MPI Tutorial

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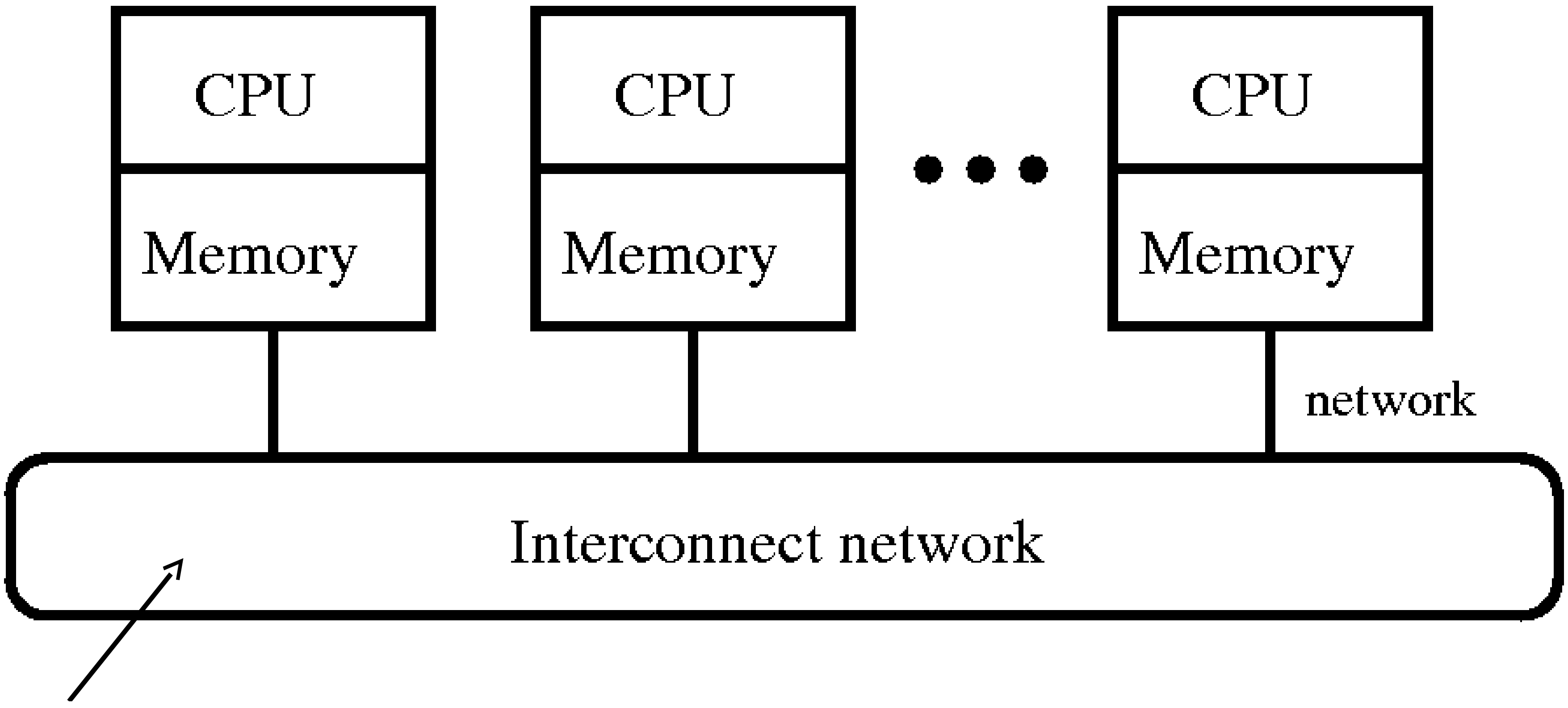
Distributed Memory

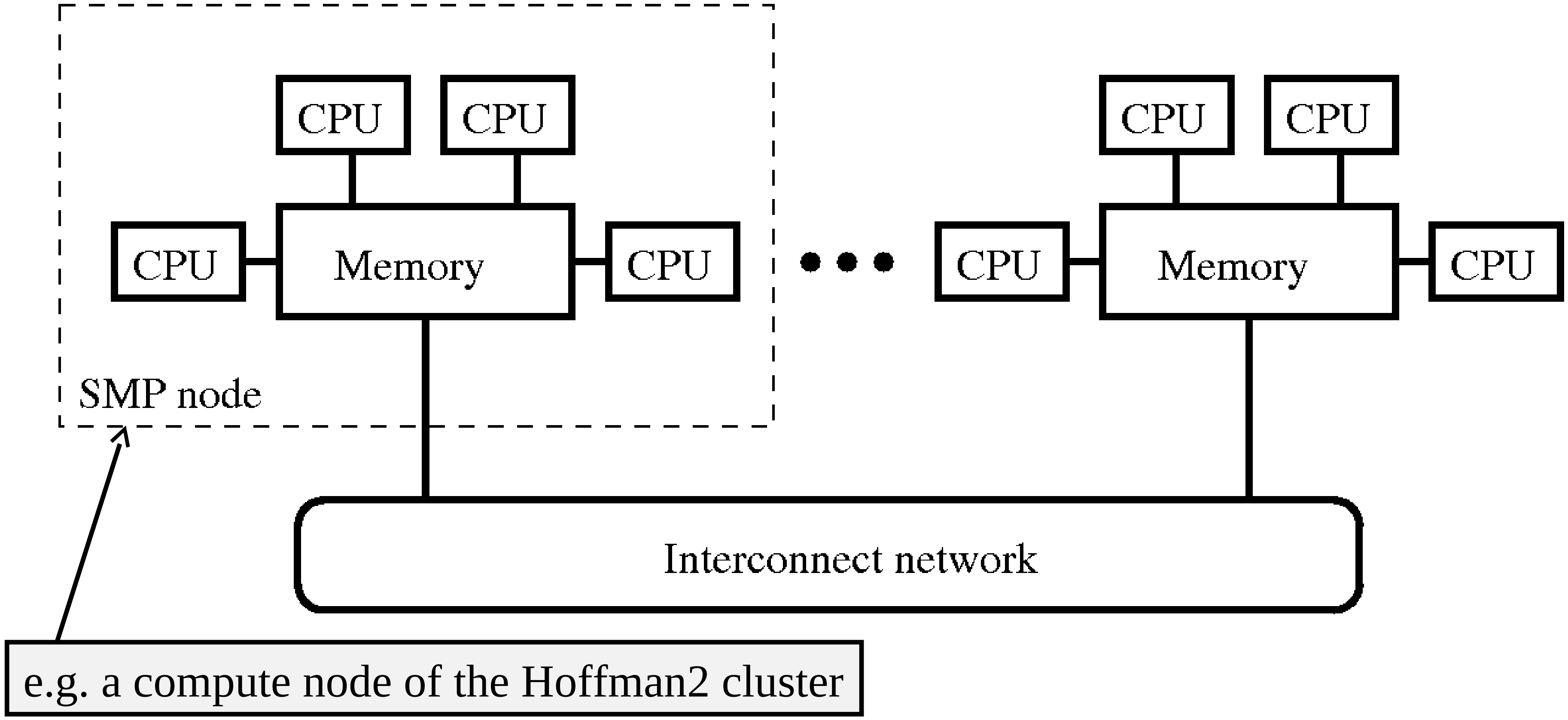
- Each CPU has its own (local) memory



This needs to be fast for parallel scalability (e.g. Infiniband, Myrinet, etc.)

