Programming for High Performance Computing

Programming Environment

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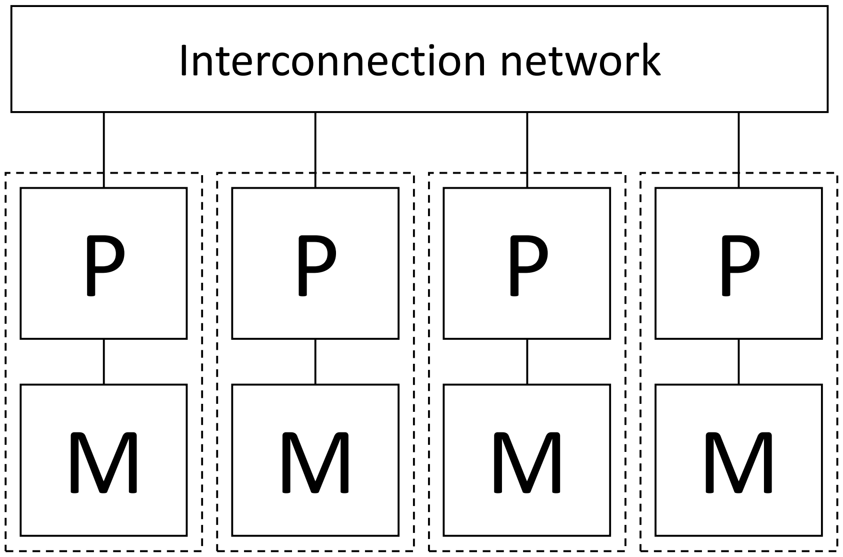
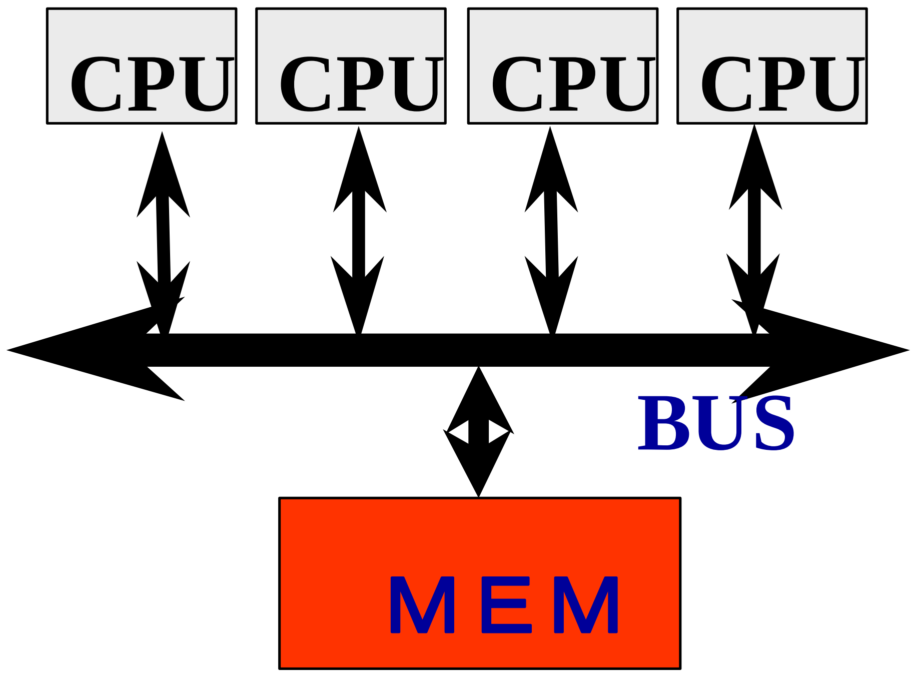
Distributed Memory Machine (PC Cluster)

- A distributed memory machine consists of computers (compute nodes) connected by a interconnection network
  - A compute node consists of a CPU and memory
- A parallel program is executed on each machine, communicating data by the network



Shared Memory Machine



◆Parallel machine such that CPUs access the same memory

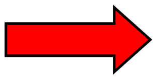
◆Parallel program is executed by accessing the data on the shared memory to communicate each other

◆Large scale server, multicore CPU

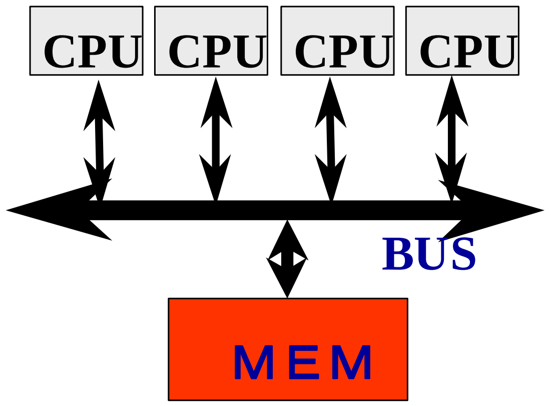
◆UMA (uniform memory access) and NUMA (non-uniform memory access)

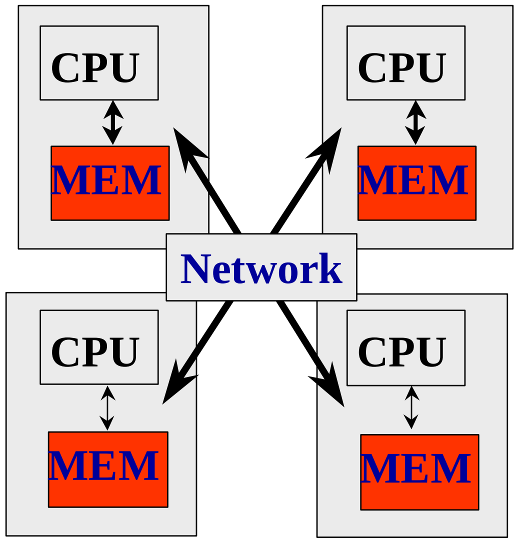
Benefit of parallel processing

- Increase computational power
  - More than one CPU
- Increase memory BW
  - Each CPU can access each memory
- Increase I/O BW
  - Each CPU can access each storage in parallel
- Increase cache/memory size
  - Even though the data size does not fit in the cache size in a single processor, the cache memory can be efficiently used by dividing the data in the problem
- Cost effective
  - When using microprocessors



PC Cluster Technology





Parallel Programming (1)

- Message passing programming
  - For Distributed memory machines
    - Can be used for shared memory machines
  - Complicated and rather difficult
  - Data transfer should be programmed
  - Scalable in terms of # processors

