MPI: The Message-Passing Interface

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Recommended Reading

- W. Gropp, E. Lusk and A. Skjellum: "Using MPI: Portable Parallel Programming with the Message-Passing Interface", 2nd Edn., MIT Press, 1999.
- W. Gropp, T. Hoefler, R. Thakur and E. Lusk: "Using Advanced MPI: Modern Features of the Message-Passing Interface", MIT Press, 2014.
- G. Karypis, V. Kumar et al. "Introduction to Parallel Computing", 2nd Edn., Benjamin/Cummings, 2003 (Chapter 6).
- MPI homepage (incl. MPICH user guide): `http://www.mcs.anl.gov/mpi/`
- MPI forum (for official standards, incl. MPI-3): `http://www.mpi-forum.org/`

Outline

- Introduction to MPI
- MPI for PC clusters (MPICH)
- Basic features
- Non-blocking sends and receives
- Collective operations
- Advanced features of MPI

Introduction to MPI

- MPI (Message-Passing Interface) is a standard library of functions for sending and receiving messages on parallel/distributed computers or workstation clusters.
- C/C++ and Fortran interfaces available.
- MPI is independent of any particular underlying parallel machine architecture.
- Processes communicate with each other by using the MPI library functions to send and receive messages.
- Now on its third major version, with each version incorporating the functionality of the previous version but adding additional features.
- Over 300 functions in standard; only 6 needed for basic communication.

MPI for PC clusters (MPICH) I

- MPICH is installed on the lab machines. The `corona` machines should always be available, but please run CPU-intensive MPI jobs outside of lab hours.
- Set up a file called `hosts`, e.g.
  ```
  corona01.doc.ic.ac.uk
  corona02.doc.ic.ac.uk
  ```
- Make sure you can `ssh` to the machines: e.g.
  ```
  ssh corona01.doc.ic.ac.uk uptime
  ```
  (see CSG pages on `ssh` for help if this fails).

MPI for PC clusters (MPICH) II

- Compile your C program:
  ```
  % mpicc sample.c -o sample
  ```
- Or for C++ source:
  ```
  % mpic++ sample.cxx -o sample
  ```
- Run your program:
  ```
  % mpiexec -machinefile hosts -np 4 ./sample
  ```


Basic features: First and last MPI calls

- **Initialise MPI**:
  ```
  int MPI_Init(int *argc, char ***argv);
  ```
  e.g.:
  ```
  int main(int argc, char *argv[]) {
    if (MPI_Init(&argc,&argv)!=MPI_SUCCESS) {
      ... error ...
    } ...etc...
  }
  ```
- **Shutdown MPI**:
  ```
  int MPI_Finalize(void);
  ```
  e.g. `MPI_Finalize();`

Basic features: The environment

- **Rank identification**:
  ```
  int MPI_Comm_rank(MPI_Comm comm, int *rank);
  ```
  e.g.:
  ```
  int rank;
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  ```
- **Find number of processes**:
  ```
  int MPI_Comm_size(MPI_Comm comm, int *size);
  ```
  e.g.:
  ```
  int size;
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  ```

A very basic C++ example

```
#include <iostream>
#include "mpi.h"
using namespace std;

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);
  cout << "[" << rank << "] of " << size << " processors
     reporting!" << endl;
  MPI_Finalize();

  return 0;
}
```


Basic features I

- **Sending a message (blocking)**:

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

e.g.:

```
#define TAG_PI 100

double pi = 3.1415926535;

MPI_Send(&pi, 1, MPI_DOUBLE, 0, TAG_PI,
  MPI_COMM_WORLD);
```


Basic features II

- **Receiving a message (blocking)**

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

e.g.:

```
double num;
MPI_Status status;

MPI_Recv(&num, 1, MPI_DOUBLE,
  MPI_ANY_SOURCE, MPI_ANY_TAG,
  MPI_COMM_WORLD, &status);
```


Basic features III

- Receive status information includes:

```
status.count       = message length
status.MPI_SOURCE  = message sender
status.MPI_TAG     = message tag
```

- Note the special tags:

```
MPI_ANY_SOURCE     MPI_ANY_TAG
```

Basic features: Data types

- MPI datatypes include:

MPI_CHAR	MPI_BYTE
MPI_SHORT	MPI_INT
MPI_LONG	MPI_FLOAT
MPI_DOUBLE	MPI_PACKED
MPI_UNSIGNED	MPI_UNSIGNED_CHAR
MPI_UNSIGNED_LONG	MPI_UNSIGNED_SHORT

- It is possible to create other user-defined datatypes.

