# MPI

https://github.com/ResearchComputing/RMACC_2015/MPI/MPI.pdf

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# Overview

- Background
- MPI
- Programming Models
- Data Types
- Communications
- Point to Point Communications
- Collective Communications
- Topologies
- Parallel IO

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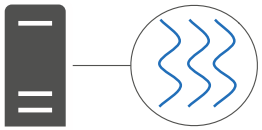
# Parallelism

Parallelism can be achieved across many levels

- Nodes – MPI

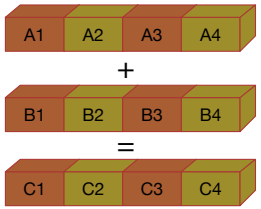
- Threads – OpenMP



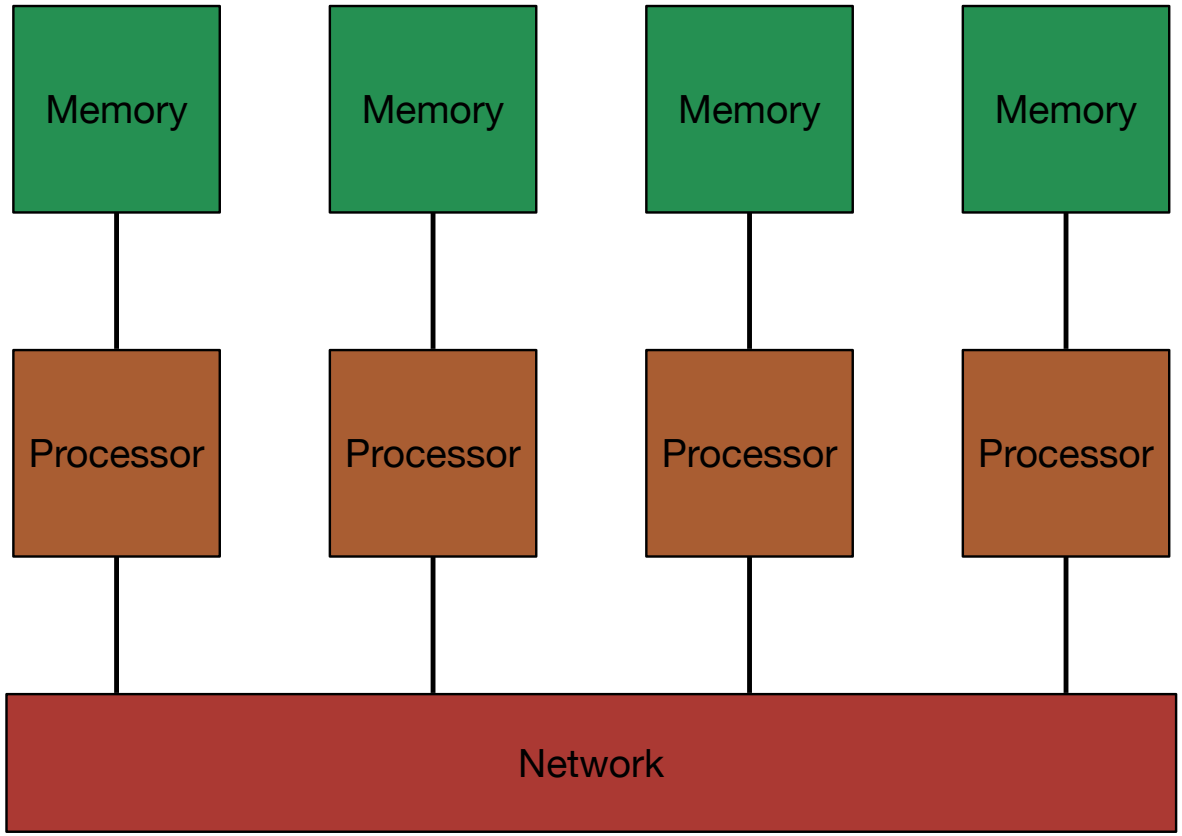
- Instructions – ILP

```
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 I

- 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.

# Message Passing II

- 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

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# Programming Models

- Single Program Multiple Data (SPMD)
  - Same program runs on each process.
- Multiple Programs Multiple Data (MPMD)
  - Different programs runs on each process.

# Programming in MPI

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).

# Execution

Once your program has compiled you can run it with:

- Through a batch system (SLURM for example).