Hybrid Model

- Shared-memory within a node
- Distributed-memory across nodes



Today’s Topics

- What is MPI
- Message passing basics
- Point to point communication
- Collective communication
- Derived data types
- Examples

MPI = Message Passing Interface

- API for distributed-memory programming
  - parallel code that runs across multiple computers (nodes)
  - http://www.mpi-forum.org/
- De facto industry standard
  - available on (almost) every parallel computer for scientific computing
- Use from C/C++, Fortran, Python, R, ...
- More than 200 routines
- Using only 10 routines are enough in many cases
  - Problem dependent

Clarification

- You can mix MPI and OpenMP in one program
- You *could* run multiple MPI processes on a single CPU
  - e.g. debug MPI codes on your laptop
  - An MPI job can span across multiple computer nodes (distributed memory)
- You *could* run multiple OpenMP threads on a single CPU
  - e.g. debug OpenMP codes on your laptop

MPI Facts

- High-quality implementation available for free
  - Easy to install one on your desktop/laptop
  - OpenMPI: http://www.open-mpi.org/
  - MPICH2: http://www.mcs.anl.gov/research/projects/mpich2/
- Installation Steps
  - download the software
  - (assuming you already have C/C++/Fortran compilers)
  - On Mac or Linux: “configure, make, make install”

Communicator

- A group of processes
  - processes are numbered 0,1,.. to N-1
- Default communicator
  - MPI_COMM_WORLD
  - contains all processes
- Query functions:
  - How many processes in total?

    MPI_Comm_size(MPI_COMM_WORLD, &nproc)
  - What is my process ID?

    MPI_Comm_rank(MPI_COMM_WORLD, &rank)

  …

Hello world (C)

```
#include "mpi.h”                         // MPI header file
#include <stdio.h>
main(int argc, char *argv[])
{
    int np, pid;
    MPI_Init(&argc, &argv);         // initialize MPI

    MPI_Comm_size(MPI_COMM_WORLD, &np);
    MPI_Comm_rank(MPI_COMM_WORLD, &pid);
    printf("N. of procs = %d, proc ID = %d\n", np, pid);

    MPI_Finalize();                      // clean up
}
```

Hello world (Fortran)

```
program hello
      Use mpi
      integer :: ierr,np,pid
      call mpi_init(ierr)
      call mpi_comm_size(MPI_COMM_WORLD,np,ierr)
      call mpi_comm_rank(MPI_COMM_WORLD,pid,ierr)
      write(*,'("np = ",i2,2x,"id = ",i2)') np,pid
      call mpi_finalize(ierr)
end program hello
```

☞ When possible, use “use mpi”, instead of “include ‘mpif.h’”

Error checking

- Most MPI routines returns an error code
  - C routines as the function value
  - Fortran routines in the last argument
- Examples
  - Fortran

    ```
    MPI_Comm_rank(MPI_COMM_WORLD, myid, ierr)
    ```
  - C/C++

    ```
    int ierr = MPI_Comm_rank(MPI_COMM_WORLD, &myid);
    ```

MPI built-in data types

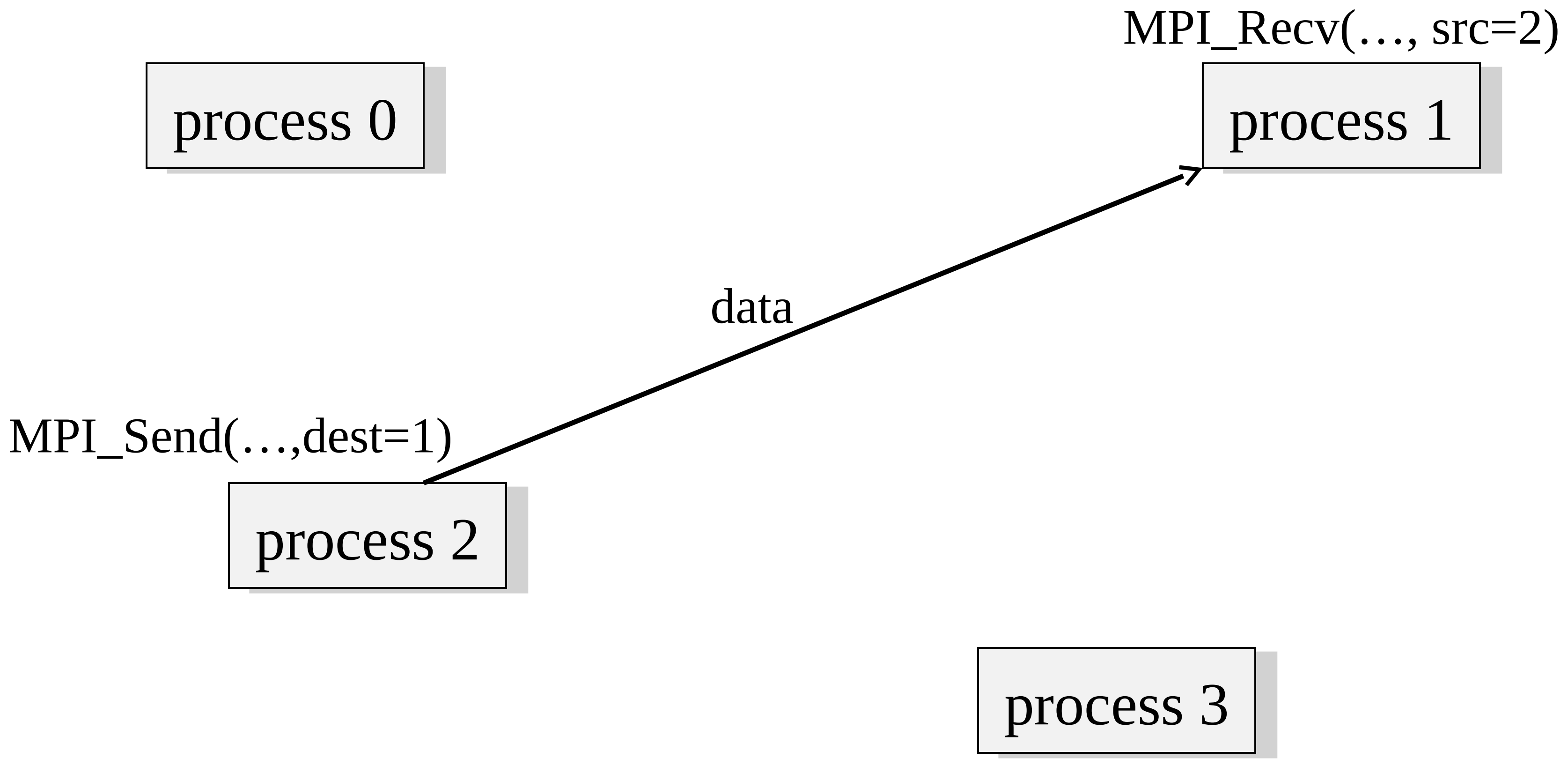
C/C++	**Fortran**
MPI_CHAR	MPI_CHARACTER
MPI_INT	MPI_INTEGER
MPI_FLOAT	MPI_REAL
MPI_DOUBLE	MPI_DOUBLE_PRECISION
…	…

- See MPI standard for a complete list
- New types can be (recursively) created/defined
  - based on existing types
  - called “derived data type”
  - discussed later

Today’s Topics

- Message passing basics
- Point to point communication
- Collective communication
- Derived data types
- Examples

Point to point communication



MPI_Send: send data to another process

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

Arguments	Meanings
buf	starting address of send buffer
count	# of elements
data_type	data type of each send buffer element
dest	processor ID (rank) destination
tag	message tag
comm	communicator

Examples:

```
C/C++:  MPI_Send(&x,1,MPI_INT,5,0,MPI_COMM_WORLD);
Fortran:MPI_Send(x,1,MPI_INTEGER,5,0,MPI_COMM_WORLD,ierr)
```

MPI_Recv: receive data from another process

MPI_Recv(buf, count, datatype, src, tag, comm, status)

Arguments	**Meanings**
buf	starting address of send buffer
count	# of elements
datatype	data type of each send buffer element
src	processor ID (rank) destination
tag	message tag
comm	communicator
status	status object (an integer array in Fortran)

Examples:

```
C/C++:   MPI_Recv(&x,1,MPI_INT,5,0,MPI_COMM_WORLD,&stat);
Fortran: MPI_Recv(x,1,MPI_INTEGER,5,0,MPI_COMM_WORLD,stat,ierr)
```

