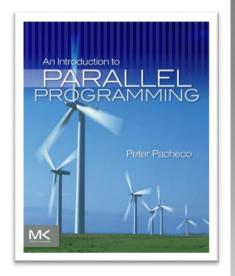
高性能计算程序设计 基础

任课教师: 黄聃 (Huang, Dan)



An Introduction to Parallel Programming Peter Pacheco



Chapter 3

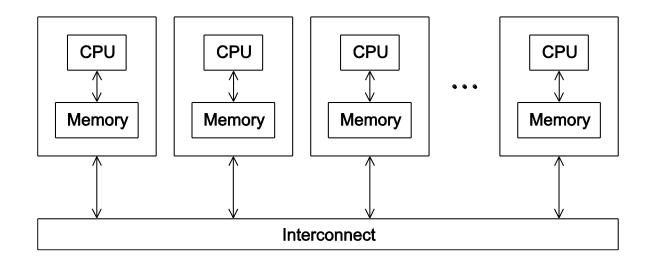
Distributed Memory Programming with MPI



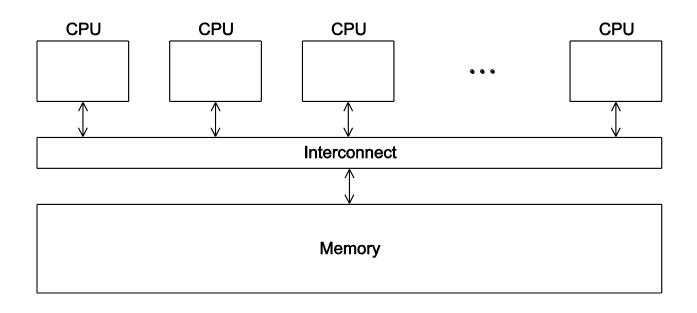
Roadmap

- Writing your first MPI program.
- Using the common MPI functions.
- The Trapezoidal Rule in MPI.
- Collective communication.
- MPI derived datatypes.
- Performance evaluation of MPI programs.
- Parallel sorting.
- Safety in MPI programs.

A distributed memory system



A shared memory system



Hello World!

```
#include <stdio.h>
int main(void) {
   printf("hello, world\n");
   return 0;
}
```



(a classic)

Finding Out About the Environment

- Two important questions that arise early in a parallel program are:
 - How many processes are participating in this computation?
 - Which one am I?
- MPI provides functions to answer these questions:
 - MPI_Comm_size reports the number of processes.
 - MPI_Comm_rank reports the rank, a number between 0 and size-1, identifying the calling process

Identifying MPI processes

 Common practice to identify processes by nonnegative integer ranks.

• p processes are numbered 0, 1, 2, .. p-1

Our first MPI program

```
1 #include < stdio.h>
 2 #include <string.h> /* For strlen
3 #include <mpi.h> /* For MPI functions, etc */
   const int MAX STRING = 100;
   int main(void) {
      char
                 greeting[MAX_STRING];
               comm_sz; /* Number of processes */
      int
             my rank; /* My process rank
      int
11
12
      MPI_Init(NULL, NULL);
      MPI_Comm_size(MPI_COMM_WORLD, &comm_sz);
      MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
14
15
      if (my rank != 0) {
16
         sprintf(greeting, "Greetings from process %d of %d!",
17
18
               my_rank, comm_sz);
         MPI\_Send(greeting, strlen(greeting)+1, MPI\_CHAR, 0, 0,
19
20
               MPI COMM WORLD):
21
      } else {
22
         printf("Greetings from process %d of %d!\n", my_rank, comm_sz);
         for (int q = 1; q < comm_sz; q++) {
            MPI_Recv(greeting, MAX_STRING, MPI_CHAR, q,
24
               0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
26
            printf("%s\n", greeting);
27
28
      MPI_Finalize();
30
31
      return 0:
      /* main */
```



Set MPICH2 Path

- Then add the following at
- the end of your ~/.bashrc file and source it with the command
- source ~/.bashrc (or log in again).
- #-----
- # MPICH2 setup
- export PATH=/opt/MPICH2/bin:\$PATH
- export MANPATH= =/opt/MPICH2/bin :\$MANPATH
- export LD_LIBRARY_PATH=/opt/MPICH2/bin:\$LD_LIBRARY_PATH
- #-----
- Some logging and visulaization help:
- You can Link with the libraries -Ilmpe -Impe to enable logging and the MPE environment. Then run the program as usual and a log file will be produced. The log file can be visualized using the jumpshot program that comes bundled with MPICH2.

Compilation

wrapper script to compile source file mpicc -g -Wall -o mpi_hello mpi_hello.c produce create this executable file name debugging (as opposed to default a.out) information turns on all warnings

Setup Multiple Computer Environment

Create a file called say "machines" containing the list of machines:

athena.cs.siu.edu oscarnode1.cs.siu.edu

.

oscarnode8.cs.siu.edu

Establish network environments

mpdboot -n 9 -f machines

mpdtrace

mpdallexit

Execution

mpiexec -n <number of processes> <executable>

mpiexec -n 4 ./mpi_hello

run with 4 processes

Execution

```
mpiexec -n 1 ./mpi_hello
```

Greetings from process 0 of 1!

```
mpiexec -n 4 ./mpi_hello
```

Greetings from process 0 of 4!

Greetings from process 1 of 4!

Greetings from process 2 of 4!

Greetings from process 3 of 4!

MPI Programs

- Written in C.
 - Has main.
 - Uses stdio.h, string.h, etc.
- Need to add mpi.h header file.
- Identifiers defined by MPI start with "MPI_".
- First letter following underscore is uppercase.
 - For function names and MPI-defined types.
 - Helps to avoid confusion.

MPI Components

- MPI_Init
 - Tells MPI to do all the necessary setup.

- MPI_Finalize
 - Tells MPI we're done, so clean up anything allocated for this program.

```
int MPI_Finalize(void);
```

Basic Outline

```
#include <mpi.h>
int main(int argc, char* argv[]) {
   /* No MPI calls before this */
   MPI_Init(&argc, &argv);
   MPI_Finalize();
   /* No MPI calls after this */
   . . .
   return 0;
```

Communicators

- A collection of processes that can send messages to each other.
- MPI_Init defines a communicator that consists of all the processes created when the program is started.

Called MPI COMM WORLD.

Communicators



```
int MPI_Comm_size(
     MPI_Comm comm /* in */,
     int* comm_sz_p /* out */);

number of processes in the communicator
```

```
#include "mpi.h"
#include <stdio.h>
#include <math.h>
#define MAXSIZE 1000
void main(int argc, char *argv)
     int myid, numprocs;
      int data[MAXSIZE], i, x, low, high, myresult, result;
     char fn[255];
     char *fp;
      MPI_Init(&argc, &argv);
      MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
      MPI_Comm_rank(MPI_COMM_WORLD,&myid);
      if (myid == 0) { /* Open input file and initialize data */
               strcpy(fn,getenv("HOME"));
               strcat(fn,"/MPI/rand data.txt");
               if ((fp = fopen(fn,"r")) == NULL) {
                               printf("Can't open the input file: %s\n\n", fn);
                               exit(1);
               for(i = 0; i < MAXSIZE; i++) fscanf(fp,"%d", &data[i]);
      MPI_Bcast(data, MAXSIZE, MPI_INT, 0, MPI_COMM_WORLD); /* broadcast data */
     x = n/nproc; /* Add my portion Of data */
     low = myid * x;
     high = low + x;
      for(i = low; i < high; i++)
               myresult += data[i];
      printf("I got %d from %d\n", myresult, myid); /* Compute global sum */
      MPI_Reduce(&myresult, &result, 1, MPI_INT, MPI_SUM, 0, MPI_COMM_WORLD);
     if (myid == 0) printf("The sum is %d.\n", result);
     MPI Finalize();
```

Sample MPI program

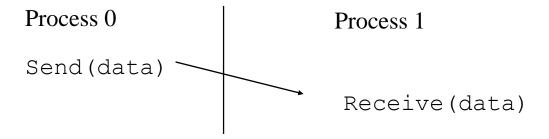
SPMD

- Single-Program Multiple-Data
- We compile <u>one</u> program.
- Process 0 does something different.
 - Receives messages and prints them while the other processes do the work.