```
login01 ~$ srun -n 1 ./a.out
```

- Through `mpiexec`.

```
node0001 ~$ mpiexec -n 1 ./a.out
```

# Login to Janus

1. Log in to Janus.

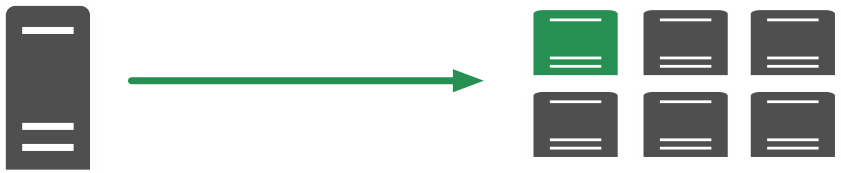
```
laptop ~$ ssh user0000@tutorial-login.rc.colorado.edu
```

2. Load the slurm and intel module.

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

3. Start a compute job.

```
[user0000@tutorial-login ~]$ sinteractive  \
                             -t 02:00:00 -N 1    \
                             --reservation=rmacc-tutorials
```



# 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`).

# Additional Functions

- Determine the processor name (hostname)
  `MPI_Get_processor_name(node, nlen, ierr)`
- Determine the MPI version (and sub-version)
  `MPI_Get_version(ver, sub_ver, ierr)`

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

# Exercise

- **Write a hello world program that outputs:**
  - Rank
  - Processor name
  - MPI version

  There is a template in `mpi_ver.f90`.

All of the examples taught are online, in a github repository:
`https://github.com/ResearchComputing/RMACC_2015`

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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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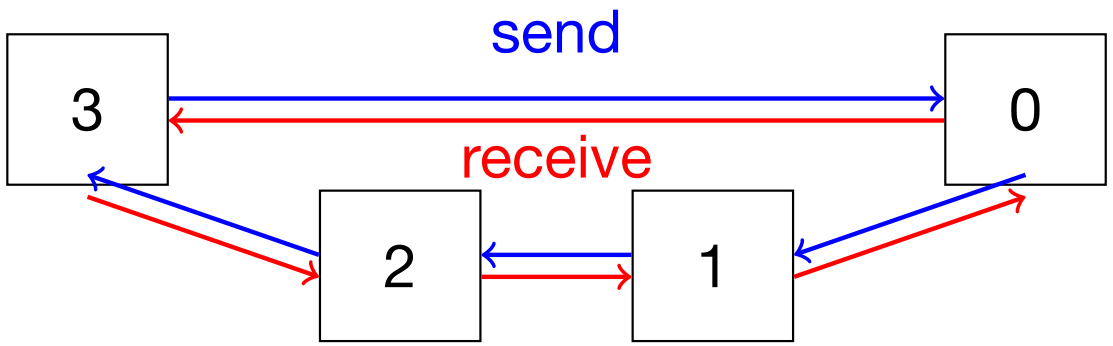
# Point to Point Communications

## Sending Data In A Ring

Sending $n$ elements to the left (rank +1) receive N elements from the right (rank -1).




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

# Blocking Send & Receive

- Blocking Send `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.
- Blocking 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.

# Blocking Send

```
MPI_Send(buf, count, data_type, dest, tag, comm, ierr)
```

| | |
|---|---|
| buf | Beginning address of data. |
| count | Length of the source array (in elements). |
| data_type | MPI type of data. |
| dest | Processor number of destination. |
| tag | Message tag. |
| comm | Communicator. |
| ierr | Error status. |

Example:

```
MPI_Send(data, 10, MPI_INT, 1, 1, MPI_COMM_WORLD, ierr)
```

# Blocking Receive

