MPI Tutorial

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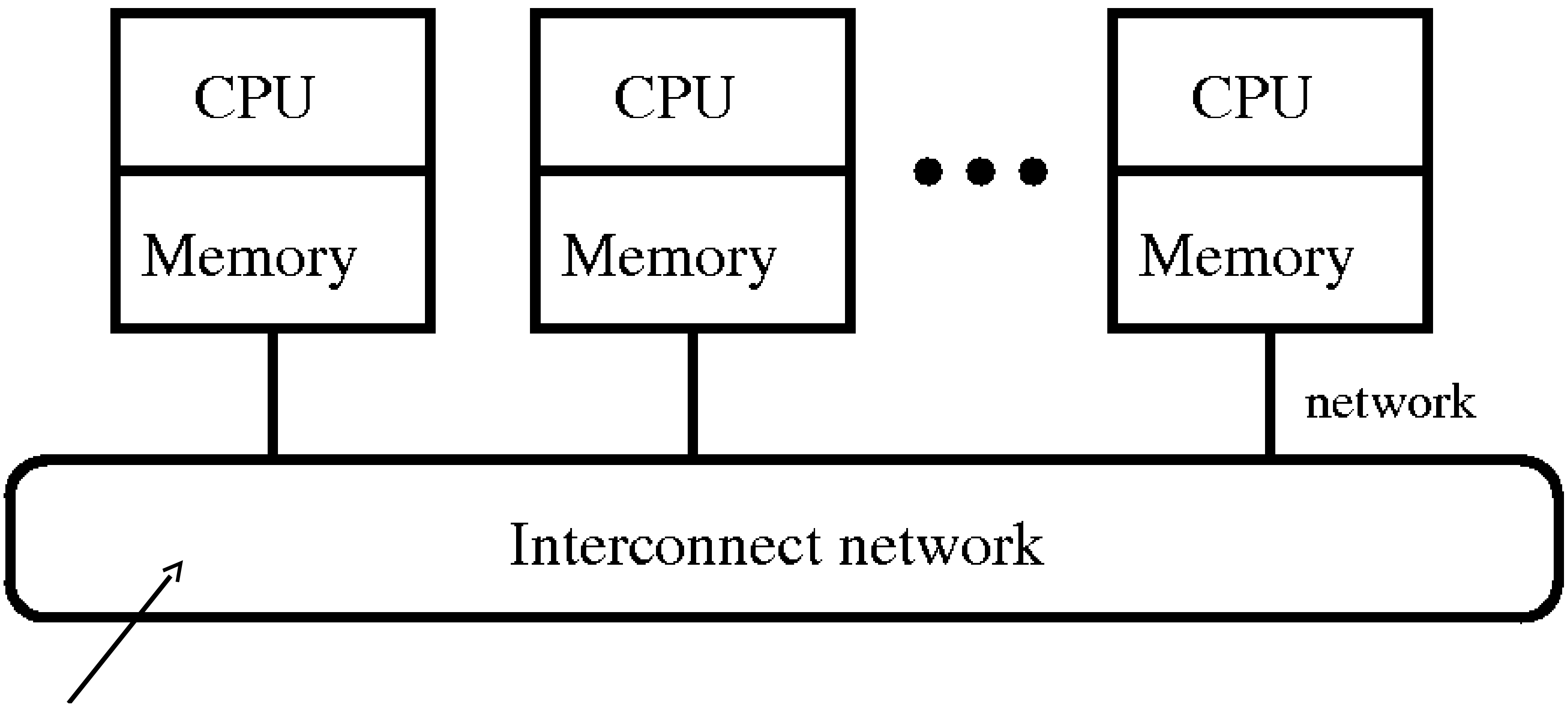
Distributed Memory