Notes on MPI_Recv

- A message is received when the followings are matched:
  - Source (sending process ID/rank)
  - Tag
  - Communicator (e.g. MPI_COMM_WORLD)
- Wildcard values may be used:
  - MPI_ANY_TAG

    (don’t care what the tag value is)
  - MPI_ANY_SOURCE

    (don’t care where it comes from; always receive)

Send/recv example (C)

- Send an integer array f[N] from process 0 to process 1

```
int f[N], src=0, dest=1;
MPI_Status status;
// ...
MPI_Comm_rank( MPI_COMM_WORLD, &rank);

if (rank == src)                    // process "dest" ignores this
      MPI_Send(f, N, MPI_INT, dest, 0, MPI_COMM_WORLD);

if (rank == dest)                        // process "src" ignores this
      MPI_Recv(f, N, MPI_INT, src, 0, MPI_COMM_WORLD, &status);
//...
```

Send/recv example (F90)

- Send an integer array f(1:N) from process 0 to process 1

```
integer f(N), status(MPI_STATUS_SIZE), rank, src=0, dest=1,ierr
// ...
call MPI_Comm_rank( MPI_COMM_WORLD, rank,ierr);

if (rank == src) then                    !process “dest” ignores this
      call MPI_Send(f, N, MPI_INT, dest, 0, MPI_COMM_WORLD,ierr)
end if

if (rank == dest) then                   !process “src” ignores this
      call MPI_Recv(f, N, MPI_INT, src, 0, MPI_COMM_WORLD,
status,ierr)
end if
//...
```

Send/Recv example (cont'd)

- Before

process 0 (send)	process 1 (recv)

f[0]=0
f[1]=1
f[2]=2
	f[0]=0
	f[1]=0
	f[2]=0

- After

process 0 (send)	process 1 (recv)

f[0]=0
f[1]=1
f[2]=2
	f[0]=0
	f[1]=1
	f[2]=2

Blocking

- Function call does not return until the communication is complete
- MPI_Send and MPI_Recv are blocking calls
- Calling order matters
  - it is possible to wait indefinitely, called “deadlock”
  - improper ordering results in serialization (loss of performance)

Deadlock

- This code always works:

```
MPI_Comm_rank(comm, &rank);

 if (rank == 0) {
     MPI_Send(sendbuf, cnt, MPI_INT, 1, tag, comm);
     MPI_Recv(recvbuf, cnt, MPI_INT, 1, tag, comm, &stat);
} else {  // rank==1
     MPI_Recv(recvbuf, cnt, MPI_INT, 0, tag, comm, &stat);
     MPI_Send(sendbuf, cnt, MPI_INT, 0, tag, comm);
}
```

Deadlock

- This code deadlocks:

```
MPI_Comm_rank(comm, &rank);

if (rank == 0) {
    MPI_Recv(recvbuf, cnt, MPI_INT, 1, tag, comm, &stat);
    MPI_Send(sendbuf, cnt, MPI_INT, 1, tag, comm);
} else { /* rank==1 */
    MPI_Recv(recvbuf, cnt, MPI_INT, 0, tag, comm, &stat);
    MPI_Send(sendbuf, cnt, MPI_INT, 0, tag, comm);
}
```

reason: MPI_Recv on process 0 waits indefinitely and never returns.

Non-blocking

- Function call returns immediately, without completing data transfer
  - Only “starts” the communication (without finishing)
  - MPI_Isend and MPI_Irecv
  - Need an additional mechanism to ensure transfer completion (MPI_Wait)
- Avoid deadlock
- Possibly higher performance
- Examples: MPI_Isend & MPI_Irecv

MPI_Isend

MPI_Isend(buf, count, datatype, dest, tag, comm, request)

- Similar to MPI_Send, except the last argument “request”
- Typical usage:

```
MPI_Request request_X, request_Y;
MPI_Isend(..., &request_X);
MPI_Isend(…, &request_Y);

//... some ground-breaking computations ...

MPI_Wait(&request_X, ...);
MPI_Wait(&request_Y,…);
```

MPI_Irecv

MPI_Irecv(buf, count, datatype, src, tag, comm, request)

- Similar to MPI_Recv, except the last argument “request”
- Typical usage:

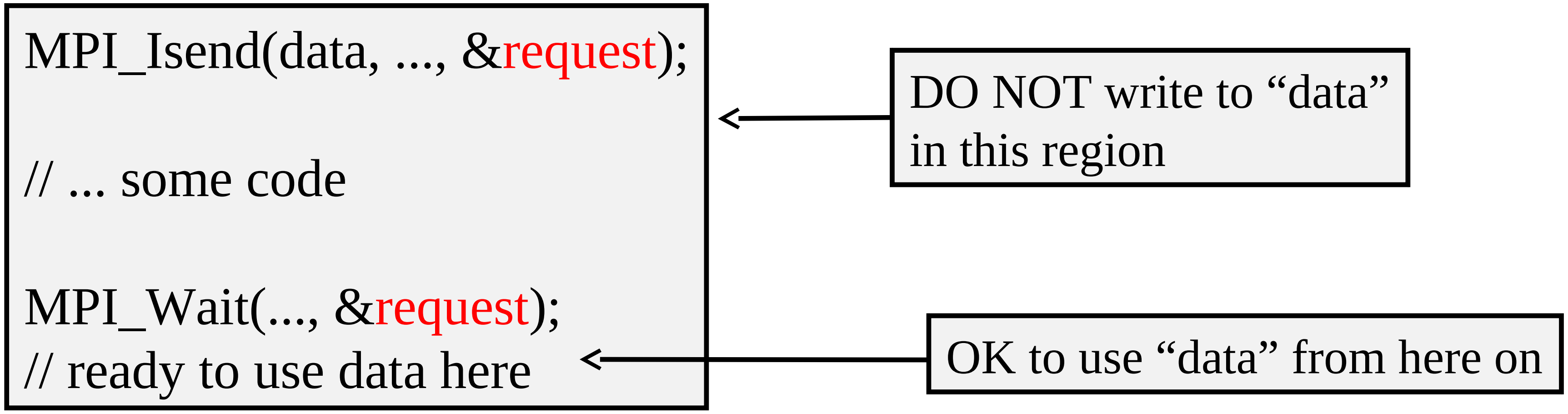
```
MPI_Request request_X, request_Y;
MPI_Irecv(..., &request_X);
MPI_Irecv(…, &request_Y);

//... more ground-breaking computations ...

MPI_Wait(&request_X, ...);
MPI_Wait(&request_Y,…);
```

Caution about MPI_Isend and MPI_Irecv

- The sending process should not access the send buffer until the send completes



```
MPI_Isend(data, ..., &request);

// ... some code

MPI_Wait(..., &request);
// ready to use data here
```

DO NOT write to “data” in this region

OK to use “data” from here on

MPI_Wait

MPI_Wait(MPI_Request, MPI_Status)

- Wait for an MPI_Isend/recv to complete
- Use the same “request” used in an earlier MPI_Isend or MPI_Irecv
- If they are multiple requests, one can use

  MPI_Waitall(count, request[], status[]);

  request[] and status[] are arrays.