```
MPI_Recv(buf, count, data_type, source, tag, &
         comm, status, ierr)
```

| | |
|---|---|
| buf | Beginning address of data. |
| count | Length of the source array (in elements). |
| data_type | MPI type of data. |
| dest | Processor number of destination. |
| tag | Message tag. |
| comm | Communicator. |
| status | Status object. |
| ierr | Error status. |

Example:

```
MPI_Recv(data, 10, MPI_INT, 0, 1, MPI_COMM_WORLD, &
         stat, ierr)
```

# Receive Wildcards & Status

- Can receive from any source, using `MPI_ANY_SOURCE`.

```
MPI_Recv(data, 10, MPI_INT, MPI_ANY_SOURCE, &
         1, MPI_COMM_WORLD, stat, ierr)
```

- Can receive from any tag, using `MPI_ANY_TAG`.

```
MPI_Recv(data, 10, MPI_INT, MPI_ANY_SOURCE, &
         MPI_ANY_TAG, MPI_COMM_WORLD, stat, ierr)
```

- Can ignore the status, using `MPI_STATUS_IGNORE`.

```
MPI_Recv(data, 10, MPI_INT, MPI_ANY_SOURCE, &
         MPI_ANY_TAG, MPI_COMM_WORLD,       &
         MPI_STATUS_IGNORE, ierr)
```

# Status Structure

- In C it is a typedef structure.
- In Fortran it is an array.

C

```c
typedef struct _MPI_Status {
  int count;
  int cancelled;
  int MPI_SOURCE;
  int MPI_TAG;
  int MPI_ERROR;
} MPI_Status;

MPI_Status status;
source = status.MPI_SOURCE;
```

Fortran

```fortran
integer :: status(MPI_STATUS_SIZE)
source = status(MPI_SOURCE)
tag    = status(MPI_TAG)
```

# 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.

# Exercise

- **Write a ring program that outputs:**
  - The total number of processors
  - Rank
  - Local sum
- **Run the program with different array sizes:**
  - $N = 10$
  - $N = 100000$

There is a template in `ring.f90`.

# 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.

# Exercise

- **Fix the ring program so that it is no longer in a deadlock.**
- **Run the program with different array sizes:**
  - $N = 10$
  - $N = 100000$

There is a template in `ring_fixed.f90`.

# Overview

# 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.

Example:

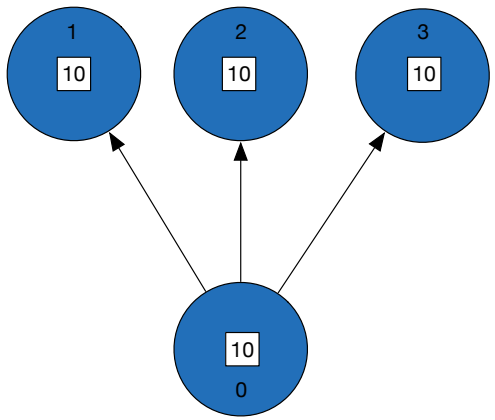
```
MPI_Barrier(MPI_COMM_WORLD, ierr)
```

# 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. |




Example:

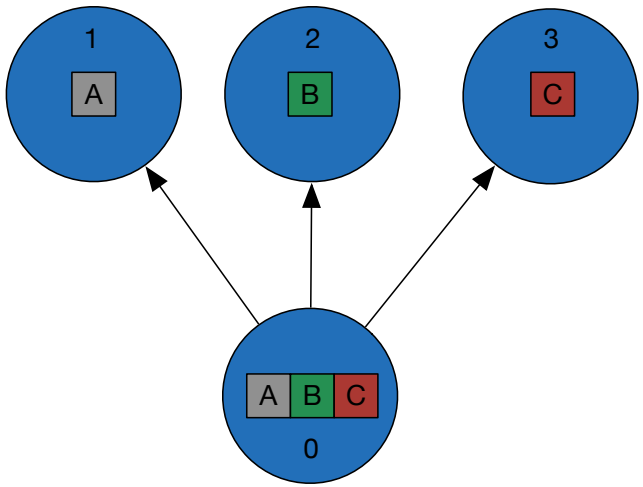
```
MPI_Bcast(data, 10, MPI_INT, 0, MPI_COMM_WORLD, ierr)
```

# Exercise

- **Write a program that broadcasts a files information:**
  - Rank
  - File size

  There is a template in `bstat.c`.

# Scatter I

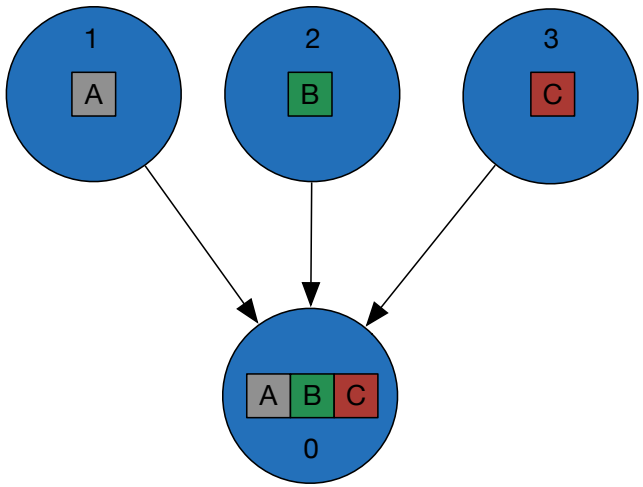