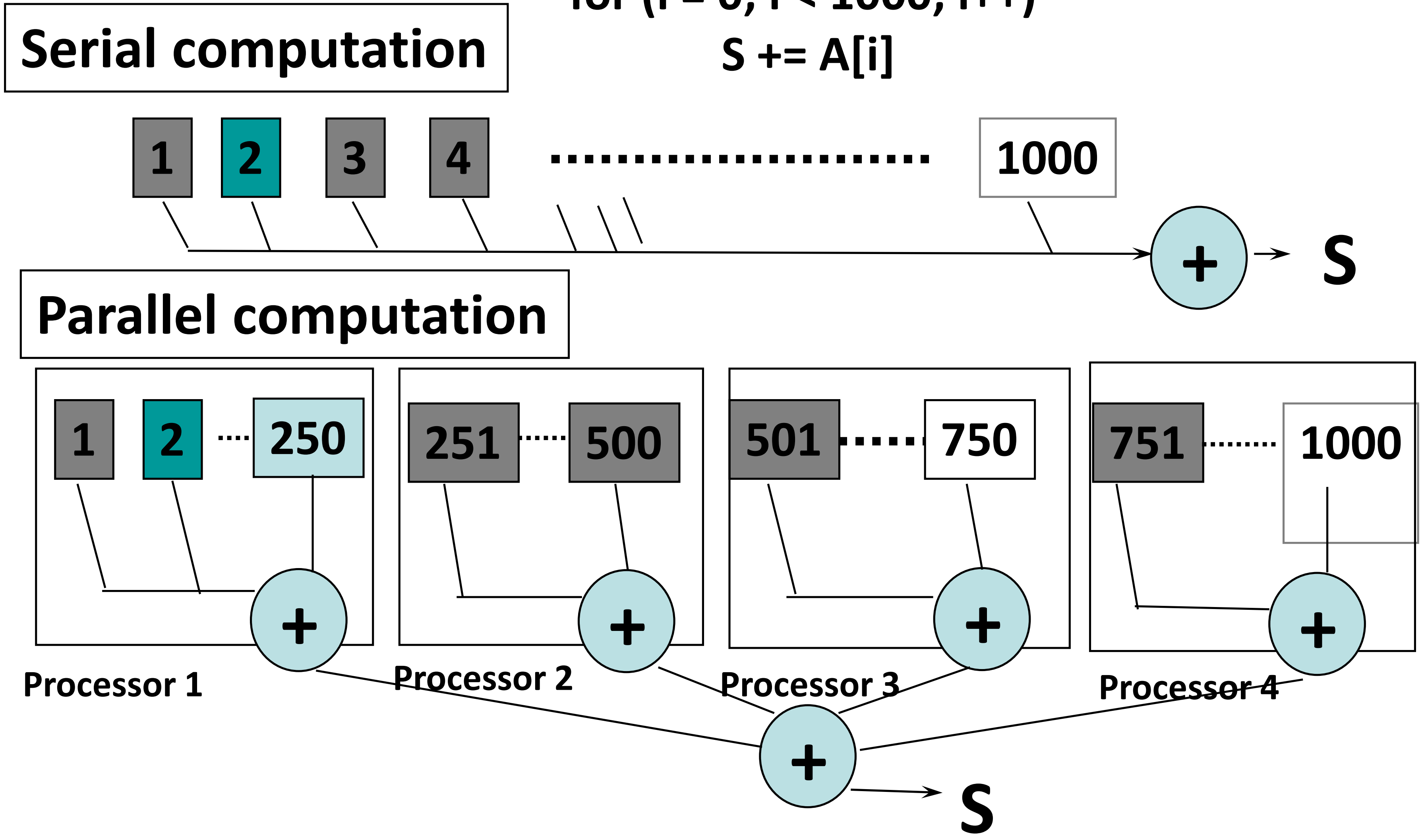
- Shared memory programming
  - For shared memory machines
    - Can be used for distributed shared memory (DSM) system on distributed memory machines
  - Easy to program (incremental from serial program)
  - Data transfer is taken care by the system
  - Often not scalable in terms of # processors

Parallel Programming (2)

- Message passing programming
  - MPI, PVM
- Shared memory programming
  - Multithread programming
    - Pthread, Solaris thread, NT thread
  - OpenMP
    - Annotation for parallel execution
    - Thread control, … for shared memory machines
  - High Performance Fortran (HPF)
    - Annotation for parallel execution
    - Parallel construct
    - Distribution of array, … for distributed memory machines
  - XcalableMP, X10, Chapel, Co-Array Fortran, Unified Parallel C, Titanium
- Automatic parallelization
  - Parallelize serial programs by compiler
    - Parallelization analysis by compiler is limited
    - Sometimes hint is required for parallelization by annotation
- Fancy parallel programming languages

Example of parallel computing

```
for (i = 0; i < 1000; i++)
        S += A[i]
```



Multithread Programming

- Thread creation

Pthread, Solaris thread

```
for (t = 1; t < n_thd; t++)
   pthread_create(&th[t], NULL, thd_main, t)
thd_main(0);
for (t = 1; t < n_thd; t++)
   pthread_join(th[t]);
```

- Divide the summation loop
- Atomic addition

```
double s;  /* global */
pthread_mutex_t mutex
   = PTHREAD_MUTEX_INITIALIZER;
int n_thd; /* number of threads */
void *thd_main(void *a)
{ int c, b, e, i, id = a;  double ss;
  c = 1000 / n_thd;
  b = c * id;
  e = b + c;
  ss = 0.0;
  for (i = b; i < e; i++) ss += a[i];
  pthread_mutex_lock(&mutex);
  s += ss;
  pthread_mutex_unlock(&mutex);
}
```

Programming in OpenMP

Just it is!

```
#pragma omp parallel for reduction(+:s)
  for (i = 0; i < 1000; i++) s += a[i];
```

About OpenMP

- Parallel programming model for shared memory machine
  - Extend the base languages (Fortran/C/C++) by using directive

- Specification discussed internationally (mainly US compiler vendors)
  - Oct. 1997 Fortran ver.1.0 API
  - Oct. 1998 C/C++ ver.1.0 API
  - July 2013 OpenMP 4.0

- URL
  - http://www.openmp.org/

Programming in MPI

- MPI (Message Passing Interface)
- Standard programming model for distributed memory machines
  - Required for more than 100 nodes
  - Complicated but required for performance
    - Like assembly language

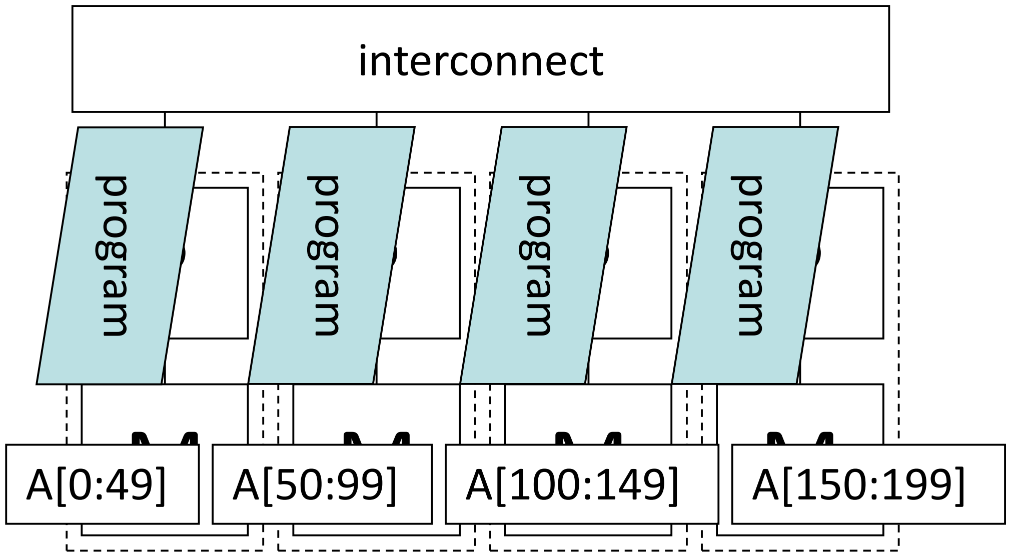
- Message passing (point-to-point communication)
  - Send/Receive
- Collective communication
  - Summation, …

MPI – The Message Passing Interface

- Standard of message passing interface
- MPI-1.0 released in 1994
  - Portable parallel library, application
  - 8 communication modes, collective communication, communication domain, process topology
  - Defined more than 100 interfaces
  - C, C++, Fortran
  - Specification http://www.mpi-forum.org/
    - MPI-3.0 released in September, 2012
  - Japanese translation http://phase.hpcc.jp/phase/mpi-j/ml/

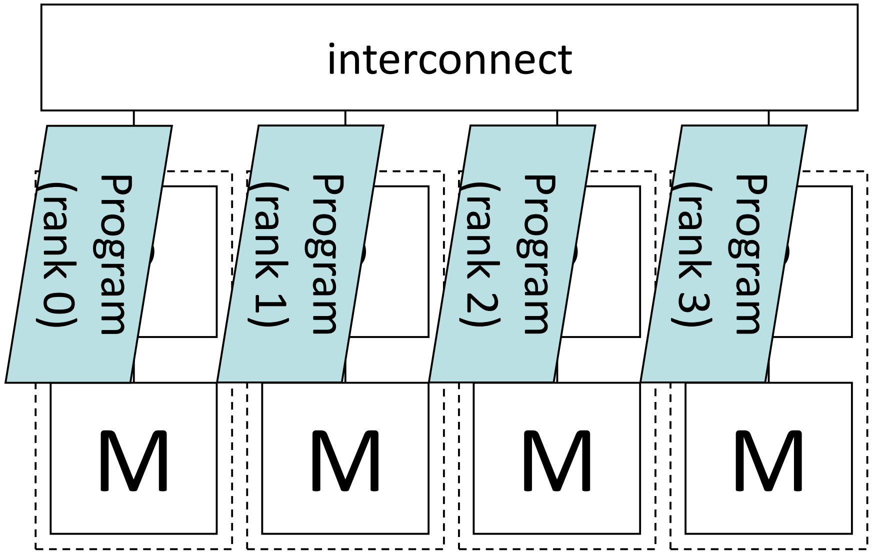
SPMD – Single Program, Multiple Data

- Parallel execution of the same single program independently (cf. SIMD)
- The same program but processes different data
- Parallel program is interacted with each other by message exchange



