

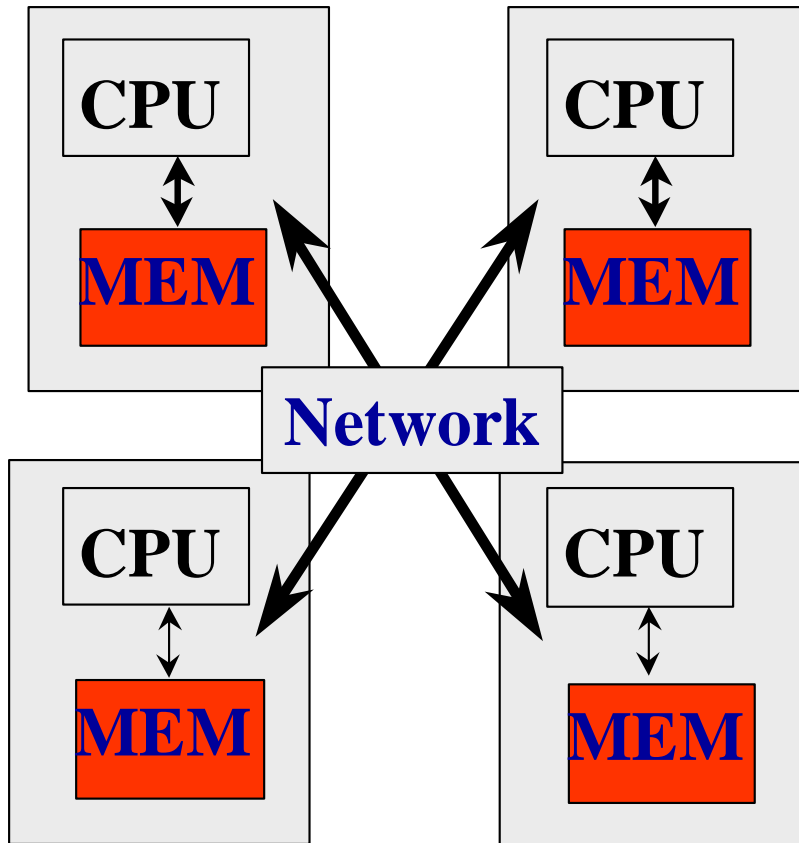
# Programming for High Performance Computing

Programming Environment

Jan 17, 2013

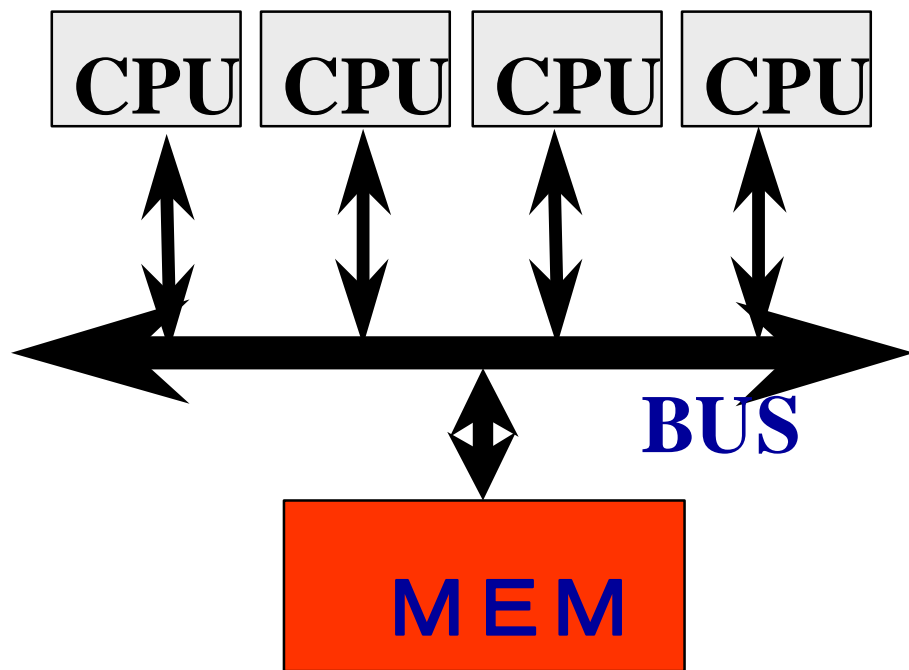
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# Distributed Memory Machine



- ◆ Parallel machine that consists computers (CPU and memory) connected by a network
- ◆ Parallel program is executed on each machine, communicating data (message) by the network
- ◆ MPP (Massively Parallel Processor)
  - ◆ Using proprietary technology
- ◆ PC Cluster
  - ◆ Using commodity technology