The if-else construct makes our program SPMD.

MPI Basic Send/Receive

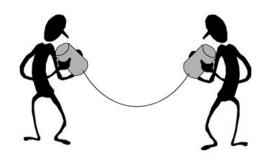
We need to fill in the details in



- Things that need specifying:
 - How will "data" be described?
 - How will processes be identified?
 - How will the receiver recognize/screen messages?
 - What will it mean for these operations to complete?

Communication

```
int MPI_Send(
```



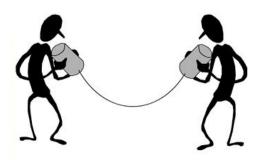
MPI Datatypes

- The data in a message to send or receive is described by a triple (address, count, datatype), where
- An MPI datatype is recursively defined as:
 - predefined, corresponding to a data type from the language (e.g., MPI_INT, MPI_DOUBLE)
 - a contiguous array of MPI datatypes
 - a strided block of datatypes
 - an indexed array of blocks of datatypes
 - an arbitrary structure of datatypes
- There are MPI functions to construct custom datatypes, in particular ones for subarrays
- May hurt performance if datatypes are complex

Data types

MPI datatype	C datatype
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_LONG_LONG	signed long long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	
MPI_PACKED	

Communication



MPI Tags

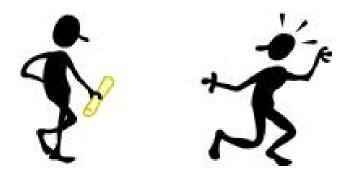
- Messages are sent with an accompanying user-defined integer tag, to assist the receiving process in identifying the message
- Messages can be screened at the receiving end by specifying a specific tag, or not screened by specifying MPI_ANY_TAG as the tag in a receive
- Some non-MPI message-passing systems have called tags "message types". MPI calls them tags to avoid confusion with datatypes

Message matching

```
MPI_Send(send_buf_p, send_buf_sz, send_type, dest, send_tag,
        send_comm);
                              Count of data
                MPI_Send
                src = q
MPI_Recv(recv_buf_p, recv_buf_sz, recv_type, src, recv_tag
         recv_comm, &status);
```

Receiving messages

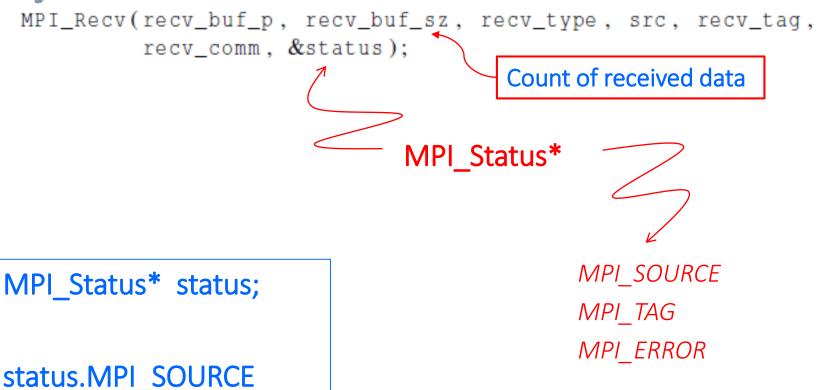
- A receiver can get a message without knowing:
 - the amount of data in the message,
 - the sender of the message, (MPI_ANY_SOURCE)
 - or the tag of the message. (MPI_ANY_TAG)



status_p argument

status.MPI TAG

How receiver finds out the sender, tag if they are not needed by the receiver

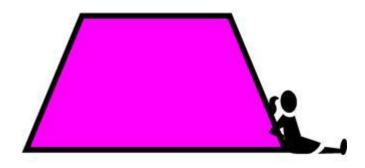


How much data am I receiving?



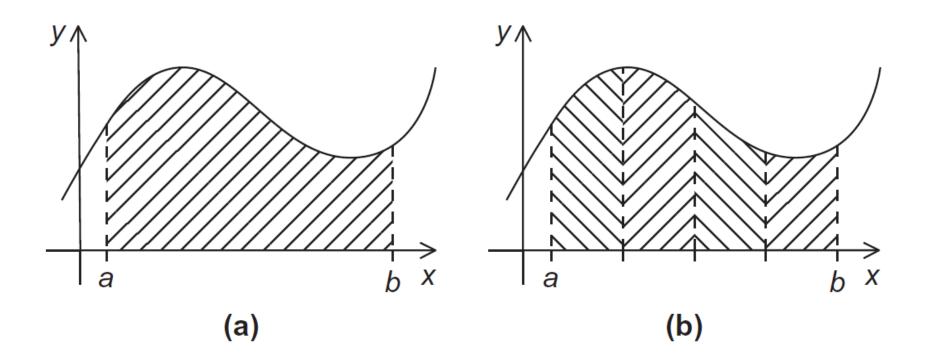
Issues with send and receive

- Exact behavior is determined by the MPI implementation.
- MPI_Send (locally blocking with buffer copied to internal storage or block starts transmission) may behave differently with regard to buffer size, cutoffs and blocking.
- MPI_Recv always blocks until a matching message is received.
- Non-blocking MPI_Isend and MPI_Irecv, immediate return.
- Know your implementation; don't make assumptions!



Trapezoidal rule in mpi 基于MPI的梯形积分法

The Trapezoidal Rule



The Trapezoidal Rule(梯形积分法)

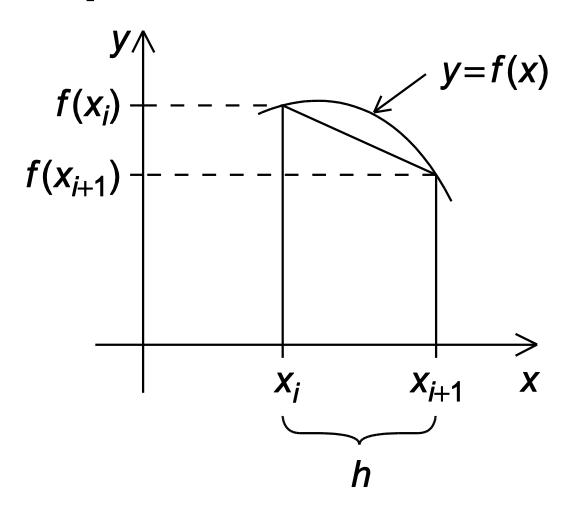
Area of one trapezoid
$$=\frac{h}{2}[f(x_i)+f(x_{i+1})]$$

$$h = \frac{b-a}{n}$$

$$x_0 = a$$
, $x_1 = a + h$, $x_2 = a + 2h$, ..., $x_{n-1} = a + (n-1)h$, $x_n = b$

Sum of trapezoid areas = $h[f(x_0)/2 + f(x_1) + f(x_2) + \dots + f(x_{n-1}) + f(x_n)/2]$

One trapezoid



Pseudo-code for a serial program

```
/* Input: a, b, n */
h = (b-a)/n;
approx = (f(a) + f(b))/2.0;
for (i = 0; i \le n-1; i++)
   x i = a + i*h;
   approx += f(x i);
approx = h*approx;
```

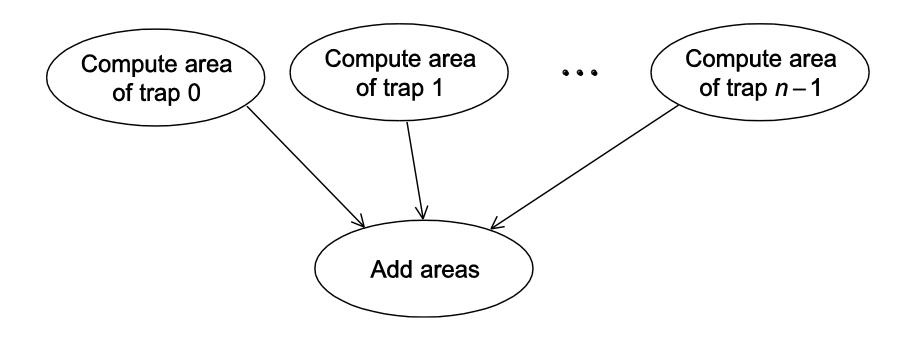
Parallelizing the Trapezoidal Rule

- 1. Partition problem solution into tasks.
- 2. Identify communication channels between tasks.
- 3. Aggregate tasks into **composite tasks**.
- 4. Map composite tasks to cores.