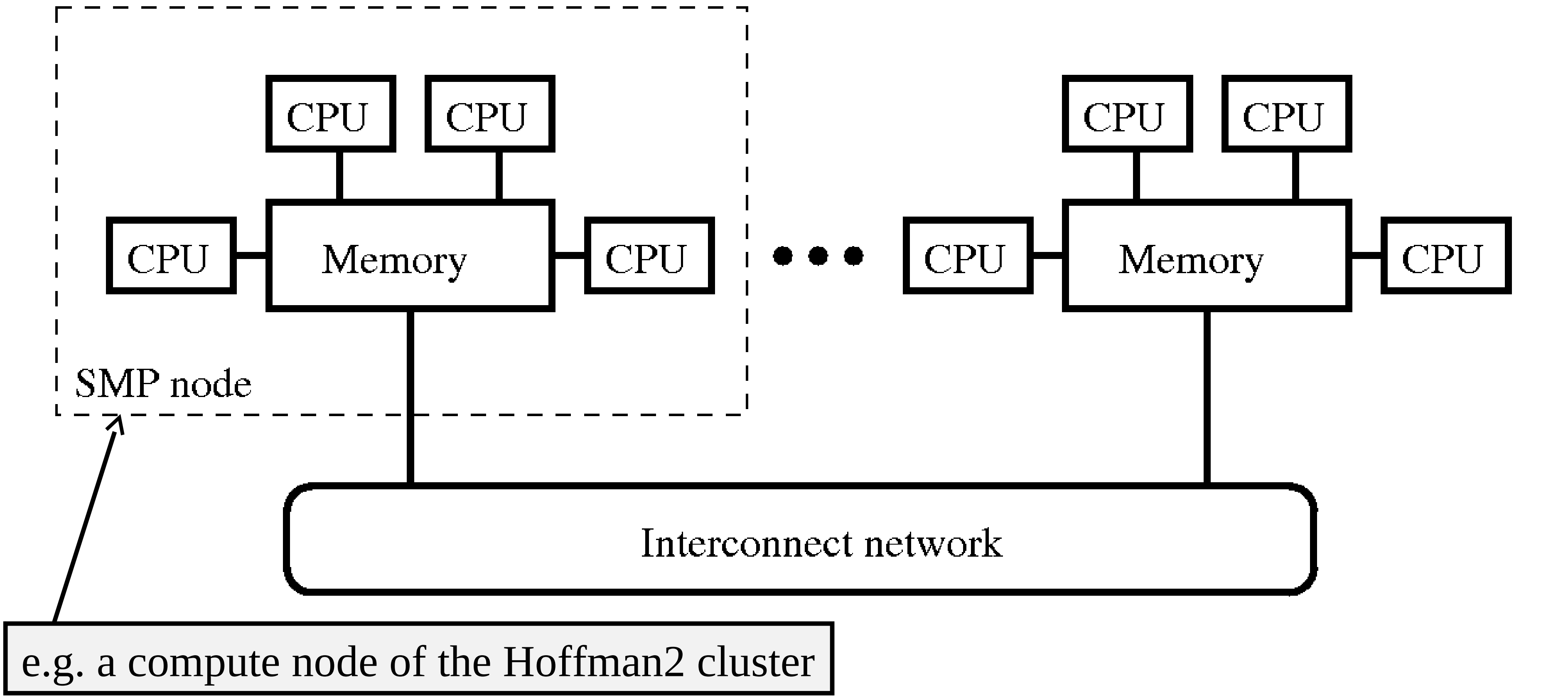
- Each CPU has its own (local) memory



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 = <u>M</u>essage <u>P</u>assing <u>I</u>nterface

- 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

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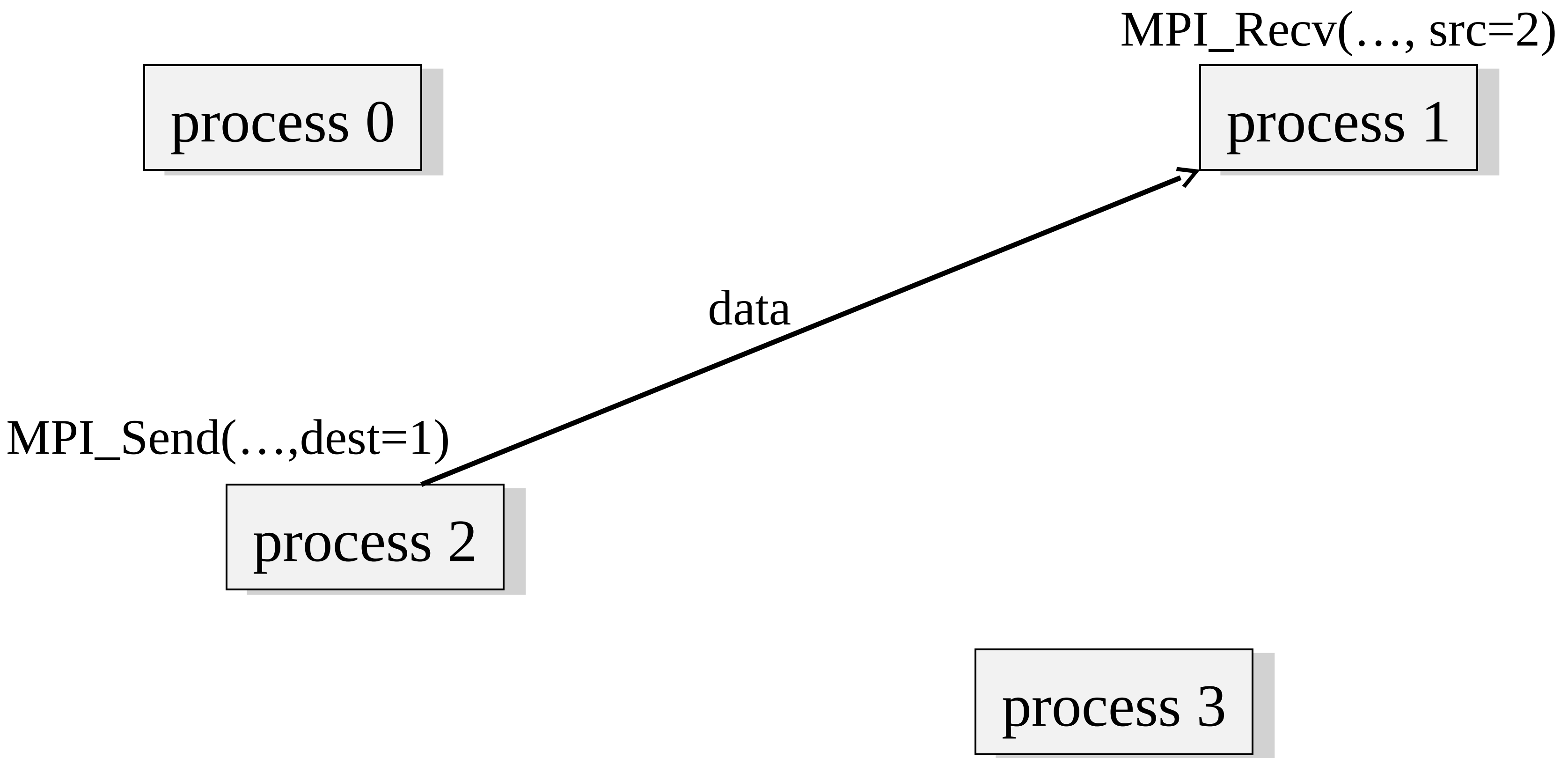
Point to point communication



