Message Passing Interface (MPI)

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What is MPI?

A message-passing library specification for explicitly programming message-passing systems.

- Fully featured
  - point-to-point, collective, and one-sided communications
  - I/O routines and profiling interface
- Multiple language bindings
  - C, C++ and Fortran
- Available on many platforms
  - Production grade implementations on supercomputers
  - Open source implementations (*e.g.* Open MPI) on Linux and Windows
- Has been stable for many years:
  - MPI 2.0 was released in 1996, and it lasted 16 years
  - MPI 3.0 was released in Sept. 2012 (Manual 852 pages)

Features of MPI

- *Point-to-Point Communications*
  - Structured buffers and derived data types, heterogeneity
  - many modes: blocking vs non-blocking vs synchronous, ready vs buffered
- *Collective Communications*
  - Both built-in and user-defined collective operations
  - Large number of data movement routines
  - Subgroups defined directly or by topology
  - Built-in support for grids and graphs
- *One-Sided Communications*
  - Allow remote memory access
- *Others*
  - Message security, thread safety
  - Profiling hooks, error control

MPI for Beginners

One need not master all parts of MPI to use it. These six functions allow you to write many programs:

- `MPI_Init` — starting MPI
- `MPI_Finalize` — exiting MPI
- `MPI_Comm_size` — the number of processes
- `MPI_Comm_rank` — the id of *this* process
- `MPI_Send` — sending a message
- `MPI_Recv` — receiving a message

"Hello world!" in MPI

- C Version:

```
#include "mpi.h"
int main(int argc, char **argv) {
  MPI_Init(&argc, &argv);
  printf("Hello world!\n");
  MPI_Finalize();
  return 0;
}
```

- C++ Version:

```
#include "mpi++.h"
int main(int argc, char **argv) {
  MPI::Init(argc, argv);
  cout << "Hello world!" << endl;
  MPI::Finalize();
  return 0;
}
```

`MPI_Init()` and `MPI_Finalize()` must be included in every MPI program.

"Hello world!" in MPI (Version 2)

```
#include "mpi.h"
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);
  printf("Hello world! I'm %d of %d\n", rank, size);
  MPI_Finalize();
  return 0;
}
```

Communication in MPI takes place with respect to *communicators*.

- `MPI_COMM_WORLD` is the default communicator, it contains all MPI processes. User can define other communicators.
- `MPI_Init()` and `MPI_Finalize()` must be called by *all* processes.

Basic Send/Receive

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

```
int MPI_Recv(void *buf, int count, MPI_Datatype type, int src,
             int tag, MPI_Comm comm, MPI_Status *st)
```

- `buf` — initial address of send/receive buffer
- `count, type` — number of and type of elements to be sent/received
- `dest, src` — rank of destination and source processes; a special value for `src` is `MPI_ANY_SOURCE`
- `tag` — message tag
- `comm` — communicator
- `st` — status of the receive command; its info includes `MPI_SOURCE`, `MPI_TAG`, `MPI_ERROR`, and message length

A Simple Send/Receive Program

```
#include <mpi.h>

int main(int argc, char **argv) {
  int i, rank, size, dest, to, src, from;
  int count, tag, st_count, st_src, st_tag;
  double data[100];
  MPI_Status st;

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  printf("Process %d of %d is alive\n", rank, size);
  src = 0; dest = size - 1;

  if (rank == src) {
    to = dest;
    tag = 2001;
    count = 100;
    for (i = 0; i < 100; i++)
      data[i] = i;
    MPI_Send(data, count, MPI_DOUBLE, to, tag, MPI_COMM_WORLD);
  }
```


A Simple Send/Receive Program (cont.)

```
  else if (rank == dest) {
    from = MPI_ANY_SOURCE;
    tag = MPI_ANY_TAG;
    count = 100;
    MPI_Recv(data, count, MPI_DOUBLE, from, tag, MPI_COMM_WORLD, &st);
    MPI_Get_count(&st, MPI_DOUBLE, &st_count);
    st_src = status.MPI_SOURCE;
    st_tag = status.MPI_TAG;
    printf("Status info: source = %d, tag = %d, count = %d\n",
           st_src, st_tag, st_count);

    printf(" %d received: ", rank);
    for (i = 0; i < st_count; i++)
      printf("%lf ", data[i]);
    printf("\n");
  }
  MPI_Finalize();
  return 0;
}
```


Non-Blocking Send and Receive

```
int MPI_ISend(void *buf, int count, MPI_Datatype type, int dest,
              int tag, MPI_COMM comm, MPI_Request *req)
```

```
int MPI_IRecv(void *buf, int count, MPI_Datatype type, int src,
              int tag, MPI_COMM comm, MPI_Request *req)
```

Both routines create and allocate a *request object* and return a pointer to it in the `req` variable.