Parallel pseudo-code

```
Get a, b, n;
      h = (b-a)/n;
      local_n = n/comm_sz;
4
      local_a = a + my_rank*local_n*h;
5
      local_b = local_a + local_n*h;
6
      local_integral = Trap(local_a, local_b, local_n, h);
      if (my rank != 0)
8
         Send local integral to process 0;
9
      else /* my_rank == 0 */
10
         total integral = local integral;
11
         for (proc = 1; proc < comm sz; proc++) {
12
            Receive local integral from proc;
13
            total_integral += local_integral;
14
15
16
      if (my_rank == 0)
17
         print result;
```

Tasks and communications for Trapezoidal Rule



First version (1) 程序3-2

```
int main(void) {
      int my_rank, comm_sz, n = 1024, local_n;
      double a = 0.0, b = 3.0, h, local_a, local_b;
      double local int, total int;
5
      int source:
6
      MPI Init(NULL, NULL);
      MPI Comm rank (MPI COMM WORLD, &my rank);
9
      MPI Comm size (MPI COMM WORLD, &comm sz);
10
      h = (b-a)/n; /* h is the same for all processes */
11
      local_n = n/comm_sz; /* So is the number of trapezoids */
12
13
14
      local a = a + my rank*local n*h;
15
      local b = local a + local n*h;
16
      local int = Trap(local a, local b, local n, h);
17
18
      if (my rank != 0) {
         MPI Send(&local int, 1, MPI DOUBLE, 0, 0,
19
20
               MPI COMM WORLD);
```

First version (2)

```
21
      } else {
22
         total int = local int;
23
         for (source = 1; source < comm_sz; source++) {</pre>
24
             MPI Recv(&local int, 1, MPI DOUBLE, source, 0,
25
                   MPI_COMM_WORLD , MPI_STATUS_IGNORE );
26
             total int += local int;
27
28
29
30
      if (mv rank == 0) {
31
         printf("With n = %d trapezoids, our estimate\n", n);
32
         printf("of the integral from %f to %f = %.15e\n",
33
              a, b, total int);
34
35
      MPI Finalize();
36
      return 0:
37
        main */
```

First version (3)

```
double Trap(
         double left endpt /* in */,
         double right_endpt /* in */,
         int trap_count /* in */,
         double base_len /* in */) {
6
      double estimate, x;
      int i:
8
9
      estimate = (f(left\_endpt) + f(right\_endpt))/2.0;
      for (i = 1; i \le trap_count - 1; i++)
10
11
         x = left endpt + i*base len;
12
        estimate += f(x);
13
14
      estimate = estimate * base len;
15
16
      return estimate:
17
    /* Trap */
```

Dealing with I/O

```
#include < stdio.h>
#include <mpi.h>
                                  Each process just
int main(void) {
                                  prints a message.
   int my_rank, comm_sz;
   MPI_Init(NULL, NULL);
   MPI_Comm_size(MPI_COMM_WORLD, &comm_sz);
   MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
   printf("Proc %d of %d > Does anyone have a toothpick?\n",
         my rank, comm sz);
   MPI Finalize();
   return 0;
   /* main */
```

Running with 6 processes

```
Proc 0 of 6 > Does anyone have a toothpick?

Proc 1 of 6 > Does anyone have a toothpick?

Proc 2 of 6 > Does anyone have a toothpick?

Proc 4 of 6 > Does anyone have a toothpick?

Proc 3 of 6 > Does anyone have a toothpick?

Proc 5 of 6 > Does anyone have a toothpick?
```

unpredictable output

Input

- Most MPI implementations only allow process 0 in MPI_COMM_WORLD access to stdin.
- Process 0 must read the data (scanf) and send to the other processes.

```
MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
MPI_Comm_size(MPI_COMM_WORLD, &comm_sz);
Get_data(my_rank, comm_sz, &a, &b, &n);
h = (b-a)/n;
. . .
```

Function for reading user input

```
void Get input(
     int my_rank /* in */,
     int comm_sz /*in */,
     double* a_p /* out */,
     double* b p /* out */,
     int* np /* out */) {
  int dest;
   if (my_rank == 0) {
     printf("Enter a, b, and n\n");
     scanf("%lf %lf %d", a_p, b_p, n_p);
     for (dest = 1; dest < comm sz; dest++)
        MPI_Send(a_p, 1, MPI_DOUBLE, dest, 0, MPI_COMM_WORLD);
        MPI Send(b p, 1, MPI DOUBLE, dest, 0, MPI COMM WORLD);
        MPI Send(n p, 1, MPI INT, dest, 0, MPI COMM WORLD);
  else { /* my\_rank != 0 */}
     MPI_Recv(a_p, 1, MPI_DOUBLE, 0, 0, MPI_COMM_WORLD,
           MPI STATUS IGNORE);
     MPI_Recv(b_p, 1, MPI_DOUBLE, 0, 0, MPI_COMM_WORLD,
           MPI STATUS IGNORE);
     MPI_Recv(n_p, 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
           MPI STATUS IGNORE);
  /* Get_input */
```

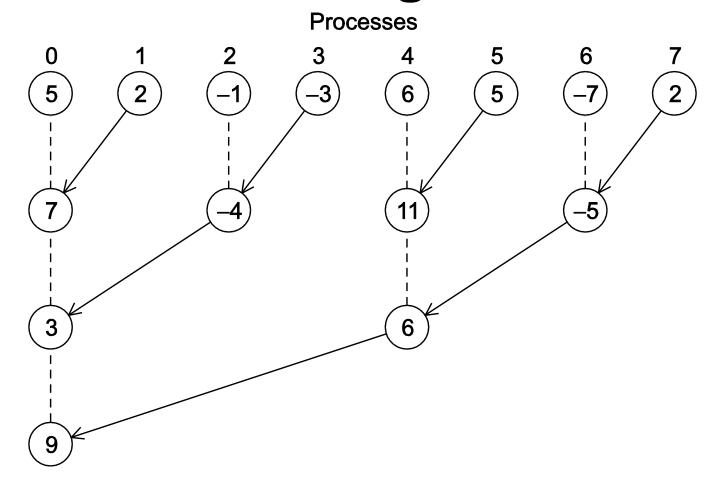
Collective communication

Tree-structured communication

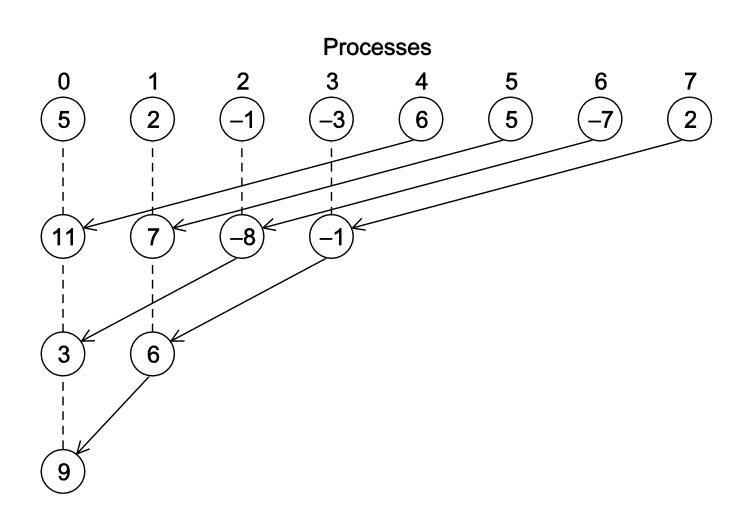
- In the first phase:
 - (a) Process 1 sends to 0, 3 sends to 2, 5 sends to 4, and 7 sends to 6.
 - (b) Processes 0, 2, 4, and 6 add in the received values.
 - (c) Processes 2 and 6 send their new values to processes 0 and 4, respectively.
 - (d) Processes 0 and 4 add the received values into their new values.