```
MPI_Scatter(sendbuf, sendcount, sendtype, &
            recvbuf, recvcount, recvtype, &
            root, comm, ierr)
```

# Scatter II

| | |
|---|---|
| sendbuf | Beginning address of send data. |
| sendcount | Number of elements sent to each process. |
| sendtype | Datatype of send buffer elements. |
| recvbuf | Address of receive buffer. |
| recvcount | Number of elements in receive buffer. |
| recvtype | Datatype of receive buffer elements. |
| root | Rank of sending process. |
| comm | Communicator. |
| ierr | Error status. |

# Gather I

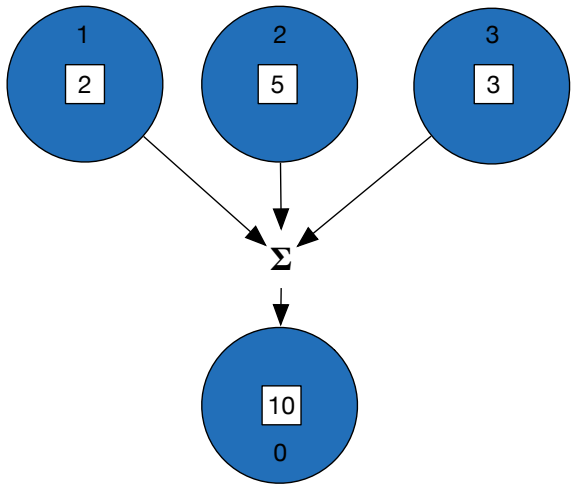