This object is useful for future testing and waiting for the finish of the non-blocking operation:

```
int MPI_Test(MPI_Request *reg, int *flag, MPI_Status *st)
int MPI_Wait(MPI_Request *reg, MPI_Status *st)
```

- If the value of `flag` is `true`, the operation has completed.

Combined Send/Receive

```
int MPI_Sendrecv(void *sbuf, int scnt, MPI_Datatype stype, int dest,
                 int stag, void *rbuf, int rcnt, MPI_Type rtype,
                 int src, int rtag, MPI_COMM comm, MPI_Status *st)
```

The routine performs both a send and a receive. Advantages over pair of send and receive:

- avoids deadlock
- does not require data buffering

Other Send Routines

- Synchronous Sends — Won't complete until the corresponding receive has been posted:

```
int MPI_Ssend(...)
int MPI_Issend(...)
```

- Ready Sends — Assume the corresponding receive has been posted; otherwise they are errorous:

```
int MPI_Rsend(...)
int MPI_Irsend(...)
```

- Buffered Sends — If the corresponding receive has not been posted, the system must buffer the data and return; it's the user's responsibility to allocate the buffer:

```
int MPI_Bsend(...)
int MPI_Ibsend(...)
```

Collective Communications

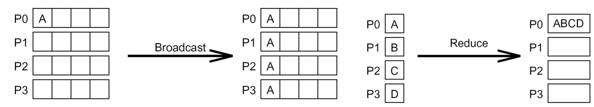
MPI Collective communications are coordinated among a group of processes, as specified by communicator.

- Message tags are not used
- All collective operations are blocking
- All processes in the communicator group must call the collective operation

Categories:

- One-to-All Broadcast
- All-to-One Reduction
- Scatter and Gather
- Prefix Scan
- All-to-All Broadcast & Reduction

Basic Broadcast and Reduce




```
int MPI_Bcast(void* buf, int cnt, MPI_Datatype type, int root,
              MPI_Comm comm)
```

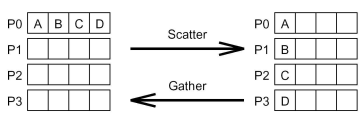
```
int MPI_Reduce(void* sbuf, void* rbuf, int cnt, MPI_Datatype type,
               MPI_Op op, int root, MPI_Comm comm)
```

- The reduce routine take can take the following built-in collective operators:

  MPI_SUM MPI_MAX MPI_LAND MPI_BAND MPI_LXOR MPI_MAXLOC
  MPI_PROD MPI_MIN MPI_LOR MPI_BOR MPI_BXOR MPI_MINLOC

- It can also take user-defined reduction functions.

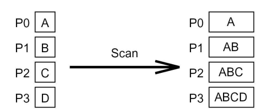
Scatter and Gather




```
int MPI_Scatter(void* sbuf, int scnt, MPI_Datatype stype,
                void *rbuf, int rcnt, MPI_Datatype rtype,
                int source, MPI_Comm comm)
```

```
int MPI_Gather(void* sbuf, int scnt, MPI_Datatype stype,
               void *rbuf, int rcnt, MPI_Datatype rtype,
               int target, MPI_Comm comm)
```

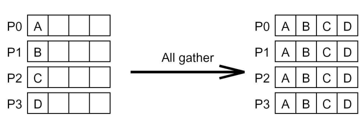

Prefix Scan

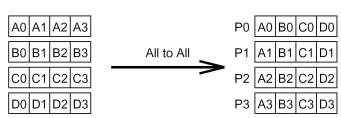



```
int MPI_Scan(void* sbuf, void *rbuf, int cnt, MPI_Datatype stype,
             MPI_Op op, MPI_Comm comm)
```


All-Version and V-Version Routines

- All-versions deliver results to all participating processes.





  MPI_ALLGATHER MPI_ALLREDUCE MPI_ALLTOALL

- V-versions allow the chunks to have different sizes.