- 2. (a) Process 4 sends its newest value to process 0.
 - (b) Process 0 adds the received value to its newest value.

A tree-structured global sum



An alternative tree-structured global sum



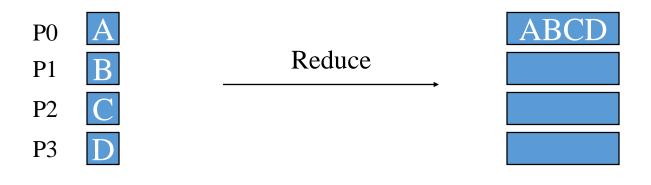
MPI_Reduce

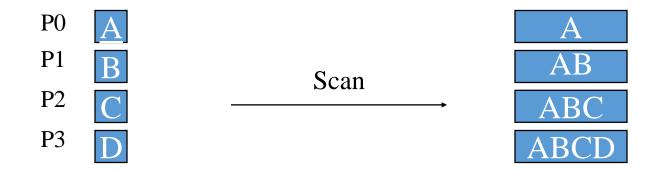
```
\label{eq:mpi_reduce} \begin{split} \texttt{MPI\_Reduce}(\&\texttt{local\_int}\,,\,\,\&\texttt{total\_int}\,,\,\,1\,,\,\,\texttt{MPI\_DOUBLE}\,,\,\,\texttt{MPI\_SUM}\,,\,\,0\,,\\ \texttt{MPI\_COMM\_WORLD}\,); \end{split}
```

Predefined reduction operators in MPI

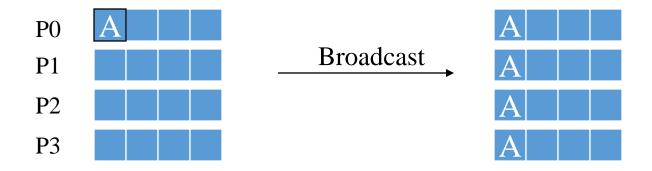
Operation Value	Meaning
MPI_MAX	Maximum
MPI_MIN	Minimum
MPI_SUM	Sum
MPI_PROD	Product
MPI_LAND	Logical and
MPI_BAND	Bitwise and
MPI_LOR	Logical or
MPI_BOR	Bitwise or
MPI_LXOR	Logical exclusive or
MPI_BXOR	Bitwise exclusive or
MPI_MAXLOC	Maximum and location of maximum
MPI_MINLOC	Minimum and location of minimum

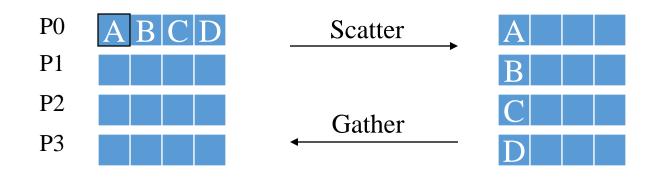
Collective Data Movement





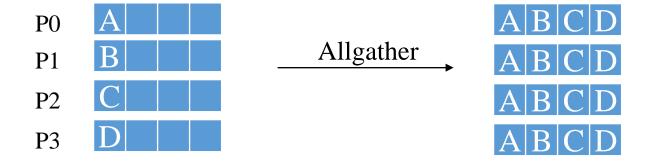
Collective Data Movement





Alltoall

Collective Data Movement





- <u>All</u> the processes in the communicator must call the same collective function.
 - For example, a program that attempts to match a call to MPI_Reduce on one process with a call to MPI_Recv on another process is erroneous, and, in all likelihood, the program will hang or crash.

- The arguments passed by each process to an MPI collective communication must be "compatible."
 - For example, if one process passes in 0 as the dest_process and another passes in 1, then the outcome of a call to MPI_Reduce is erroneous, and, once again, the program is likely to hang or crash.

 The output_data_p argument is only used on dest_process.

 However, all of the processes still need to pass in an actual argument corresponding to output_data_p, even if it's just NULL.

 Point-to-point communications are matched on the basis of tags and communicators.

- Collective communications don't use tags.
- They're matched solely on the basis of the communicator and the order in which they're called (调用顺序).

Example (1)

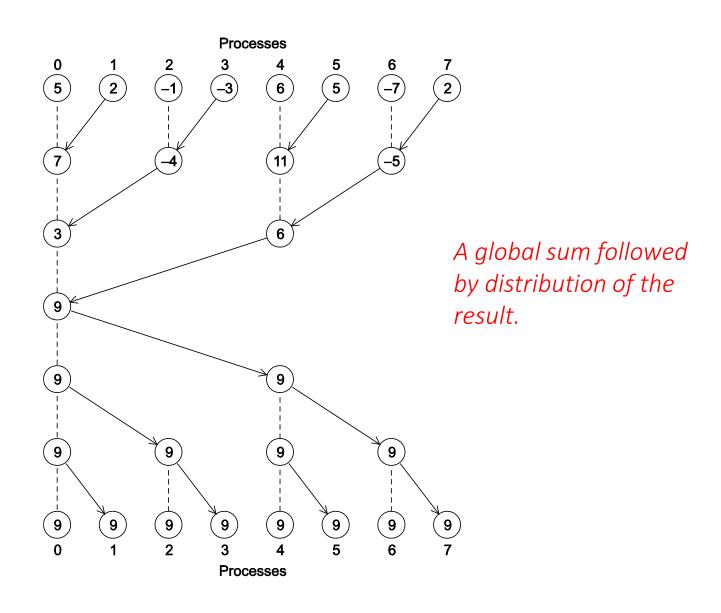
Time	Process 0			Process 1	Process 2			
0	a = 1; c = 2			a = 1; c = 2	a = 1; c = 2			
1	MPI_Reduce(&a,	&b,)	MPI_Reduce(&c, &d,)	MPI_Reduce(&a, &b,)			
2	MPI_Reduce(&c,	&d,)	MPI_Reduce(&a, &b,)	MPI_Reduce(&c, &d,)			

$$b = 4$$
, $d = 5$

Multiple calls to MPI_Reduce,
Suppose that each process calls
MPI_Reduce with operator MPI_SUM,
and destination process 0.

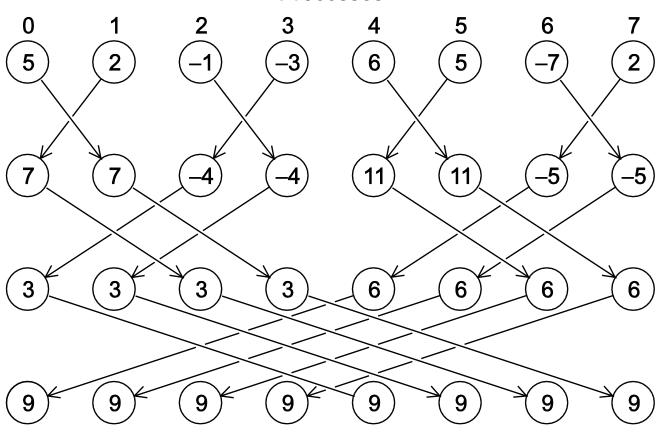
MPI_Allreduce

 Useful in a situation in which all of the processes need the result of a global sum in order to complete some larger computation.