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
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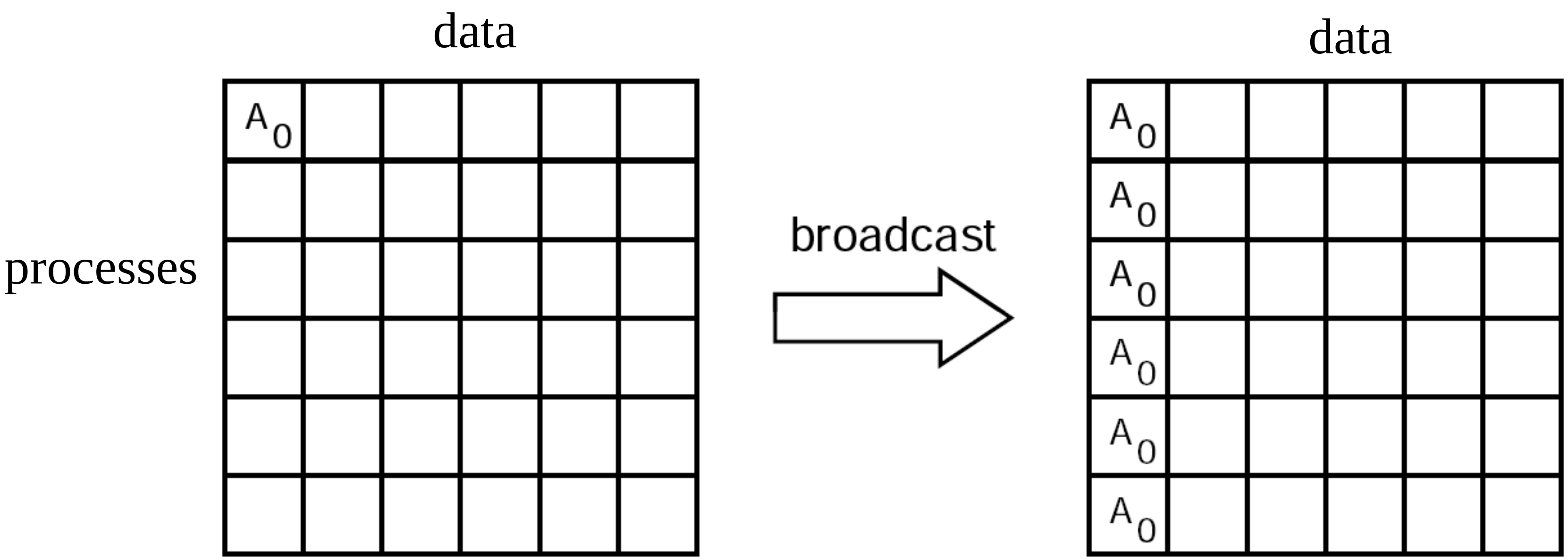
Collective communication