# Shared Memory Machine



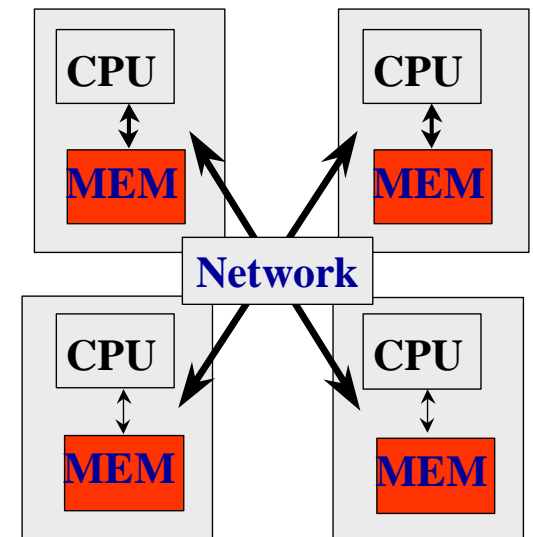
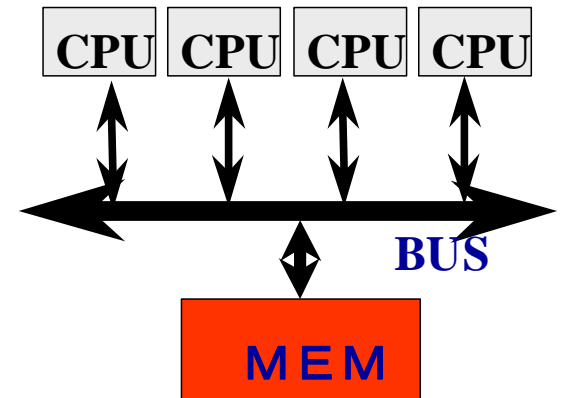
- ◆ Parallel machine such that CPUs access the same memory
- ◆ Parallel program is executed by accessing the data on the shared memory to communicate each other
- ◆ Large scale server, multicore CPU
- ◆ UMA (uniform memory access) and NUMA (non-uniform memory access)

# 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

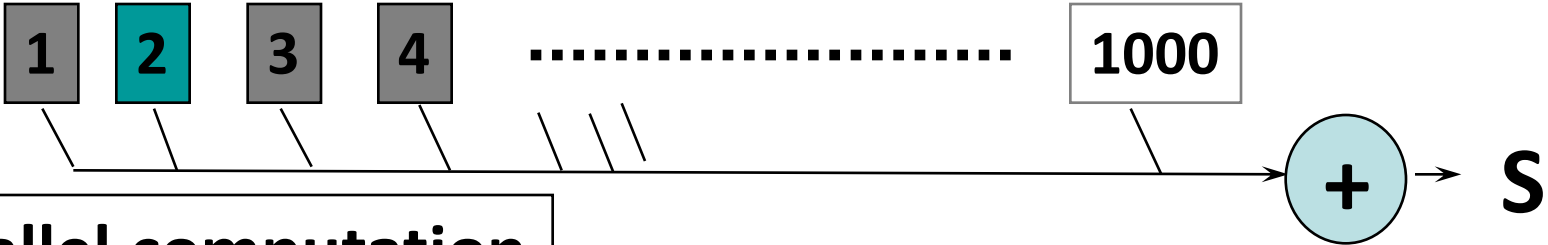
# Parallel Programming (2)

- 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
  - HPF
    - Annotation for parallel execution
    - Parallel construct
    - Distribution of array, ... for distributed memory machines
- 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