Other variants of MPI Send/Recv

- MPI_Sendrecv
  - send and receive in one call
- Mixing blocking and non-blocking calls
  - e.g. MPI_Isend + MPI_Recv
- MPI_Bsend
  - buffered send
- MPI_Ibsend
- … (see MPI standard for more)

Today’s Topics

- Message passing basics
  - communicators
  - data types
- Point to point communication
- Collective communication
- Derived data types
- Examples

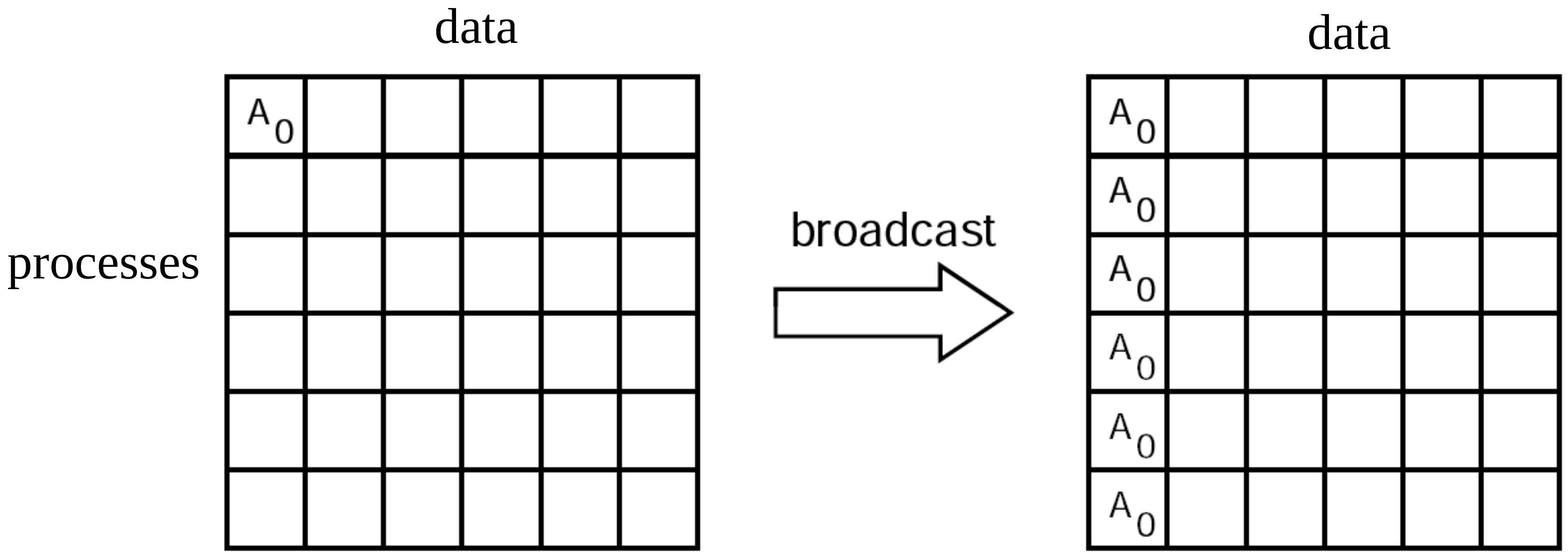
Collective communication

- One to all
  - MPI_Bcast, MPI_Scatter
- All to one
  - MPI_Reduce, MPI_Gather
- All to all
  - MPI_Alltoall

MPI_Bcast

MPI_Bcast(buffer, count, datatype, root, comm)

Broadcasts a message from “root” process to all other processes in the same communicator



MPI_Bcast Example

- Broadcast 100 integers from process “3” to all other processes

C/C++

```
MPI_Comm comm;
int array[100];
//...
MPI_Bcast( array, 100, MPI_INT, 3, comm);
```

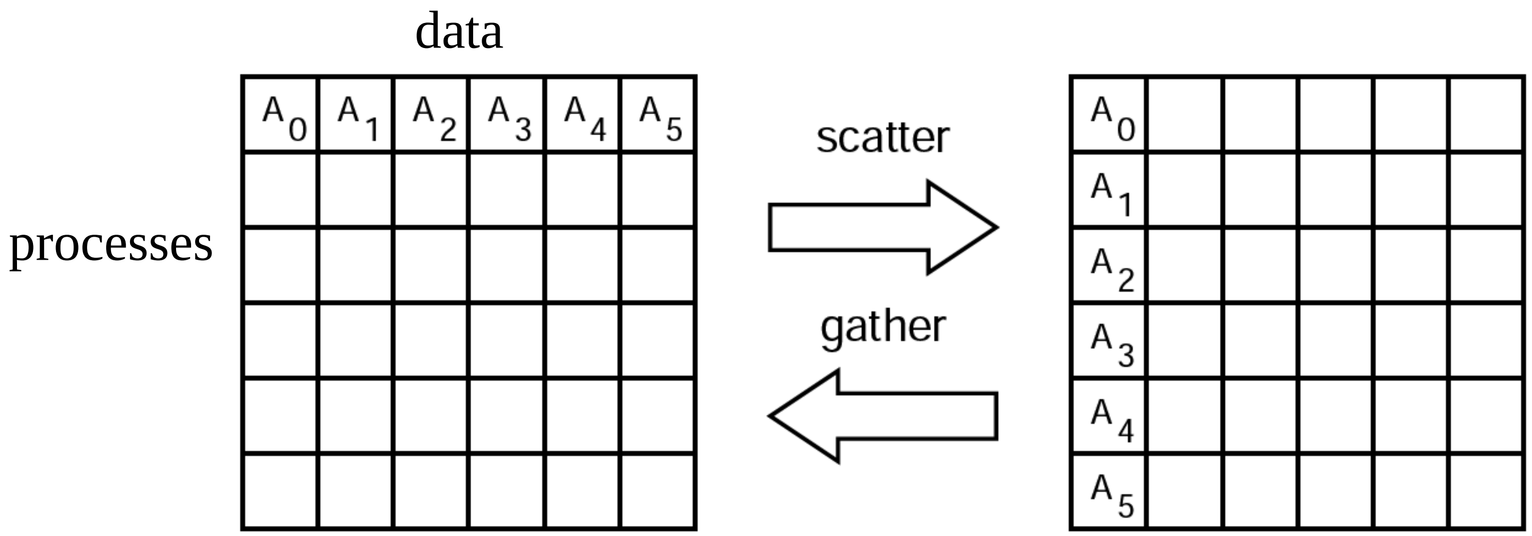
Fortran

```
INTEGER comm
integer array(100)
//...
call MPI_Bcast( array, 100, MPI_INTEGER, 3, comm,ierr)
```

MPI_Gather & MPI_Scatter

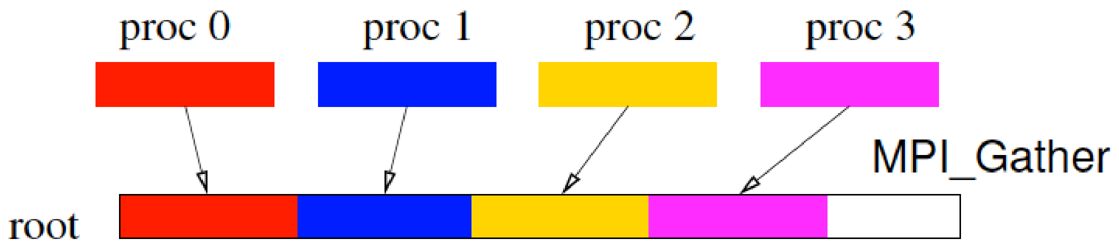
MPI_Gather (sbuf, scnt, stype, rbuf, rcnt, rtype, root, comm)

MPI_Scatter(sbuf, scnt, stype, rbuf, rcnt, rtype, root, comm)



☞ When gathering, make sure the root process has big enough memory to hold the data (especially when you scale up the problem size).

