Message Passing Programming with MPI

What is MPI?

MPI Forum

- ❑ First message-passing interface standard.
- ❑ Sixty people from forty different organisations.
- ❑ Users and vendors represented, from the US and Europe.
- ❑ Two-year process of proposals, meetings and review.
- ❑ *Message Passing Interface* document produced.

Goals and Scope of MPI

- ❑ MPI's prime goals are:
  - To provide source-code portability.
  - To allow efficient implementation.
- ❑ It also offers:
  - A great deal of functionality.
  - Support for heterogeneous parallel architectures.

Header files

- C:
```
#include <mpi.h>
```
- Fortran:
```
include ‘mpif.h’
```

MPI Function Format

- C:
```
error = MPI_Xxxxx(parameter, ...);

MPI_Xxxxx(parameter, ...);
```
- Fortran:
```
CALL MPI_XXXXX(parameter, ..., IERROR)
```

Handles

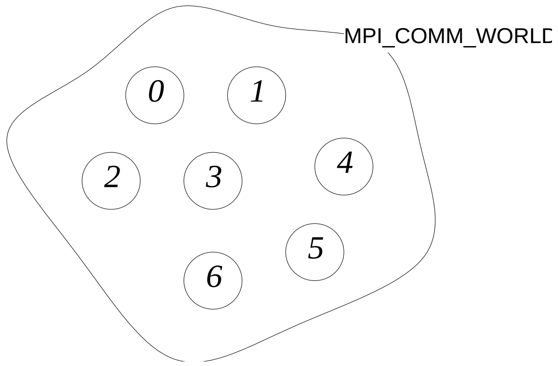
- MPI controls its own internal data structures.
- MPI releases `handles’ to allow programmers to refer to these.
- C handles are of defined **`typedefs`.**
- Fortran handles are **`INTEGER`**s.

Initialising MPI

- C:
```
int MPI_Init(int *argc, char ***argv)
```
- Fortran:
```
MPI_INIT(IERROR)
   INTEGER IERROR
```
- Must be the first MPI procedure called.

MPI_COMM_WORLD

Communicators



Rank

- How do you identify different processes in a communicator?

```
MPI_Comm_rank(MPI_Comm comm, int *rank)

MPI_COMM_RANK(COMM, RANK, IERROR)
   INTEGER COMM, RANK, IERROR
```

- The rank is not the PE number.

Size

- How many processes are contained within a communicator?

```
MPI_Comm_size(MPI_Comm comm, int *size)

MPI_COMM_SIZE(COMM, SIZE, IERROR)
   INTEGER COMM, SIZE, IERROR
```

Exiting MPI

- C:

```
int MPI_Finalize()
```

- Fortran:

```
MPI_FINALIZE(IERROR)
   INTEGER IERROR
```

- Must be the last MPI procedure called.

Exercise: Hello World

The minimal MPI program

- ❑ Write a minimal MPI program which prints ``hello world''.
- ❑ Compile it.
- ❑ Run it on a single processor.
- ❑ Run it on several processors in parallel.
- ❑ Modify your program so that only the process ranked 0 in **`MPI_COMM_WORLD`** prints out.
- ❑ Modify your program so that the number of processes is printed out.

Messages

Messages

- ❑ A message contains a number of elements of some particular datatype.
- ❑ MPI datatypes:
  - Basic types.
  - Derived types.
- ❑ Derived types can be built up from basic types.
- ❑ C types are different from Fortran types.

MPI Basic Datatypes - C

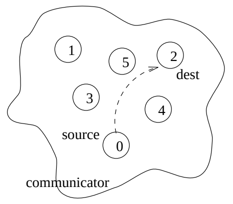
MPI Datatype	C datatype
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long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

MPI Basic Datatypes - Fortran

MPI Datatype	Fortran Datatype
MPI_INTEGER	INTEGER
MPI_REAL	REAL
MPI_DOUBLE_PRECISION	DOUBLE PRECISION
MPI_COMPLEX	COMPLEX
MPI_LOGICAL	LOGICAL
MPI_CHARACTER	CHARACTER(1)
MPI_BYTE	
MPI_PACKED	

Point-to-Point Communication

Point-to-Point Communication



- ❑ Communication between two processes.
- ❑ Source process sends message to destination process.
- ❑ Communication takes place within a communicator.
- ❑ Destination process is identified by its rank in the communicator.

Communication modes

Sender mode	Notes
Synchronous send	Only completes when the receive has completed.
Buffered send	Always completes (unless an error occurs), irrespective of receiver.
Standard send	Either synchronous or buffered.
Ready send	Always completes (unless an error occurs), irrespective of whether the receive has completed.
Receive	Completes when a message has arrived.