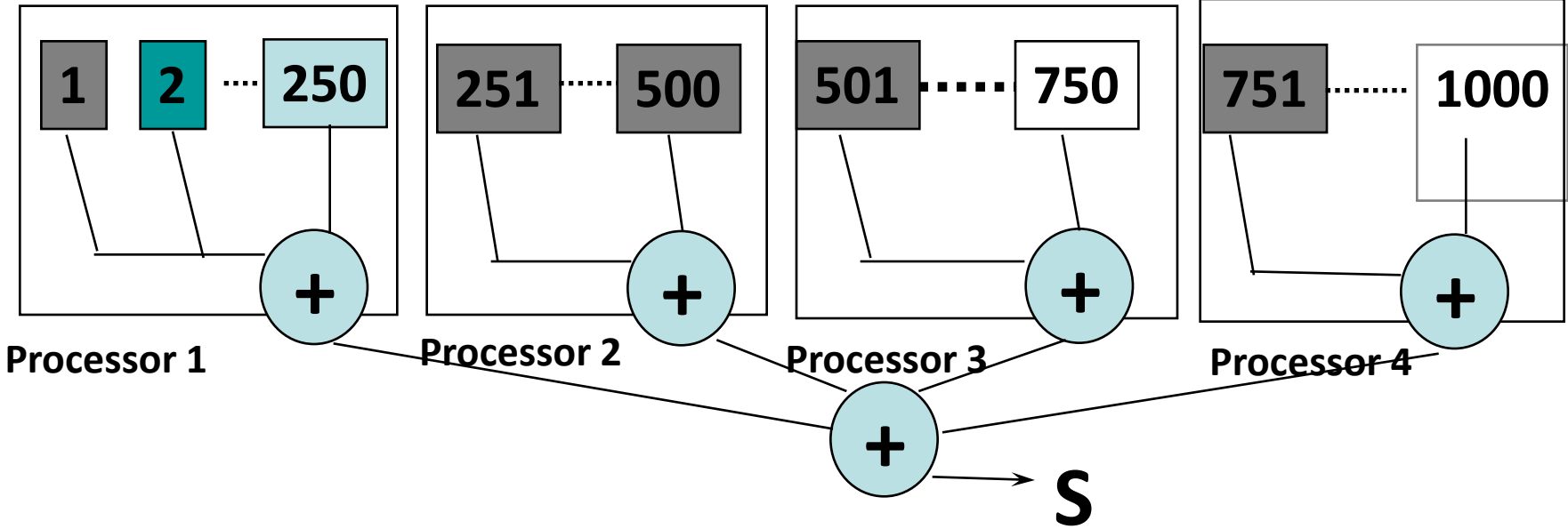
# Example of parallel computing

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

**Serial computation**



**Parallel computation**



# Multithread Programming

- Thread creation

## Pthread, Solaris thread

```
for (t = 1; t < n_thd; t++){
    r = pthread_create(thd_main, t)
}
thd_main(0);
for (t = 1; t < n_thd; t++)
    pthread_join();
```

- Divide the summation loop
- Atomic addition

```
double s; /* global */
int n_thd; /* number of threads */
int thd_main(int id)
{ int c, b, e, i; 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_lock();
  s += ss;
  pthread_unlock();
  return (0);
}
```



# 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 2011 OpenMP 3.1
- URL
  - <http://www.openmp.org/>

# Programming in MPI

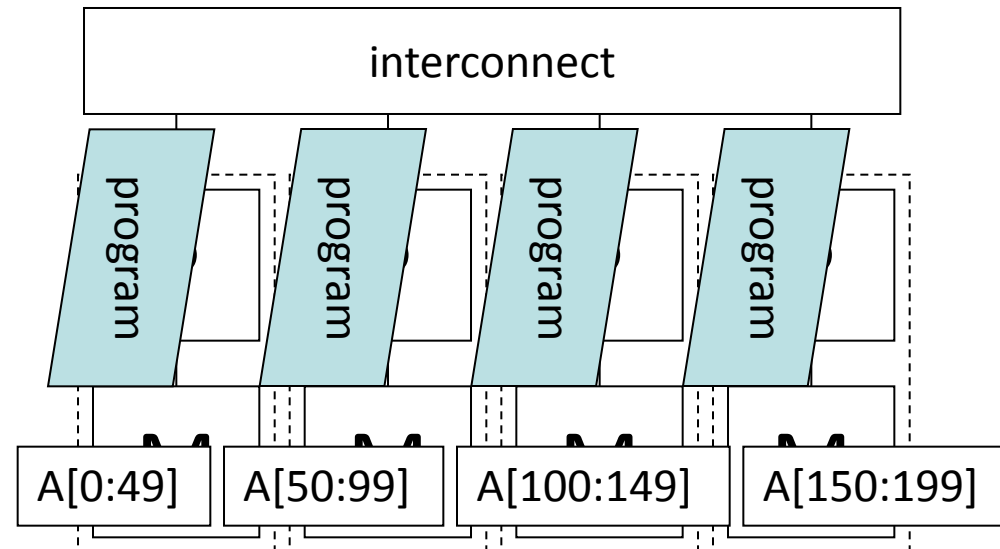
- MPI (Message Passing Interface)
- Standard programming model for distributed memory machines
  - Required for more than 100 nodes
  - Complicated but required for performance
    - Like assembly language
- Message passing (point-to-point communication)
  - Send/Receive
- Collective communication
  - 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/>

