Masterpraktikum - Scientific Computing, High Performance Computing

Message Passing Interface (MPI)

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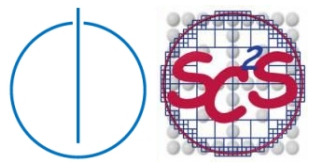

Outline

- Hello World
- P2P communication
- Collective operations
- Virtual topologies and communicators

Hello World

```
#include <mpi.h>
void 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! (rank %d of %d)", rank,
size);
   MPI_Finalize();
}
```

- compile
  `mpicc -o hello hello.c`
- execute
  `mpirun -np number_of_processes ./hello`

Hello World

```
#include <mpi.h>
void 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! (rank %d of %d)", rank,
size);
   MPI_Finalize();
}
```

- `int MPI_Comm_size(MPI_Comm comm, int *size)`
  Returns the number of processes in the communicator
  - `MPI_COMM_WORLD` : Predefined standard communicator. Includes all processes of a parallel application.
- `int MPI_Comm_rank(MPI_Comm comm, int *size)`
  Returns the process number of the executing process.

Point-to-Point Communication

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

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

- Blocking operations (return when buffer can be reused)
- `rank` (dest/source) and `tag` of send- and recieve-call must match
- Wildcards for recieve-calls
  - `MPI_ANY_SOURCE`, `MPI_ANY_TAG`, `MPI_STATUS_IGNORE`
- Messages with same destination rank do **not** overtake each other (order preservation)

MPI Datatypes

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	unsigned int
...	
MPI_FLOAT	float
MPI_DOUBLE	double

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Point-to-Point Communication

Example: ring.c

```
...
int rank, size, dest, src;
double *s_buf, *r_buf;
MPI_Status status;
...
dest = (rank + 1) % size;
src = (rank - 1 + size) % size;
MPI_Send(s_buf,2,MPI_DOUBLE,dest,0,MPI_COMM_WORLD);
MPI_Recv(r_buf,2,MPI_DOUBLE,src,0,MPI_COMM_WORLD,&status);
...
```

Point-to-Point Communication

Example: ring.c

```
...
int rank, size, dest, src;
double *s_buf, *r_buf;
MPI_Status status;
...
dest = (rank + 1) % size;
src = (rank - 1 + size) % size;
MPI_Send(s_buf,2,MPI_DOUBLE,dest,0,MPI_COMM_WORLD);
MPI_Recv(r_buf,2,MPI_DOUBLE,src,0,MPI_COMM_WORLD,&status);
...
```

Deadlock!

Non-blocking Communication

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

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

- Returns immediately
- Separates communication into three phases
  - (1) initiate communication
  - (2) do something else
  - (3) wait for communication to complete
- `MPI_Request`-object is used to test / wait for completition.

Non-blocking Communication

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

- Waits until pending communication is finished.

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

- Tests if pending communication is finished.

Other routines

- `MPI_Waitall`, `MPI_Testall`
- `MPI_Waitany`, `MPI_Testany`
- `MPI_Waitsome`, `MPI_Testsome`

Collective Operations

- Three types of collective operations
  - Synchronization (`MPI_Barrier`, ...)
  - Communication (`MPI_Bcast`, ...)
  - Reduction (`MPI_Allreduce`, ...)
- Must be executed by all processes of the communicator
- All collective operations are blocking operations
- MPI 3.0 will contain non-blocking collective operations