- 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);
```

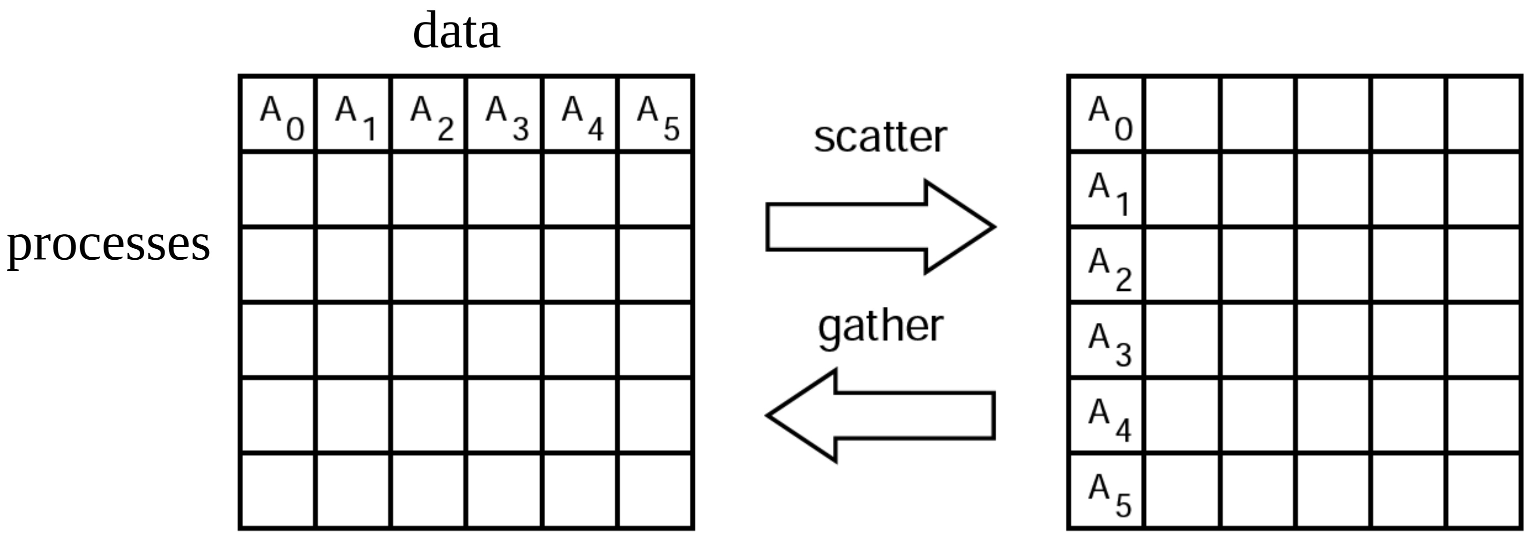
Fortran

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

MPI_Gather & MPI_Scatter

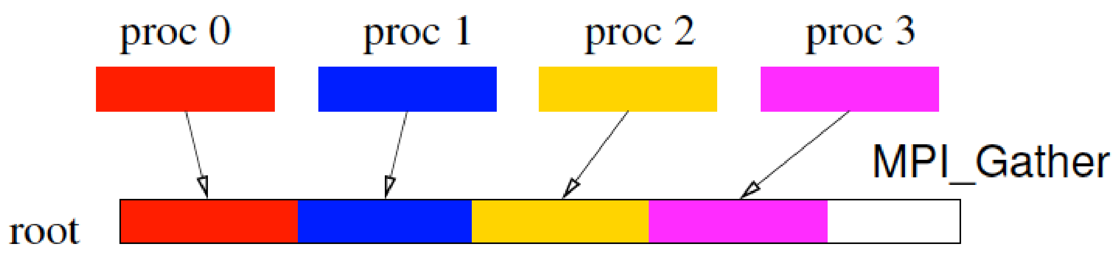
MPI_Gather (sbuf, scnt, stype, rbuf, rcnt, rtype, root, comm)

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

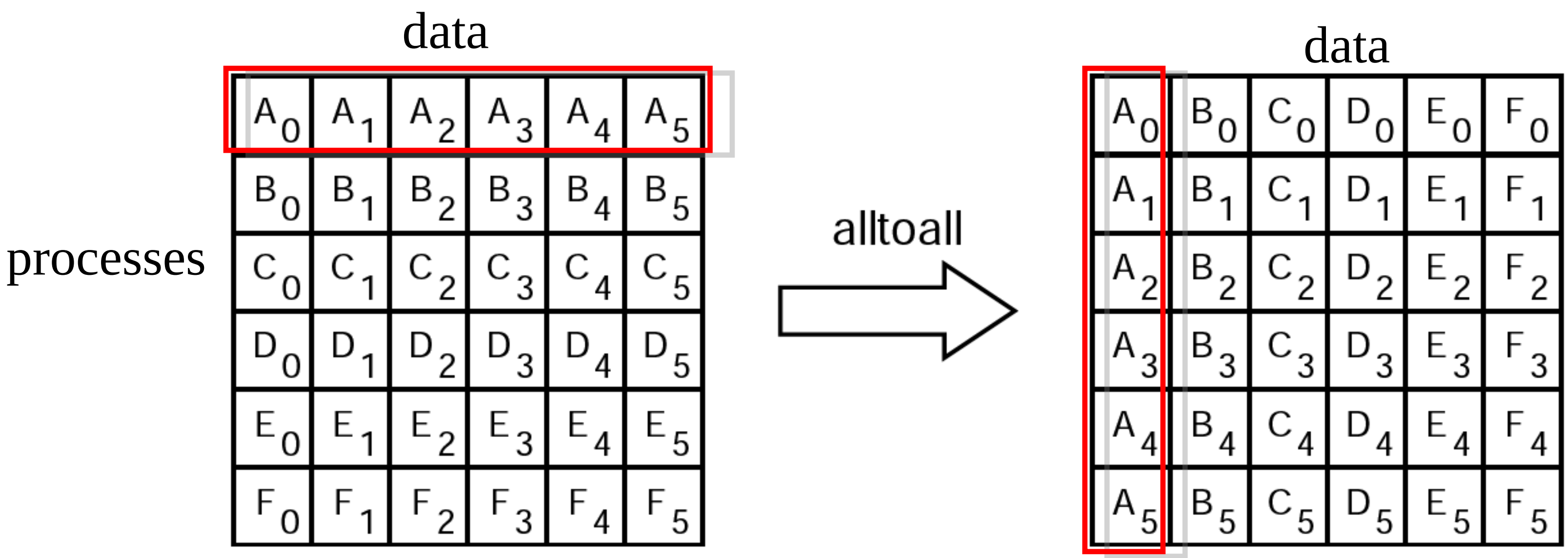
- Variable data size
  - MPI_Gatherv
  - MPI_Scatterv
- Gather + broadcast (in one call)
  - MPI_Allgather
  - MPI_Allgatherv

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:



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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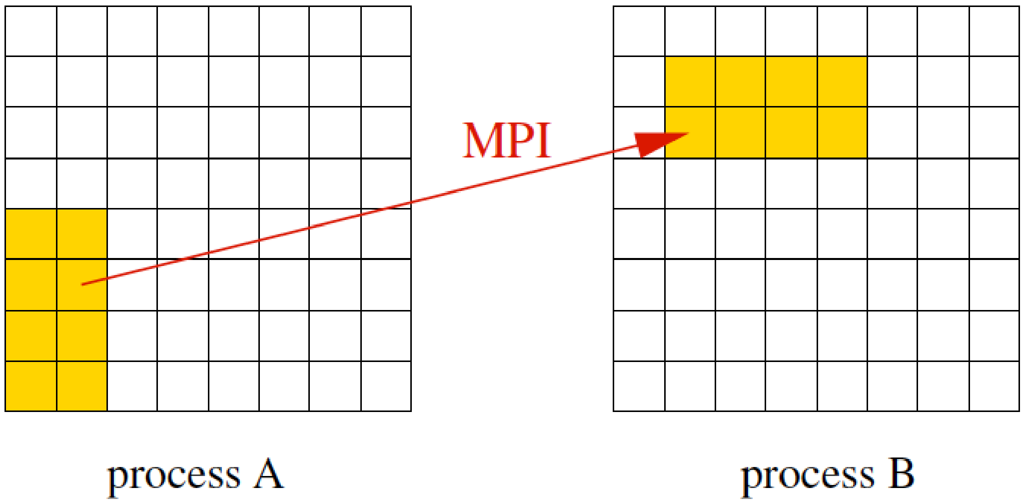
Derived Data Type

- 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

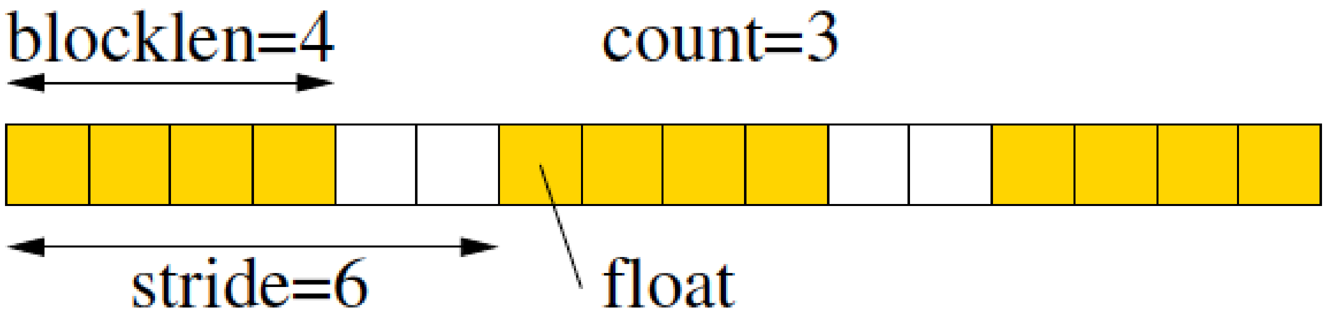
is equivalent to