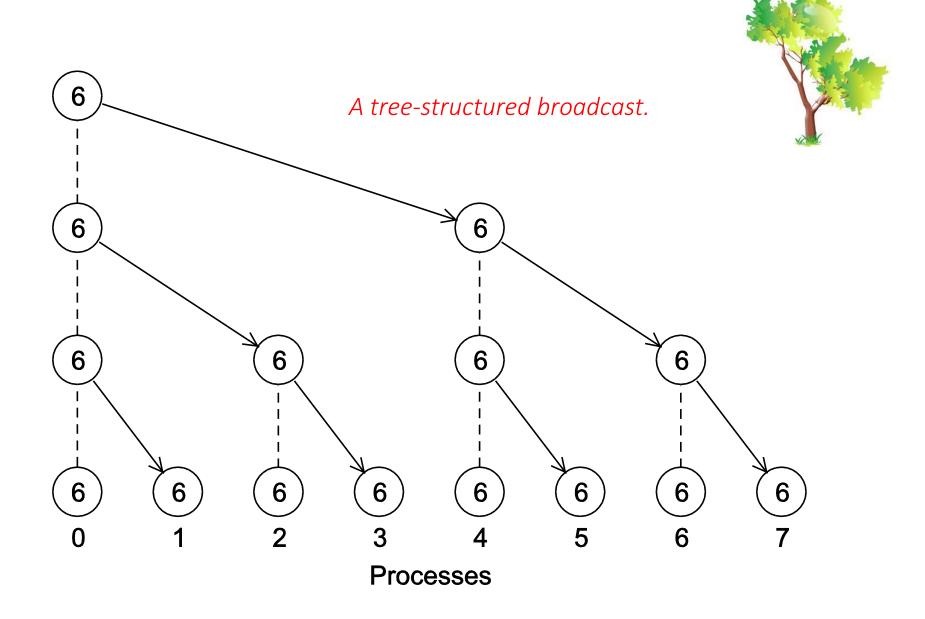
Processes



A butterfly-structured global sum.

Broadcast

 Data belonging to a single process is sent to all of the processes in the communicator.



A version of Get_input that uses MPI Bcast

```
void Get input(
     int my_rank /* in */,
     int comm_sz /* in */,
     double * a_p /* out */,
     double* b_p /* out */,
     int * n_p /* out */) {
  if (my_rank == 0) {
     printf("Enter a, b, and n\n");
     scanf("%lf %lf %d", a_p, b_p, n_p);
  MPI_Bcast(a_p, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
  MPI_Bcast(b_p, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
  MPI_Bcast(n_p, 1, MPI_INT, 0, MPI_COMM_WORLD);
 /* Get_input */
```

Data distributions

$$\mathbf{x} + \mathbf{y} = (x_0, x_1, \dots, x_{n-1}) + (y_0, y_1, \dots, y_{n-1})$$

$$= (x_0 + y_0, x_1 + y_1, \dots, x_{n-1} + y_{n-1})$$

$$= (z_0, z_1, \dots, z_{n-1})$$

$$= \mathbf{z}$$

Compute a vector sum.

Serial implementation of vector addition

```
void Vector_sum(double x[], double y[], double z[], int n) {
  int i;

for (i = 0; i < n; i++)
    z[i] = x[i] + y[i];
} /* Vector_sum */</pre>
```

Different partitions of a 12component vector among 3 processes

	Components											
								Block-cyclic				
Process	Block				Cyclic				Blocksize = 2			
0	0	1	2	3	0	3	6	9	0	1	6	7
1	4	5	6	7	1	4	7	10	2	3	8	9
2	8	9	10	11	2	5	8	11	4	5	10	11

Partitioning options

- Block partitioning
 - Assign blocks of consecutive components to each process.
- Cyclic partitioning
 - Assign components in a round robin fashion.
- Block-cyclic partitioning
 - Use a cyclic distribution of blocks of components.

Parallel implementation of vector addition

Scatter

 MPI_Scatter can be used in a function that reads in an entire vector on process 0 but only sends the needed components to each of the other processes.

Reading and distributing a vector

```
void Read_vector(
     double local a[] /* out */,
              local n /*in */,
     int
     int
              n /* in */,
     char vec name [] /* in */,
     int my rank /*in */,
     MPI Comm comm /*in */) {
  double* a = NULL;
  int i;
  if (my rank == 0) {
     a = malloc(n*sizeof(double));
     printf("Enter the vector %s\n", vec_name);
     for (i = 0; i < n; i++)
        scanf("%lf", &a[i]);
     MPI_Scatter(a, local_n, MPI_DOUBLE, local_a, local_n, MPI_DOUBLE,
           0. \text{comm});
     free(a);
  } else {
     MPI Scatter(a, local n, MPI DOUBLE, local a, local n, MPI DOUBLE,
           0, comm);
  /* Read vector */
```

Gather

 Collect all of the components of the vector onto process 0, and then process 0 can process all of the components.

Print a distributed vector (1)

```
void Print_vector(
    double local_b[] /* in */,
    int local n /*in */,
    int
              /* in */,
    char title[] /* in */,
    int
       my_rank /* in */,
    MPI Comm comm /*in */) {
  double* b = NULL;
  int i;
```

Print a distributed vector (2)

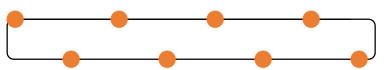
```
if (my_rank == 0) 
  b = malloc(n*sizeof(double));
  MPI_Gather(local_b, local_n, MPI_DOUBLE, b, local_n, MPI_DOUBLE,
         0, comm);
  printf("%s\n", title);
   for (i = 0; i < n; i++)
      printf("%f ", b[i]);
  printf("\n");
  free(b);
} else {
  MPI_Gather(local_b, local_n, MPI_DOUBLE, b, local_n, MPI_DOUBLE,
         0. \text{comm});
/* Print_vector */
```

Allgather

- Concatenates the contents of each process' send_buf_p and stores this in each process' recv_buf_p.
- As usual, recv_count is the amount of data being received from each process.

AllGather

Ring Algorithm



 $T_{ring} = \alpha (p-1) + \beta n (p-1)/p$

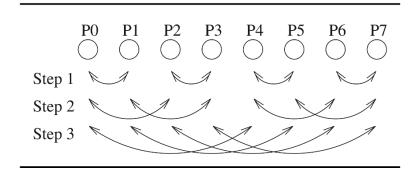
α: latency

β: time to transmit a byte

n: number of bytes of all processes

p: number of processes

Recursive Doubling Algorithm



$$T_{rec-dbl} = \alpha \lg(p) + \beta n (p-1)/p$$

- At time t: send the data you received at time t-1 to your right, and receive new data from your left.
- At time 0, send your original data
- Optimal bandwidth, high latency

- At time t: process i exchanges
 (send/recv) all your current data (its
 original data plus anything received so
 far) with process i±2^t
- Data exchanged at each step: n/p,
 2n/p, 4n/p,..., 2^{|g(p)-1} n/p
- Tricky for non-power-of-two

AllGather Performance

 Similar ideas are used in other collectives (e.g. recursive halving instead of recursive doubling for reduce-scatter) with different local computations (e.g. for allreduce, perform a local reduction at each step instead of concatenating data as in allgather)

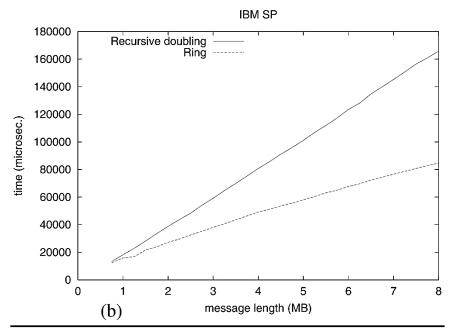


Fig. 5 Ring algorithm versus recursive doubling for long-message allgather (64 nodes). The size on the x-axis is the total amount of data gathered on each process.