MPI_Gather Example



```
MPI_Comm comm;
int np, myid, sendarray[N], root;
double *rbuf;
MPI_Comm_size( comm, &np);      // # of processes
MPI_Comm_rank( comm, &myid);  // process ID
if (myid == root)                          // allocate space on process root
      rbuf = new double [np*N];

MPI_Gather( sendarray, N, MPI_INT, rbuf, N, MPI_INT,
                        root, comm);
```

Variations of MPI_Gather/Scatter

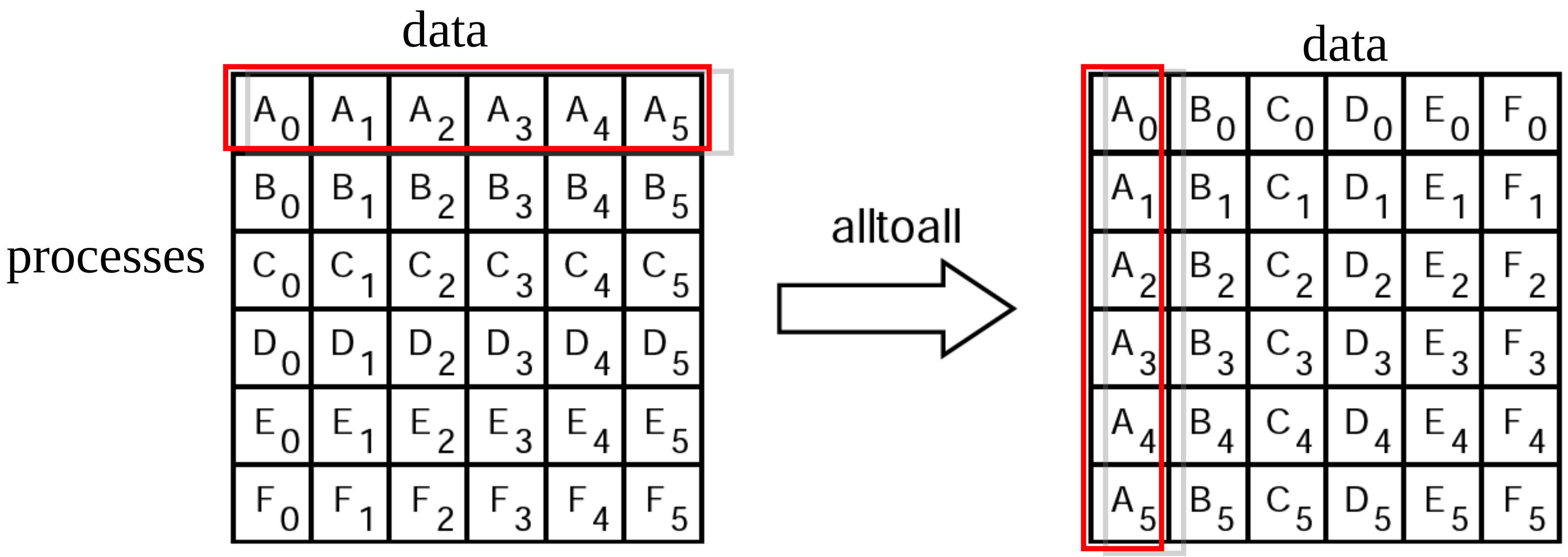
- Variable data size
  - MPI_Gatherv
  - MPI_Scatterv
- Gather + broadcast (in one call)
  - MPI_Allgather
  - MPI_Allgatherv

MPI_Alltoall

MPI_Alltoall(send_buf, send_count, send_data_type,

recv_buf, recv_count, recv_data_type, comm)

The j-th block send_buf from process i is received by process j and is placed in the i-th block of rbuf:



$$\begin{array}{cccccc} A_0 & A_1 & A_2 & A_3 & A_4 & A_5 \\ B_0 & B_1 & B_2 & B_3 & B_4 & B_5 \\ C_0 & C_1 & C_2 & C_3 & C_4 & C_5 \\ D_0 & D_1 & D_2 & D_3 & D_4 & D_5 \\ E_0 & E_1 & E_2 & E_3 & E_4 & E_5 \\ F_0 & F_1 & F_2 & F_3 & F_4 & F_5 \end{array} \xrightarrow{\text{alltoall}} \begin{array}{cccccc} A_0 & B_0 & C_0 & D_0 & E_0 & F_0 \\ A_1 & B_1 & C_1 & D_1 & E_1 & F_1 \\ A_2 & B_2 & C_2 & D_2 & E_2 & F_2 \\ A_3 & B_3 & C_3 & D_3 & E_3 & F_3 \\ A_4 & B_4 & C_4 & D_4 & E_4 & F_4 \\ A_5 & B_5 & C_5 & D_5 & E_5 & F_5 \end{array}$$

MPI_Reduce

MPI_Reduce (send_buf, recv_buf, data_type, OP, root, comm)

- Apply operation OP to send_buf from all processes and return result in the recv_buf on process “root”.
- Some predefined operations:

Operations (OP)	Meaning
MPI_MAX	maximum value
MPI_MIN	minimum value
MPI_SUM	sum
MPI_PROD	products
…	

(see MPI standard for more predefined reduce operations)

MPI_Reduce example

- Parallel vector inner product:

$$a \leftarrow x \cdot y$$

```
// loc_sum = local sum
float loc_sum = 0.0;          // probably should use double
for (i = 0; i < N; i++)
      loc_sum += x[i] * y[i];

// sum = global sum
MPI_Reduce(&loc_sum, &sum, 1, MPI_FLOAT, MPI_SUM,
                          root, MPI_COMM_WORLD);
```

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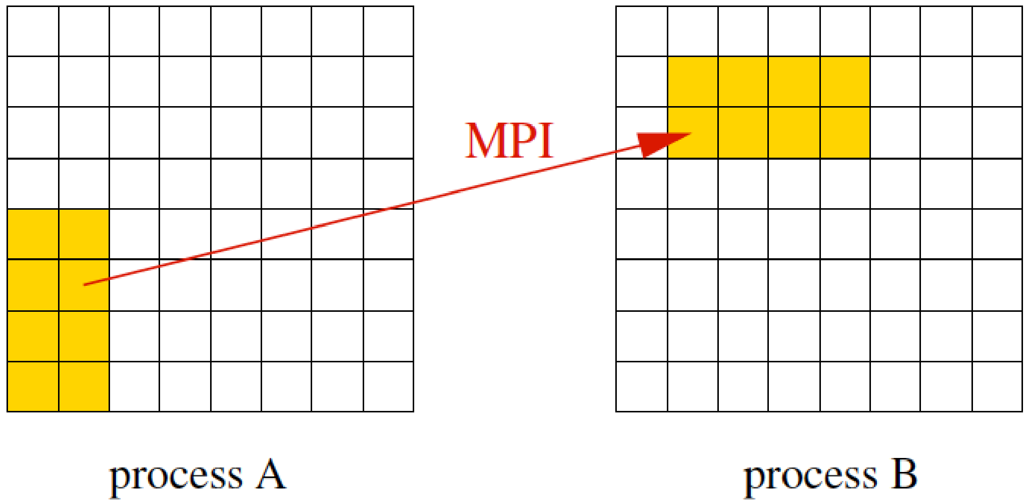
Derived Data Type

- Define data objects of various sizes and shapes (memory layout)
- Example
  - The send and recv ends have same data size but different memory layouts



memory layout

Data Type Constructors

Constructors	**Usage**
Contiguous	contiguous chunk of memory
Vector	strided vector
Hvector	strided vector in bytes
Indexed	variable displacement
Hindexed	variable displacement in bytes
Struct	fully general data type

MPI_Type_contiguous

MPI_Type_contiguous(count, old_type, newtype)

- Define a contiguous chunk of memory
- Example – a memory block of 10 integers

```
int a[10];
MPI_Datatype intvec;
MPI_Type_contiguous(10, MPI_INT, &intvec);
MPI_Type_commit(&intvec);
MPI_Send(a, 1, intvec, ...); /* send 1 10-int vector */
```

new type

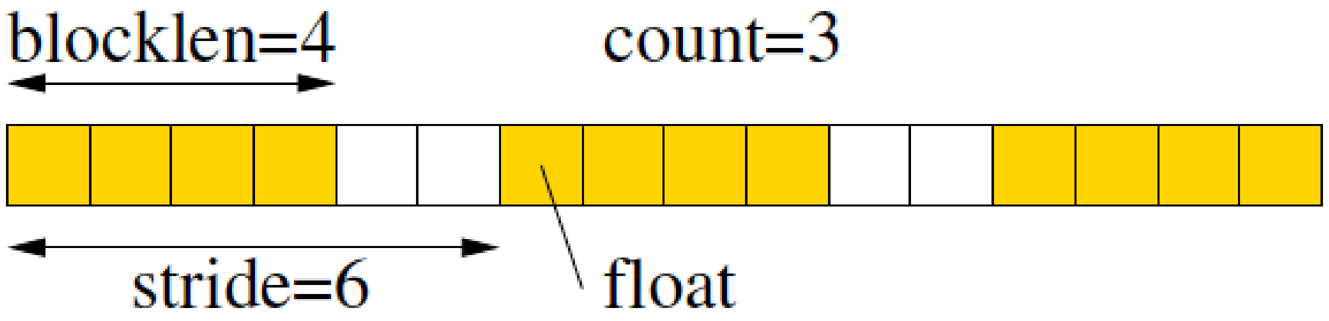
is equivalent to

```
MPI_Send(a, 10, MPI_INT,...); /* send 10 ints */
```