```
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.

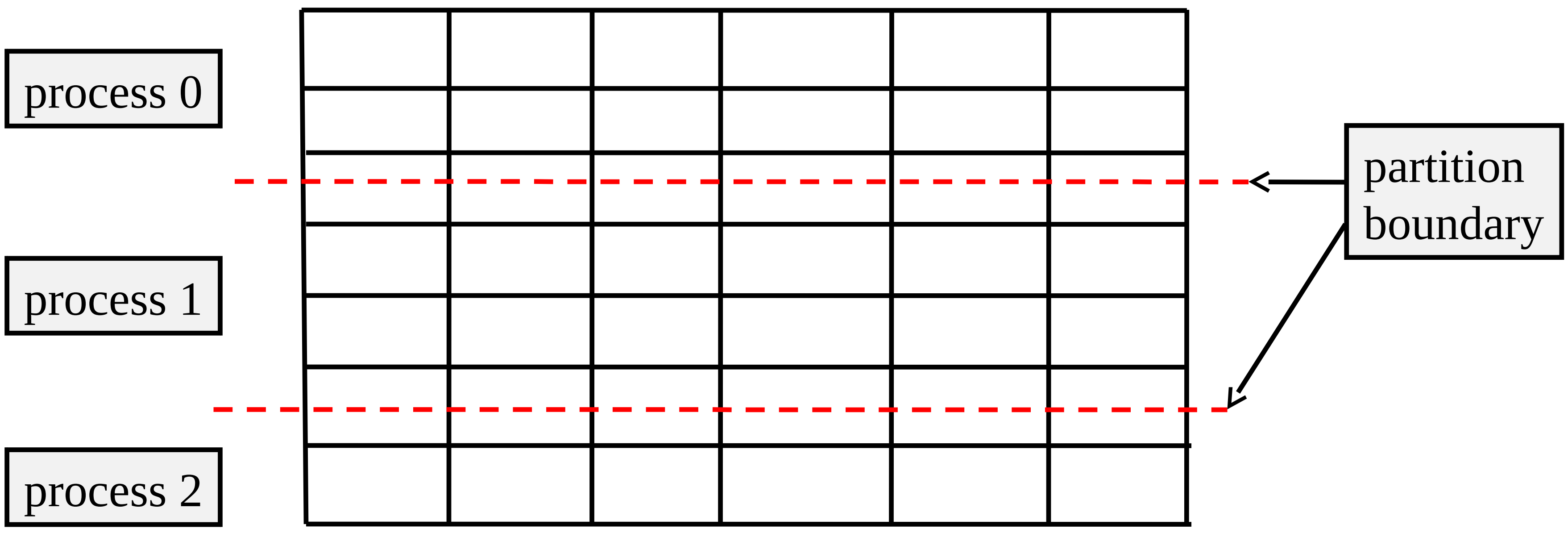
Examples

- Poisson equation
- Fast Fourier Transform (FFT)

Poisson equation (or any elliptic PDE)