Thakur, Rajeev, Rolf Rabenseifner, and William Gropp. "Optimization of collective communication operations in MPICH." *The International Journal of High Performance Computing Applications* 19.1 (2005): 49-66



MPI Derived Datatype

Derived datatypes

- Used to represent any collection of data items in memory by storing both the types of the items and their relative locations in memory.
- The idea is that if a function that sends data knows this information about a collection of data items, it can collect the items from memory before they are sent.
- Similarly, a function that receives data can distribute the items into their correct destinations in memory when they're received.

Derived datatypes

- Formally, consists of a sequence of basic MPI data types together with a displacement for each of the data types.
- Trapezoidal Rule example:

Variable	Address		
a	24		
b	40		
n	48		

 $\{(MPI_DOUBLE, 0), (MPI_DOUBLE, 16), (MPI_INT, 24)\}$

MPI_Type create_struct

 Builds a derived datatype that consists of individual elements that have different basic types.

MPI_Get_address

- Returns the address of the memory location referenced by location_p.
- The special type MPI_Aint is an integer type that is big enough to store an address on the system.

```
int MPI_Get_address(
    void* location_p /* in */,
    MPI_Aint* address_p /* out */);
```

MPI_Type_commit

 Allows the MPI implementation to optimize its internal representation of the datatype for use in communication functions.

```
int MPI_Type_commit(MPI_Datatype* new_mpi_t_p /* in/out */);
```

MPI_Type_free

• When we're finished with our new type, this frees any additional storage used.

```
int MPI_Type_free(MPI_Datatype* old_mpi_t_p /* in/out */);
```

Get input function with a derived datatype (1)

Get input function with a derived datatype (2)

Get input function with a derived datatype (3)

```
void Get_input(int my_rank, int comm_sz, double* a_p, double* b_p,
      int* n_p) {
   MPI Datatype input mpi t;
                                                             Address
                                                    Variable
                                                                24
   Build_mpi_type(a_p, b_p, n_p, &input_mpi_t);
                                                       а
                                                                40
                                                       b
   if (my rank == 0) 
                                                                48
                                                       n
      printf("Enter a, b, and n\n");
      scanf("%lf %lf %d", a_p, b_p, n_p);
                                                              MPI Bcast
   MPI_Bcast(a_p, 1, input_mpi_t, 0, MPI_COMM_WORLD);
                                                                 OS
                                                            b
                                                                 buffer
  MPI Type free(&input mpi t);
  /* Get_input */
                                                      Network interface
```

Difference with C Struct

```
struct range integral t {
                                                               struct range integral t* range p
                                                    a
         double a;
                                                   b
         double b;
                              new or malloc
         int n;
       };
 int main () {
                                                                                  int main () {
   double a;
                  a
                                                       a
                                                                                    double a;
                                   a
                                                       b
                                   b
   double b;
                                                                                    double b;
  int n;
                                                                                    int n;
                                Buffer
                                                     Buffer
 };
                                                                                  };
MPI_Type_create_struct
                                                                      MPI Type create struct
       Send by Proc 0
                                                                               Recv by Proc 1
```

- MPI_Type_contiguous (int count, MPI_Datatype datatype, MPI_Datatype *newtype);
 - count elements of the same datatype forming a contiguous chunk in the memory
- Input datatype can be a derived datatype
 - End of one element of the derived datatype has to be exactly at the beginning of the next element of the derived datatype

```
int myvec[4];
MPI_Type_contiguous ( 4, MPI_INT, &mybrandnewdatatype);
MPI_Type_commit ( &mybrandnewdatatype );
MPI Send ( myvec, 1, mybrandnewdatatype, ... );
```

- MPI_Type_vector(int count, int blocklength, int stride, MPI_Datatype datatype, MPI_Datatype *newtype);
 - count blocks of blocklength elements of the same datatype
 - Between the start of each block there are stride elements of the same datatype

- MPI_Type_indexed(int count, int blocklengths[], int displacements[], MPI_Datatype datatype, MPI_Datatype
 *newtype);
 - The number of elements per block do not have to be identical
 - *displacements* gives the distance from the 'base' to the beginning of the block in multiples of the used datatype

```
count = 3
blocklengths[0] = 2 displacements[0] = 0
blocklengths[1] = 1 displacements[1] = 3
blocklengths[2] = 4 displacements[2] = 5
```

- MPI_Type_create_subarray (int ndims, int sizes[], int subsizes[], int starts[], int order, MPI_Datatype datatype,MPI_Datatype *newtype);
 - Define sub-matrices of n-dimensional data
 - sizes[]: dimension of the entire matrix
 - subsizes[]: dimensions of the submatrix described by the derived data type
 - starts[]: array describing the beginning of the submatrices
 - Order: MPI_ORDER_C for row-major order or MPI_ORDER_FORTRAN for column-major data

Example

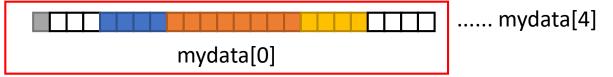
_								
	1	2	3	4	5	6	7	8
	9	10	11	12	13	14	15	16
	17	18	19	20	21	22	23	24
	25	26	27	28	29	30	31	32
	33	34	35	36	37	38	39	40
	41	42	43	44	45	46	47	48
	49	50	51	52	53	54	55	56
	57	58	59	60	61	62	63	64
ı								

Dimension 1

Dimension 0

Problem of derived datatype

```
typedef struct {
   char a;
   int b;
   double c;
   float d;
} mystruct;
mystruct mydata[5];
```



• If we just want to send elements **b** and **c** of the structure?

Problem of derived datatype

```
MPI Get address (&(mydata[0], &baseaddr);
MPI_Get_address ( &(mydata[0].b, &addr1);
MPI_Get_address ( &(mydata[0].c, &addr2);
displ(0) = addr1 - baseaddr;
displ[1] = addr2 - baseaddr;
dtype[0] = MPI INT; blength[0] = 1;
dtype[1] = MPI DOUBLE; blength[1] = 1;
MPI_Type_create_struct (2,blength,displ,dtype,&newtype);
MPI Type commit (&newtype);
MPI Send (mydata, 1, newtype,...); //it is ok if we send one struct instance.
MPI_Send (mydata, 5, newtype, ...) //If send more instances, received data will be wrong
    Memory layout
    What we send is
                                                          ..... mydata[4]

    What we wanted to send is
```

Problem of derived datatype

- Solution to the problem
- MPI_Type_create_resized (MPI_Datatype datatype, MPI_Aint lb, MPI_Aint extent, MPI_Datatype *newtype);
 - Reset the low-bound and up-bound marker of a derived datatype



Performance evaluation

Elapsed parallel time

 Returns the number of seconds that have elapsed since some time in the past.