MPI_Type_vector

MPI_Type_vector(count, blocklen, stride, old_type, newtype)

To create a strided vector (i.e. with "holes"):



```
MPI_Datatype yellow_vec;
MPI_Type_vector(3, 4, 6, MPI_FLOAT, &yellow_vec);
MPI_Type_commit(&yellow_vec);
```

Commit and Free

- A new type needs to be committed before use

  MPI_Type_commit(datatype)
- Once committed, it can be used many times
- To destroy a data type, freeing the memory:

  MPI_Type_free(datatype)

☞ If you repeatedly (e.g. in iterations) create MPI types, make sure you free them when they are no longer in use. Otherwise you may have memory leak.

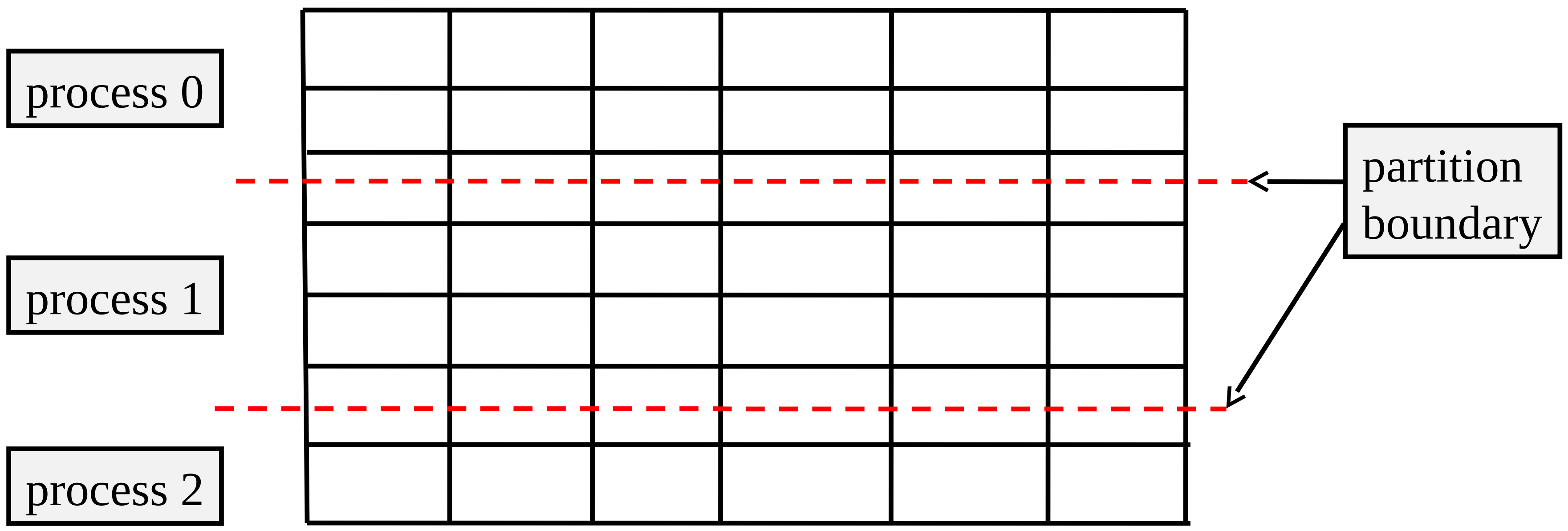
Examples

- Poisson equation
- Fast Fourier Transform (FFT)

Poisson equation (or any elliptic PDE)

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = R(x, y)$$

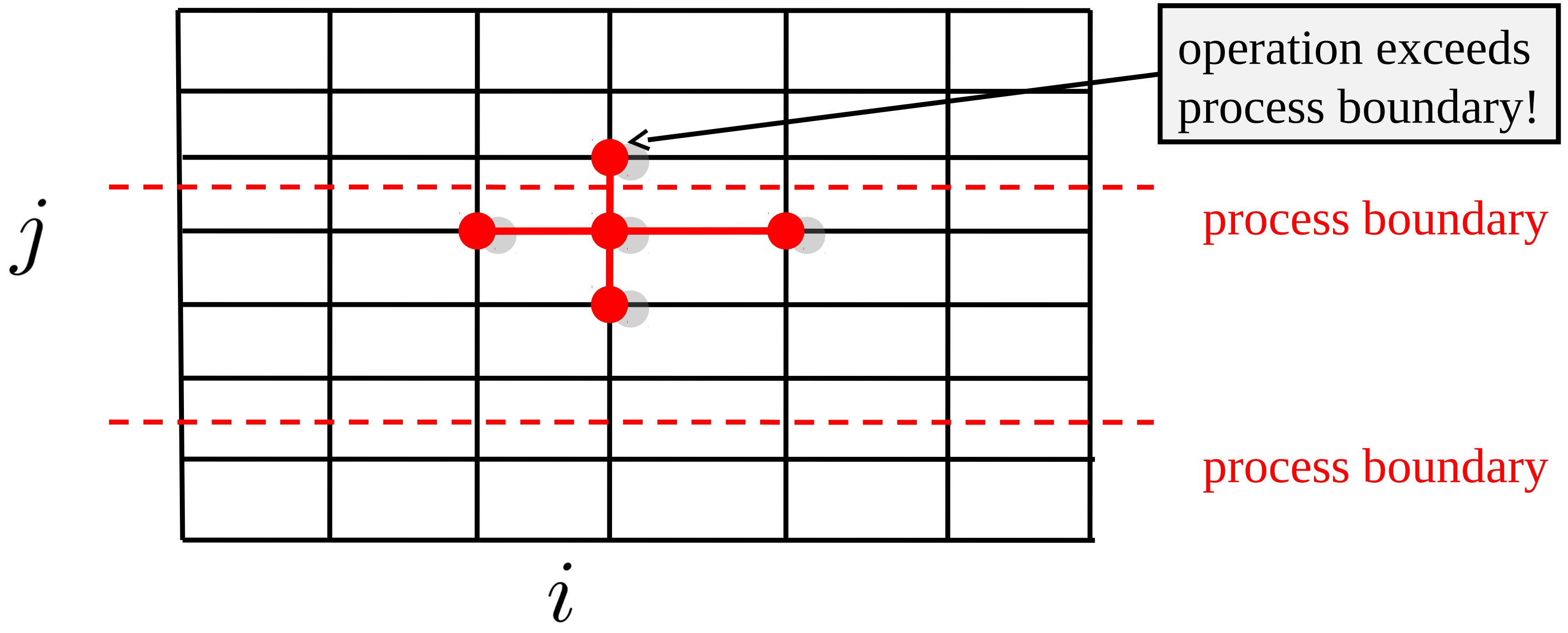
Computational grid:



Poisson equation

Jacobi iterations (as an example)