```
MPI_Gather(sendbuf, sendcount, sendtype, &
           recvbuf, recvcount, recvtype, &
            root, comm, ierr)
```

# Gather II

| | |
|---|---|
| sendbuf | Beginning address of send data. |
| sendcount | Number of elements sent to each process. |
| sendtype | Datatype of send buffer elements. |
| recvbuf | Address of receive buffer. |
| recvcount | Number of elements for any single receive. |
| recvtype | Datatype of receive buffer elements. |
| root | Rank of receiving process. |
| comm | Communicator. |
| ierr | Error status. |

# Reduction I




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

# Reduction II

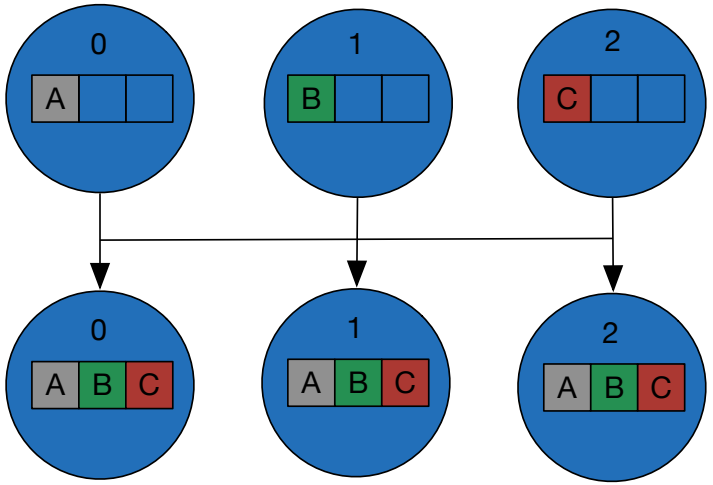
| | |
|---|---|
| sendbuf | Beginning address of send data. |
| recvbuf | Address of receive buffer. |
| count | Number of elements in the send buffer. |
| datatype | Datatype of elements. |
| op | Reduce operation. |
| root | Rank of receiving process. |
| comm | Communicator. |
| ierr | Error status. |

# Reduction Operations

| Name | Meaning |
|---|---|
| MPI_MAX | maximum |
| MPI_MIN | minimum |
| MPI_SUM | sum |
| MPI_PROD | product |
| MPI_LAND | logical and |
| MPI_BAND | bit-wise and |
| MPI_LOR | logical or |
| MPI_BOR | bit-wise or |
| MPI_LXOR | logical xor |
| MPI_BXOR | bit-wise xor |
| MPI_MAXLOC | max value and location |
| MPI_MINLOC | min value and location |

In addition, users may define their own operations that can be overloaded to operate.

# All Gather I




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

# All Gather II

| | |
|---|---|
| sendbuf | Beginning address of send data. |
| sendcount | Number of elements in the send buffer. |
| sendtype | Datatype of send buffer elements. |
| recvbuf | Address of receive buffer. |
| recvcount | Number of elements for any single receive. |
| recvtype | Datatype of receive buffer elements. |
| root | Rank of receiving process. |
| comm | Communicator. |
| ierr | Error status. |

# Overview

# Topologies

A topology is an extra, optional attribute that one can give to an intra-communicator; topologies cannot be added to inter-communicators. A topology can provide a convenient naming mechanism for the processes of a group (within a communicator), and additionally, may assist the runtime system in mapping the processes onto hardware.[1]

- Distribute Processors.
- Cartesian Topology.
- Processor Coordinates.

[1] MPI 1.1 Documentation

# Distribute Processors

Create a balanced distribution of processes per coordinate direction.

```
MPI_Dims_create(nnodes, ndims, dims, ierr)
```

| | |
|---|---|
| nnodes | Number of nodes in a grid. |
| ndims | Number of Cartesian dimensions. |
| dims | Integer array of size ndims specifying the number of processors in each dimension. |
| ierr | Error status. |

# Cartesian Topology.

Makes a new communicator to which Cartesian topology information has been attached.

```
MPI_Cart_create(comm_old, ndims, dims, periods, &
                reorder, comm_cart, ierr)
```

| | |
|---|---|
| nnodes | Input communicator. |
| ndims | Number of Cartesian dimensions. |
| dims | Integer array of size ndims specifying the number of processors in each dimension. |
| period | Logical array of size ndims specifying whether the grid is periodic (true) or not (false) in each dimension. |
| reorder | Ranking may be reordered (true) or not (false). |
| cart_comm | Communicator with new Cartesian topology. |
| ierr | Error status. |

# Processor Coordinates.

Determines process coords in Cartesian topology given rank in group.