MPI Sender Modes

OPERATION	MPI CALL
Standard send	MPI_SEND
Synchronous send	MPI_SSEND
Buffered send	MPI_BSEND
Ready send	MPI_RSEND
Receive	MPI_RECV

Sending a message

- C:

```
int MPI_Ssend(void *buf, int count,
              MPI_Datatype datatype,
              int dest, int tag,
              MPI_Comm comm)
```

- Fortran:

```
MPI_SSEND(BUF, COUNT, DATATYPE, DEST,
          TAG,COMM, IERROR)
   <type> BUF(*)
   INTEGER COUNT, DATATYPE, DEST, TAG
   INTEGER COMM, IERROR
```

Receiving a message

- C:

```
int MPI_Recv(void *buf, int count,
        MPI_Datatype datatype,
        int source, int tag,
        MPI_Comm comm, MPI_Status *status)
```

- Fortran:

```
MPI_RECV(BUF, COUNT, DATATYPE, SOURCE,
           TAG, COMM, STATUS, IERROR)
<type> BUF(*)
INTEGER COUNT, DATATYPE, SOURCE, TAG, COMM,
       STATUS(MPI_STATUS_SIZE),IERROR
```

Synchronous Blocking Message-Passing

- Processes synchronise.
- Sender process specifies the synchronous mode.
- Blocking – both processes wait until the transaction has completed.

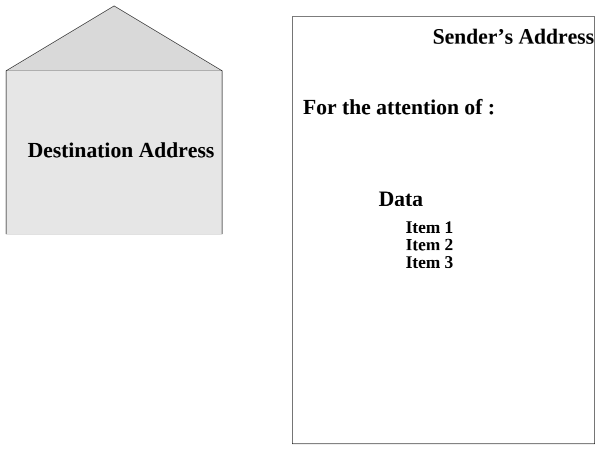
For a communication to succeed:

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

Wildcarding

- ❑ Receiver can wildcard.
- ❑ To receive from any source – **`MPI_ANY_SOURCE`**
- ❑ To receive with any tag – **`MPI_ANY_TAG`**
- ❑ Actual source and tag are returned in the receiver's **`status`** parameter.

Communication Envelope



Commmunication Envelope Information

- ❑ Envelope information is returned from **`MPI_RECV`** as **`status`**
- ❑ Information includes:
  - Source: **`status.MPI_SOURCE`** or **`status(MPI_SOURCE)`**
  - Tag: **`status.MPI_TAG`** or **`status(MPI_TAG)`**
  - Count: **`MPI_Get_count`** or **`MPI_GET_COUNT`**

Received Message Count

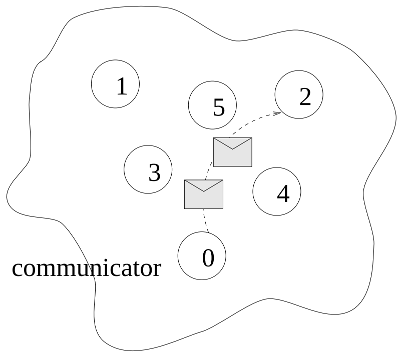
- C:

```
int MPI_Get_count(MPI_Status *status,
                  MPI_Datatype datatype,
                  int *count)
```

- Fortran:

```
MPI_GET_COUNT(STATUS, DATATYPE, COUNT,
              IERROR)
INTEGER STATUS(MPI_STATUS_SIZE), DATATYPE,
        COUNT, IERROR
```

Message Order Preservation



- Messages do not overtake each other.
- This is true even for non-synchronous sends.

Exercise - Ping pong

- Write a program in which two processes repeatedly pass a message back and forth.
- Insert timing calls to measure the time taken for one message.
- Investigate how the time taken varies with the size of the message.

Timers

- C:

```
double MPI_Wtime(void);
```

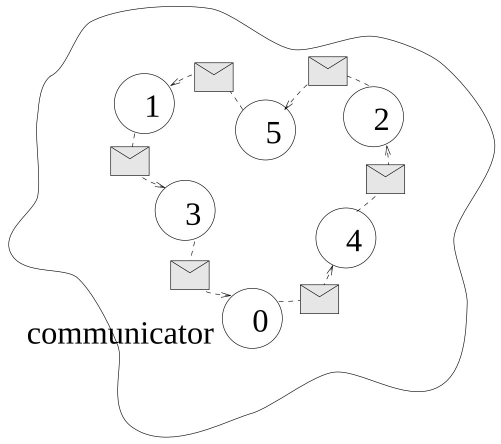
- Fortran:

```
DOUBLE PRECISION MPI_WTIME()
```

- Time is measured in seconds.
- Time to perform a task is measured by consulting the timer before and after.
- Modify your program to measure its execution time and print it out.

