High-Performance Computing

- Distributed Memory Programming with MPI -

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Outline

Overview of MPI

Basic MPI

- Hello world
- basic MPI functions
- example: trapezoidal rule

Intermediate MPI

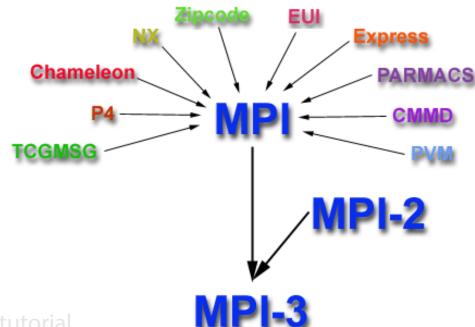
- collective communication
- derived datatypes
- performance measurements
- example: parallel sorting
- safety in MPI programs

Advanced MPI (in future supplement to these slides)

- non-blocking peer-to-peer communication
- one-sided communication
- I/O

The Message Passing Interface (MPI)

- Messages are transported between processes by explicit cooperation of sending and receiving processes
- Increasing popularity in the 1980s and early 90s
 - numerous vendor-specific libraries, but no standard
 - limited portability of code between different machines
 - differences in features, efficiency, price



The Message Passing Interface (MPI)

- Need for a common standard recognized in 1992
- First drafts in 1992, final standard of MPI-1.0 in 1994
- Today, MPI the most widely used standard for message passing
 - MPI is a specification for users and developers of a message passing library (not a library itself)
 - defines C and Fortran interfaces

There exist several widely used implementations, e.g.

- OpenMPI, Intel MPI, MPICH, MVAPICH, ...
- vendors can innovate in the implementation, e.g. offloading part of MPI functions to network cards (e.g. broadcast, barrier)

Standard has been extended over time

- initially rather simple
- over time, more complex features added, latest MPI-3.1 standard has 800+ pages

Hello World!

/* This is a short program */
#include <stdio.h>

int main(int argc, char* argv[]) {
 printf("hello, world\n");

```
return 0;
}
```



Identifying MPI processes

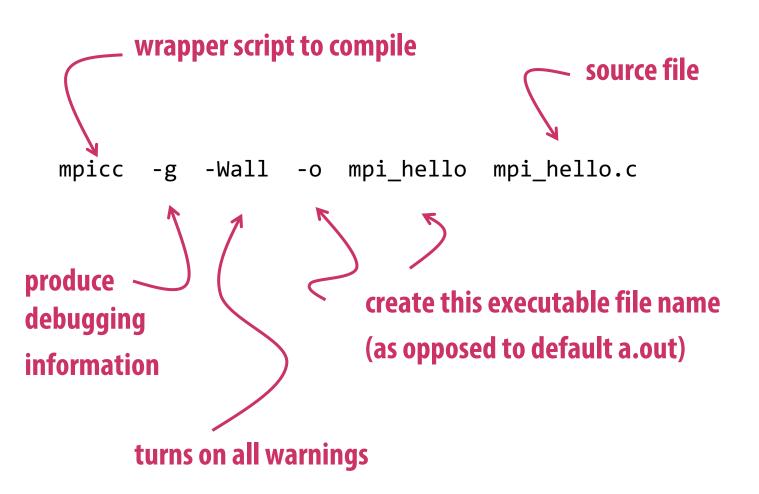
- Common practice to identify processes by nonnegative integer numbers, denoted as ranks
 - p processes are numbered 0, 1, 2, .. p-1
 - rank 0 is typically reserved for the "master process"
- Processes can query their own rank and the total number of ranks at runtime