```
MPI_Cart_coords(comm, rank, maxdims, coords, ierr)
```

| | |
|---|---|
| comm | Communicator with Cartesian structure. |
| rank | Rank of a process within group of comm. |
| maxdims | Length of vector coord in the calling program. |
| coords | Integer array containing the Cartesian coordinates of specified processors. |
| ierr | Error status. |

# Example

Problem

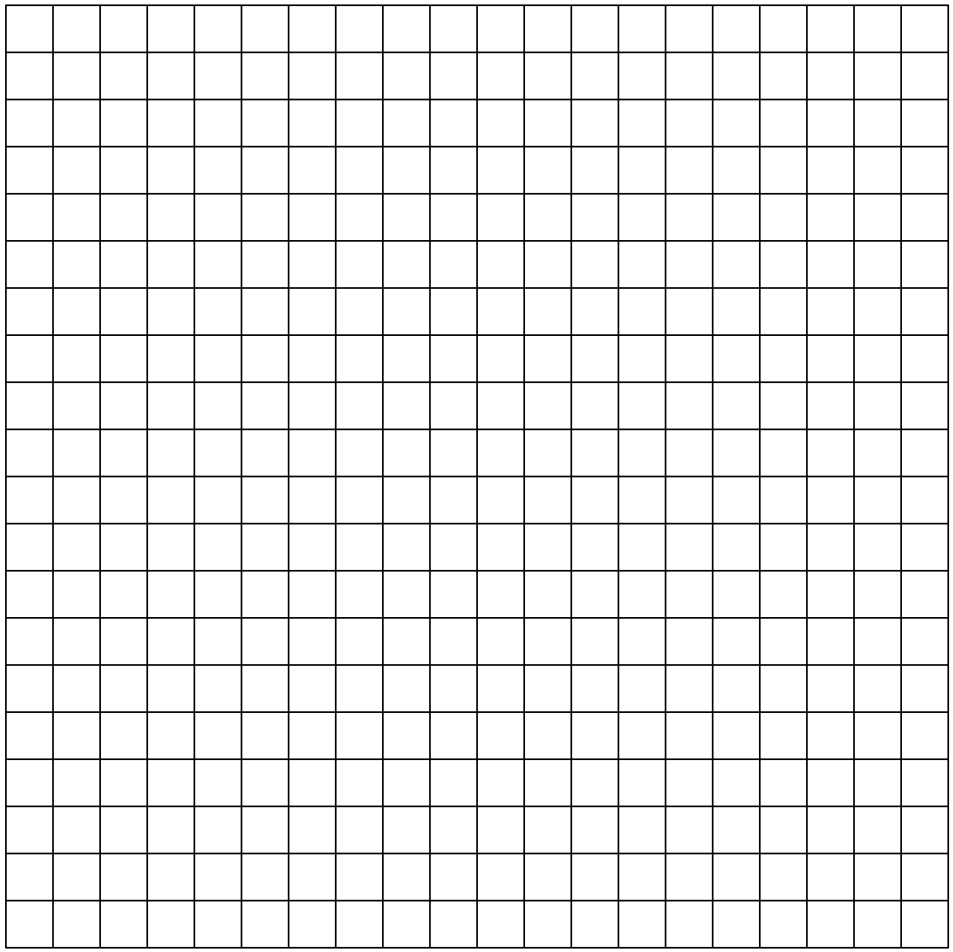
- Global domain of $20 \times 20$.
- $4$ MPI processors.

Steps in the solution:

- Domain decomposition in MPI.
- Generate local matrix.

The full solution is in `hdf_pwrite.f90`.

# Global Grid:



Split the process up across the dimensions.