Non-Blocking Communications

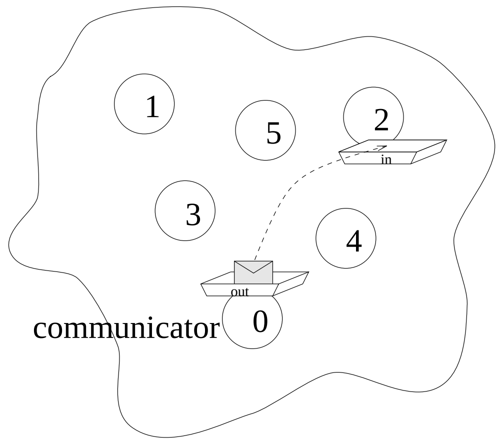
Deadlock



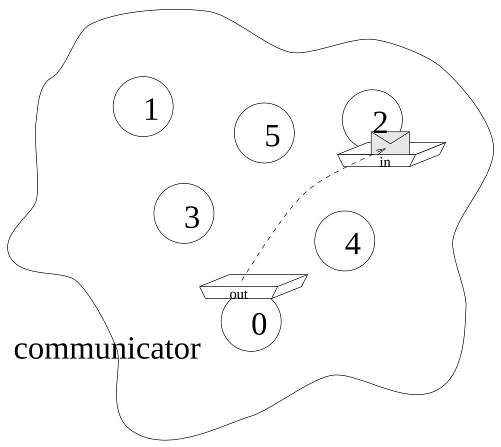
Non-Blocking Communications

- ❑ Separate communication into three phases:
- ❑ Initiate non-blocking communication.
- ❑ Do some work (perhaps involving other communications?)
- ❑ Wait for non-blocking communication to complete.

Non-Blocking Send



Non-Blocking Receive



Handles used for Non-blocking Comms

- datatype – same as for blocking (**`MPI_Datatype`** or **`INTEGER`**).
- communicator – same as for blocking (**`MPI_Comm`** or **`INTEGER`**).
- request – **`MPI_Request`** or **`INTEGER`**.
- A *request handle* is allocated when a communication is initiated.

Non-blocking Synchronous Send

- C:

```
int MPI_Issend(void* buf, int count,
           MPI_Datatype datatype, int dest,
           int tag, MPI_Comm comm,
           MPI_Request *request)

int MPI_Wait(MPI_Request *request,
         MPI_Status *status)
```

- Fortran:

```
MPI_ISSEND(buf, count, datatype, dest,
               tag, comm, request, ierror)

MPI_WAIT(request, status, ierror)
```

Non-blocking Receive

- C:

```
int MPI_Irecv(void* buf, int count,
             MPI_Datatype datatype, int src,
             int tag, MPI_Comm comm,
             MPI_Request *request)

int MPI_Wait(MPI_Request *request,
             MPI_Status *status)
```

- Fortran:

```
MPI_IRECV(buf, count, datatype, src,
           tag,comm, request, ierror)

MPI_WAIT(request, status, ierror)
```

Blocking and Non-Blocking

- Send and receive can be blocking or non-blocking.
- A blocking send can be used with a non-blocking receive, and vice-versa.
- Non-blocking sends can use any mode - synchronous, buffered, standard, or ready.
- Synchronous mode affects completion, not initiation.

Communication Modes

NON-BLOCKING OPERATION	MPI CALL
Standard send	MPI_ISEND
Synchronous send	MPI_ISSEND
Buffered send	MPI_IBSEND
Ready send	MPI_IRSEND
Receive	MPI_IRECV

Completion

- Waiting versus Testing.
- C:

```
int MPI_Wait(MPI_Request *request,
             MPI_Status *status)
int MPI_Test(MPI_Request *request,
             int *flag,
             MPI_Status *status)
```

- Fortran:

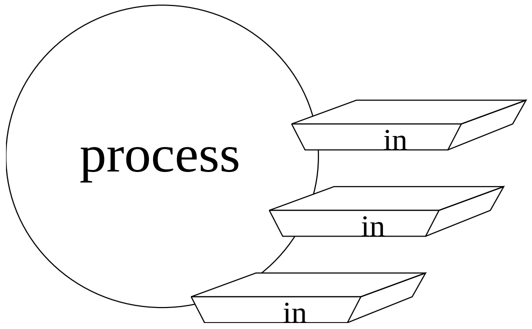
```
MPI_WAIT(handle, status, ierror)

MPI_TEST(handle, flag, status, ierror)
```

Multiple Communications

- Test or wait for completion of one message.
- Test or wait for completion of all messages.
- Test or wait for completion of as many messages as possible.

Testing Multiple Non-Blocking Comms



Exercise

Rotating information around a ring

- Arrange processes to communicate round a ring.
- Each process stores a copy of its rank in an integer variable.
- Each process communicates this value to its right neighbour, and receives a value from its left neighbour.
- Each process computes the sum of all the values received.
- Repeat for the number of processes involved and print out the sum stored at each process.