Average/least/most execution time spent by individual process

```
int myrank, numprocs;
double mytime, maxtime, mintime, avgtime; /*variables used for gathering timing statistics*/
MPI Comm rank(MPI COMM WORLD, &myrank); MPI Comm size(MPI COMM WORLD, &numprocs);
MPI Barrier(MPI COMM WORLD); /*synchronize all processes*/
mytime = MPI Wtime(); /*get time just before work section */
work();
mytime = MPI Wtime() - mytime; /*get time just after work section*/ /*compute max, min, and average timing
statistics*/
MPI Reduce(&mytime, &maxtime, 1, MPI DOUBLE, MPI MAX, 0, MPI COMM WORLD);
MPI_Reduce(&mytime, &mintime, 1, MPI_DOUBLE, MPI_MIN, 0,MPI_COMM_WORLD);
MPI_Reduce(&mytime, &avgtime, 1, MPI_DOUBLE, MPI_SUM, 0,MPI_COMM_WORLD);
if (myrank == 0) {
           avgtime /= numprocs;
           printf("Min: %lf Max: %lf Avg: %lf\n", mintime, maxtime, avgtime);
```

Elapsed serial time

- In this case, you don't need to link in the MPI libraries.
- Returns time in microseconds elapsed from some point in the past.

```
#include "timer.h"
. . .
double now;
. . .
GET_TIME(now);
```



Elapsed serial time

```
#include "timer.h"
. . .
double start, finish;
. . .
GET_TIME(start);
/* Code to be timed */
. . .
GET_TIME(finish);
printf("Elapsed time = %e seconds\n", finish-start);
```

MPI_Barrier

- Ensures that no process will return from calling it until every process in the communicator has started calling it.
- Blocks until all processes in the group of the communicator comm call it.



MPI_Barrier

```
double local_start, local_finish, local_elapsed, elapsed;
. . .
MPI Barrier(comm);
local start = MPI Wtime();
/* Code to be timed */
. . .
local finish = MPI Wtime();
local_elapsed = local_finish - local_start;
MPI Reduce(&local elapsed, &elapsed, 1, MPI DOUBLE,
  MPI MAX, 0, comm);
if (my rank == 0)
  printf("Elapsed time = %e seconds\n", elapsed);
```

Run-times of serial and parallel matrix-vector multiplication

	Order of Matrix							
comm_sz	1024	2048	4096	8192	16,384			
1	4.1	16.0	64.0	270	1100			
2	2.3	8.5	33.0	140	560			
4	2.0	5.1	18.0	70	280			
8	1.7	3.3	9.8	36	140			
16	1.7	2.6	5.9	19	71			

(Seconds)

Speedup

$$S(n, p) = \frac{T_{\text{serial}}(n)}{T_{\text{parallel}}(n, p)}$$

Efficiency

$$E(n,p) = \frac{S(n,p)}{p} = \frac{T_{\text{serial}}(n)}{p \times T_{\text{parallel}}(n,p)}$$

Speedups of Parallel Matrix-Vector Multiplication

	Order of Matrix					
comm_sz	1024	2048	4096	8192	16,384	
1	1.0	1.0	1.0	1.0	1.0	
2	1.8	1.9	1.9	1.9	2.0	
4	2.1	3.1	3.6	3.9	3.9	
8	2.4	4.8	6.5	7.5	7.9	
16	2.4	6.2	10.8	14.2	15.5	

Efficiencies of Parallel Matrix-Vector Multiplication

	Order of Matrix					
comm_sz	1024	2048	4096	8192	16,384	
1	1.00	1.00	1.00	1.00	1.00	
2	0.89	0.94	0.97	0.96	0.98	
4	0.51	0.78	0.89	0.96	0.98	
8	0.30	0.61	0.82	0.94	0.98	
16	0.15	0.39	0.68	0.89	0.97	

Scalability

 A program is scalable if the problem size can be increased at a rate so that the efficiency doesn't decrease as the number of pro



Scalability

 Programs that can maintain a constant efficiency without increasing the problem size are sometimes said to be strongly scalable.

 Programs that can maintain a constant efficiency if the problem size increases at the same rate as the number of processes are sometimes said to be weakly scalable.

A parallel sorting algorithm

Sorting

- n keys and p = number of processes.
- n/p keys assigned to each process.
- No restrictions on which keys are assigned to which processes.
- When the algorithm terminates:
 - The keys assigned to each process should be sorted in (say) increasing order.
 - If 0 ≤ q < r < p, then each key assigned to process q should be less than or equal to every key assigned to process r.

Serial bubble sort

```
void Bubble_sort(
     int a[] /* in/out */,
     int n /* in */) {
  int list_length, i, temp;
  for (list_length = n; list_length \geq 2; list_length--)
     for (i = 0; i < list_length -1; i++)
        if (a[i] > a[i+1]) {
           temp = a[i];
           a[i] = a[i+1];
           a[i+1] = temp;
  /* Bubble_sort */
```

Odd-even transposition sort

- A sequence of phases.
- Even phases, compare swaps:

$$(a[0], a[1]), (a[2], a[3]), (a[4], a[5]), \dots$$

Odd phases, compare swaps:

$$(a[1], a[2]), (a[3], a[4]), (a[5], a[6]), \dots$$

Example

Start: 5, 9, 4, 3

Even phase: compare-swap (5,9) and (4,3) getting the list 5, 9, 3, 4

Odd phase: compare-swap (9,3) getting the list 5, 3, 9, 4

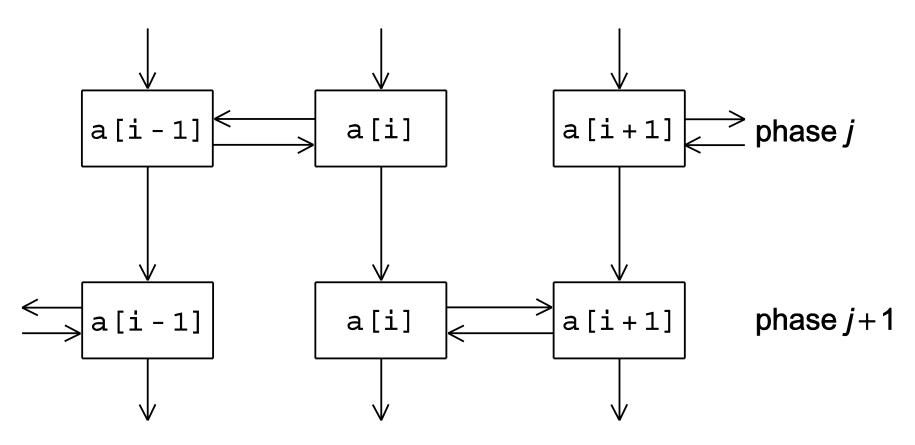
Even phase: compare-swap (5,3) and (9,4) getting the list 3, 5, 4, 9

Odd phase: compare-swap (5,4) getting the list 3, 4, 5, 9

Serial odd-even transposition sort

```
void Odd even sort(
      int a [] /* in/out */,
      int n /* in */) {
   int phase, i, temp;
  for (phase = 0; phase < n; phase++)
      if (phase % 2 == 0) { /* Even phase */
         for (i = 1; i < n; i += 2)
            if (a[i-1] > a[i]) {
              temp = a[i];
               a[i] = a[i-1];
              a[i-1] = temp;
      } else { /* Odd phase */
         for (i = 1; i < n-1; i += 2)
            if (a[i] > a[i+1]) {
              temp = a[i];
               a[i] = a[i+1];
               a[i+1] = temp;
  /* Odd_even_sort */
```

Communications among tasks in odd-even sort



Tasks determining a[i] are labeled with a[i].