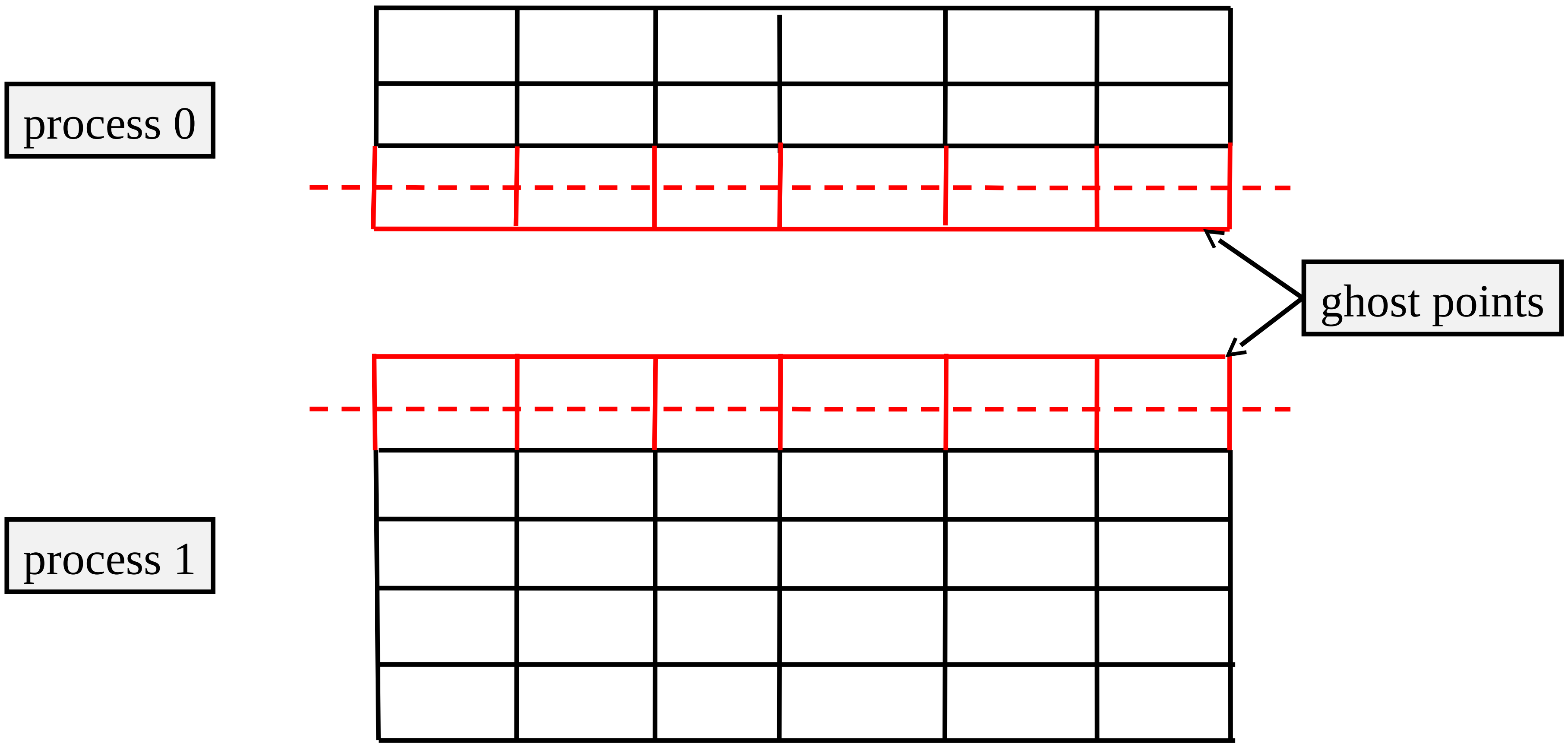
$$f_{i,j}^{k+1} = \frac{1}{4}(f_{i+1,j}^{k} + f_{i-1,j}^{k} + f_{i,j+1}^{k} + f_{i,j-1}^{k})$$



One solution is to introduce "ghost points" (see next slide)

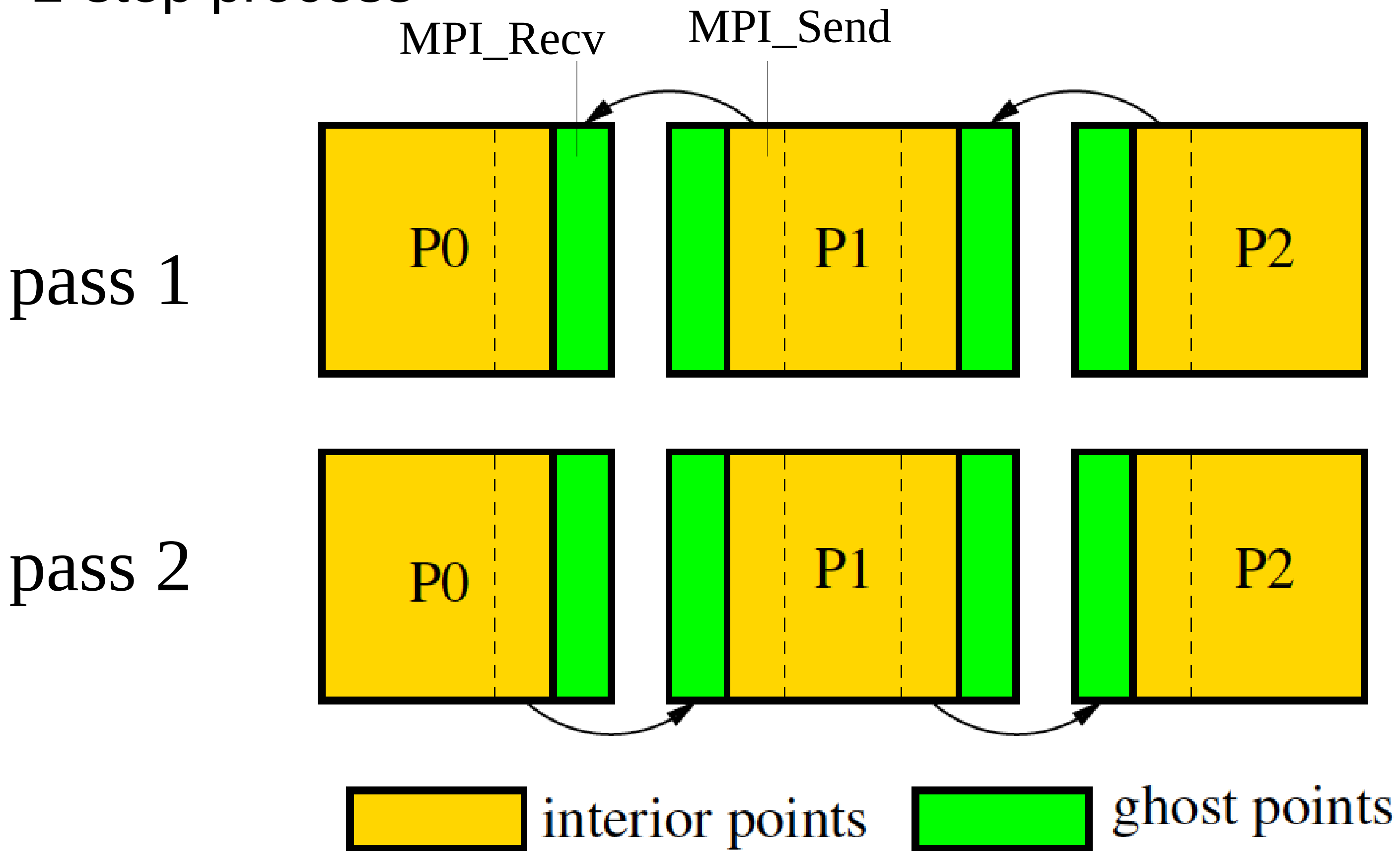
Ghost points

Redundant copy of data held on neighboring processes



Update ghost points in one iteration

- 2-step process



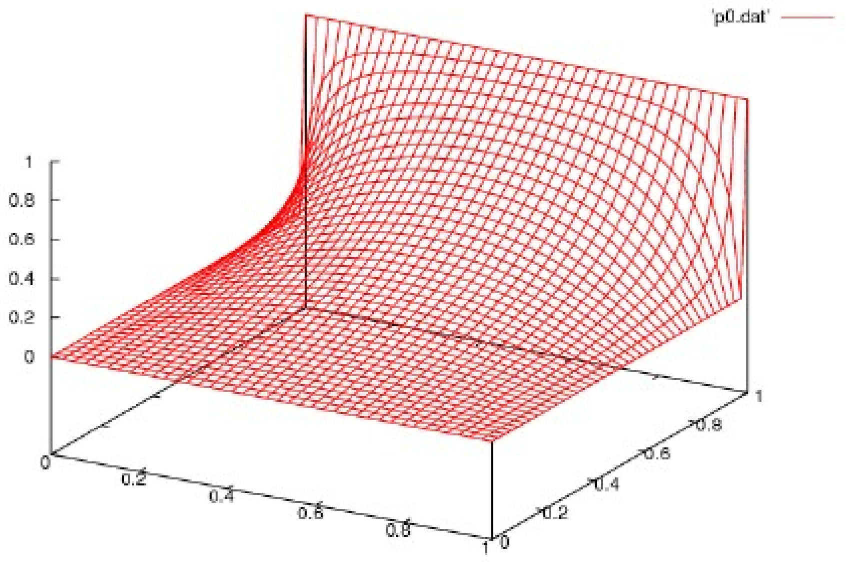
- Repeat for many iterations until convergence