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

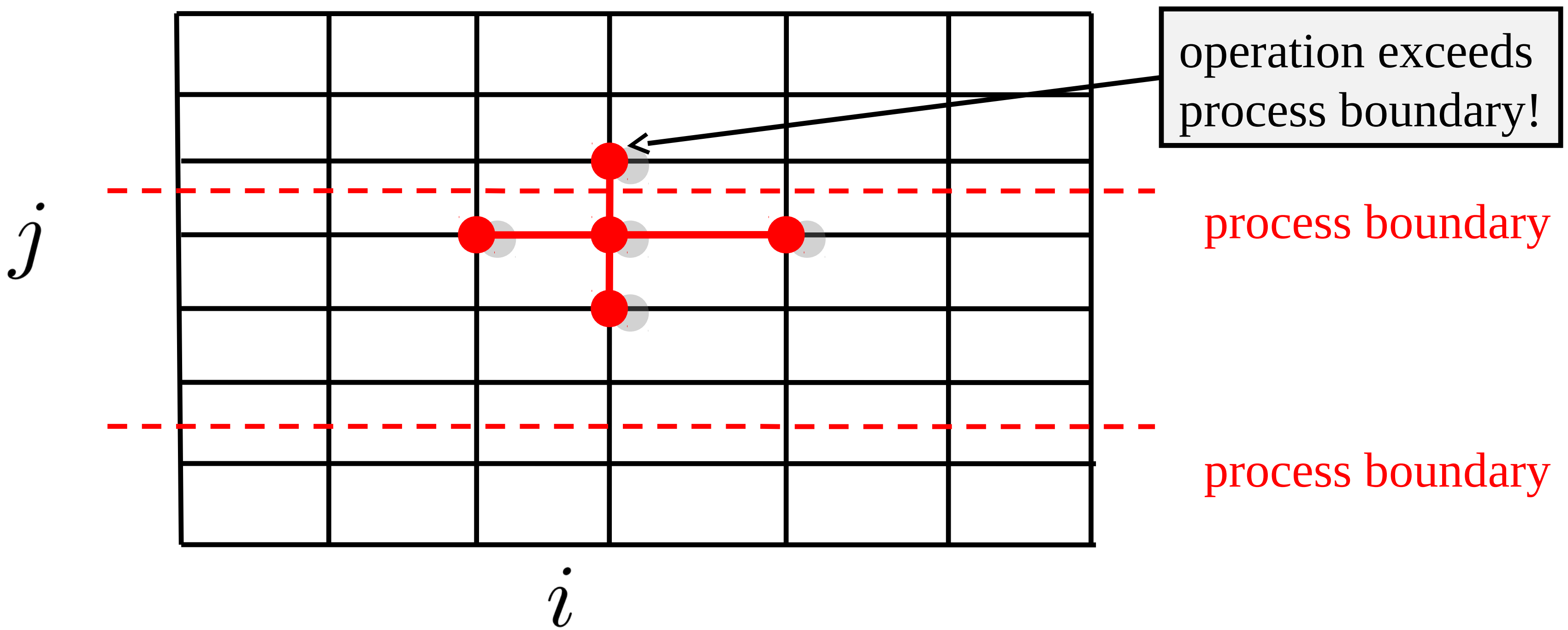
Computational grid:



Poisson equation

Jacobi iterations (as an example)

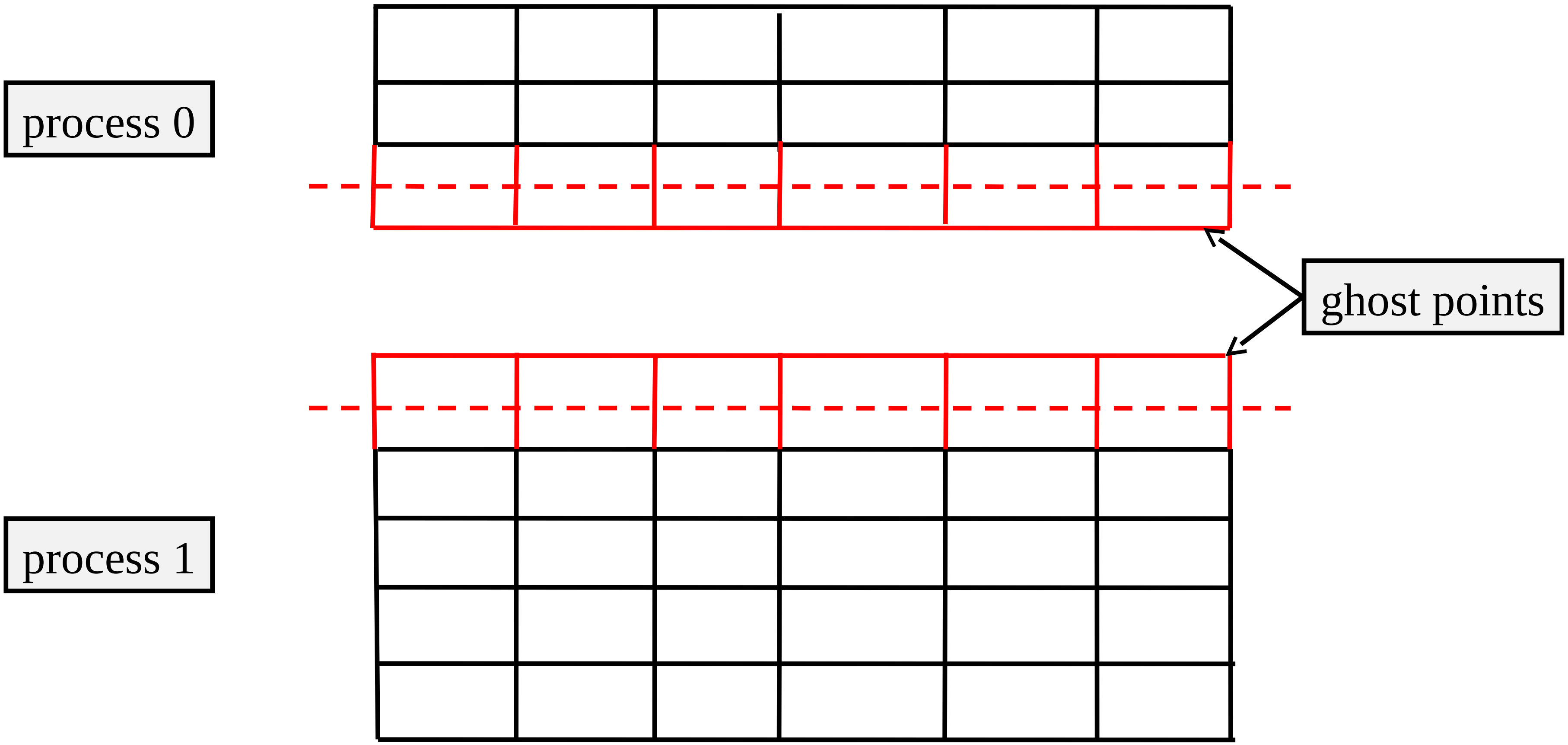
$$f_{i,j}^{k+1} = \frac{1}{4}(f_{i+1,j}^{k} + f_{i-1,j}^{k} + f_{i,j+1}^{k} + f_{i,j-1}^{k})$$