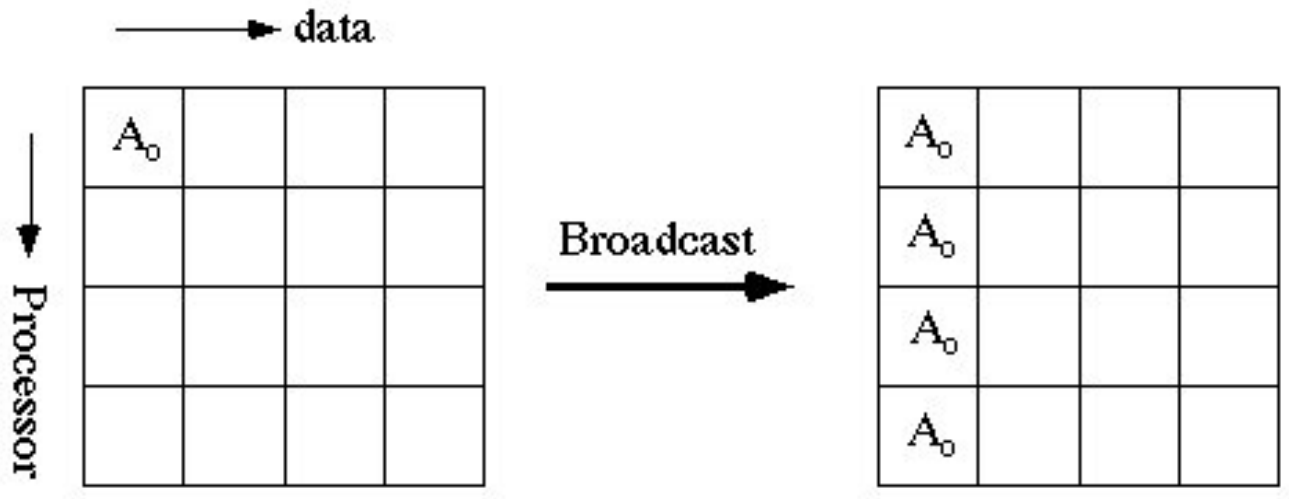
Collective Operations

```
MPI_Barrier (MPI_Comm comm);
```

- Blocks until **all** processes of the communicator have reached the barrier.

Collective Operations

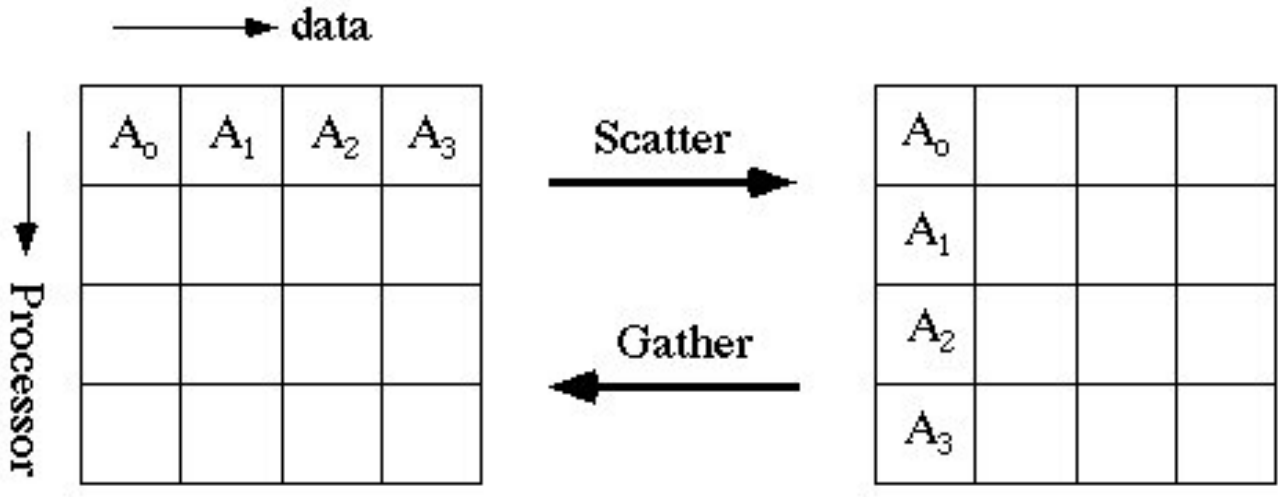
```
MPI_Bcast (void *buf, int count, MPI_Datatype dtype,
int root, MPI_Comm comm);
```