A simple C message-passing example

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

int main(int argc, char *argv[])
{
  char msg[20], smsg[20];
  int rank, size, src, dest, tag;
  MPI_Status status;
  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  if (size!=2) {
    MPI_Abort(MPI_COMM_WORLD, 1);
    return 1;
  }
```


A simple C message-passing example

```
  src  = 1;
  dest = 0;
  tag  = 999;
  if (rank==src) {
    strcpy(msg, "Hello World");
    MPI_Send(msg, 12, MPI_BYTE, dest, tag, MPI_COMM_WORLD);
  } else {
    MPI_Recv(smsg, 12, MPI_BYTE, src, tag, MPI_COMM_WORLD, &status);
    if (strcmp(smsg, "Hello World"))
      fprintf(stderr, "Message is wrong !\n");
    else
      fprintf(stdout, "Message(%s) %d->%d OK !\n", smsg, src, dest);
  }
  MPI_Finalize();
  return 0;
}
```


Non-blocking sends/receives I

- **Non-blocking send/receive**:

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

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

Non-blocking sends/receives II

- **Wait for send/receive completion**:

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

int MPI_Waitall(int count,
  MPI_Request *array_of_requests,
  MPI_Status *array_of_statuses);
```

- **Non-blocking probe for a message**:

```
int MPI_Iprobe(int source, int tag,
  MPI_Comm comm, int *flag,
  MPI_Status *status);
```

- `flag` is set if message waiting
- `status` has details of message

Collective operations

- Often need to communicate between groups of processes rather than just one-to-one, and MPI defines a large number of collective operations to enable this.
- These groups communicate using specific communicators rather than the message tags used in one-to-one communication.
- Three classes of collective operations:
  - Data movement
  - Collective computation
  - Explicit synchronisation
- Note that all collective operations are blocking operations within the particpating communication group.

Creating your own communicators

- You create your own communicators by splitting up pre-existing communicators:

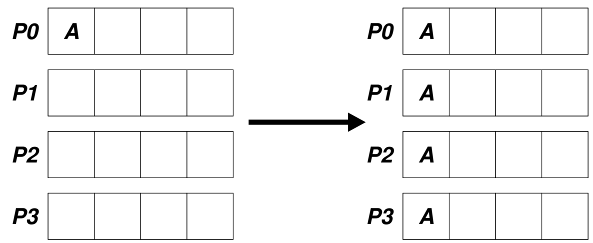
```
int new_group_size = 3;
int new_group_members[] = {1,3,5};
MPI_Group all, some;
MPI_Comm subset;

MPI_Comm_group(MPI_COMM_WORLD, &all);
MPI_Group_incl(all, new_group_size,
  new_group_members, &some);
MPI_Comm_create(MPI_COMM_WORLD, some,
  &subset);
```

- The complementary function, `MPI_Group_excl`, also exists.

Data movement operations I

- **Broadcasting**:




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

Data movement operations II

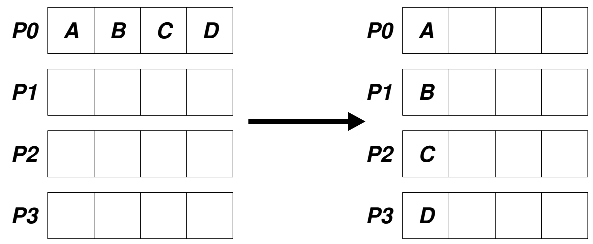
- **Multicasting**:
  Most elegant way is to create a communicator for a subset of the MPI processes, and broadcast to that subset:

```
int new_group_size = 3;
int new_group_members[] = {1,3,5};
MPI_Group all, some;
MPI_Comm subset;

MPI_Comm_group(MPI_COMM_WORLD, &all);
MPI_Group_incl(all, new_group_size,
  new_group_members, &some);
MPI_Comm_create(MPI_COMM_WORLD, some,
  &subset);
MPI_Bcast(buffer, ... , subset);
```