  MPI_ALLGATHERV MPI_GATHERV MPI_ALLTOALLV

Example: Collective Communication

```
#include <mpi.h>
int main(int argc, char **argv) {
  int rank, size, myn, i, N;
  double *vector, *myvec, sum, mysum, total;

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  MPI_Comm_size(MPI_COMM_WORLD, &size);

  /* In the root process read the vector length, initialize
     the vector and determine the sub-vector sizes */
  if (rank == 0) {
    printf("Enter the vector length : ");
    scanf("%d", &N);
    vector = (double *)malloc(sizeof(double) * N);
    for (i = 0, sum = 0; i < N; i++)
      vector[i] = 1.0;
    myn = N / size;
  }

  MPI_Bcast(&myn, 1, MPI_INT, 0, MPI_COMM_WORLD);
```

Example: Collective Communication (cont.)

```
  myvec = (double *)malloc(sizeof(double)*myn);
  MPI_Scatter(vector, myn, MPI_DOUBLE, myvec, myn, MPI_DOUBLE,
              0, MPI_COMM_WORLD);

  /* Find the local sum, then the global sum of the vectors */
  for (i = 0, mysum = 0; i < myn; i++)
    mysum += myvec[i];
  MPI_Allreduce(&mysum, &total, 1, MPI_DOUBLE, MPI_SUM, MPI_COMM_WORLD);

  /* Multiply the local part of the vector by the global sum */
  for (i = 0; i < myn; i++)
    myvec[i] *= total;
  MPI_Gather(myvec, myn, MPI_DOUBLE, vector, myn, MPI_DOUBLE,
             0, MPI_COMM_WORLD);

  if (rank == 0)
    for (i = 0; i < N; i++)
      printf("[%d] %f\n", rank, vector[i]);
  MPI_Finalize();
  return 0;
}
```


One-Sided Communications

(*A.k.a.* Remote memory access or RMA.)

- Allow one process to specify all communication parameters, both for the sending side and for the receiving side.
- De-couple communication of data and syncrhonization between sender and receiver.
- The semantics is *very* complicated.

Sample Routines:

- `MPI_Put` — remote write
- `MPI_Get` — remote read
- `MPI_Accumulate` — remote update
- `MPI_Compare_and_swap` — remote atomic swap

One-Sided Communications (cont.)

- One-sided communications can only access data in specific memory regions called "*windows*", which have to be explicitly created.

```
MPI_Win_create(...)
```

- One-sided communications can only occur during specific temporal intervals called "*epochs*", which are bracketed with synchronization calls.

```
MPI_Win_lock(...)

... // RMA operation here

MPI_Win_unlock(...)
```


Example: One-Sided Communication

Process A:

```
int n;
MPI_WIN nwin;

MPI_Win_create(&n, sizeof(int), 1, MPI_INFO_NULL, MPI_COMM_WORLD, &nwin);
...
n = 1000; /* local update */
MPI_Barrier(MPI_COMM_WORLD);
...
```

Process B:

```
int n;
MPI_WIN nwin;

MPI_Win_create(MPI_BOTTOM, 0, 1, MPI_INFO_NULL, MPI_COMM_WORLD, &nwin);
...
MPI_Barrier(MPI_COMM_WORLD);
MPI_Win_lock(MPI_LOCK_EXCLUSIVE, 0, 0, nwin);
MPI_Get(&n, 1, MPI_INT, 0, 0, 1, MPI_INT, nwin); /* remote read */
MPI_Win_unlock(MPI_LOCK_EXCLUSIVE, 0, 0, nwin);
```


File I/O

```
int MPI_File_open(MPI_Comm comm, char *filename, int amode,
                  MPI_Info info, MPI_File *fh)
```

```
int MPI_File_close(MPI_File *fh)
```

- Both routines are collective routines:
  – Input parameters (except `info`) must have the same values;
  – `MPI_File_close` implies a `MPi_File_sync`.
- However, it's possible to open a file to just one process — by using `MPI_COMM_SELF` as `comm`'s value.
- File access modes include the usual choices, *e.g.*, *read-only*, *read-write*, *append*, etc.
- File Info is for advanced uses (i.e. passing optimization hints). For normal cases, just use `MPI_INFO_NULL`.