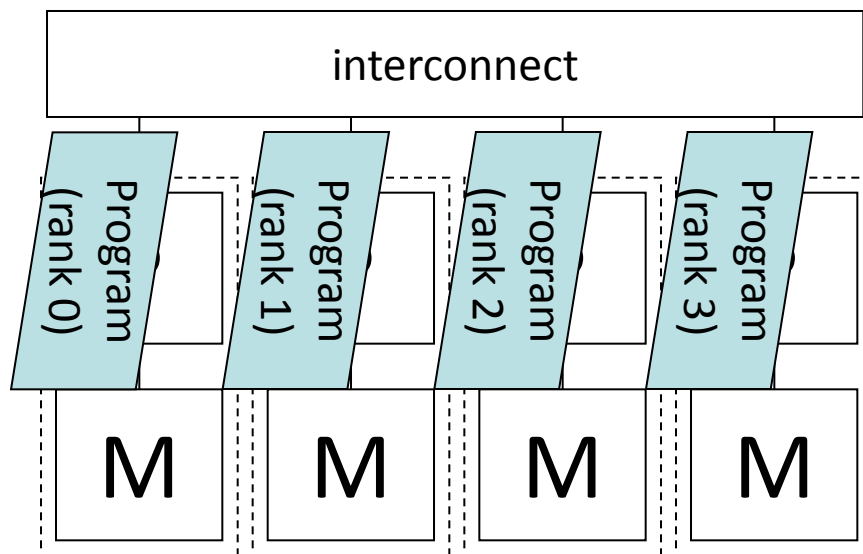
# SPMD – Single Program, Multiple Data

- 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



# 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

# Communicator (2)

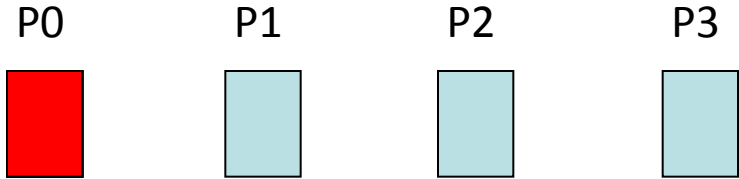
- “Scope” of collective communication (communication domain)
- Can divide set of processes
  - Two thirds of processes compute weather forecast, the rest one third compute the initial condition of the next iteration
- Intra-communicator and inter-communicator



# 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

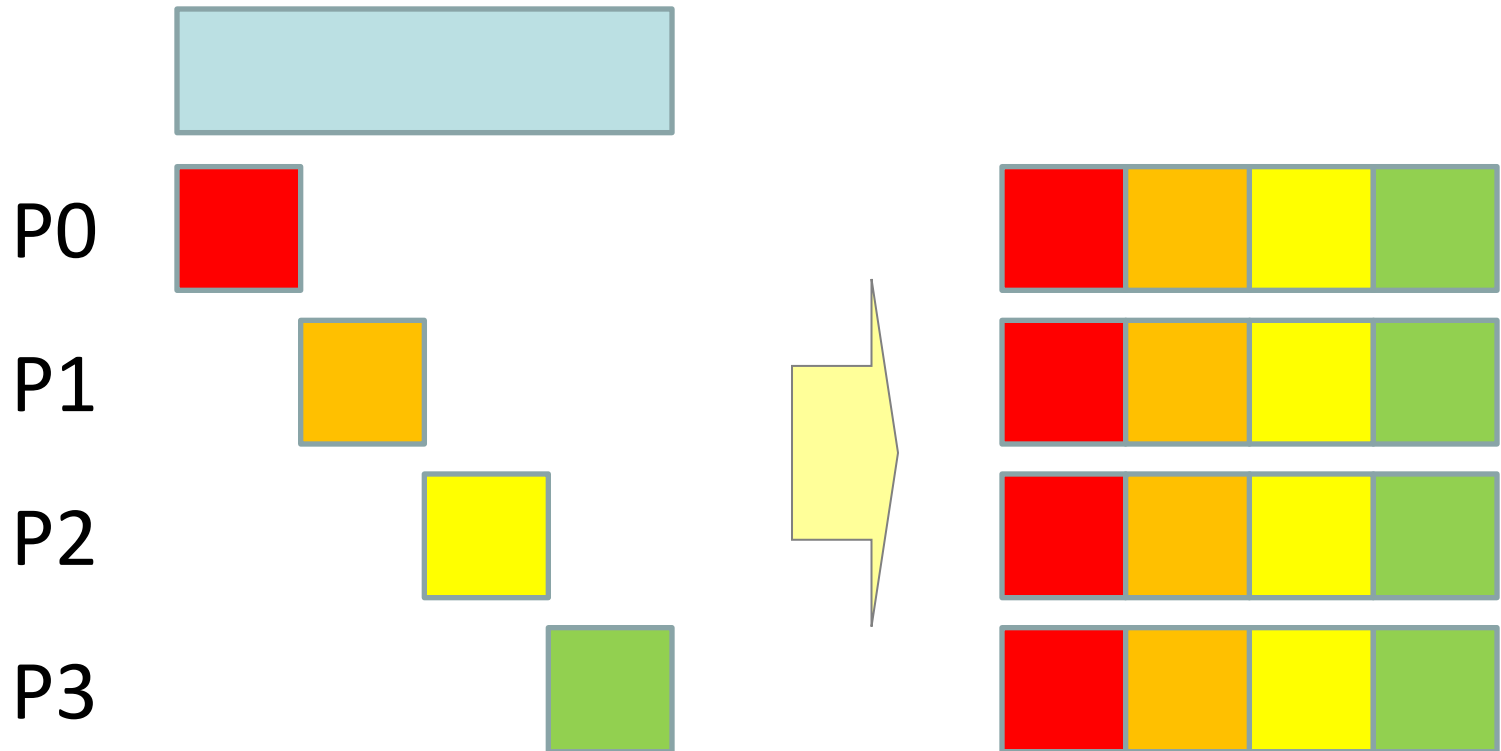


- Alltoall

- Scatter/gather data from all processes to all processes
- Distributed matrix transpose  $A[:,*] \rightarrow A^T[:,*]$  (: means this dimension is distributed)