Derived Datatypes

MPI Datatypes

- Basic types
- Derived types
  - vectors
  - structs
  - others

Derived Datatypes - *Type*

basic datatype 0	displacement of datatype 0
basic datatype 1	displacement of datatype 1
...	...
basic datatype n-1	displacement of datatype n-1

Contiguous Data

- The simplest derived datatype consists of a number of contiguous items of the same datatype.
- C:

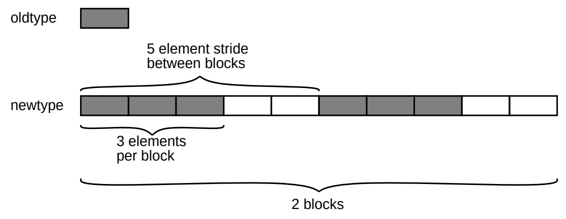
```
int MPI_Type_contiguous(int count,
MPI_Datatype oldtype, MPI_Datatype *newtype)
```

- Fortran:

```
MPI_TYPE_CONTIGUOUS(COUNT, OLDTYPE, NEWTYPE,
                    IERROR)
  INTEGER COUNT, OLDTYPE, NEWTYPE, IERROR
```

Vector Datatype Example

A 3X2 block of a 5X5 Fortran array



- **`count = 2`**
- **`stride = 5`**
- **`blocklength = 3`**

Constructing a Vector Datatype

- C:

```
int MPI_Type_vector (int count,
     int blocklength, int stride,
     MPI_Datatype oldtype,
     MPI_Datatype *newtype)
```

- Fortran:

```
  MPI_TYPE_VECTOR (COUNT, BLOCKLENGTH,
     STRIDE, OLDTYPE, NEWTYPE, IERROR)
```

Extent of a Datatatype

- C:

```
int MPI_Type_extent (MPI_Datatype datatype,
                     MPI_Aint *extent)
```

- Fortran:

```
MPI_TYPE_EXTENT( DATATYPE, EXTENT,
                 IERROR)
INTEGER DATATYPE, EXTENT, IERROR
```

Address of a Variable

- C:

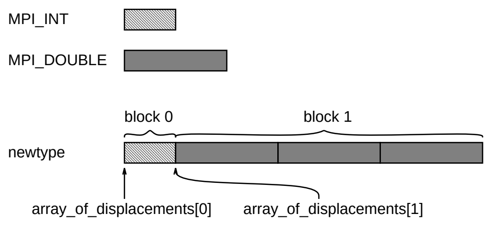
```
int MPI_Address (void *location, MPI_Aint
             *address)
```

- Fortran:

```
MPI_ADDRESS( LOCATION, ADDRESS, IERROR)

<type> LOCATION (*)
INTEGER ADDRESS, IERROR
```

Struct Datatype Example



- `count = 2`
- `array_of_blocklengths[0] = 1`
- `array_of_types[0] = MPI_INT`
- `array_of_blocklengths[1] = 3`
- `array_of_types[1] = MPI_DOUBLE`

Constructing a Struct Datatype

- C:

```
int MPI_Type_struct (int count,
   int *array_of_blocklengths,
   MPI_Aint *array_of_displacements,
   MPI_Datatype *array_of_types,
   MPI_Datatype *newtype)
```

- Fortran:

```
MPI_TYPE_STRUCT (COUNT,
   ARRAY_OF_BLOCKLENGTHS,
   ARRAY_OF_DISPLACEMENTS,
   ARRAY_OF_TYPES, NEWTYPE, IERROR)
```

Committing a datatype

- ❑ Once a datatype has been constructed, it needs to be committed before it is used.
- ❑ This is done using **`MPI_TYPE_COMMIT`**
- ❑ C:

```
int MPI_Type_commit (MPI_Datatype *datatype)
```

- ❑ Fortran:

```
MPI_TYPE_COMMIT (DATATYPE, IERROR)
   INTEGER DATATYPE, IERROR
```

Exercise

Derived Datatypes

- ❑ Modify the passing-around-a-ring exercise.
- ❑ Calculate two separate sums:
  - rank integer sum, as before
  - rank floating point sum
- ❑ Use a *struct* datatype for this.

Virtual Topologies

Virtual Topologies

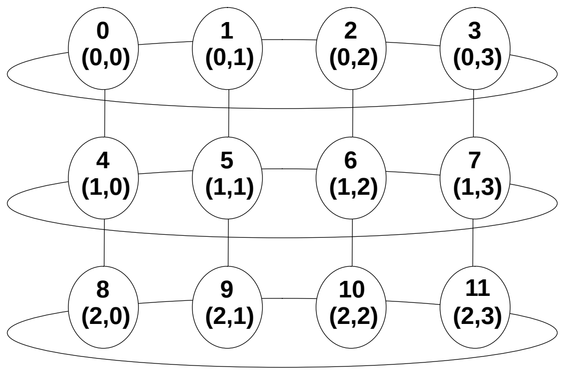
- ❑ Convenient process naming.
- ❑ Naming scheme to fit the communication pattern.
- ❑ Simplifies writing of code.
- ❑ Can allow MPI to optimise communications.

How to use a Virtual Topology

- Creating a topology produces a new communicator.
- MPI provides ``mapping functions''.
- Mapping functions compute processor ranks, based on the topology naming scheme.

