope have been buffered in matching receive buffer or temporary system buffer.
  - Can complete as soon as the message was buffered, even if no matching receive has been executed by the receiver.
  - MPI buffers or not, depending on availability of space.
  - **Non-local**: successful completion of the send operation may depend on the occurrence of a matching receive.
- `MPI_Recv()`
  - The opposite of `MPI_Send()`.
  - Does not return until the message data has been copied into the destination buffer.
  - Stalls progress of program **but**:
    - Blocking sends and receives enforce process synchronization.
    - Enforces consistency of data.

Sending Data In A Ring

Sending n elements to the $rank + 1$ receive n elements from the $rank - 1$.

- Store them in an array of size $nprocs \times n$.
- Sum up and print the local results.



Ring Data Nprocs = 4, N = 3

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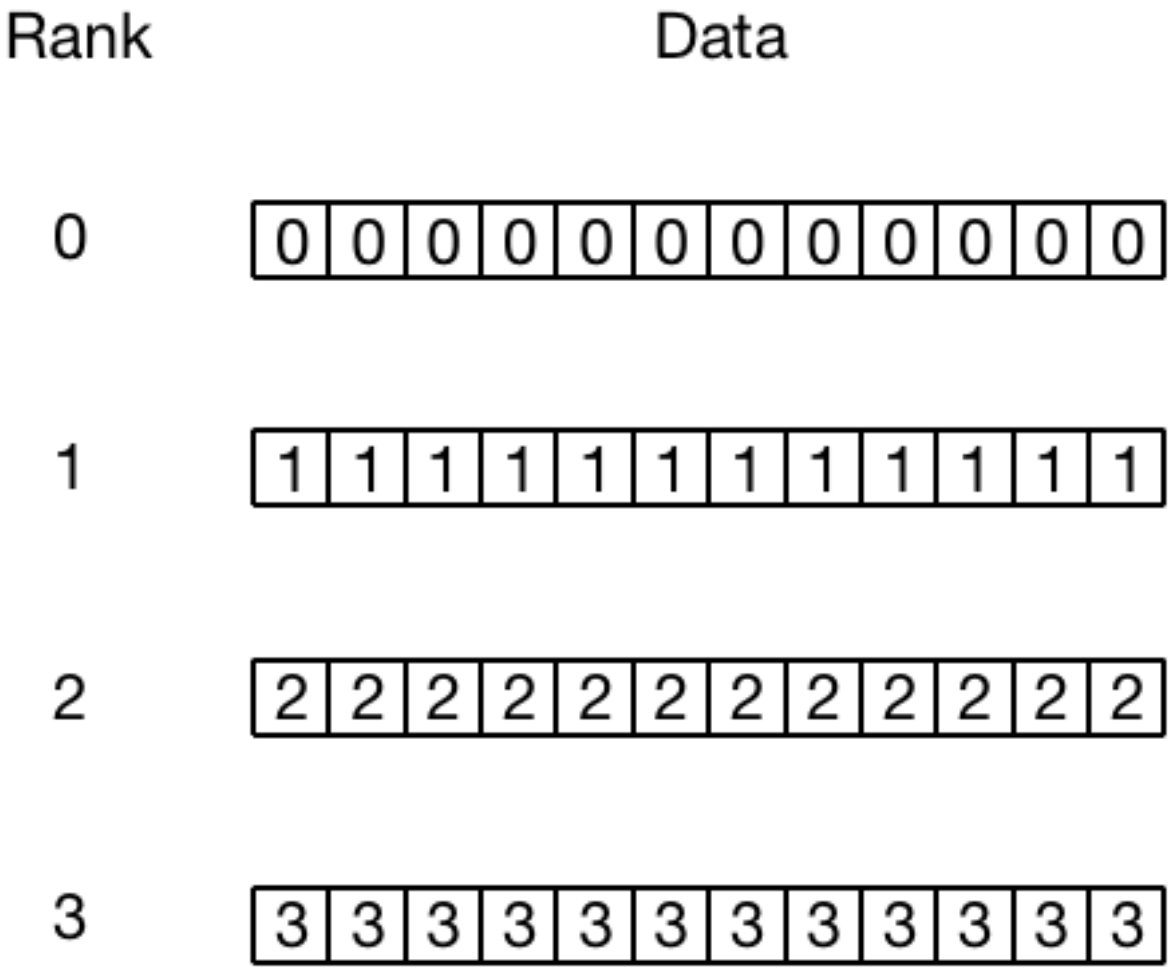
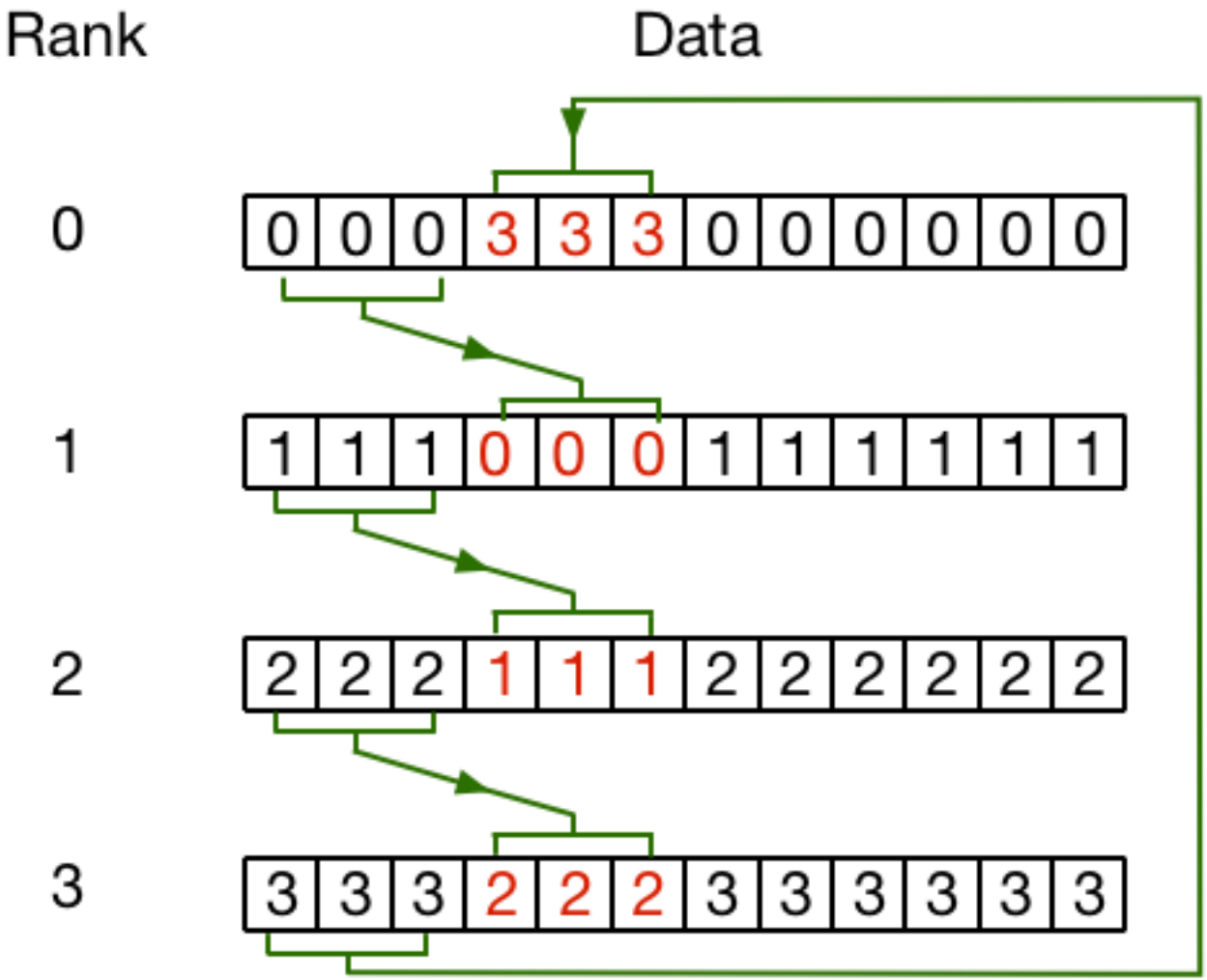