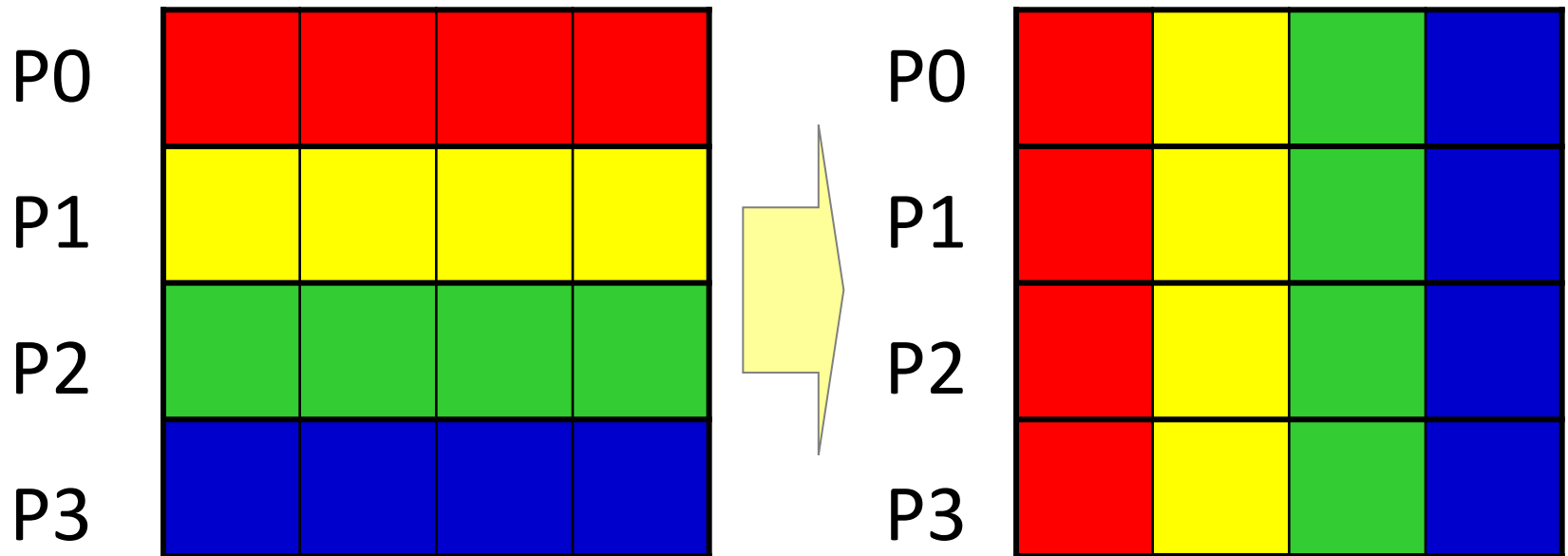
# allgather

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



# alltoall

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



# 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)
- 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 (2)

- 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-recv, complete-recv
- 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

# 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**();

# Operation for communicator

- int **MPI\_Comm\_size**(MPI\_Comm *comm*, int *\*size*);

- Returns the total number of processes *size* in the communicator *comm*

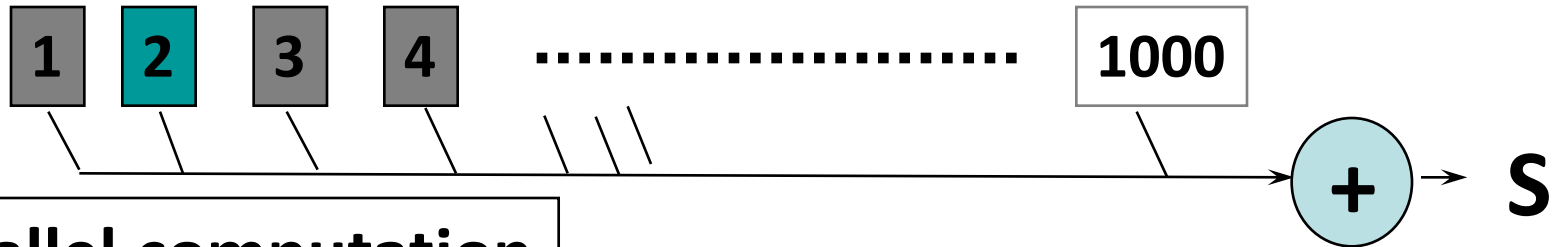
- int **MPI\_Comm\_rank**(MPI\_Comm *comm*, int *\*rank*);