Example: Reading From a File

```
int main(int argc, char *argv[])
{
  int size, rank, buf[2];
  MPI_File fh;
  MPI_Status st;

  MPI_Init(&argc, &argv);
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);

  MPI_File_open(MPI_COMM_WORLD, argv[1], MPI_MODE_RDONLY,
                MPI_INFO_NULL, &fh);
  MPI_File_set_view(fh, 0, MPI_INT, MPI_INT, "native", MPI_INFO_NULL);
  MPI_File_read(fh, buf, 2, MPI_INT, &st);
  MPI_File_close(&fh);

  printf("rank=%d: buf=[%d,%d]\n", rank, buf[0], buf[1]);
  MPI_Finalize();
  return 0;
}
```

Example: Writing to a File

```c
int main(int argc, char *argv[])
{
  int cnt=4, buf[4], i, rank;
  char fname[10];
  MPI_File fh;
  MPI_Status st;

  MPI_Init(&argc,&argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  for (i=0; i<cnt; i++) buf[i] = rank*100 + i;
  sprintf(fname, "%s.%d", "test", rank);

  MPI_File_open(MPI_COMM_SELF, fname, MPI_MODE_CREATE|MPI_MODE_RDWR,
                MPI_INFO_NULL, &fh);
  MPI_File_set_view(fh, 0, MPI_INT, MPI_INT, "native", MPI_INFO_NULL);
  MPI_File_write(fh, buf, cnt, MPI_INT, &st);
  MPI_File_close(&fh);

  MPI_Finalize();
  return 0;
}
```


File View

```c
int MPI_File_set_view(MPI_File fh, MPI_Offset disp, MPI_Datatype etype,
                      MPI_Datatype ftype, char *datarep, MPI_Info info)
```

This routine sets individual process's view of the data in the file.

- `disp` — displacement. Specifies where within the file to start access. Useful for reading different sections to different processes.
- `etype` — elementary datatype.
- `ftype` — file type. For advanced uses. Specifies gaps between desirable data items. For simple cases, just use the same value as `etype`.
- `datarep` — data representation. Normally just use `"native"`.

Open MPI

An open-source implementation of MPI.

- Comprehensive — support many platforms (including GPUs)
- Flexible — lots of user-level configuration/tuning controls
- High-Performance — used by many TOP500 supercomputers

(The name 'Open MPI' can be shortend to OMPI, but *not* to OpenMPI.)

The steps to use Open MPI:

- Creating a hostfile
- Compiling a program
- Running a program

Optionally, one can also create an appfile.

Open MPI: Creating a Hostfile

A hostfile contains a list of computer names.

Example:

```
linux> cat myhosts
# a line starting with # is a comment
african
chatham
chinstrap
...
```

- The MPI program must be accessible by the same pathname on all host computers.
- The environment variable `OMPI_MCA_orte_default_hostfile` can be set to point to a default hostfile.
- It's a good idea to create multiple host files for different number of hosts: *e.g.* `mpihost2`, `mpihost4`, `mpihost8`, etc.

Open MPI: Compiling a Program

The command: **mpicc**

Example:

```
linux> mpicc -o ring ring.c
```

- mpicc is just a gcc wrapper:

```
linux> mpicc --showme
gcc -I/usr/lib/openmpi/include -I/usr/lib/openmpi/include/openmpi
-pthread -L/usr/lib/openmpi/lib -lmpi -lopen-rte -lopen-pal -ldl
-Wl,--export-dynamic -lnsl -lutil -lm -ldl
```


Open MPI: Running a Program

The command:

```
mpirun -host <hostnames> -n <#process> <program>
mpirun -hostfile <hostfile> -n <#process> <program>
```

Example:

```
linux> mpirun -n 4 ring
linux> mpirun -host african -n 4 ring
linux> mpirun -host african,chatham -n 4 ring
linux> mpirun -hostfile host2 -n 4 ring
linux> mpirun -hostfile host4 -n 4 ring
```

- If there is no host or hostfile specified, the program will run on the console computer.
- The number of processes do not need to match the number of hosts.
- If a default hostfile exists, the `-hostfile` switch can be omitted.

Open MPI: Running a Program (cont.)

Open MPI also supports master/slave programs:

Example:

```
linux> mpirun -hostfile myhosts -n 1 master -n 4 slave
```

This command will run one copy of 'master' and four copies of 'slave'.

Creating an Appfile

mpirun command-line parameters can be saved in an appfile; and a program can be executed from an appfile.

Example:

```
linux> cat myapp
# execute 4 copies of 'ring' on 2 hosts
-host african,chatham -n 4 ring
linux> mpirun -app myapp
```