Ring Data Nprocs = 4, N = 3



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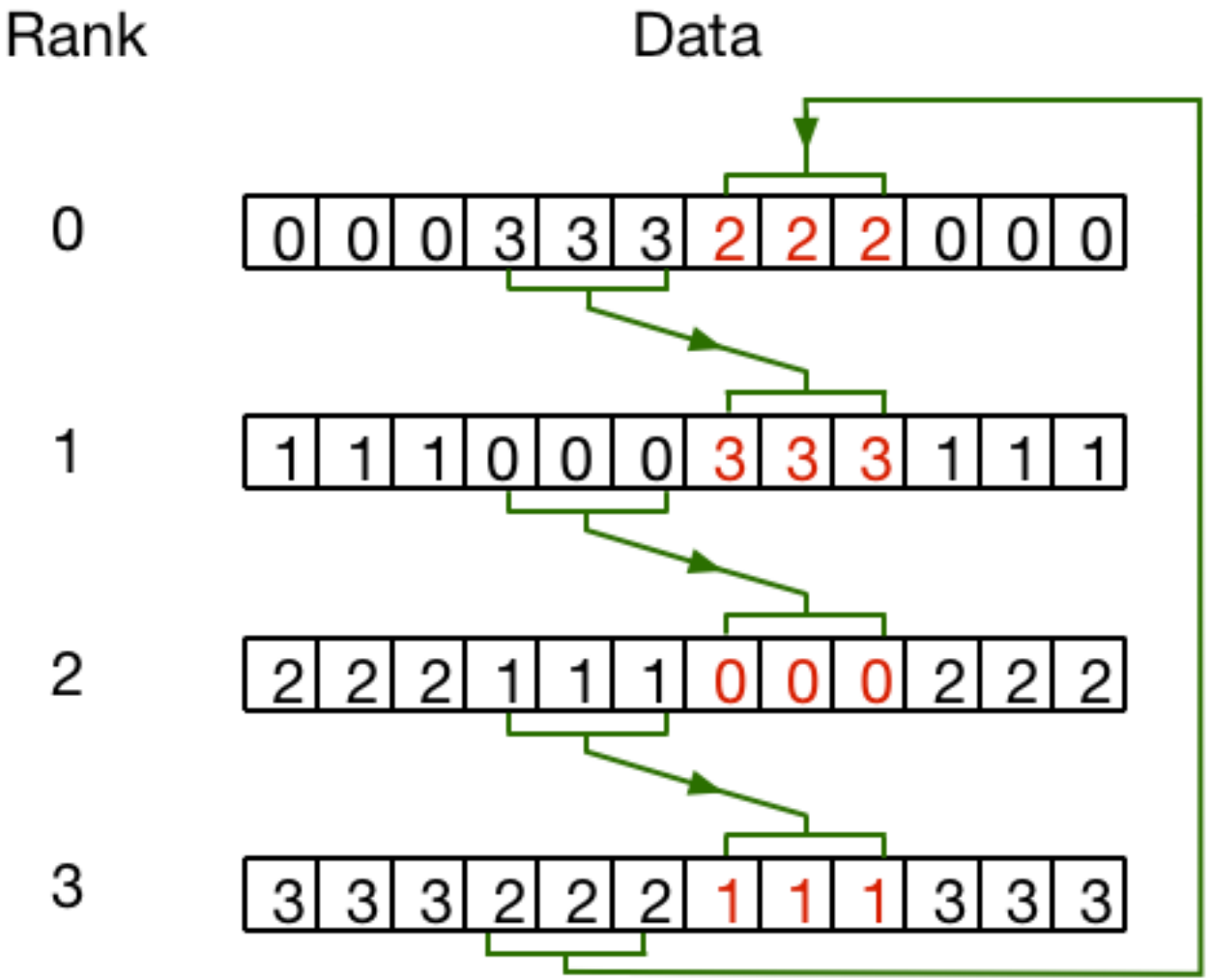
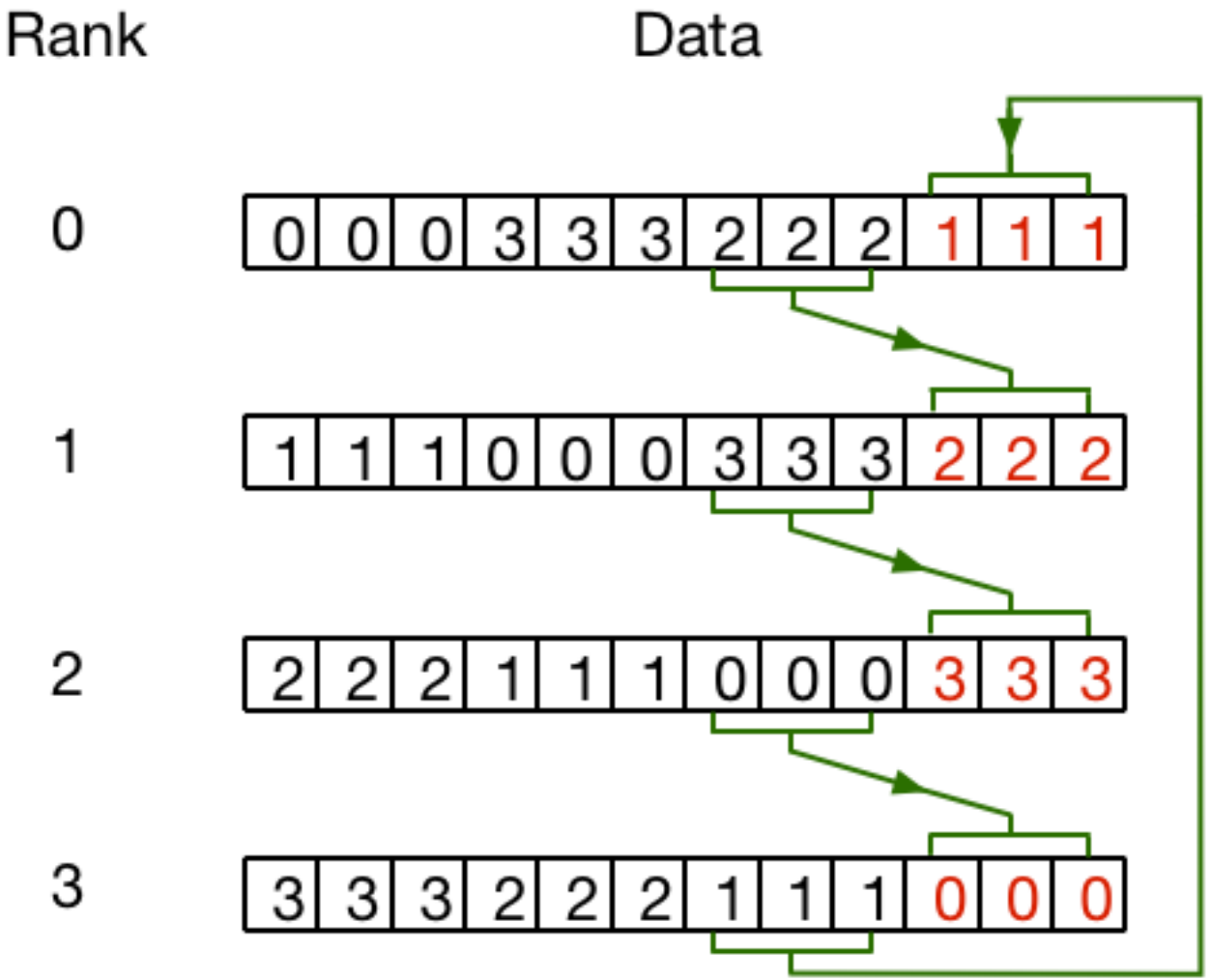