- Returns the process rank *rank* in the communicator *comm*

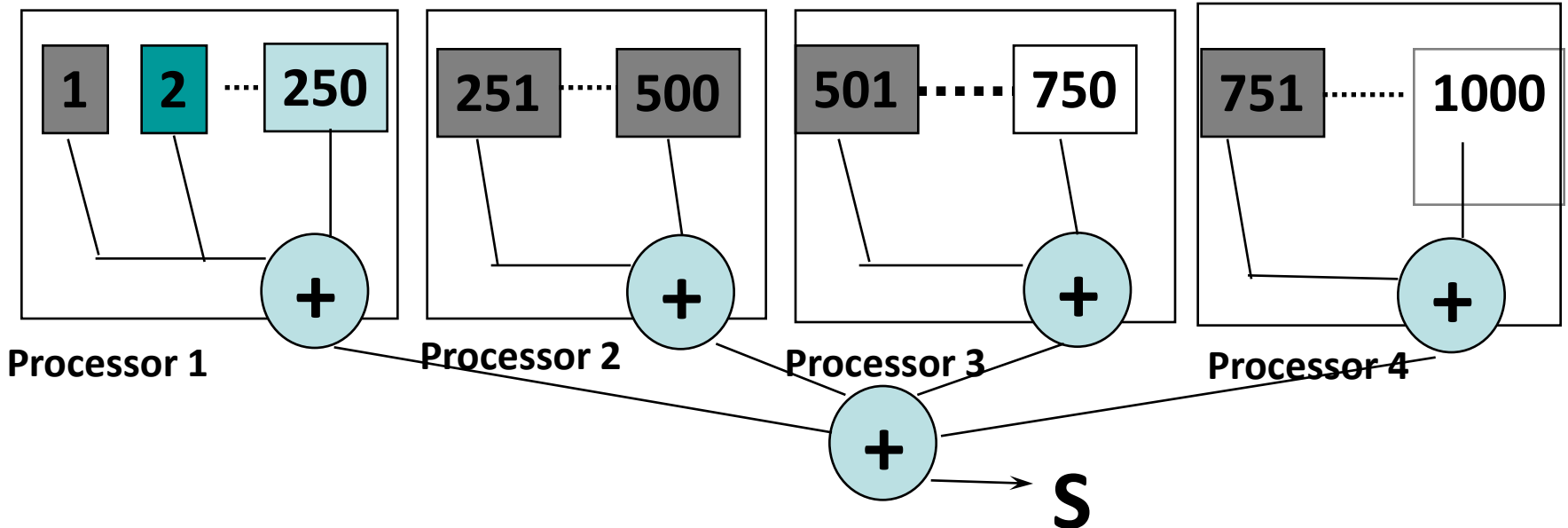
# Sample program (2): summation

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

**Serial computation**



**Parallel computation**



```
#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 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;
```

```
sum = 0.0;
```

```
for (i = myid + 1; i <= n; i += numprocs){
```

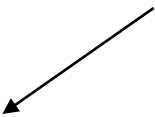
```
    x = h * (i - 0.5);
```

```
    sum += f(x);
```

```
}
```

```
mypi = h * sum;
```

for (i = 1; i <= n; i++)

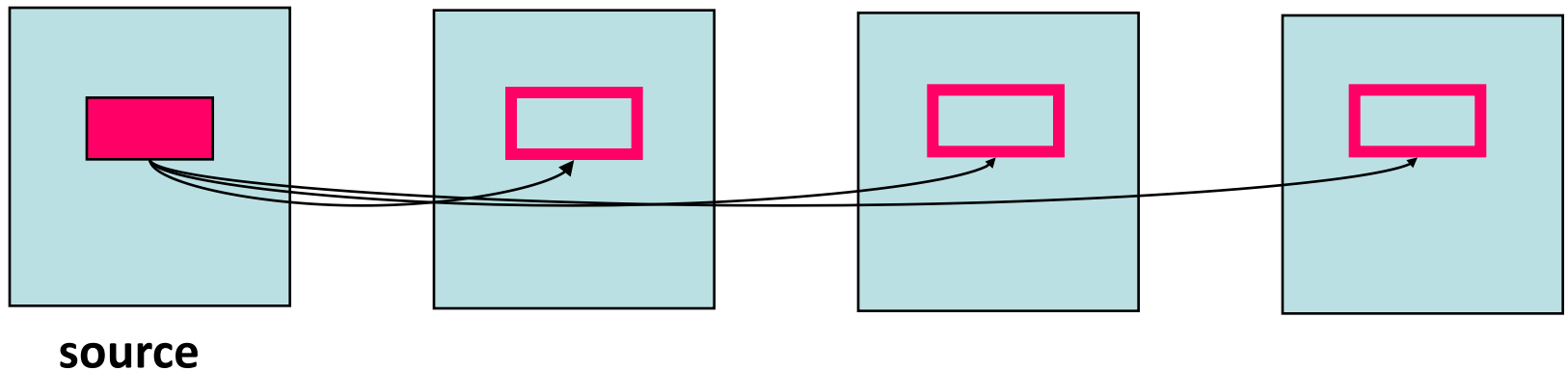


```
MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE,  
            MPI_SUM, 0, MPI_COMM_WORLD);
```