```
integer, parameter :: ndims = 2      ! Number of dims
integer            :: id             ! Rank/ID
integer            :: nprocs         ! Number of procs
integer            :: m_dims(ndims) ! MPI Cart dims

m_dims = (/ 0, 0 /)
call MPI_Comm_rank(MPI_COMM_WORLD, id, ierr)
call MPI_Comm_size(MPI_COMM_WORLD, nprocs, ierr)
call MPI_Dims_create(nprocs, ndims, m_dims, ierr)

if (id .eq. 0) then
    write(6, *) 'Processor dims/decomposition: ' m_dims
end if
```

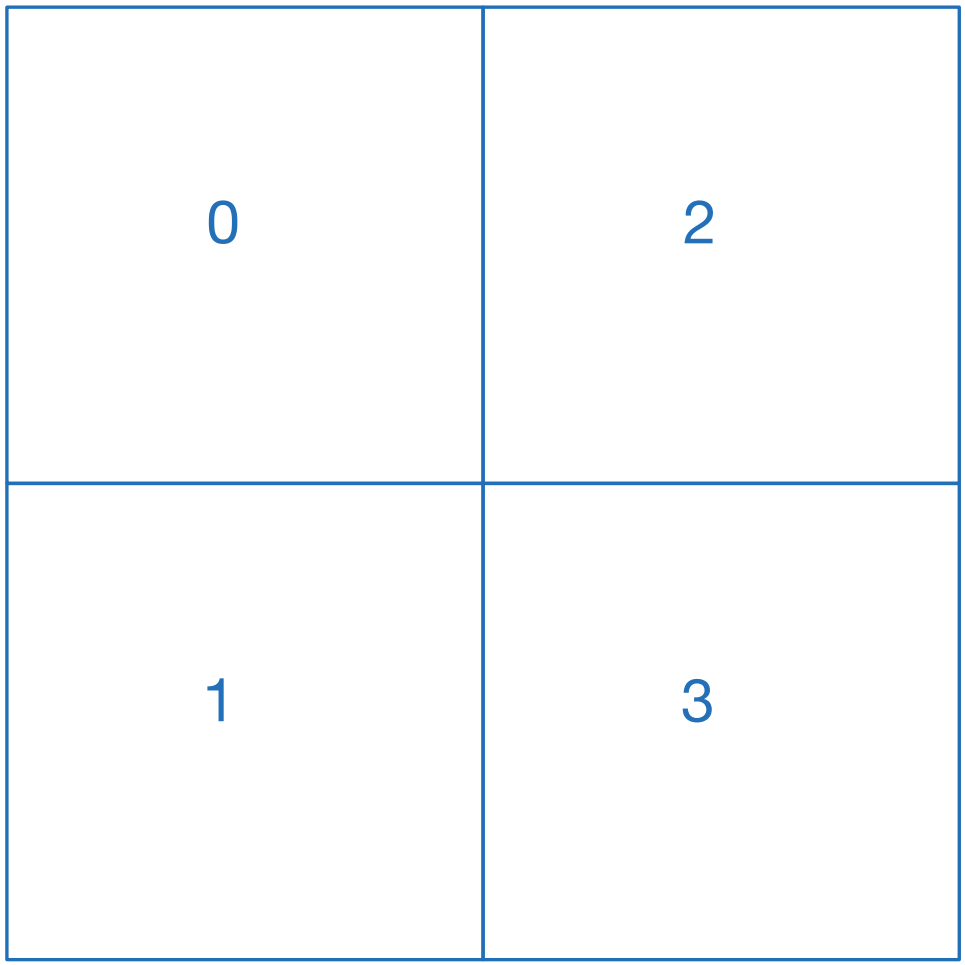
Create a new communicator for this decomposition, also obtain our new rank.

```
logical                 :: is_periodic(ndims)
logical                 :: reorder
integer                 :: MPI_COMM_2D

is_periodic = .false.
reorder     = .false.

call MPI_Cart_create(MPI_COMM_WORLD, ndims, m_dims, &
                     is_periodic, reorder,          &
                     MPI_COMM_2D, ierr)
call MPI_Comm_rank(MPI_COMM_2D, id, ierr)
```

Query our new processor Cartesian coordinates.