Ring Data Nprocs = 4, N = 3



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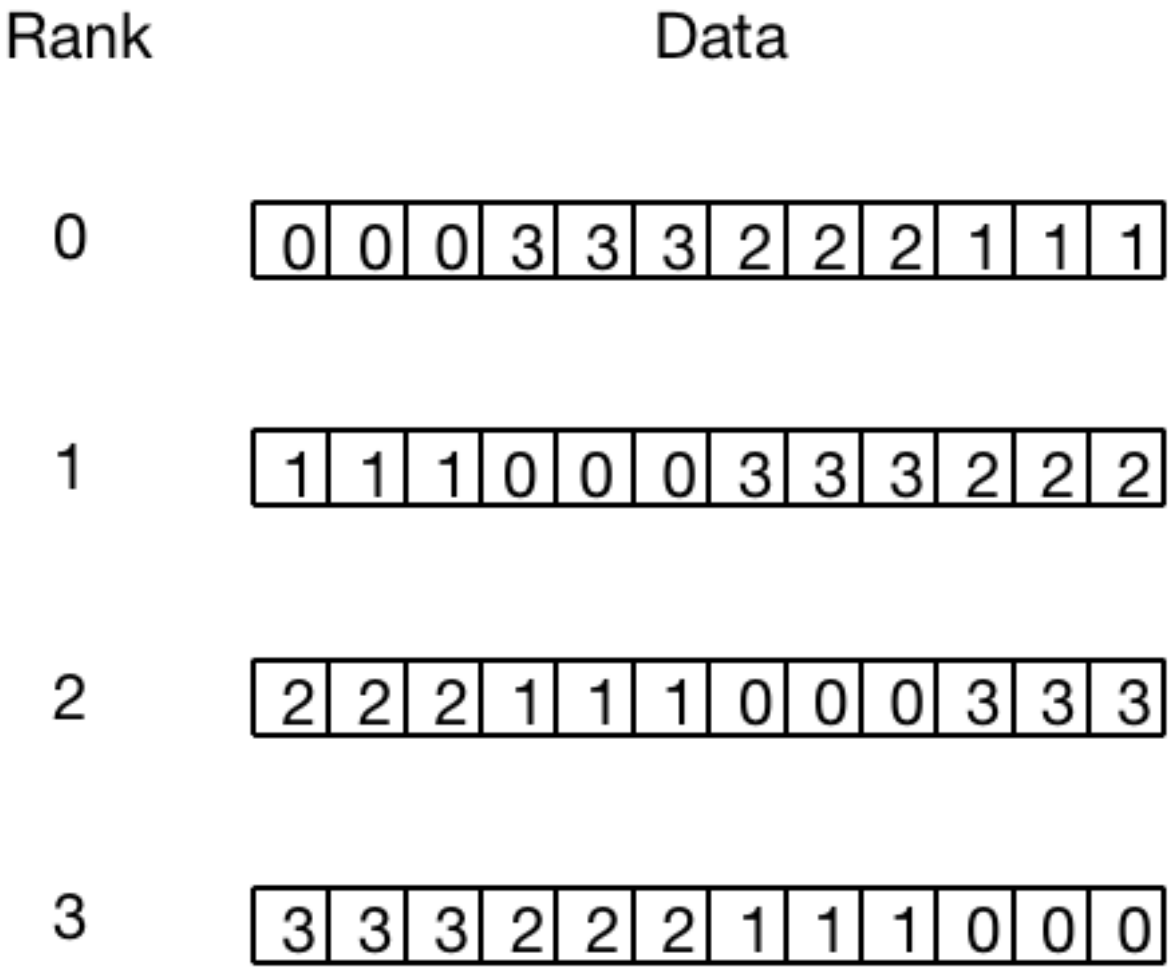

For Success

- Sender must specify a valid destination rank.
- Receiver must specify a valid source rank.
- The communicator must be the same.
- Tags must match.
- Message data types must match.
- Receiver's buffer must be large enough.

Ring Program

The program `ring.c` has been written using blocking `MPI_Send/Recv()`.
Compile and run the program with different array sizes:

- $N = 10$
- $N = 100000$

Deadlocks

A process waiting for a condition that will never become true.

- Easy to write send/receive code that deadlocks
  - Two processes: both receive before send.
  - Send tag does not match receive tag.
  - Process sends message to wrong destination process.

Non-Blocking Send & Receive

Non-Blocking Send `MPI_Isend()` and Receive `MPI_Irecv()`.

- Same syntax as `MPI_Send()/MPI_Recv()` with the addition of a request handle.
- Request handle (`integer` in Fortran; `MPI_Request` in C) is used to check for completeness of the send.
- These calls returns immediately.
- Data in the buffer may not be accessed until the user has completed the send/receive operation.
- The send is completed by a successful call to `MPI_Test()` or a call to `MPI_Wait()`.