# broadcast

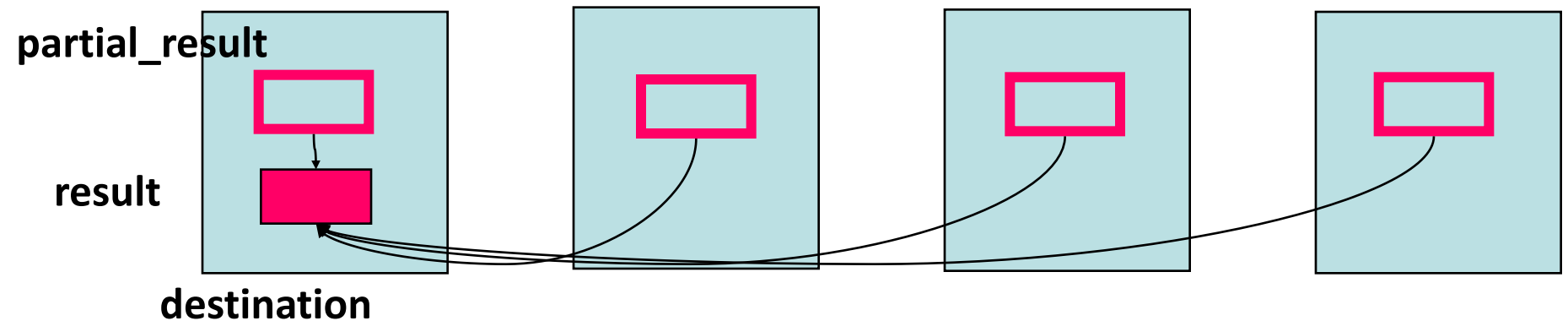
```
MPI_Bcast(  
  void    *data_buffer, // address of source and destination buffer of data  
  int     count,        // data counts  
  MPI_Datatype data_type, // data type  
  int     source,       // source process rank  
  MPI_Comm communicator // communicator  
);
```



It should be executed on all processes in the communicator

# Reduction

```
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**

```
/* 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);
}
```

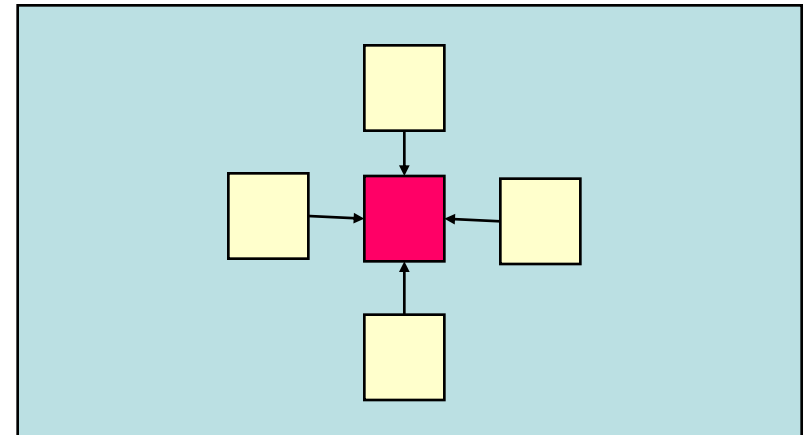
```

/* 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);
}

```

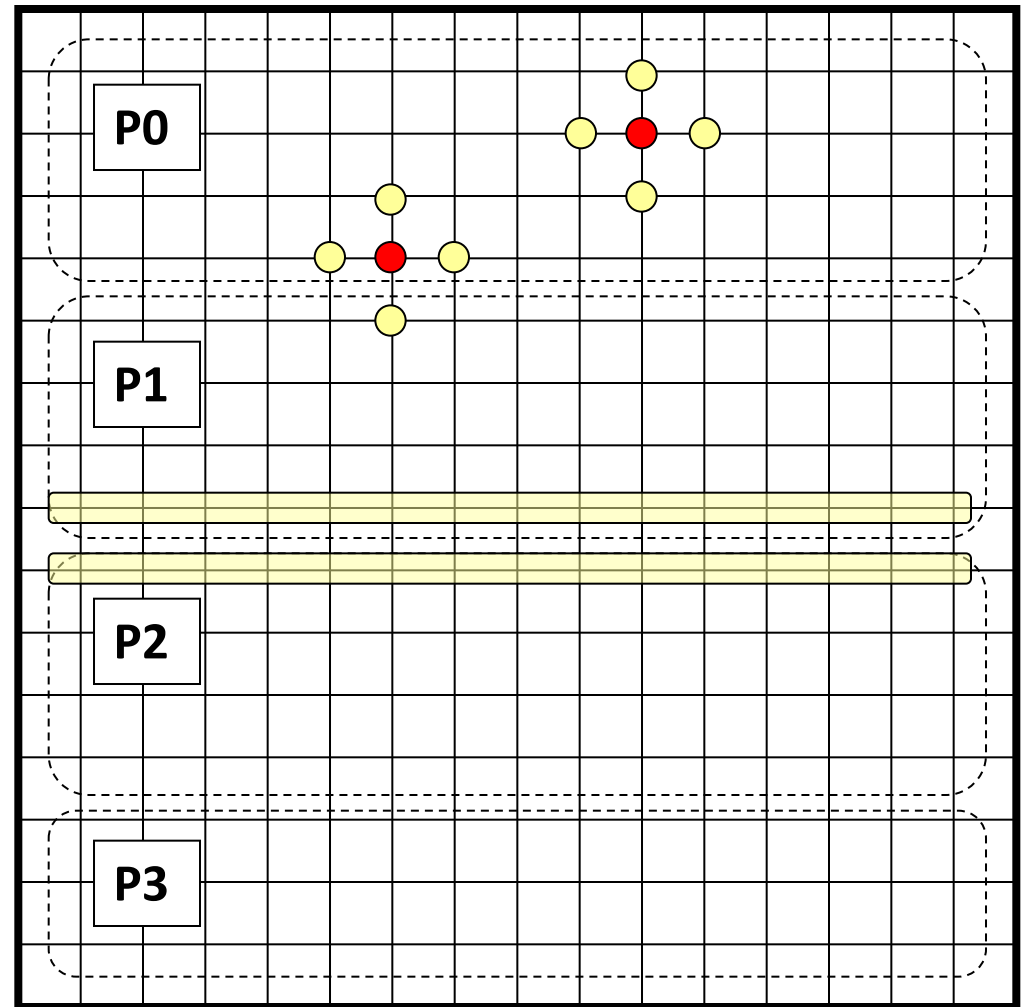
# Sample program (4): laplace

- 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



# Blocking point-to-point communication

- Send/Receive