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

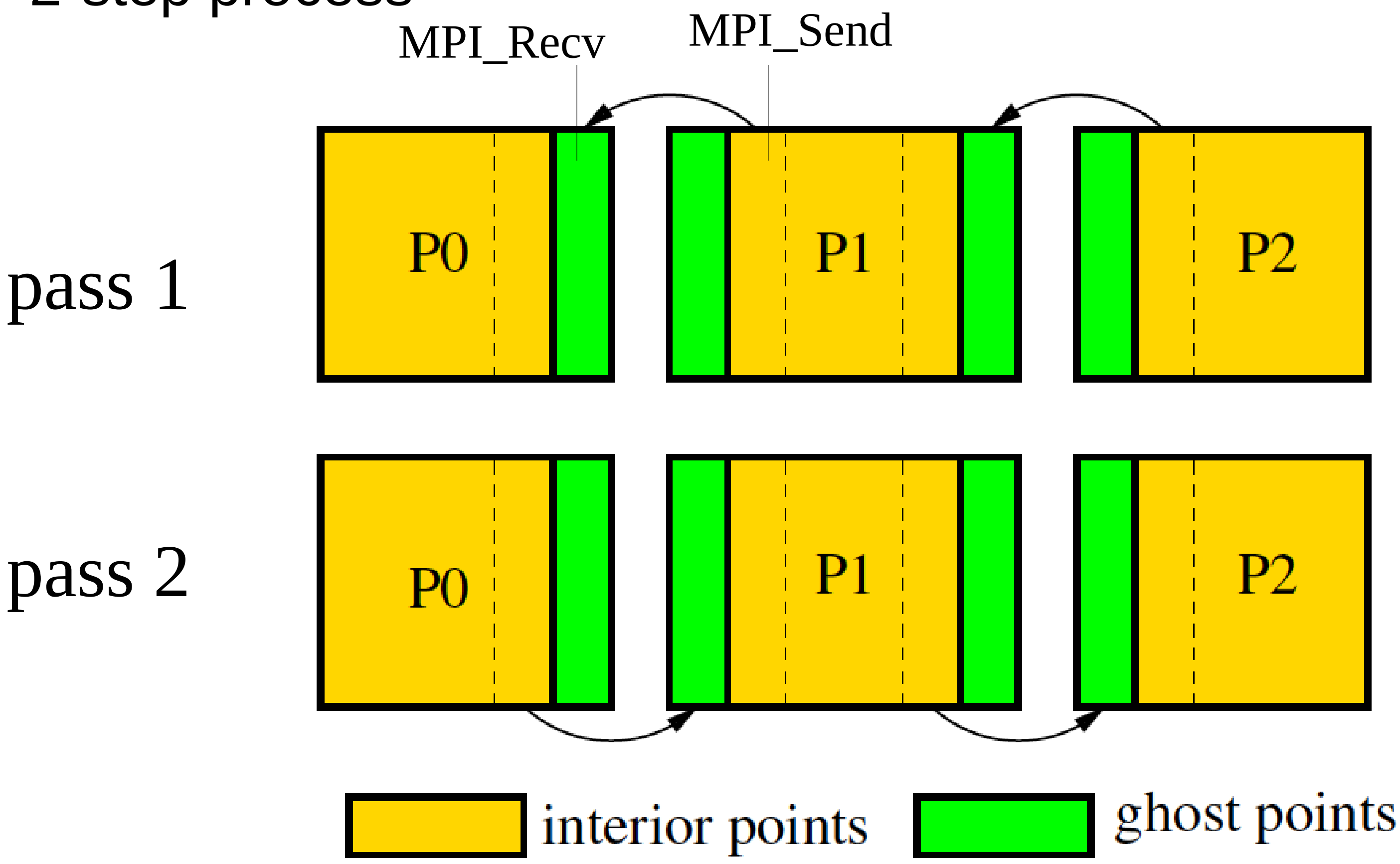
Ghost points

Redundant copy of data held on neighboring processes



Update ghost points in one iteration

- 2-step process



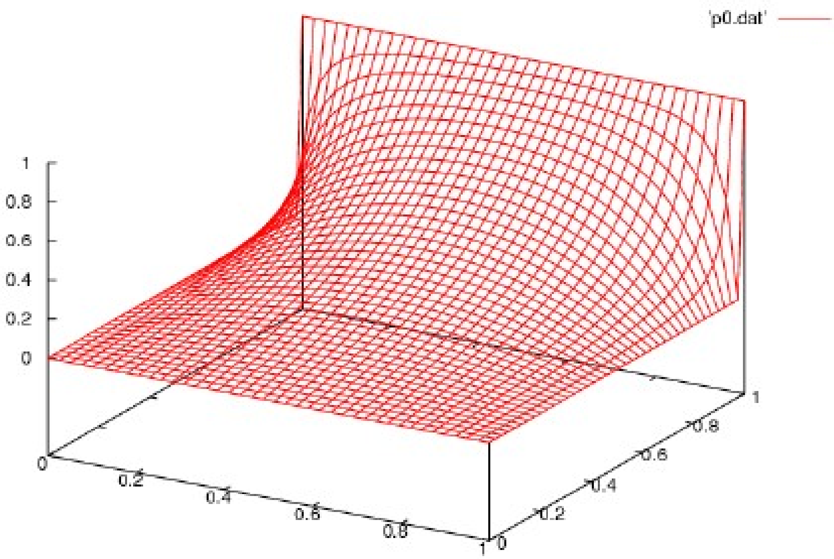
- Repeat for many iterations until convergence