Example

A 2-dimensional Cylinder



Topology types

- Cartesian topologies
  - each is "connected" to its neighbours in a virtual grid.
  - boundaries can be cyclic, or not.
  - processes are identified by cartesian coordinates.
- Graph topologies
  - general graphs
  - not covered here

Creating a Cartesian Virtual Topology

- C:

```
int MPI_Cart_create(MPI_Comm comm_old,
      int ndims, int *dims, int *periods,
      int reorder, MPI_Comm *comm_cart)
```

- Fortran:

```
MPI_CART_CREATE(COMM_OLD, NDIMS, DIMS,
      PERIODS, REORDER, COMM_CART, IERROR)

INTEGER COMM_OLD, NDIMS, DIMS(*), COMM_CART,
        IERROR
LOGICAL PERIODS(*), REORDER
```

Balanced Processor Distribution

- C:

```
int MPI_Dims_create(int nnodes, int ndims,
                    int *dims)
```

- Fortran:

```
MPI_DIMS_CREATE(NNODES, NDIMS, DIMS, IERROR)

INTEGER NNODES, NDIMS, DIMS(*), IERROR
```

Example

- Call tries to set dimensions as close to each other as possible.

dims before the call	function call	dims on return
(0, 0)	MPI_DIMS_CREATE(6, 2, dims)	(3, 2)
(0, 0)	MPI_DIMS_CREATE(7, 2, dims)	(7, 1)
(0, 3, 0)	MPI_DIMS_CREATE(6, 3, dims)	(2, 3, 1)
(0, 3, 0)	MPI_DIMS_CREATE(7, 3, dims)	erroneous call

- Non zero values in dims sets the number of processors required in that direction.

WARNING:- make sure dims is set to 0 before the call!

Cartesian Mapping Functions

Mapping process grid coordinates to ranks

- C:

```
int MPI_Cart_rank(MPI_Comm comm,
                     int *coords, int *rank)
```

- Fortran:

```
MPI_CART_RANK (COMM, COORDS, RANK, IERROR)

INTEGER COMM, COORDS(*), RANK, IERROR
```

Cartesian Mapping Functions

Mapping ranks to process grid coordinates

- C:

```
int MPI_Cart_coords(MPI_Comm comm, int rank,
                     int maxdims, int *coords)
```

- Fortran:

```
MPI_CART_COORDS(COMM, RANK, MAXDIMS,
                      COORDS, IERROR)

INTEGER COMM, RANK, MAXDIMS, COORDS(*),
        IERROR
```

Cartesian Mapping Functions

Computing ranks of neighbouring processes

- C:

```
int MPI_Cart_shift(MPI_Comm comm,
          int direction, int disp,
          int *rank_source, int *rank_dest)
```

- Fortran:

```
MPI_CART_SHIFT(COMM, DIRECTION, DISP,
          RANK_SOURCE, RANK_DEST, IERROR)

INTEGER  COMM, DIRECTION, DISP,RANK_SOURCE,
          RANK_DEST, IERROR
```

Cartesian Partitioning

- Cut a grid up into `slices'.
- A new communicator is produced for each slice.
- Each slice can then perform its own collective communications.
- **`MPI_Cart_sub`** and **`MPI_CART_SUB`** generate new communicators for the slices.

Partitioning with MPI_CART_SUB

- C:

```
int MPI_Cart_sub (MPI_Comm comm,
      int *remain_dims, MPI_Comm *newcomm)
```

- Fortran:

```
MPI_CART_SUB (COMM, REMAIN_DIMS, NEWCOMM,
                IERROR)

INTEGER COMM, NEWCOMM, IERROR
LOGICAL REMAIN_DIMS(*)
```

Exercise

- Rewrite the exercise passing numbers round the ring using a one-dimensional ring topology.
- Rewrite the exercise in two dimensions, as a torus. Each row of the torus should compute its own separate result.

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Collective Communications

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Collective Communication

- ❑ Communications involving a group of processes.
- ❑ Called by all processes in a communicator.
- ❑ Examples:
  - Barrier synchronisation.
  - Broadcast, scatter, gather.
  - Global sum, global maximum, etc.

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Characteristics of Collective Comms

- ❑ Collective action over a communicator.
- ❑ All processes must communicate.
- ❑ Synchronisation may or may not occur.
- ❑ All collective operations are blocking.
- ❑ No tags.
- ❑ Receive buffers must be exactly the right size.

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Barrier Synchronisation

- ❑ C:

```
int MPI_Barrier (MPI_Comm comm)
```

- ❑ Fortran:

```
MPI_BARRIER (COMM, IERROR)
INTEGER COMM, IERROR
```

Broadcast

- C:

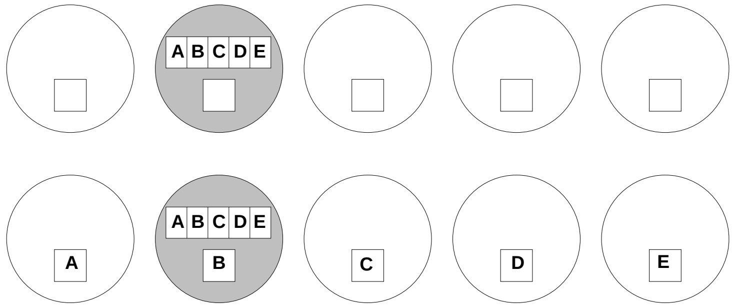
```
int MPI_Bcast (void *buffer, int count,
           MPI_Datatype datatype, int root,
           MPI_Comm comm)
```