Parallel odd-even transposition sort

	Process				
Time	0	1	2	3	
Start	15, 11, 9, 16	3, 14, 8, 7	4, 6, 12, 10	5, 2, 13, 1	
After Local Sort	9, 11, 15, 16	3, 7, 8, 14	4, 6, 10, 12	1, 2, 5, 13	
After Phase 0	3, 7, 8, 9	11, 14, 15, 16	1, 2, 4, 5	6, 10, 12, 13	
After Phase 1	3, 7, 8, 9	1, 2, 4, 5	11, 14, 15, 16	6, 10, 12, 13	
After Phase 2	1, 2, 3, 4	5, 7, 8, 9	6, 10, 11, 12	13, 14, 15, 16	
After Phase 3	1, 2, 3, 4	5, 6, 7, 8	9, 10, 11, 12	13, 14, 15, 16	

Pseudo-code

```
Sort local keys;
for (phase = 0; phase < comm_sz; phase++) {
   partner = Compute_partner(phase, my_rank);
   if (I'm not idle) {
      Send my keys to partner;
      Receive keys from partner;
      if (my_rank < partner)</pre>
         Keep smaller keys;
      else
         Keep larger keys;
```

Compute_partner

```
if (phase % 2 == 0) /* Even phase */
  if (my_rank % 2 != 0) /* Odd rank */
     partner = my_rank - 1;
  else
                            /* Even rank */
     partner = my_rank + 1;
                       /* Odd phase */
else
   if (my_rank % 2 != 0)  /* Odd rank */
     partner = my_rank + 1;
  else
                            /* Even rank */
     partner = my_rank - 1;
if (partner == -1 || partner == comm_sz)
  partner = MPI_PROC_NULL;
```

- The MPI standard allows MPI_Send to behave in two different ways:
 - it can simply copy the message into an MPI managed buffer and return,
 - or it can block until the matching call to MPI Recv starts.

- Many implementations of MPI set a threshold at which the system switches from buffering to blocking.
- Relatively small messages will be buffered by MPI_Send.
- Larger messages, will cause it to block.

 If the MPI_Send executed by each process blocks, no process will be able to start executing a call to MPI_Recv, and the program will hang or deadlock.

 Each process is blocked waiting for an event that will never happen.

• A program that relies on MPI provided buffering is said to be unsafe.

 Such a program may run without problems for various sets of input, but it may hang or crash with other sets.

Sources of Deadlocks

- Send a large message from process 0 to process 1
 - If there is insufficient storage at the destination, the send must wait for the user to provide the memory space (through a receive)
- What happens with this code?

Process 0	Process 1	
Send(1)	Send(0)	
Recv(1)	Recv(0)	

• This is called "unsafe" because it depends on the availability of system buffers in which to store the data sent until it can be received

Some Solutions to the "unsafe" Problem

Order the operations more carefully:

Process 0	Process 1
Send(1)	Recv(0)
Recv(1)	Send(0)

Supply receive buffer at same time as send:

```
Process 0 Process 1

Sendrecv(1) Sendrecv(0)
```

More Solutions to the "unsafe" Problem

Supply own space as buffer for send

Process 0	Process 1	
Bsend(1)	Bsend(0)	
Recv(1)	Recv(0)	

Use non-blocking operations:

Process 0	Process 1		
Isend(1)	Isend(0)		
Irecv(1)	Irecv(0)		
Waitall	Waitall		

MPI_Ssend

- An alternative to MPI_Send defined by the MPI standard.
- The extra "s" stands for synchronous and MPI_Ssend is guaranteed to block until the matching receive starts.

Restructuring communication

```
\label{eq:mpi_send} \begin{split} \text{MPI\_Send(msg, size, MPI\_INT, (my\_rank+1) \% comm\_sz, 0, comm);} \\ \text{MPI\_Recv(new\_msg, size, MPI\_INT, (my\_rank+comm\_sz-1) \% comm\_sz,} \\ 0, comm, MPI\_STATUS\_IGNORE. \end{split}
```



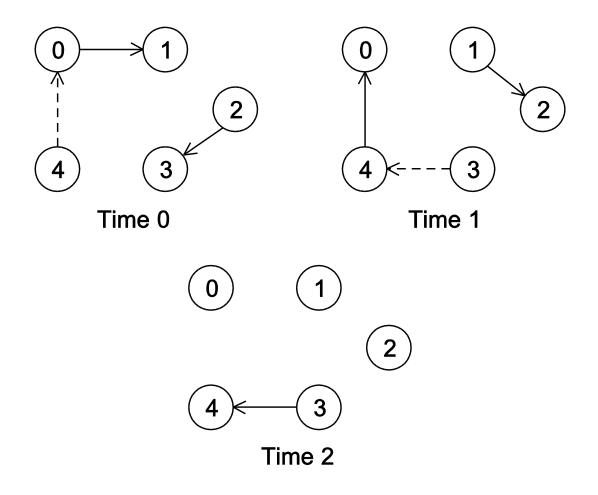
MPI_Sendrecv

- An alternative to scheduling the communications ourselves.
- Carries out a blocking send and a receive in a single call.
- The dest and the source can be the same or different.
- Especially useful because MPI schedules the communications so that the program won't hang or crash.

MPI_Sendrecv

```
int MPI_Sendrecv(
     void*
                  send_buf_p /*in */,
                  send_buf_size /*in */,
     int
     MPI_Datatype send_buf_type /*in */,
                               /* in */,
     int
                  dest
     int
                               /* in */,
                  send_tag
                  recv_buf_p /* out */,
     void*
                  recv_buf_size /*in */,
     int
                  recv_buf_type /* in */,
     MPI_Datatype
     int
                                /* in */,
                  source
     int
                               /* in */,
                  recv_tag
                  communicator /*in */,
     MPI Comm
                               /* in */);
     MPI Status*
                  status p
```

Safe communication with five processes



Parallel odd-even transposition sort

```
void Merge_low(
     int my_keys[], /* in/out */
     int recv_keys[], /* in */
     int temp_keys[], /* scratch */
     int local_n /* = n/p, in */) {
  int mi, ri, ti;
  m i = r i = t i = 0;
  while (t_i < local_n) {
     if (my_keys[m_i] <= recv_keys[r_i]) {</pre>
        temp keys[t i] = my keys[m i];
        t i++; m i++;
     } else {
        temp_keys[t_i] = recv_keys[r_i];
       t_i++; r_i++;
  for (m_i = 0; m_i < local_n; m_i++)
     my keys[m_i] = temp keys[m_i];
} /* Merge_low */
```

Run-times of parallel odd-even sort

	Number of Keys (in thousands)				
Processes	200	400	800	1600	3200
1	88	190	390	830	1800
2	43	91	190	410	860
4	22	46	96	200	430
8	12	24	51	110	220
16	7.5	14	29	60	130

(times are in milliseconds)

MPI's Non-blocking Operations

Non-blocking operations return (immediately)
 "request handles" that can be tested and waited on:

One can also test without waiting:

```
MPI_Test(&request, &flag, &status);
```

Accessing the data buffer without waiting is undefined

MPI's Non-blocking Operations

• It is sometimes desirable to wait on multiple requests:

```
MPI_Waitall(count, array_of_requests,
    array_of_statuses)
MPI_Waitany(count, array_of_requests,
    &index, &status)
MPI_Waitsome(count, array_of_requests,
    array_of_indices, array_of_statuses)
```

 There are corresponding versions of test for each of these.

Concluding Remarks (1)

- MPI or the Message-Passing Interface is a library of functions that can be called from C, C++, or Fortran programs.
- A communicator is a collection of processes that can send messages to each other.
- Many parallel programs use the single-program multiple data or SPMD approach.

Concluding Remarks (2)

- Most serial programs are deterministic: if we run the same program with the same input we'll get the same output.
- Parallel programs often don't possess this property.
- Collective communications involve all the processes in a communicator.

Concluding Remarks (3)

- When we time parallel programs, we're usually interested in elapsed time or "wall clock time".
- Speedup is the ratio of the serial run-time to the parallel run-time.
- Efficiency is the speedup divided by the number of parallel processes.

Concluding Remarks (4)

- If it's possible to increase the problem size (n) so that the efficiency doesn't decrease as p is increased, a parallel program is said to be scalable.
- An MPI program is unsafe if its correct behavior depends on the fact that MPI_Send is buffering its input.