Non-Blocking Wait

Non-Blocking Wait for ISend completion `MPI_Wait()`

```
MPI_Wait(requset, status, ierr)
```

- Request is the handle returned by the non-blocking send or receive call.
- Upon return, status holds source, tag, and error code information.
- This call does not return until the non-blocking call referenced by request has completed.
- Upon return, the request handle is freed.
- If request was returned by a call to `MPI_ISend()`, return of this call indicates nothing about the destination process.

Wait for any specified send or receive to complete.

```
MPI_Waitany(count, requsets, index, status, ierr)
```

- Requests is an array of handles returned by nonblocking send or receive calls.
- Count is the number of requests.
- This call does not return until a non-blocking call referenced by one of the requests has completed.
- Upon return, index holds the index into the array of requests of the call that completed.
- Upon return, status holds source, tag, and error code information for the call that completed.
- Upon return, the request handle stored in `requests[index]` is freed.

Wait for all specified send or receive to complete.

```
MPI_Waitall(count, requsets, status, ierr)
```

- Requests is an array of handles returned by nonblocking send or receive calls.
- `Count` is the number of requests.
- This call does not return until all non-blocking call referenced by one of the `requests` has completed.
- Upon return, `status` holds source, tag, and error code information for all the call that completed.
- Upon return, the request handle stored in `requests` is freed.

Tests for the completion of a specific send or receive.

`MPI_Test(request, flag, status, ierr)`

- `Request` is a handle returned by a non-blocking send or receive call.
- Upon return, `flag` will have been set to true if the associated non-blocking call has completed. Otherwise it is set to false.
- If `flag` returns true, the request handle is freed and status contains source, tag, and error code information.
- If request was returned by a call to `MPI_Isend()`, return with flag set to true indicates nothing about the destination process.

Non-Blocking Ring

A fixed ring program called `iring.f90` uses no-blocking `MPI_ISend/IRecv()`.

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Collective Communications

- Synchronization points:
- One to all:
  - Broadcast data to all ranks.
  - Scatter (all and parts).
- All to one:
  - Gather from a group.
  - Gather varying amounts from all.
  - Reduce values on all.
- All to all
  - Gather and distribute to all.
  - Gather and distribute various amounts to all.
  - Combines values from all processes and distribute.

Synchronization

- Synchronization between MPI processes in a group.

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

comm Communicator.

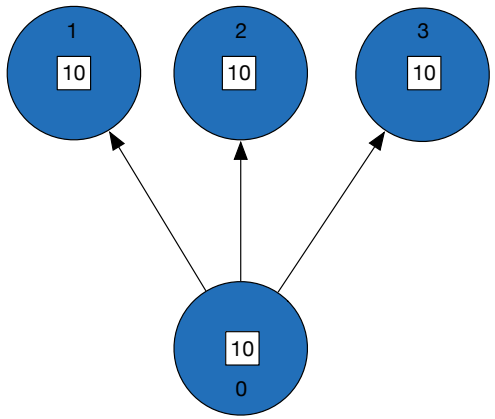
ierr Error status.

Broadcast

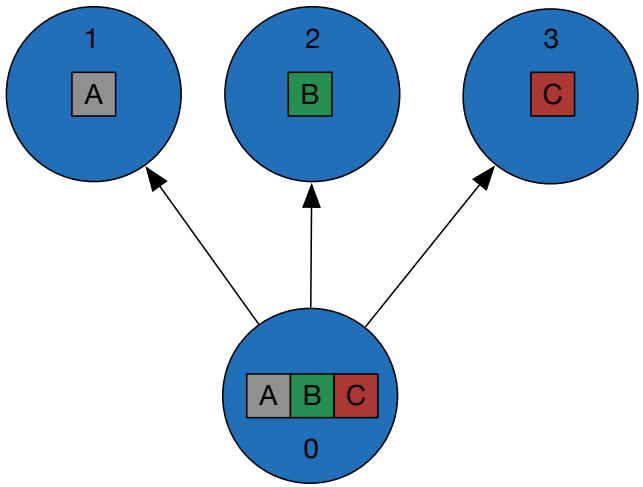
Broadcasts a message from the process with rank root to all other processes of the group.

```
MPI_Bcast(buf, count, data_type, root, comm, ierr)
```

buf	Beginning address of data.
count	Length of the source array (in elements).
data_type	MPI type of data.
root	Rank of broadcast root.
comm	Communicator.
ierr	Error status.