Poisson solution

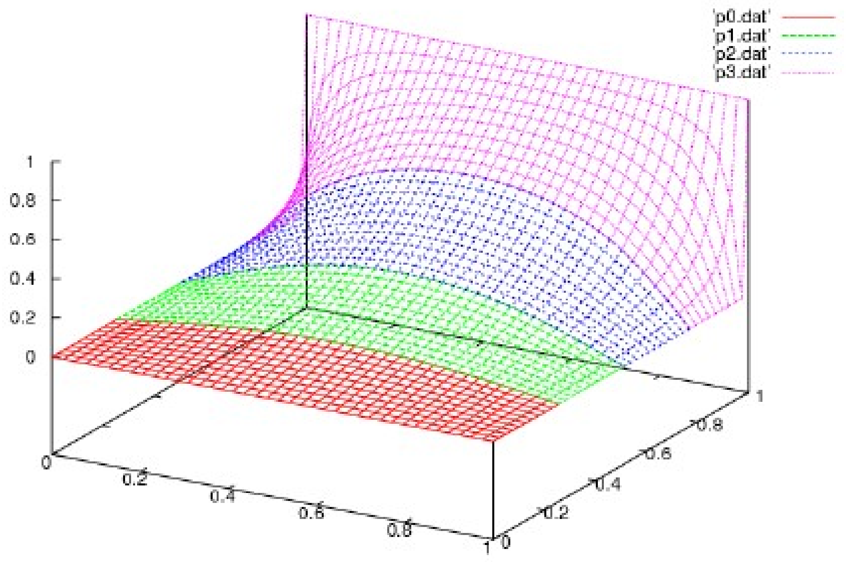
Dirichlet boundary conditions

$$\phi(x,1) = 1, \phi(x,0) = \phi(0,y) = \phi(1,y) = 0$$

1 process

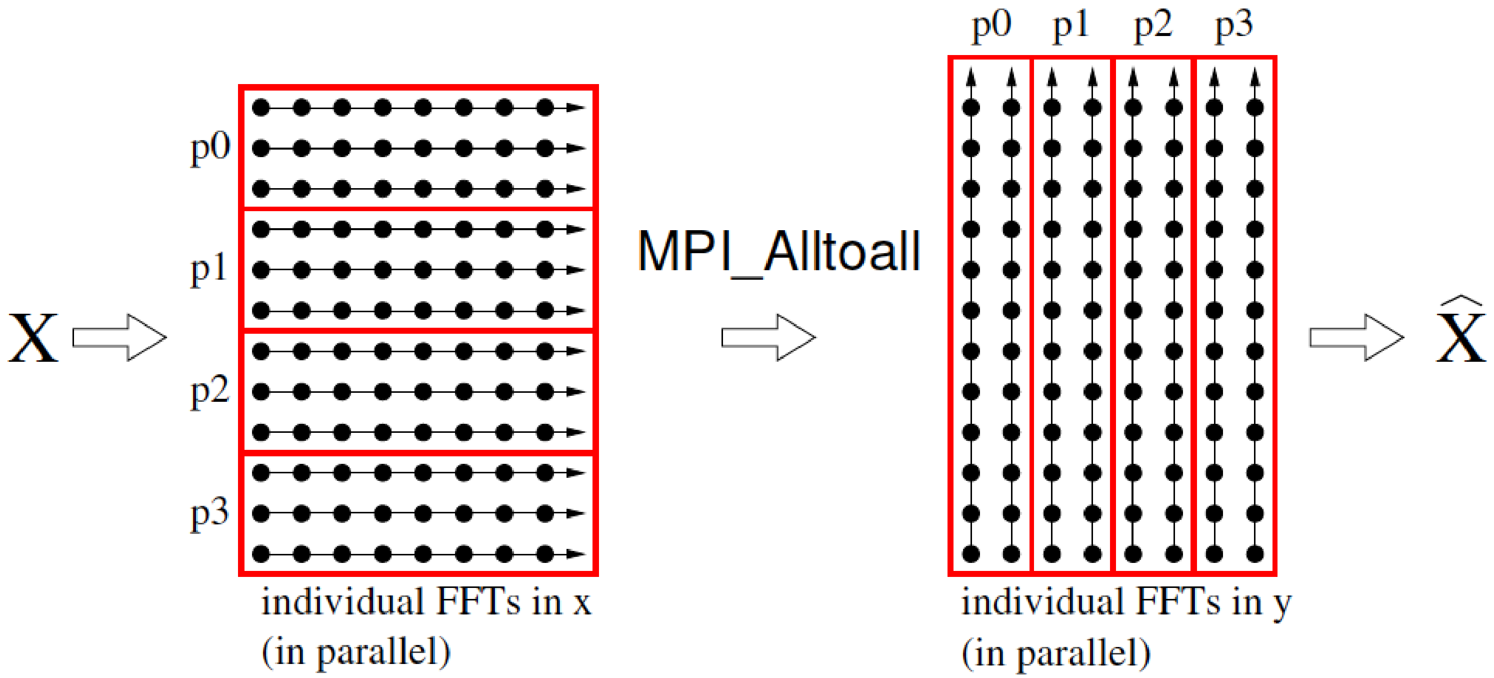


4 processes



“Parallel” FFT

$$\hat{X}(k_x, k_y) = \sum\sum X(x, y) \exp^{-i(k_x x + k_y y)}$$



Doing multiple (sequential) FFT in parallel

Timing

- MPI_Wtime
  - elapsed wall-clock time in seconds
  - Note: wall-clock time is not CPU time
- Example

```
double t1,t2;
t1 = MPI_Wtime();
//... some heavy work ...
t2 = MPI_Wtime();
printf("elapsed time = %f seconds\n", t2-t1);
Parallel
```

How to run an MPI program

- Compile

  C: mpicc foo.c

  C++: mpicxx foo.cpp

  F90: mpif90 foo.f90

☞ mpicc, mpicxx and mpif90 are sometimes called the MPI compilers (wrappers)

- Run

  mpiexec –n 4 [options] a.out

  – The options in mpiexec are implementation dependent

  – Check out the user’s manual

Summary

- MPI for distributed-memory programming
  - works on shared-memory parallel computers too
- Communicator
  - a group of processes, numbered 0,1,…,to N-1
- Data Types
  - derived types can be defined based on built-in ones
- Point-to-point Communication
  - blocking (Send/Recv) and non-blocking (Isend/Irecv)
- Collective Communication
  - gather, scatter, alltoall

Online Resources

- MPI-1 standard

  http://www.mpi-forum.org/docs/mpi-11-html/mpi-report.html

- MPI-2 standard

  http://www.mpi-forum.org/docs/mpi-20-html/mpi2-report.html

- MPI-3 standard

  http://www.mpi-forum.org/docs/mpi-3.0/mpi30-report.pdf