Our First MPI Program

```
1 #include <stdio.h>
2 #include <string.h> /* For strlen
                                                    */
3
   #include <mpi.h> /* For MPI functions. etc */
4
5
   const int MAX_STRING = 100:
6
   int main(void) {
7
8
       char
                  greeting[MAX_STRING];
                 comm_sz; /* Number of processes */
9
      int
                 my_rank; /* My process rank
       int
10
                                                    */
11
      MPI_Init(NULL. NULL):
12
      MPI_Comm_size(MPI_COMM_WORLD, &comm_sz);
13
14
      MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
15
      if (my_rank != 0) {
16
          sprintf(greeting, "Greetings from process %d of %d!",
17
                my_rank, comm_sz);
18
19
         MPI_Send(greeting, strlen(greeting)+1, MPI_CHAR, 0, 0,
                MPI_COMM_WORLD):
20
21
       } else {
          printf("Greetings from process %d of %d!\n", my_rank,
22
              comm_sz):
         for (int q = 1; q < comm_sz; q++) {
23
            MPI_Recv(greeting, MAX_STRING, MPI_CHAR, q,
24
                0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
25
26
             printf("%s\n", greeting);
27
         }
28
       }
29
      MPI_Finalize();
30
       return 0:
31
      /* main */
32
```

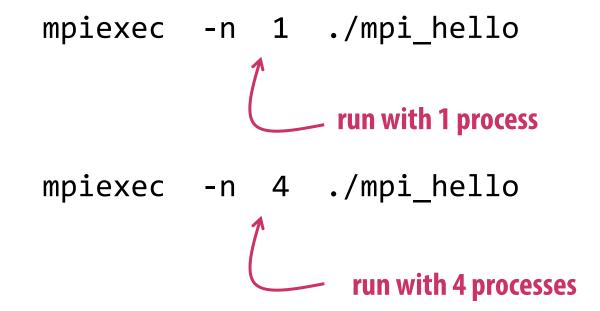


Compilation



Execution

mpiexec -n <number of processes> <executable>



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 (in this lecture, Fortran interface available too)
 - need main function
 - include headers for standard library functions, e.g., stdio.h, string.h, etc.
- MPI-specific functions declared in 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

Compilation and linking with MPI-specific libraries

- simplified with mpicc compiler wrapper
- wrapper adds required libraries automatically

MPI Program Structure

MPI_Init

- needs to be called by all ranks before using any MPI functions
- tells MPI to do all the necessary setup

```
int MPI_Init(
    int* argc_p /* in/out */,
    char*** argv_p /* in/out */);
```

MPI_Finalize

- needs to be called by all ranks at the end of the program
- frees up any resources allocated for this program

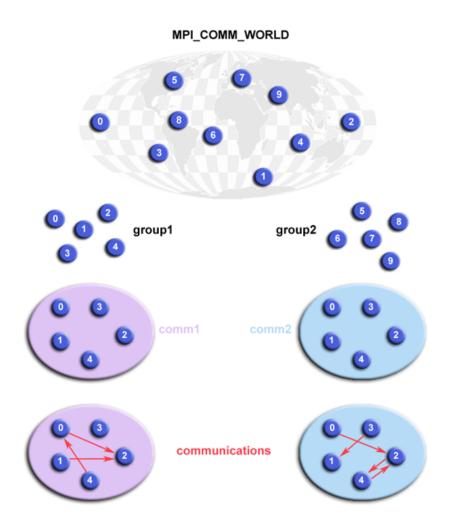
int MPI_Finalize(void);

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

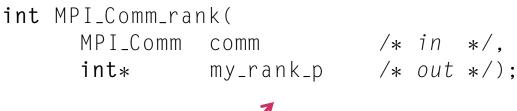
- A communicator is a group of processes that may send messages to each other
- MPI_Init creates a default communicator
 - consists of all the processes created when the program is started
 - called MPI_COMM_WORLD
- Additional communicators and groups can be created at runtime
 - simplifies repeated communication within subset of nodes (e.g. all even or all odd nodes)
 - for our basic needs typically not required



Communicators







my rank (the process making this call)

SPMD (Single-Program Multiple Data)

The code for all processes (ranks) is specified with one program

Advantages

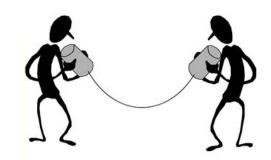
- simplified compilation, deployment and execution of code on many processors
- tailoring the execution to the available number of processes (ranks) is happens at runtime, not compile time
- Rank-specific code implemented by conditional code (if-else constructs)

Rank 0 is different

- designated Master process
- has access to standard input
- (in the hello world example: receives messages and prints them while the other processes do the work)

Communication

<pre>int MPI_Send(</pre>				
void*	msg_buf_p	/*	in	*/,
int	msg_size	/*	in	*/,
MPI_Datatype	msg_type	/*	in	*/,
int	dest	/*	in	*/,
int	tag	/*	in	*/,
MPI_Comm	communicator	/*	in	*/);