- Fortran:

```
MPI_BCAST (BUFFER, COUNT, DATATYPE, ROOT,
           COMM, IERROR)

<type> BUFFER(*)
INTEGER COUNT, DATATYPE, ROOT, COMM, IERROR
```

Scatter



Scatter

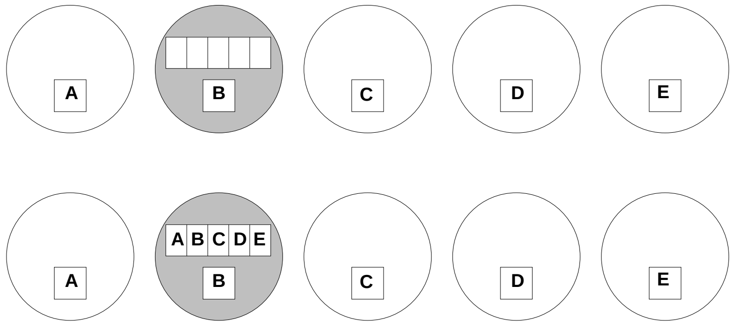
- C:

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

- Fortran:

```
   MPI_SCATTER(SENDBUF, SENDCOUNT, SENDTYPE,
               RECVBUF, RECVCOUNT, RECVTYPE,
              ROOT, COMM, IERROR)
   <type> SENDBUF, RECVBUF
   INTEGER SENDCOUNT, SENDTYPE, RECVCOUNT
   INTEGER RECVTYPE, ROOT, COMM, IERROR
```

Gather



Gather

- C:

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

- Fortran:

```
MPI_GATHER(SENDBUF, SENDCOUNT, SENDTYPE,
      RECVBUF, RECVCOUNT, RECVTYPE,
      ROOT, COMM, IERROR)
<type> SENDBUF, RECVBUF
INTEGER SENDCOUNT, SENDTYPE, RECVCOUNT
INTEGER RECVTYPE, ROOT, COMM, IERROR
```

Global Reduction Operations

- Used to compute a result involving data distributed over a group of processes.
- Examples:
  - global sum or product
  - global maximum or minimum
  - global user-defined operation

Predefined Reduction Operations

MPI Name	Function
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 exclusive OR
MPI_BXOR	Bitwise exclusive OR
MPI_MAXLOC	Maximum and location
MPI_MINLOC	Minimum and location

MPI_REDUCE

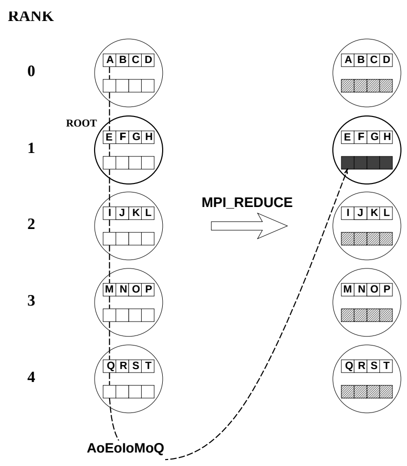
- C:

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

- Fortran:

```
MPI_REDUCE(SENDBUF, RECVBUF, COUNT,
   DATATYPE, OP, ROOT, COMM, IERROR)
<type> SENDBUF, RECVBUF
INTEGER SENDCOUNT, SENDTYPE, RECVCOUNT
INTEGER RECVTYPE, ROOT, COMM, IERROR
```

MPI_REDUCE



Example of Global Reduction

Integer global sum

- C:

```
MPI_Reduce(&x, &result, 1, MPI_INT, MPI_SUM,
           0, MPI_COMM_WORLD)
```

- Fortran:

```
CALL MPI_REDUCE(x, result, 1, MPI_INTEGER,
         MPI_SUM, 0, MPI_COMM_WORLD, IERROR)
```

- Sum of all the **`x`** values is placed in **`result.`**
- The result is only placed there on processor 0.

User-Defined Reduction Operators

- Reducing using an arbitrary operator, ■
- C - function of type **`MPI_User_function`**:

```
void my_op (void *invec,
         void *inoutvec,int *len,
         MPI_Datatype *datatype)
```

- Fortran - external subprogram of type

```
SUBROUTINE MY_OP(INVEC(*),INOUTVEC(*),
     LEN, DATATYPE)

<type> INVEC(LEN), INOUTVEC(LEN)
INTEGER LEN, DATATYPE
```

Reduction Operator Functions

- Operator function for ■ must act as:

```
for (i = 1 to len)
   inoutvec(i) = inoutvec(i) ■ invec(i)
```

- Operator ■ need not commute but must be associative.