```
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  
);
```

```
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

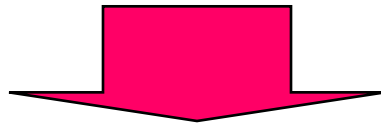
- Message is specified by address and size
  - Typed: MPI\_INT, MPI\_DOUBLE, ...
  - Binary data can be specified by MPI\_BYTE with message size in byte
- Source/destination is specified by process rank and message tag
  - MPI\_ANY\_SOURCE for any source process rank
  - MPI\_ANY\_TAG for any message tag
- Status information includes the source rank, size, tag of the received message

# 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)
```

# 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* specifies 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;
    }
}
```

```
#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 parallelize 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”

# Parallel computing in coins

- `viola0[1-6].coins.tsukuba.ac.jp` (6 node cluster)
  - 8 cores / node
    - 2.93GHz Nehalem x 2 sockets
  - 12GB memory / node
    - 1333MHz 2GB DDR3 x 3 channels x 2
  - Network bandwidth 4GB/s
    - 4x QDR Infiniband
  - Software
    - CentOS5.4
    - OpenMPI\*, MVAPICH1, MVAPICH2
      - System default is OpenMPI
      - It can be selected by `mpi-selector-menu`
    - gcc, gfortran, Sun JDK6
    - BLAS, LAPACK, ScaLAPACK

# Initial setting

- Ssh authentication setting

```
% ssh-keygen -t rsa  
% cat .ssh/id_rsa.pub >> .ssh/authorized_keys
```

- Create known hosts file (also for hostnames of IB interface such as viola01-ib0)

```
% echo StrictHostKeyChecking no >> .ssh/config  
% ssh viola01-ib0 hostname  
viola01.coins.tsukuba.ac.jp  
% ssh viola02-ib0 hostname  
viola02.coins.tsukuba.ac.jp  
...  
% ssh viola06-ib0 hostname  
viola06.coins.tsukuba.ac.jp
```



# Selection of MPI

## \$ mpi-selector-menu

Current system default: openmpi-1.3.2-gcc-x86\_64

Current user default: <none>

"u" and "s" modifiers can be added to numeric and "U" commands to specify "user" or "system-wide".

1. mvapich-1.1.0-gcc-x86\_64
  2. mvapich2-1.2-gcc-x86\_64
  3. openmpi-1.3.2-gcc-i386
  4. openmpi-1.3.2-gcc-x86\_64
- U. Unset default  
Q. Quit

Selection (1-4[us], U[us], Q): **2u**

System default is OpenMPI, no user default specified

Select MVAPICH2

# Compilation

- How to compile an MPI program

```
% mpicc -O2 a.c
```

- If you select MPI, you need to re-compile
  - Not binary compatible among OpenMPI and MVAPICH

# How to execute MPI program in OpenMPI

- Create a host file

```
% cat hosts-openmpi  
viola01-ib0 slots=8  
viola02-ib0 slots=8  
...  
viola06-ib0 slots=8
```

- Execute an MPI program (OpenMPI)

```
% mpirun -hostfile hosts-openmpi -np 48 a.out
```

# How to execute MPI program in MVAPICH

- Create a host file

```
% cat hosts  
viola01-ib0  
viola02-ib0  
...  
viola06-ib0  
% cat hosts hosts hosts hosts hosts hosts hosts hosts >  
hosts-mvapich
```

- Execute an MPI program

```
% mpirun_rsh -hostfile hosts-mvapich -np 48 a.out
```

- Note that the execution command in MVAPICH is `mpirun_rsh`

# Open source implementation

## OpenMP

- GNU GCC 4.2 or later
  - `% cc -fopenmp . . .`
- Omni OpenMP Compiler
  - <http://phase.hpcc.jp/Omni/>

## MPI

- OpenMPI
  - <http://www.openmpi.org/>
- MPICH2
  - <http://www-unix.mcs.anl.gov/mimpi/mpich2/>
- YAMPII
  - <http://www.il.is.s.u-tokyo.ac.jp/yampii/>