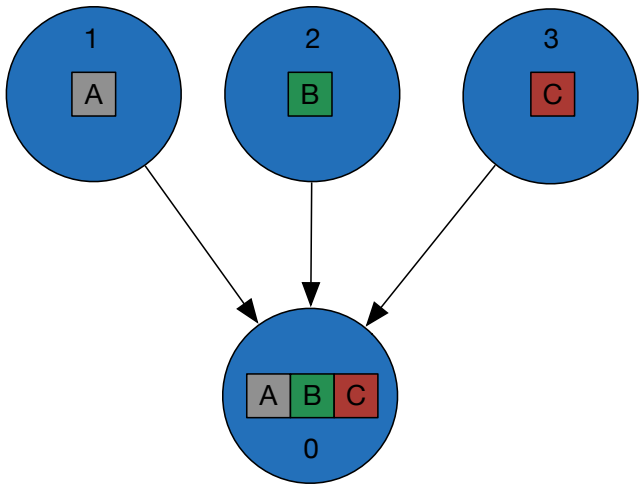


Scatter



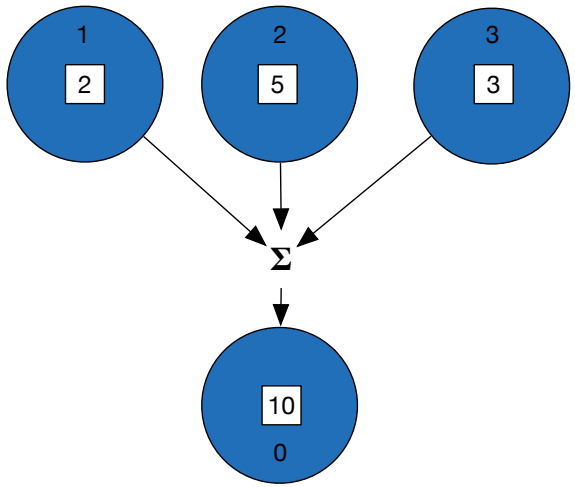

```
MPI_Scatter(sendbuf, sendcount, sendtype, &
            recvbuf, recvcount, recvtype, &
            root, comm, ierr)
```

Gather



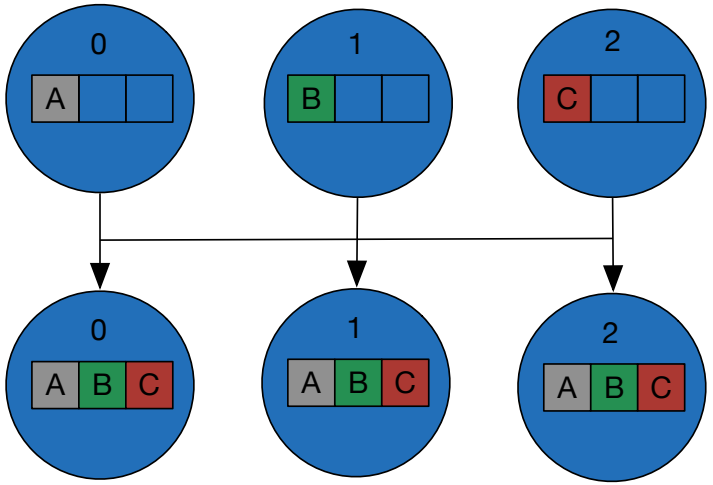

```
MPI_Gather(sendbuf, sendcount, sendtype, &
           recvbuf, recvcount, recvtype, &
            root, comm, ierr)
```

Reduction




```
MPI_Reduce(sendbuf, recvbuf, count,  &
           datatype, op, root, comm, &
           ierr)
```

All Gather




```
MPI_Allgather(sendbuf, sendcount, sendtype, &
              recvbuf, recvcount, recvtype, &
               root, comm, request, ierr)
```

All Reduce Ring

A version of the ring program called `rring.c` uses `MPI_Allreduce`.

Questions?

Online Survey

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