Registering User-Defined Operator

- Operator handles have type **`MPI_Op`** or **`INTEGER`**
- C:

```
int MPI_Op_create(MPI_User_function
      *my_op, int commute, MPI_Op *op)
```

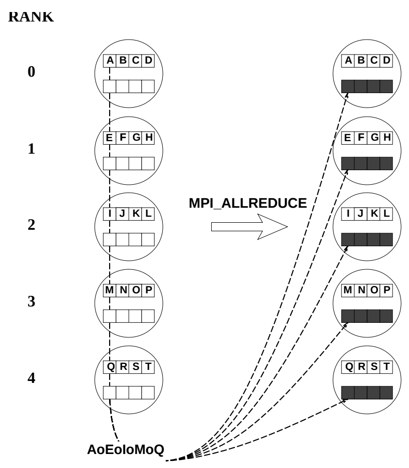
- Fortran:

```
MPI_OP_CREATE (MY_OP, COMMUTE, MPI_OP, IERROR)
EXTERNAL FUNC
LOGICAL COMMUTE
INTEGER OP, IERROR
```

Variants of MPI_REDUCE

- **`MPI_ALLREDUCE`** – no root process
- **`MPI_REDUCE_SCATTER`** – result is scattered
- **`MPI_SCAN`** – “parallel prefix”

MPI_ALLREDUCE



MPI_ALLREDUCE

Integer global sum

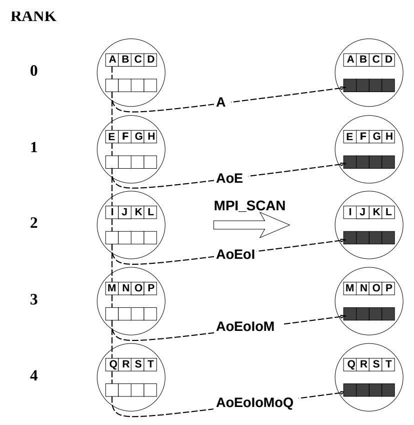
- C:

```
int MPI_Allreduce(void* sendbuf,
         void* recvbuf, int count,
         MPI_Datatype datatype,
         MPI_Op op, MPI_Comm comm)
```

- Fortran:

```
MPI_ALLREDUCE(SENDBUF, RECVBUF, COUNT,
           DATATYPE, OP, COMM, IERROR)
```

MPI_SCAN



MPI_SCAN

Integer partial sum

- C:

```
int MPI_Scan(void* sendbuf, void* recvbuf,
        int count, MPI_Datatype datatype,
        MPI_Op op, MPI_Comm comm)
```

- Fortran:

```
MPI_SCAN(SENDBUF, RECVBUF, COUNT,
      DATATYPE, OP, COMM, IERROR)
```

Exercise

- Rewrite the pass-around-the-ring program to use MPI global reduction to perform its global sums.
- Then rewrite it so that each process computes a partial sum.
- Then rewrite this so that each process prints out its partial result, in the correct order (process 0, then process 1, etc.).

Casestudy
Towards Life

The Story so Far....

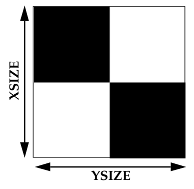
- This course has:
  - Introduced the basic concepts/primitives in MPI.
  - Allowed you to examine the standard in a comprehensive manner.
  - Not all the standard has been covered but you should now be in a good position to do so yourself.
- However the examples have been rather simple. This case study will:
  - Allow you to use all the techniques that you have learnt in one application.
  - Teach you some basic aspects of domain decomposition: how you go about parallelising a code.
  - ... other courses in EPCC do this in more detail ...

Overview

- Three part case study that puts into practice all that you learnt in this course to build a *real* application
  - each part is self contained (having completed the previous part)
  - later parts build on from earlier parts
  - extra exercises extend material and are independent
- If all parts completed you should end up with a fully working version of *the Game of Life*
- Detailed description on how to do the casestudy in notes
  - start from *scratch* – some *pseudo code* provided

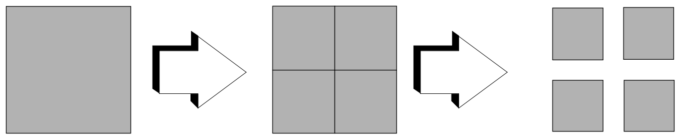
Part 1: Master–slave Model

- Create a master–slave model
  - master outputs data to file (also does work!)
  - perform a domain decomposition of *large* 2d array
  - create a chess board pattern – processors colour local domains
  - output *pgm* files – graphical result
- Can view the result using *xv*



Details

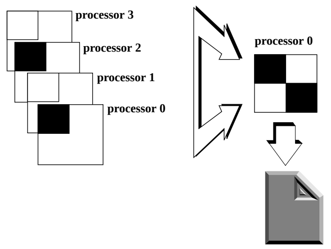
- Basically what you want to do for this part is:-
  - Create a cartesian virtual topology
  - Decompose a global array across processors



  - Processor colours in its segment according to its position
  - Create derived data type(s) to receive local arrays at the master processor – these arrays must be inserted at the correct location.
  - May need to create derived data types at the slave processors to send data to the master processor.

Details *cont.*

All processors write their data back to the master processor



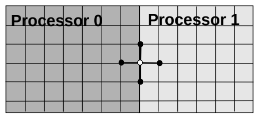
Master processor writes data to file in pgm (portable graymap) format

- ❑ view the results using xv to make sure it works

Try different numbers of processors to make sure the program works properly.