MPI execution model

- Execute the same program on each processor
  - Execution is not synchronous (if no communication happens)
- Each process has its own process rank
- Each process is communicated in MPI

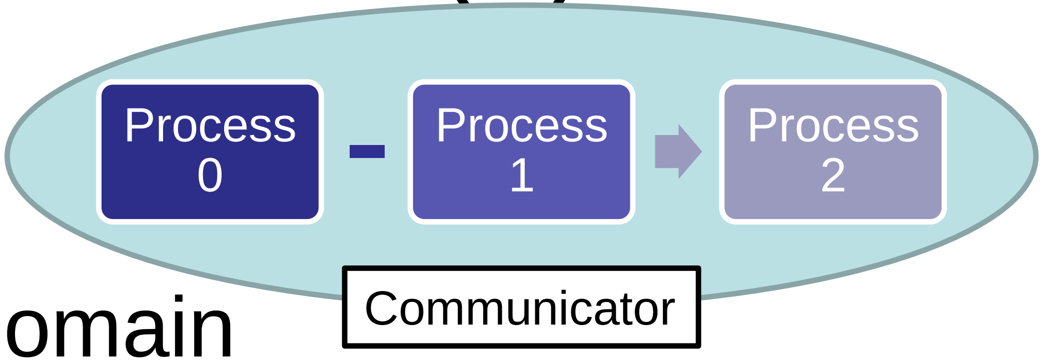


Initialization / Finalization

- int **MPI_Init**(int **argc*, char ****argv*);
  - Initialize MPI execution environment
  - All processes must call first

- int **MPI_Finalize**(void);
  - Terminate MPI execution environment
  - All processes must call before exiting

Communicator (1)



- Communication domain
  - Set of processes
  - # processes, process rank
  - Process topology
    - 1D ring, 2D mesh, torus, graph
- MPI_COMM_WORLD
  - Initial communicator including all processes

Operation for communicator

- int **MPI_Comm_size**(MPI_Comm *comm*, int **size*);
  - Returns the total number of processes *size* in the communicator *comm*
- int **MPI_Comm_rank**(MPI_Comm *comm*, int **rank*);
  - Returns the process rank *rank* in the communicator *comm*

Communicator (2)

- “Scope” of collective communication (communication domain)
- Can divide set of processes
  - Two thirds of processes compute weather forecast, the rest one third compute the initial condition of the next iteration
- Intra-communicator and inter-communicator

Sample program (1): hostname

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

int
main(int argc, char *argv[])
{
        int rank, len;
        char name[MPI_MAX_PROCESSOR_NAME];