```
integer                 :: coords(ndims)

call MPI_Cart_coords(MPI_COMM_2D, id, ndims, &
                     coords, ierr)
```

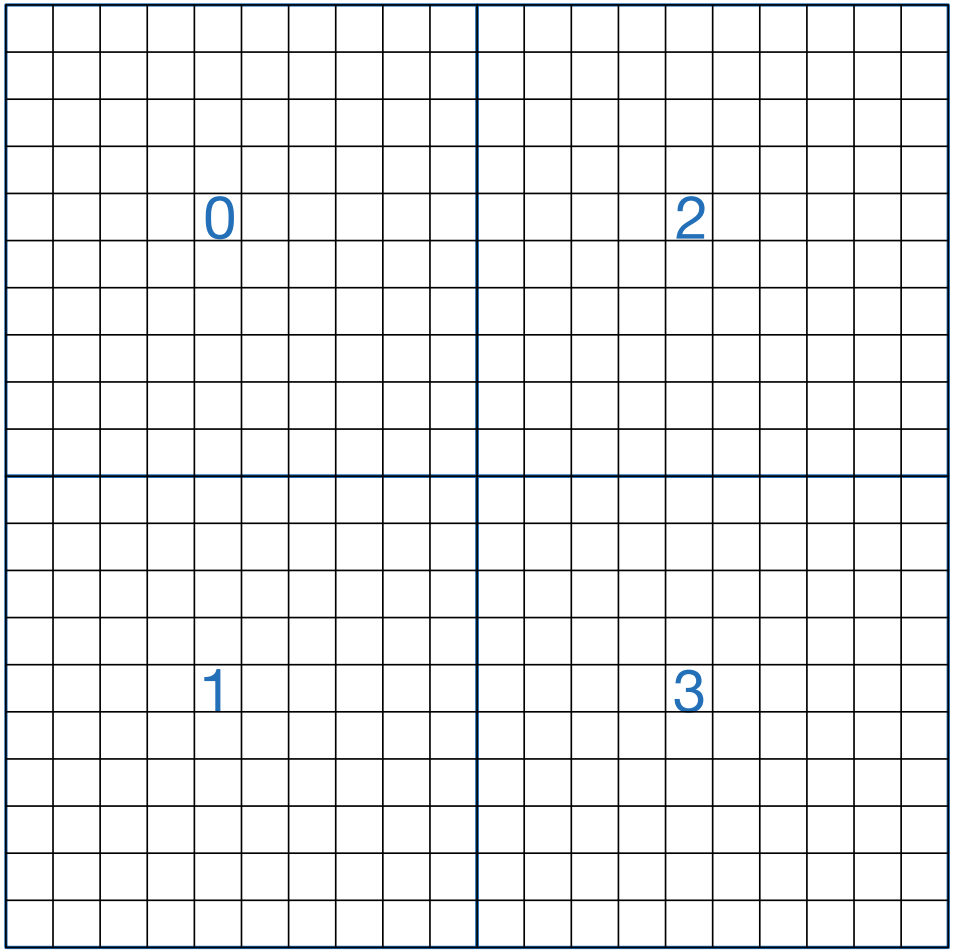
Global grid with our new processor mapping:



Decompose the global grid to our local grid.

```
integer, parameter :: g_N = 20 ! Global grid size
integer :: n(ndims)            ! Local grid size

do i = 1, ndims
    n(i) = g_N / m_dims(i)
end do
allocate(ld(n(1),n(2)), stat=ierr)
```

Global grid with our processor mapping and local grid allocations.



# Overview

# Parallel IO

- MPI-IO
- Parallel HDF5
  - MPI Properties
  - Hyperslabs

# MPI IO

MPI provides a set of file IO routines.

- `MPI_File_open()`
- `MPI_File_set_view()`
- `MPI_File_read_at()`

Be warned, these write binary data to the file.
The file will be:

- Endian dependent.
- Application specific.

**Please** consider using a higher level library.

# HDF5

HDF (Hierarchical Data Format) version 5.
*This is really a talk all to it's self.*
The easiest way to think about a HDF5 file is that it is a file system in a file. It can contain:

- Groups (directories/folders)
- Links (internal and external)
- Metadata
- Data
- Images
- Tables

# Example

Continue working through `hdf_pwrite.f90`

# Questions?

# Online Survey

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# License