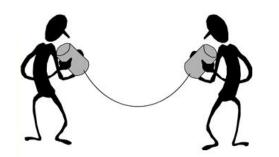
Data Types

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	iong uoubie

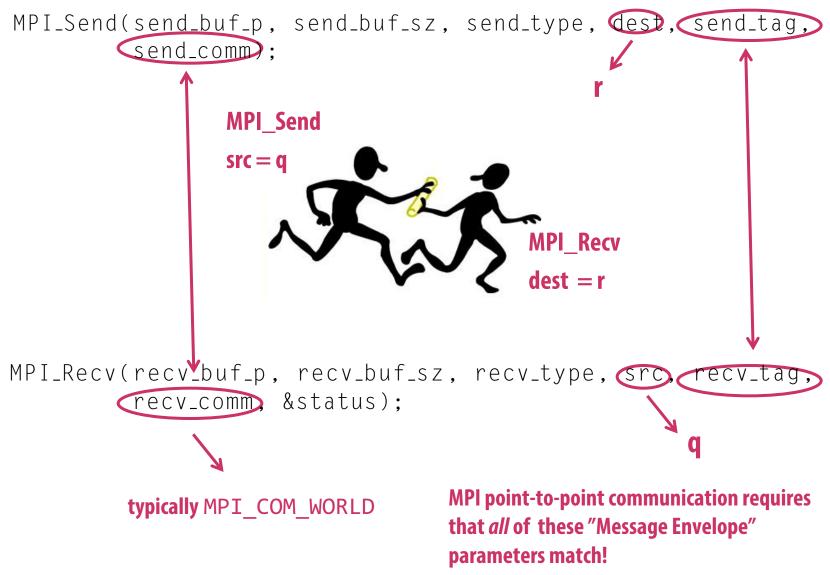
Communication

int MPI_Recv(void* msg_buf_p int buf_size MPI_Datatype buf_type int source int tag communicator /* in */, MPI_Comm MPI_Status* status_p

/* out */, /* in */, /* in */, /* in */, /* in */, /* out */);



Message Matching



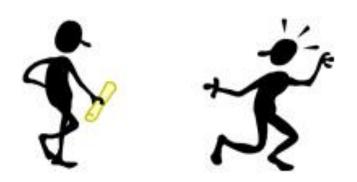
Receiving Messages

- A receiver can also receive a message without knowing ..

- the amount of data in the message,
- the sender of the message,
- or the tag of the message

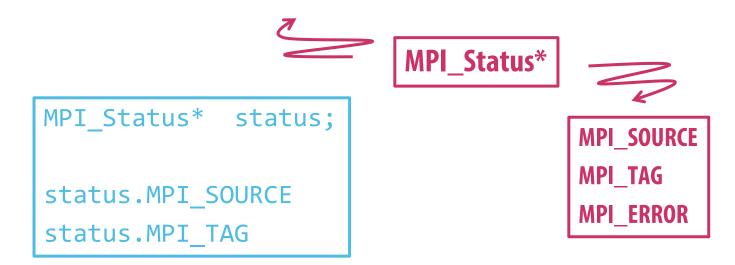
• .. by specifying wildcards for source and tag

- MPI_ANY_SOURCE
- MPI_ANY_TAG



Determine Source, Tag and Length

When using wildcards (MPI_ANY_SOURCE or MPI_ANY_TAG) the sender can use the MPI_Status* return value to identify the source, tag of a message



How Much Data am I Receiving?

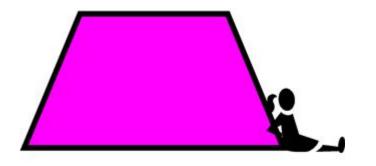
int MPI_Get_count(
 MPI_Status* status_p /* in */,
 MPI_Datatype type /* in */,
 int* count_p /* out */);



Issues with Send and Receive

- Exact behavior is determined by the MPI implementation
- MPI_Send may behave differently with regard to buffer size, cutoffs and blocking
- MPI_Recv always blocks until a matching message is received
- Know your implementation; don't make assumptions!