        MPI_Init(&argc, &argv);
        MPI_Comm_rank(MPI_COMM_WORLD, &rank);
        MPI_Get_processor_name(name, &len);
        printf("%03d %s¥n", rank, name);
        MPI_Finalize();
        return (0);
}
```

Explanation

- Include mpi.h to use MPI

- Each process executes the main function
- SPMD (single program, multiple data)
  - A single program is executed on each node
  - Each program accesses different data (ie. data in their own running process)

- Initialize the MPI process
  - **MPI_Init**

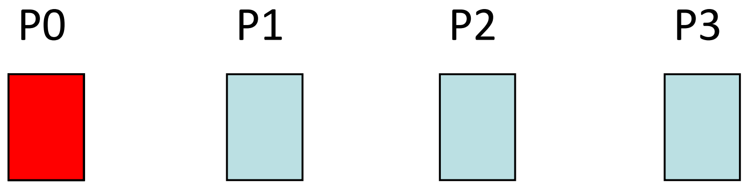
Explanation (continued)

- Obtain the process rank
  - **MPI_Comm_rank**(MPI_COMM_WORLD, &rank);
  - Obtain the self rank in the communicator MPI_COMM_WORLD
  - Communicator is an opaque object. The information can be access by API
- Obtain the node name
  - **MPI_Get_processor_name**(name, &len);
- All processes should finalize the MPI process
  MPI_Finalize();

Collective communication

- Message exchange among all processes specified by a communicator
- Barrier synchronization (no data transfer)
- Global communication
  - Broadcast, gather, scatter, gather to all, all-to-all scatter/gather
- Global reduction
  - Reduction (sum, maximum, logical and, …), scan (prefix computation)

Global communication



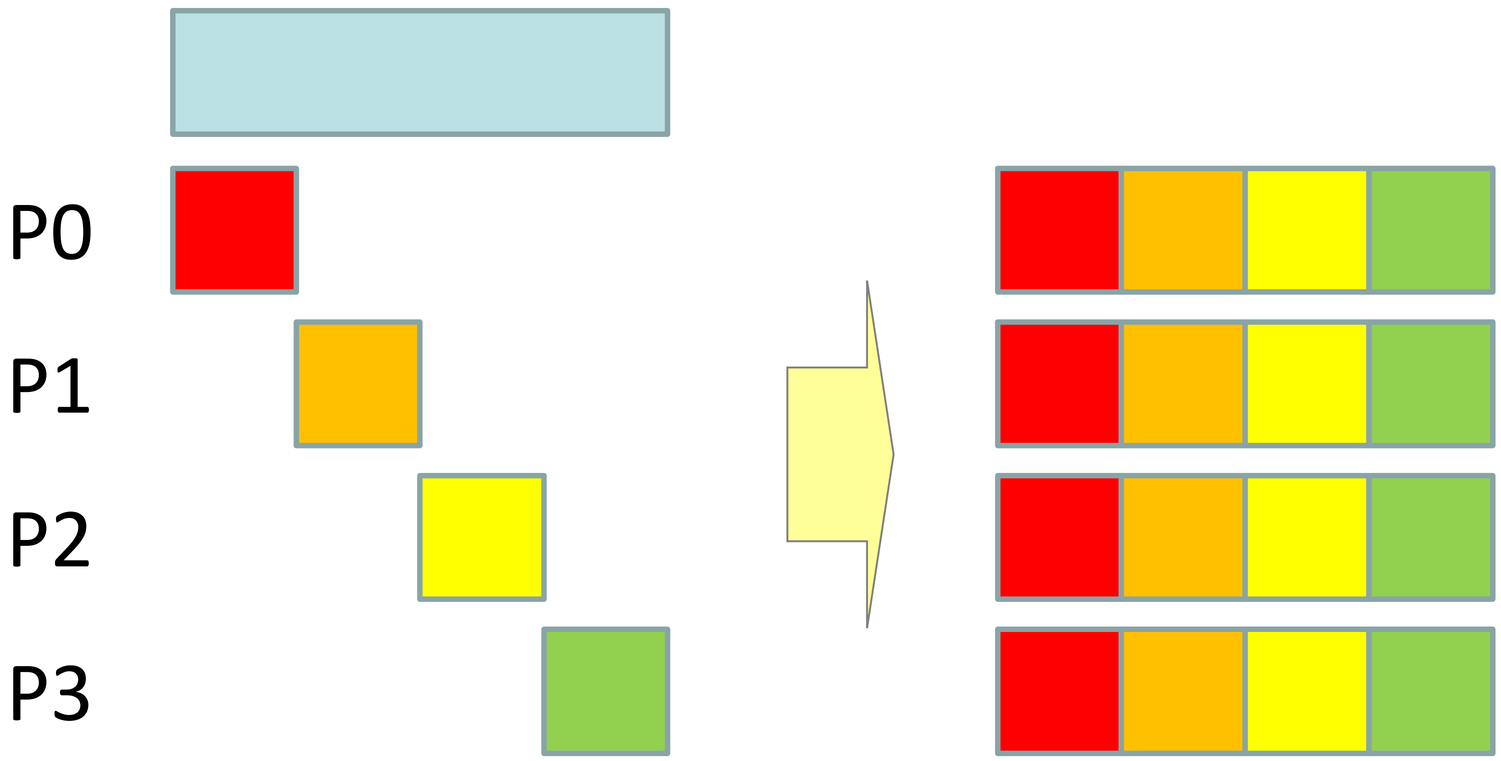
- broadcast
  - Transfer A[*] of the root process to all other processes

- gather
  - Gather sub arrays distributed among processes into a root process
  - Allgather gather sub arrays into all processes

- scatter
  - Scatter A[*] of the root process to all processes
- Alltoall
  - Scatter/gather data from all processes to all processes
  - Distributed matrix transpose A[:][*]→A^T[:][*] (: means this dimension is distributed)

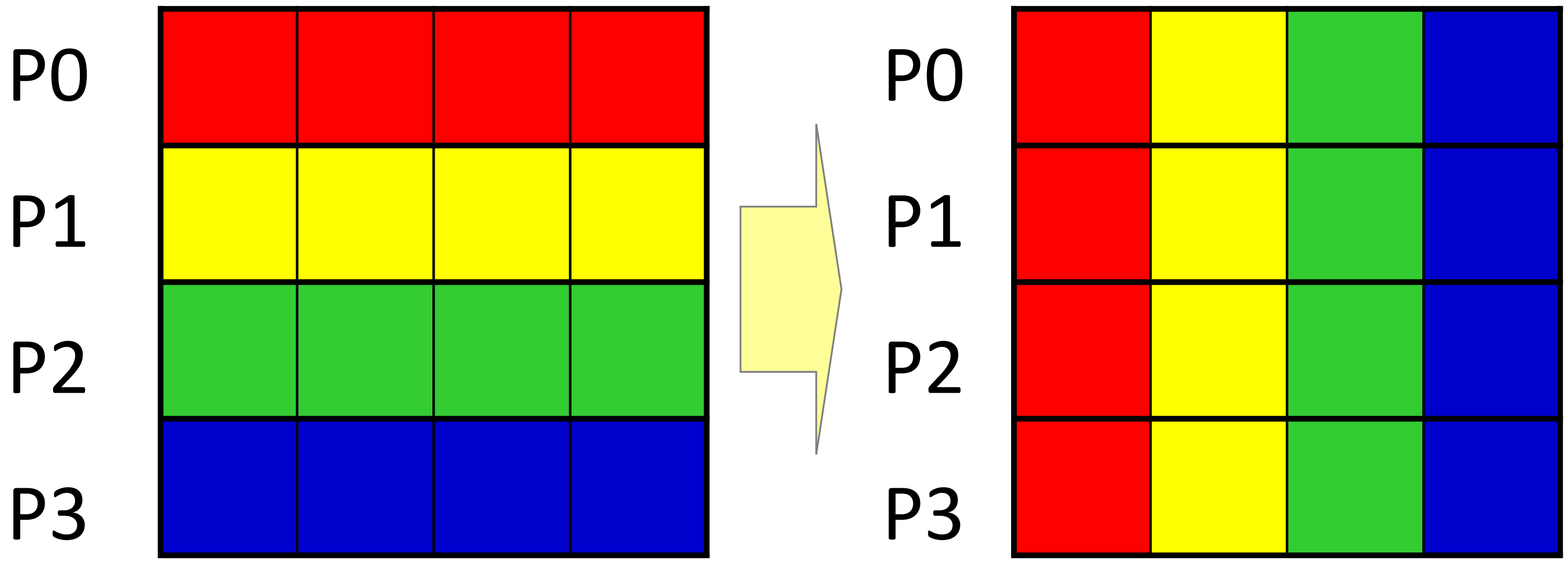
allgather

- Gather sub array of each process, and broadcast the whole array to all processes



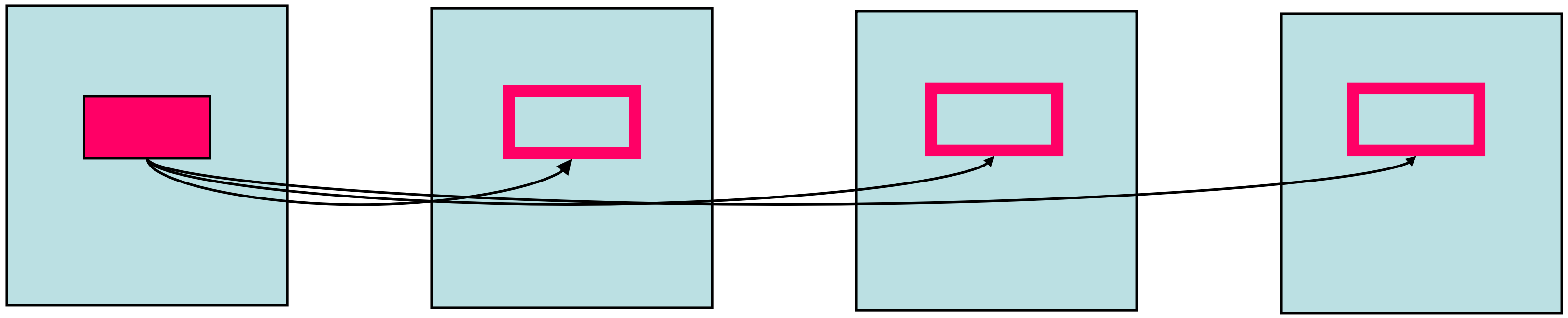
alltoall

- Matrix transformation of (row-wise) distributed 2D array



Collective communication: broadcast

```
int MPI_Bcast(
  void        *data_buffer,    // address of source and destination buffer of data
  int         count,           // data counts
  MPI_Datatype data_type,      // data type
  int         source,          // source process rank
  MPI_Comm    communicator     // communicator
);
```

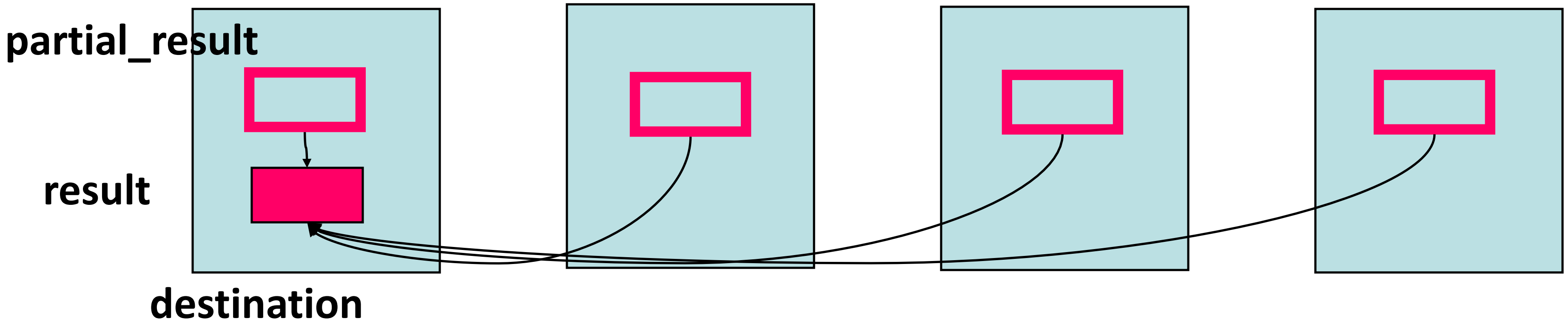


source

It should be executed on all processes in the communicator

Collective communication: Reduction