Part 2: Boundary Swaps

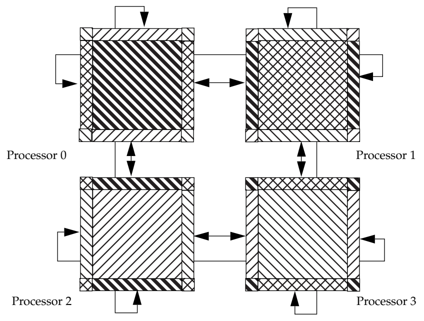
- ❑ Part 1 achieves the beginning of a decomposition.
- ❑ Lots of applications require data located on the other processor, *e.g.* finite differences.



- ❑ Instead of communicating each element of data as is needed all elements necessary are copied across. This is called a *halo region*.
- ❑ Internal points can thus be calculated without further communications. Here we will practice boundary swaps.

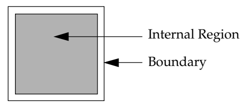
Outline Sketch

- ❑ Create a halo region.
- ❑ Perform halo swaps across processor domains.



Boundary Swaps

- ❑ To achieve this – Cheat.



Update internal regions of processor domains only.

Create derived data types to do the boundary swaps.

Halo region should be exterior to data storage – artificial.

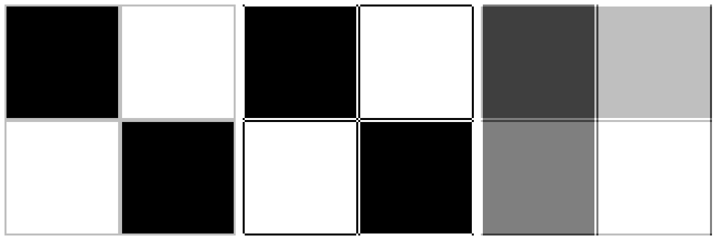
Here we want to see the result of the boundary swaps hence the halo is contained inside the data region.

This will have to be undone for the final part of this case study.

- ❑ You will be able to visualise whether the boundary swaps are being done correctly.

The Result

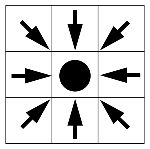
- ❑ Can *see* the result of performing the boundary swaps
  - Can make sure that the boundary swap are correct



- ❑ The underlying mechanism used here can be used in any future codes you might write....

Part 3: The game of Life

- ❑ Have all routines necessary to construct *Game of Life*.
- ❑ Simple Cellular Automata in a 2d space. State of cells at the next time step determined from a simple set of rules:



dead if cell has less than two live neighbours – lonely

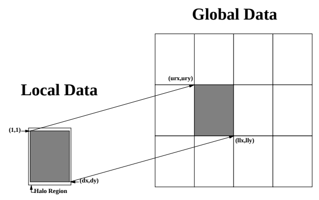
maintain state if cell has exactly two live neighbours – content

cell is born if the cell has exactly three live neighbours – ... ❤

die if the cell has more than three live neighbours – overcrowding

Procedure

- ❑ Rewrite the code from part 2 so that the halo lies outside the processor’s subdomain
  - Will need to write derived data types to transfer the internal regions, excluding the halo, of the processors to the master processor
- ❑ Must devise a mapping from local processor coordinates to global coordinates

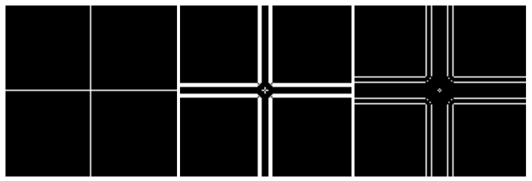


Allows global initial conditions to be output.

Results

- ❑ Output the state of the frame in pgm format at every iteration.
- ❑ Can animate the result using xv:

```
xv -expand 10 -wait 0.5 -wloop -raw *.pgm
```



Steps 0, 5 and 10 in the evolution of a 128x128 simulation.

- ❑ Good Luck.....!!

MPI on lomond

Compiling MPI Programs on lomond

- ❑ Fortran programmers use the Fortran 90 compiler
- ❑ Must include MPI library:

```
tmcc -o hello hello.c -lmpi

tmf90 -o hello hello.f -lmpi
```

Running MPI Programs on lomond

- ❑ To interactively run the executable **`hello`** on two processors in the **`fe-int`** queue:

```
lomond$ bsub -I -q fe-int -n 2 pam ./hello
```

- ❑ To run the executable **`hello`** on four processors in the **`8-course`** queue:

```
lomond$ bsub -q 8-course -c 00:10 -n 4 pam ./hello
```

  Use **`-o logfile`** to store the output in **`logfile`**

- ❑ The **`pam`** MPI job starter software is mandatory for all queues.
- ❑ The **`-c`** switch is mandatory in all queues except **`fe-int`**

Issues for Fortran Programmers

- ❑ You should use the Fortran 90 compiler - this is the preferred option, but:
- ❑ Use Fortran 90 features with care - MPI is a FORTRAN 77 library.
- ❑ In particular:
  - Do not pass array sections - whole arrays only
  - Do not use user defined data types
- ❑ You may however use Fortran 90 free-format layout for source files.

Compiling MPI Programs on lomond

- Example MPI makefiles are shown in Appendix A of the course notes.
- Similar to other makefiles.