Collective Operations

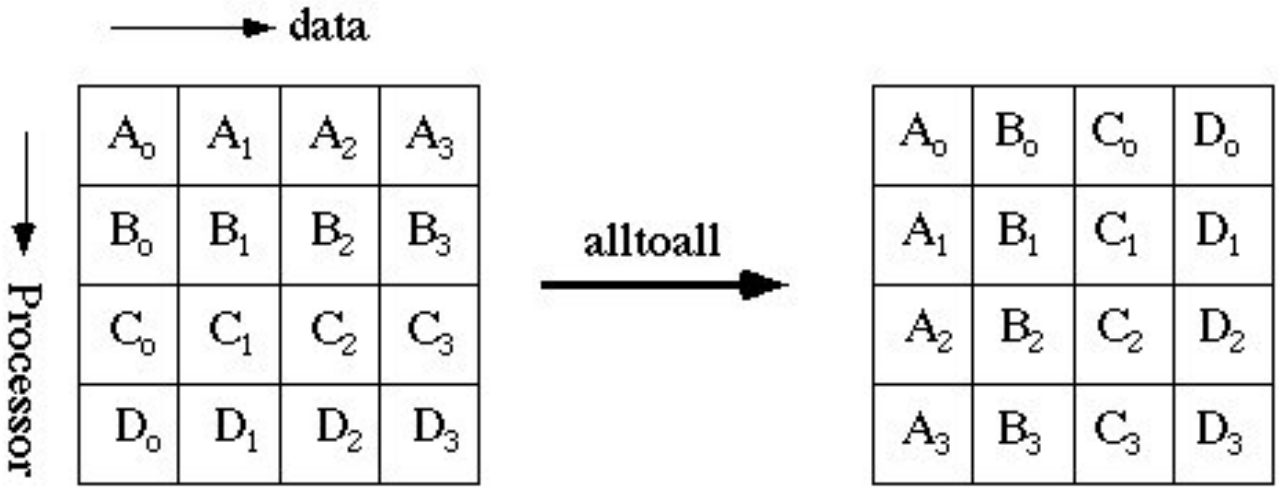
```
MPI_Gather(void *sendbuf, int sendcnt, MPI_Datatype
sendtype, void* recvbuf, int recvcnt, MPI_Datatype
recvtype, int root, MPI_Comm comm);
```

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



Collective Operations

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



Collective Operations

```
MPI_Reduce (void* sbuf, void* rbuf, int count,
MPI_Datatype dtype,MPI_Op op, int root, MPI_Comm
comm);
```

- Accumulates the elements in `sbuf` and delivers the results to process `root`.
- `MPI_Op` is a Reduction Operation Handle. Possible values:
  - MPI_MAX (Maximum)
  - MPI_MIN (Minimum)
  - MPI_SUM (Sum)
  - MPI_PROD (Product)
  - MPI_BAND (Bitwise AND)
  - ...
- Similar routines: `MPI_Allreduce`, `MPI_Reduce_scatter`

Virtual Topologies

- Processes of a communicator (e.g. `MPI_COMM_WORLD`) can be mapped to
  - a Cartesian Topology
  - a Graph Topology
- Allow convenient process naming with **cartesian process coordinates**.
- May lead to better performance (network aware programming).

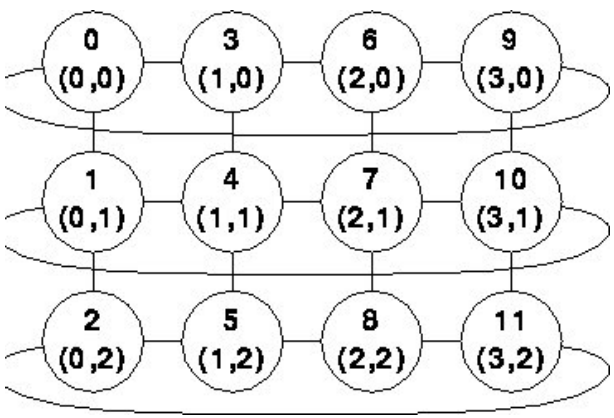
Virtual Topologies

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

- Creates a communicator with cartesian topology

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

- Cuts a grid up into “slices”.



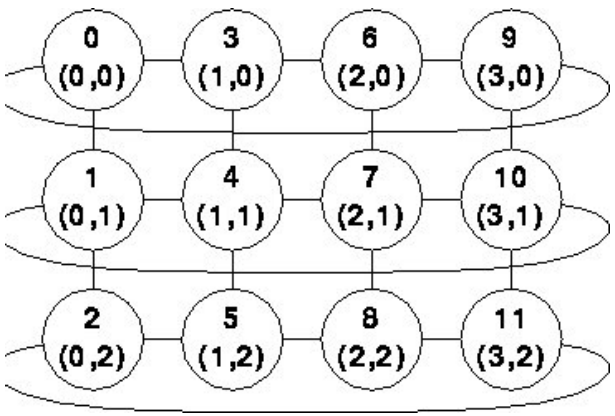
Virtual Topologies

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

- Converts grid coordinates into process rank.

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

- Returns the grid coordinates of process `rank`.



Other useful routines

```
double MPI_Wtime();
```

- Returns the elapsed time on the calling processor

Resources

- MPI 2.2 Standard
  http://www.mpi-forum.org/docs/mpi-2.2/mpi22-report.pdf
- List of MPI routines
  http://mpi.deino.net/mpi_functions/