```
int MPI_Reduce(
  void         *partial_result,        // address of input data
  void         *result,                // address of output data
  int          count,                  // data count
  MPI_Datatype data_type,              // data type
  MPI_Op       operator,               // reduce operation
  int          destination,            // destination process rank
  MPI_Comm     communicator            // communicator
);
```

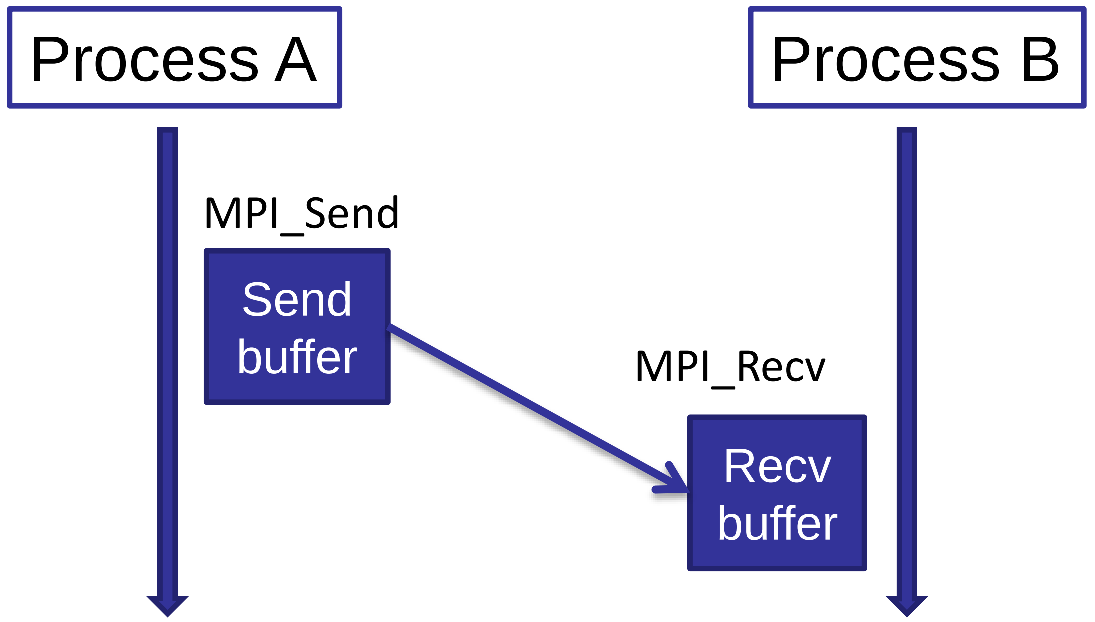


It should be executed on all processes in the communicator

MPI_Allreduce returns the result on all processes

Point-to-point communication (1)

- Data transfer among two process pair
  - Process A sends a data to process B (send)
  - Process B receives the data (from the process A) (recv)



Point-to-point communication (2)

- Data is typed
  - Basic data type, array, structure, vector, user-defined data type
- Send and the corresponding receive are specified by Communicator, message tag, process rank of source and destination

Point-to-point communication (3)

- Message is specified by address and size
  - Typed: MPI_INT, MPI_DOUBLE, …
  - Binary data can be specified by MPI_BYTE with message size in byte
- Source/destination is specified by process rank and message tag
  - MPI_ANY_SOURCE for any source process rank
  - MPI_ANY_TAG for any message tag
- Status information includes the source rank, size, tag of the received message

Blocking point-to-point communication

- Send/Receive

```
int MPI_Send(
  void          *send_data_buffer, // address of input data
  int           count,             // data count
  MPI_Datatype  data_type,         // data type
  int           destination,       // destination process rank
  int           tag,               // message tag
  MPI_Comm      communicator       // communicator
);
```

```
int MPI_Recv(
  void          *recv_data_buffer, // address of receive data
  int           count,             // data count
  MPI_Datatype  data_type,         // data type
  int           source,            // source process rank
  int           tag,               // message tag
  MPI_Comm      communicator,      // communicator
  MPI_Status    *status            // status information
);
```

Point-to-point communication (4)

- Semantics of blocking communication
  - Send call returns when the send buffer can be reused
  - Receive call returns when the receive buffer is available
- When MPI_Send(A, . . .) returns, A can be safely modified
  - It may be that A is just copied into the communication buffer of the sender
  - It does not mean message transfer completion

Non-blocking point-to-point communication

- Nonblocking communication
  - post-send, complete-send
  - post-receive, complete-receive
- Post-{send,recv} initiates the send/receive operations
- Complete-{send,recv} waits for the completion
- It enables the overlap of computation and communication to improve performance
  - Multithread programming also enables the overlapping, but nonblocking communication often more efficient

Nonblocking point-to-point communication

- MPI_Isend/Irecv initiates the communication, MPI_Wait waits for the completion in semantics of blocking communication
  - Computation and communication can be overlapped if the communication can be executed in the background

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

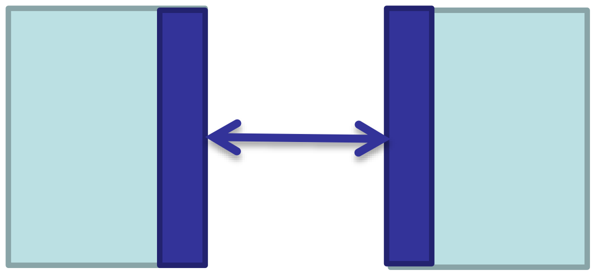
```
int MPI_Irecv( void *buf, int count, MPI_Datatype datatype,
 int source, int tag, MPI_Comm comm, MPI_Request *request )
```

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

Communication modes

- Blocking and nonblocking send operations have four communication modes
  - Standard mode
    - MPI decides whether message is buffered or not. **User should not assume it is buffered.**
  - Buffered mode
    - Outgoing message is buffered
    - Send operation is local
  - Synchronous mode
    - Send completes only if a matching receive is posted
    - Send operation is non-local
  - Ready mode
    - Send may be started only if the matching receive is posted
    - It can remove a hand-shake operation

Message exchange



- Blocking P2P