Poisson solution

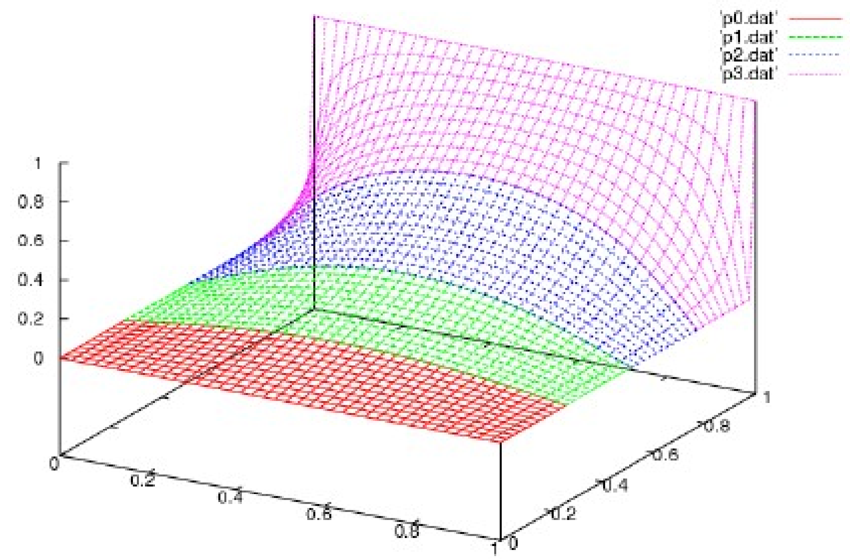
Dirichlet boundary conditions

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

1 process

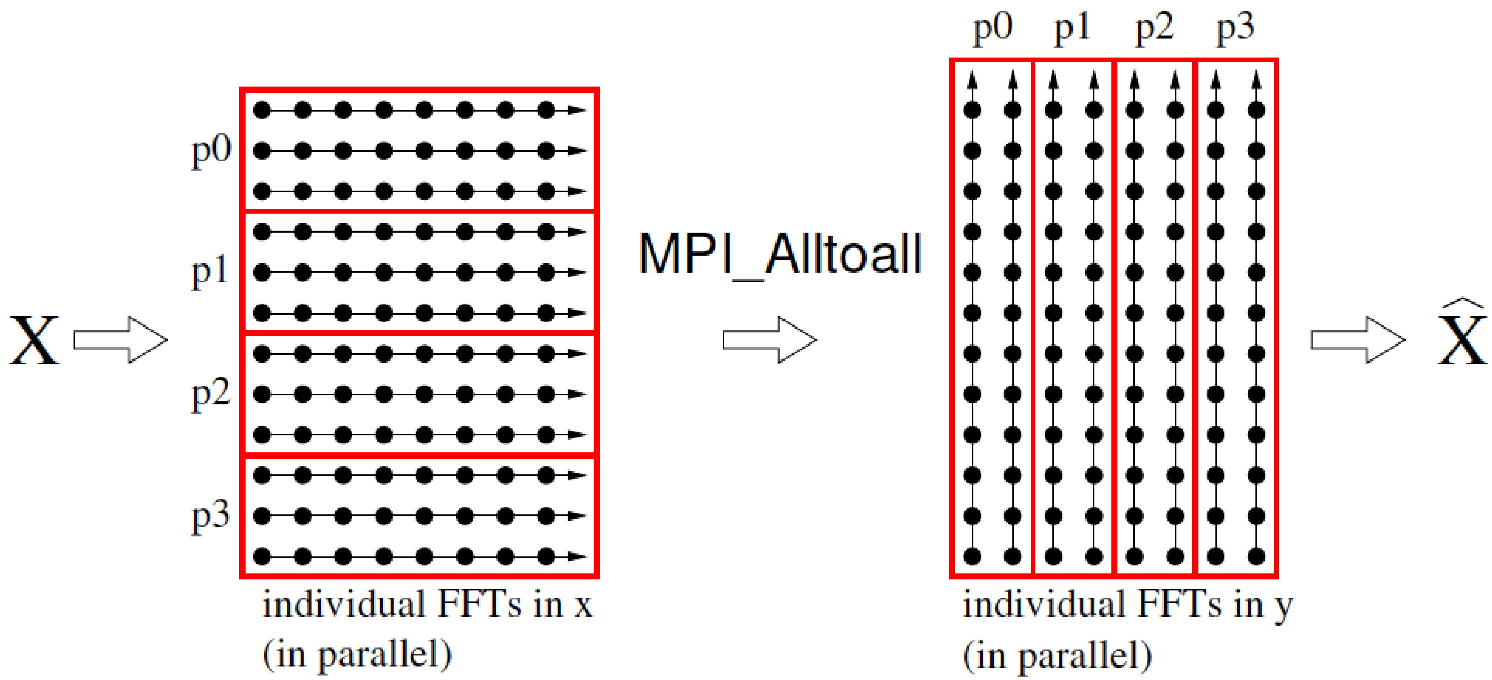


4 processes



“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