Data movement operations III

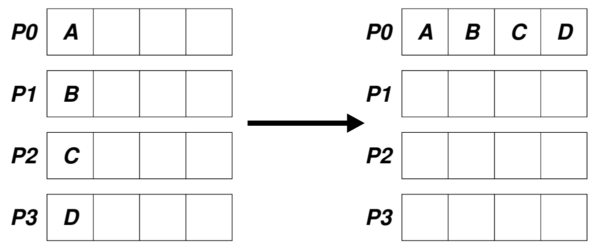
- **Scatter operation**:




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


Data movement operations IV

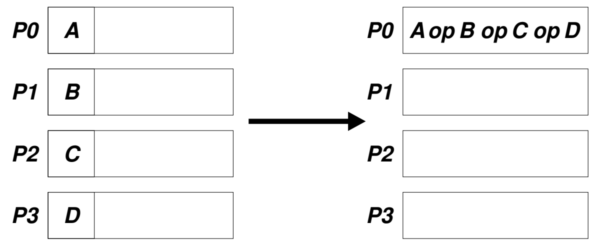
- **Gather operation**:




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


Collective computation operations

- **Reduce operation**:




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

- Useful ops include MPI_SUM, MPI_PROD, MPI_MIN and MPI_MAX.
- Can also define your own operations.

Collective operations

- There are also a large number of MPI collective operations beyond those shown here.
- Those starting with `All` deliver results to all participating processes (e.g. `MPI_Allgather`).
- Those ending with `v` allow different sizes of buffer to be sent and received (e.g. `MPI_Scatterv`).

Explicit synchronisation

- **Barrier synchronization**:
  `int MPI_Barrier(MPI_Comm comm);`
- **Timing your program**:
  `double MPI_Wtime();`

Non-contiguous data

```
int MPI_Pack_size(int incount,
  MPI_Datatype datatype, MPI_Comm comm,
  int *size);

int MPI_Pack(void* inbuf, int incount,
  MPI_Datatype datatype, void *outbuf,
  int outsize, int *position,
  MPI_Comm comm);

int MPI_Unpack(void* inbuf, int insize,
  int *position, void *outbuf, int outcount,
  MPI_Datatype datatype, MPI_Comm comm);
```


Advanced features of MPI

- MPI-2 introduces 3 new advanced features:
  - Parallel I/O
  - Remote memory operations
  - Dynamic process management

Parallel I/O

- MPI-1 relied on OS I/O functions, but MPI-2 provides `MPI_File` functions for dedicated parallel I/O:

```
int MPI_File_open(MPI_Comm comm, char *name,
  int mode, MPI_Info info, MPI_File *fh);

int MPI_File_seek(MPI_File fh,
  MPI_Offset offset, int whence);

int MPI_File_read / MPI_File_write(
  MPI_File fh, void *buf, int count,
  MPI_Datatype type, MPI_Status *status);

int MPI_File_close(MPI_File *fh);
```

- Also supports parallel I/O for non-contiguous data, non-blocking parallel I/O and shared file pointers.

Remote memory operations

- Based on *windows* into each process's address space:

```
int MPI_Put / int MPI_Get(void *srcaddr,
  int srccount, MPI_Datatype srctype,
  int targrank, MPI_Aint targdisp,
  int targcount, MPI_Datatype targtype,
  MPI_Win win);

int MPI_Accumulate(void *srcaddr,
  int srccount, MPI_Datatype srctype,
  int targrank, MPI_Aint targdisp,
  int targcount, MPI_Datatype targype,
  MPI_Op op, MPI_Win win);
```

- These operations are non-blocking.
- Note that functions like `MPI_Win_lock()` aren't shared memory locks!

Dynamic process management

- In the MPI-1 standard, the number of processors a given MPI job executes on is fixed.
- In MPI-2 supports dynamic process managment to allow:
  - New MPI processes to be spawned while an MPI program is running.
  - New MPI processes to connect to other MPI processes which are already running.
- Interesting to compare PVM with MPI-1 and MPI-2!

MPI-3 is rolling out

- MPI-3 was adopted as a standard in September 2012.
- For full specification see `http://www.mpi-forum.org/docs/`
- Includes non-blocking versions of many collective operations and various tweaks to Remote Direct Memory Access (RDMA) operations.
- Implementations ongoing.