  ```
  …
  MPI_Send(destination, data)
  MPI_Recv(sender, data)
  …
  ```

- It can be executed only if MPI_Send is bufferred
  - Unless, the **dead lock** occurs
- Or, use MPI_Sendrecv

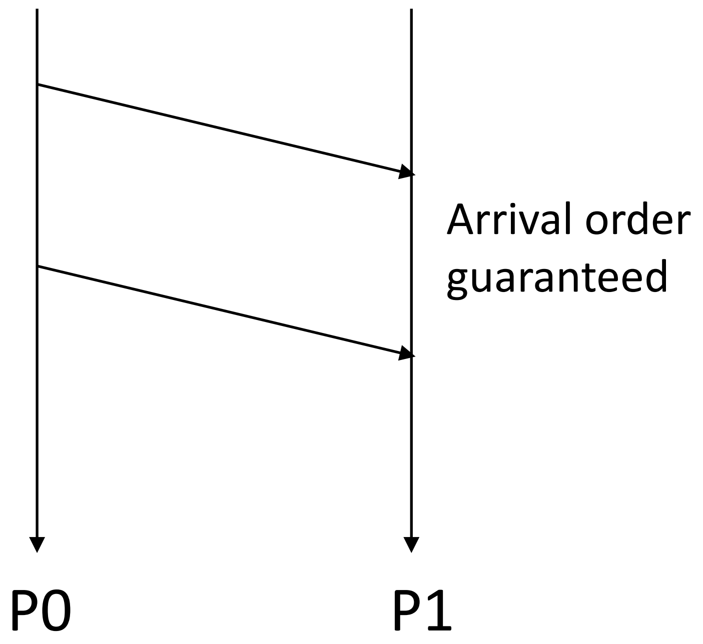
- Nonblocking P2P

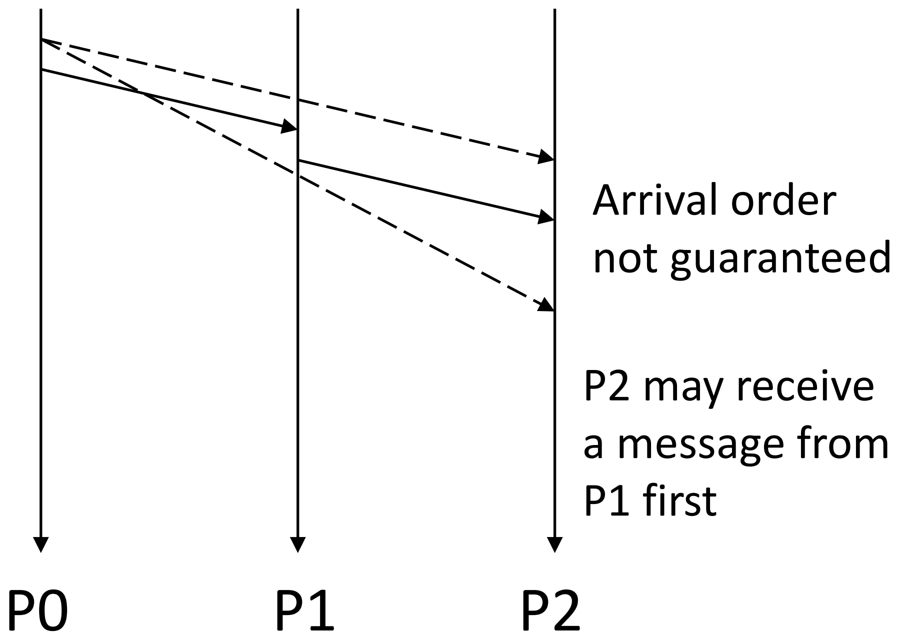
  ```
  …
  MPI_Isend(destingation, data, req)
  MPI_Recv(sender)
  MPI_Wait(req, status)
  …
  ```

- Safely executed
- Portable

Caveat (1)

- Message arrival order
  - Message is not overtaken between two processes
  - It may be overtaken among three or more

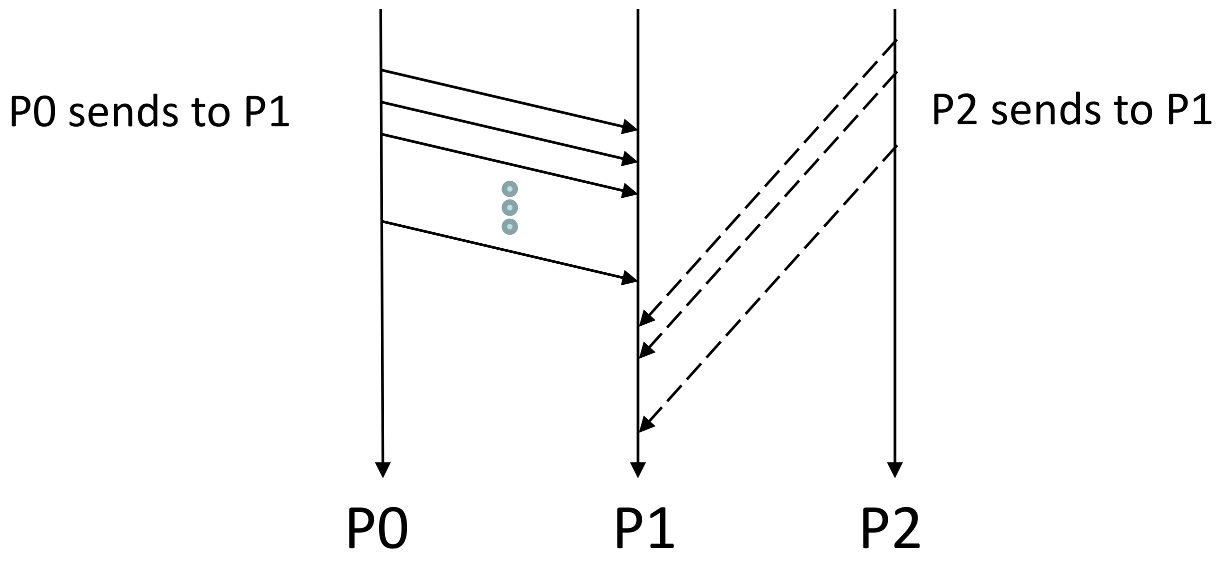




Arrival order not guaranteed
P2 may receive a message from P1 first
P0
P1
P2

Caveat (2)

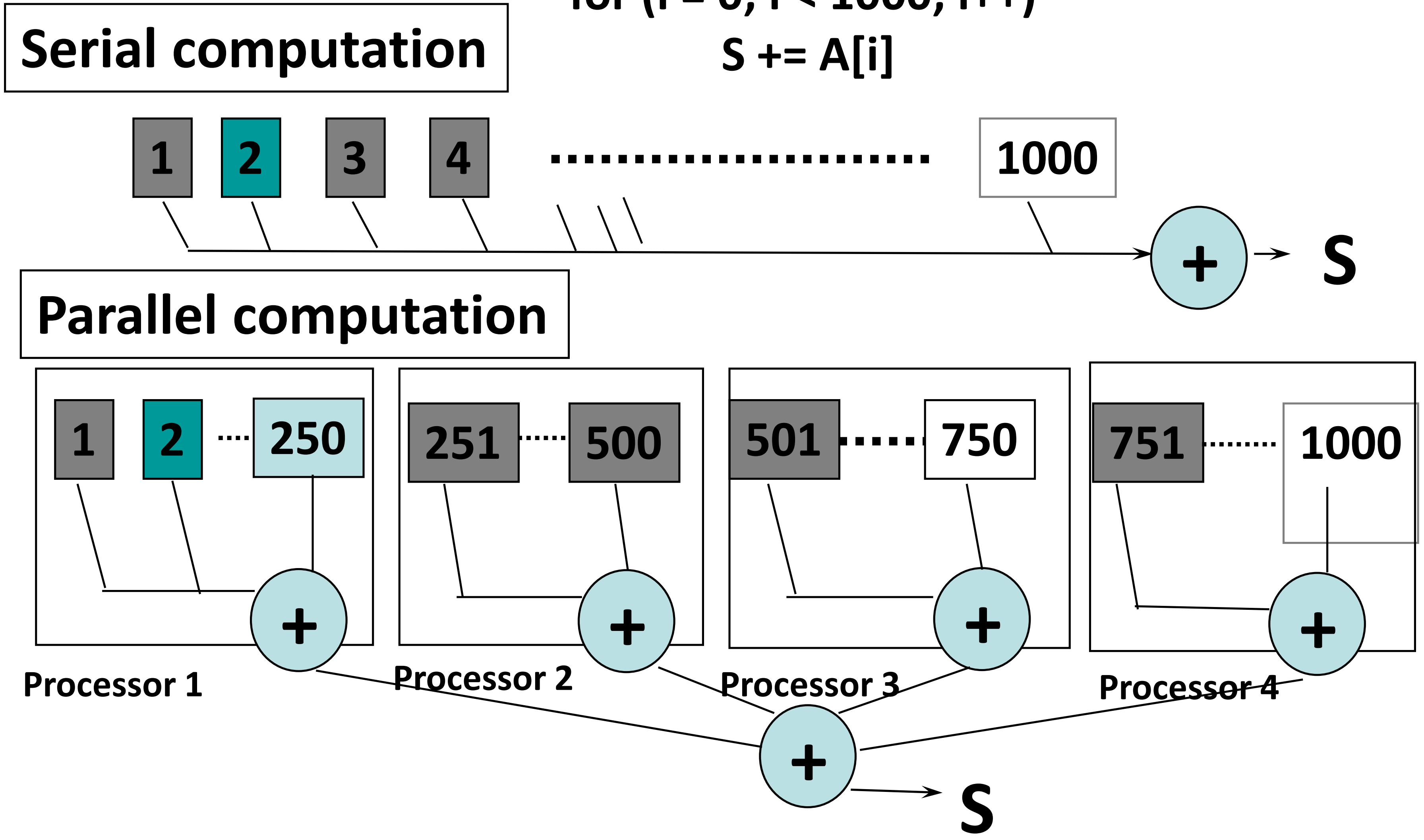
- Fairness
  - Fairness is not guaranteed in communication process



P1 may receive messages from P0 **only**

Sample program (2): summation

```
for (i = 0; i < 1000; i++)
    S += A[i]
```



```
#include <mpi.h>

double SubA[250];      // subarray of A

int main(int argc, char *argv[])
{
   double sum, mysum;

   MPI_Init(&argc,&argv);
   mysum = 0.0;
   for (i = 0; i < 250; i++)
          mysum += SubA[i];
   MPI_Reduce(&mysum, &sum, 1, MPI_DOUBLE,
          MPI_SUM, 0, MPI_COMM_WORLD);
   MPI_Finalize();
   return (0);
}
```

Explanation

- Allocate a different part of **sub-array** of A is in each process
- Computation and communication
  - Each process computes a partial sum, and communicates with all processes to sum it up by collective communication

    MPI_Reduce(&*mysum*, &*sum*, 1, MPI_DOUBLE, MPI_SUM, *0*, MPI_COMM_WORLD);
  - Combines *mysum* (an array of MPI_DOUBLE with size 1) using MPI_SUM, and returns the combined value *sum* of the root process (rank *0*)

Sample program (3): Cpi

- Calculate the PI by the integral calculus
- Test program of MPICH
  - Riemann Sum
  - Broadcast n (number of divided parts)
  - Reduce the partial sum
  - The partial sum is computed in cyclic manner

$$\pi = \int_0^1 \frac{4}{1+t^2}\,dt$$

```
…
MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);

h = 1.0 / n;                                    for (i = 1; i <= n; i++)
sum = 0.0;
for (i = myid + 1; i <= n; i += numprocs){
        x = h * (i - 0.5);
        sum += f(x);
}
mypi = h * sum;

MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE,
             MPI_SUM, 0, MPI_COMM_WORLD);
```

```
/* cpi mpi version */
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include <mpi.h>

double
f(double a)
{
	return (4.0 / (1.0 + a * a));
}

int
main(int argc, char *argv[])
{
	int n = 0, myid, numprocs, i;
	double PI25DT = 3.141592653589793238462643;
	double mypi, pi, h, sum, x;
	double startwtime = 0.0, endwtime;
	int namelen;
	char processor_name[MPI_MAX_PROCESSOR_NAME];
```

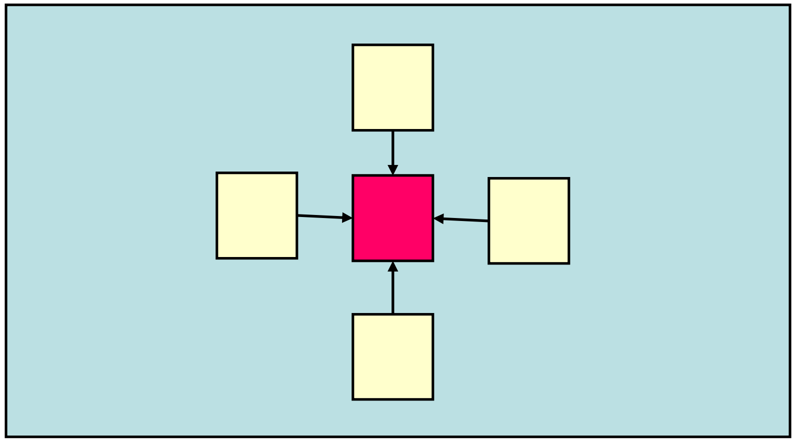
```
MPI_Init(&argc, &argv);
MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
MPI_Comm_rank(MPI_COMM_WORLD, &myid);
MPI_Get_processor_name(processor_name, &namelen);
fprintf(stderr, "Process %d on %s¥n", myid, processor_name);

if (argc > 1)
        n = atoi(argv[1]);
startwtime = MPI_Wtime();
/* broadcast 'n' */
MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
if (n <= 0) {
        fprintf(stderr, "usage: %s #partition¥n", *argv);
        MPI_Abort(MPI_COMM_WORLD, 1);
}
```

```
    /* calculate each part of pi */
    h = 1.0 / n;
    sum = 0.0;
    for (i = myid + 1; i <= n; i += numprocs){
        x = h * (i - 0.5);
        sum += f(x);
    }
    mypi = h * sum;
    /* sum up each part of pi */
    MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
    if (myid == 0) {
        printf("pi is approximately %.16f, Error is %.16f¥n",
            pi, fabs(pi - PI25DT));
        endwtime = MPI_Wtime();
        printf("wall clock time = %f¥n",
            endwtime - startwtime);
    }
    MPI_Finalize();
    return (0);
}
```

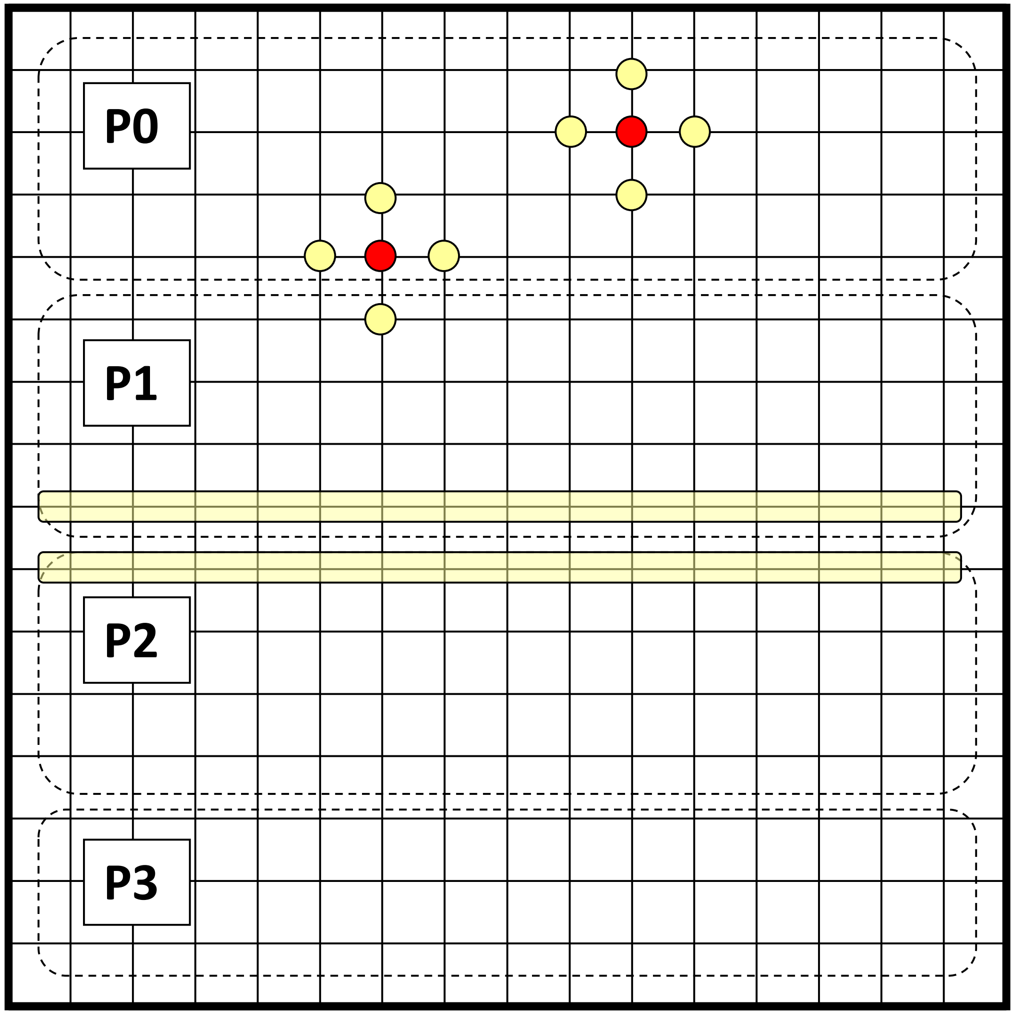
Sample program (4): laplace

- Explicit solution of Laplace equation
  - Update by averaging data of up, down, left, right four points
  - Prepare two arrays old and new to keep the old (previous) value
  - Region segmentation, region division
  - Compute the residual to check the convergence



Matrix decomposition and nearest neighbor communication

- Block distribution of 2D region
- To update boundary elements, boundary elements of neighbors are required
- Data exchange of boundary elements



Process topology

- int **MPI_Cart_create**(MPI_Comm *comm_old*, int *ndims*, int **dims*, int **periods*, int *reorder*, MPI_Comm **comm_cart*);
  - Creates *comm_cart* with *ndims* dimensional hypercube topology
  - Process size of each dimension is specified by *dims*
  - *Periods* specified whether each dimension is periodical or not
  - *Reorder* specifies whether it allows renumbering of ranks between old and new communicators

Source/destination of shift communication

- int **MPI_Cart_shift**(MPI_Comm *comm*, int *direction*, int *disp*, int **rank_source*, int **rank_dest*);
  - *Direction* spefified the dimension of shift communication
    - It is 0 to ndims-1 in ndims dimension case
  - Disp is a displacement of shift communication
  - It returns rank_source as a source rank and rank_dest as a destination rank
  - If the boundary is not periodical, it returns MPI_PROC_NULL if it exceeds the boundary

```
/* calculate process ranks for 'down' and 'up' */
MPI_Cart_shift(comm, 0, 1, &down, &up);

/* recv from down */
MPI_Irecv(&uu[x_start-1][1], YSIZE, MPI_DOUBLE, down, TAG_1,
            comm, &req1);
/* recv from up */
MPI_Irecv(&uu[x_end][1], YSIZE, MPI_DOUBLE, up, TAG_2,
            comm, &req2);

/* send to down */
MPI_Send(&u[x_start][1], YSIZE, MPI_DOUBLE, down, TAG_2, comm);
/* send to up */
MPI_Send(&u[x_end-1][1], YSIZE, MPI_DOUBLE, up, TAG_1, comm);

MPI_Wait(&req1, &status1);
MPI_Wait(&req2, &status2);
```

In a process of rank 0 and numprocs-1, MPI_Cart_shift returns MPI_PROC_NULL
No need to treat specially. MPI_Send and Irecv do not do anything if MPI_PROC_NULL is specified

```
/*
 * Laplace equation with explicit method
 */
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <mpi.h>

/* square region */
#define XSIZE 256
#define YSIZE 256
#define PI 3.1415927
#define NITER 10000
double u[XSIZE + 2][YSIZE + 2], uu[XSIZE + 2][YSIZE + 2];
double time1, time2;
void lap_solve(MPI_Comm);
int myid, numprocs;
int namelen;
char processor_name[MPI_MAX_PROCESSOR_NAME];
int xsize;
```

2D target domain
Uu is for new values

```
void
initialize()
{
        int x, y;

        /* initialization*/
        for (x = 1; x < XSIZE + 1; x++)
                for (y = 1; y < YSIZE + 1; y++)
                        u[x][y] = sin((x - 1.0) / XSIZE * PI) +
                                cos((y - 1.0) / YSIZE * PI);
        /* zero clear in the boundary */
        for (x = 0; x < XSIZE + 2; x++) {
                u [x][0] = u [x][YSIZE + 1] = 0.0;
                uu[x][0] = uu[x][YSIZE + 1] = 0.0;
        }
        for (y = 0; y < YSIZE + 2; y++) {
                u [0][y] = u [XSIZE + 1][y] = 0.0;
                uu[0][y] = uu[XSIZE + 1][y] = 0.0;
        }
}
```

```c
#define TAG_1 100
#define TAG_2 101

#ifndef FALSE
#define FALSE 0
#endif

void lap_solve(MPI_Comm comm)
{
        int x, y, k;
        double sum;
        double t_sum;
        int x_start, x_end;
        MPI_Request req1, req2;
        MPI_Status status1, status2;
        MPI_Comm comm1d;
        int down, up;
        int periods[1] = { FALSE };
```

```
/*
 * Create one dimensional cartesian topology with
 * nonperiodical boundary
 */
MPI_Cart_create(comm, 1, &numprocs, periods, FALSE, &comm1d);
/* calculate process ranks for 'down' and 'up' */
MPI_Cart_shift(comm1d, 0, 1, &down, &up);

x_start = 1 + xsize * myid;
x_end = 1 + xsize * (myid + 1);
```

- Create *comm1d* with one dimensional topology
  - The boundary is not periodical
- Obtain the *up* and *down* process rank
  - The boundary process may obtain MPI_PROC_NULL

```
for (k = 0; k < NITER; k++){
        /* old <- new */
        for (x = x_start; x < x_end; x++)
                for (y = 1; y < YSIZE + 1; y++)
                        uu[x][y] = u[x][y];

        /* recv from down */
        MPI_Irecv(&uu[x_start - 1][1], YSIZE, MPI_DOUBLE,
                  down, TAG_1, comm1d, &req1);
        /* recv from up */
        MPI_Irecv(&uu[x_end][1], YSIZE, MPI_DOUBLE,
                  up, TAG_2, comm1d, &req2);
        /* send to down */
        MPI_Send(&u[x_start][1], YSIZE, MPI_DOUBLE,
                 down, TAG_2, comm1d);
        /* send to up */
        MPI_Send(&u[x_end - 1][1], YSIZE, MPI_DOUBLE,
                 up, TAG_1, comm1d);

        MPI_Wait(&req1, &status1);
        MPI_Wait(&req2, &status2);
        /* update */
        for (x = x_start; x < x_end; x++)
                for (y = 1; y < YSIZE + 1; y++)
                        u[x][y] = .25 * (uu[x - 1][y] + uu[x + 1][y] +
                                        uu[x][y - 1] + uu[x][y + 1]);
    }
    /* check sum */
    sum = 0.0;
    for (x = x_start; x < x_end; x++)
        for (y = 1; y < YSIZE + 1; y++)
            sum += uu[x][y] - u[x][y];
    MPI_Reduce(&sum, &t_sum, 1, MPI_DOUBLE, MPI_SUM, 0, comm1d);
    if (myid == 0)
        printf("sum = %g¥n", t_sum);
    MPI_Comm_free(&comm1d);
}
```

```
int
main(int argc, char *argv[])
{
	MPI_Init(&argc, &argv);
	MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
	MPI_Comm_rank(MPI_COMM_WORLD, &myid);
	MPI_Get_processor_name(processor_name, &namelen);
	fprintf(stderr, "Process %d on %s¥n", myid, processor_name);

	xsize = XSIZE / numprocs;
	if ((XSIZE % numprocs) != 0)
		MPI_Abort(MPI_COMM_WORLD, 1);
	initialize();
	MPI_Barrier(MPI_COMM_WORLD);
	time1 = MPI_Wtime();
	lap_solve(MPI_COMM_WORLD);
	MPI_Barrier(MPI_COMM_WORLD);
	time2 = MPI_Wtime();
	if (myid == 0)
		printf("time = %g¥n", time2 - time1);
	MPI_Finalize();
	return (0);
}
```

Things to improve

- This program allocates the whole array although it is not necessary
  - When the partial array is allocated, the index of array should be computed from global index to local index
  - This is essential to solve large-scale problem using distributed memory machine
- Two dimensional distribution of 2D array is more efficient than one dimensional distribution
  - Reduce the communication size
  - Can be parallelized by more number of processors

Summary

- Parallel computing is indispensable to achieve high performance

- OpenMP is easy, but may be efficient up to 16 processors
- For more number of processors, MPI is only the choice
  - Tradeoff between the programming cost and execution time
  - We expect a new programming language that replaces MPI for longer term

- It is not *too* difficult to parallelize scientific applications
  - It has inherent data parallelism
  - Most scientific applications can be parallelized in some "parallelization patterns"

Open source implementation

OpenMP

- GNU GCC 4.2 or later

  ```
  % cc -fopenmp . . .
  ```

- Omni OpenMP Compiler
  - http://phase.hpcc.jp/Omni/

MPI

- OpenMPI
  - http://www.open-mpi.org/
- MPICH2
  - http://www-unix.mcs.anl.gov/mpi/mpich2/
- YAMPII
  - http://www.il.is.s.u-tokyo.ac.jp/yampii/