TRAPEZOIDAL RULE IN MPI

The Trapezoidal Rule

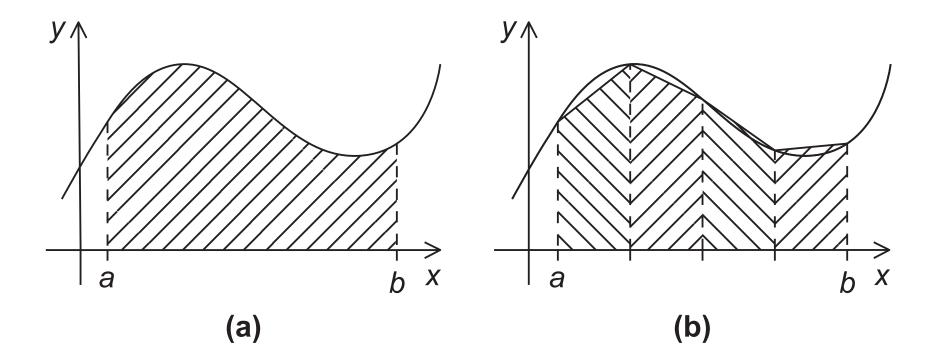


Figure 3.3

One Trapezoid

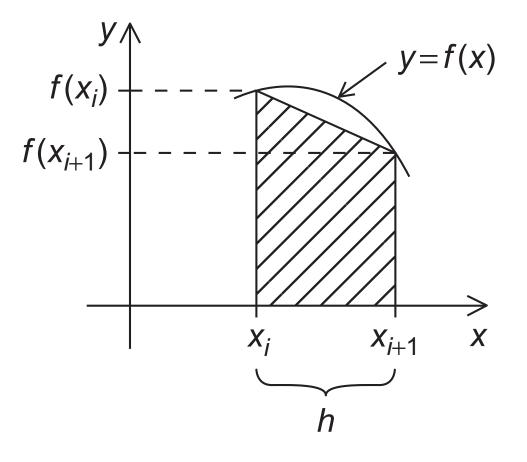


Figure 3.4



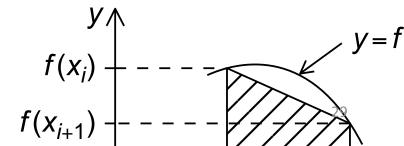
Area of one trapezoid
$$= \frac{h}{2} [f(x_i) + f(x_{i+1})].$$

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

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

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

Pseudo-Code for a Serial Program

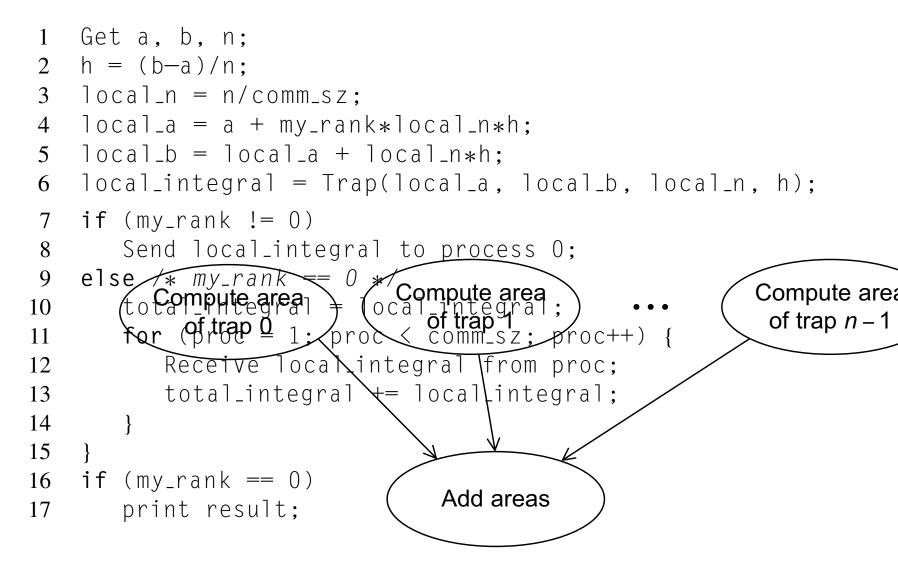


Parallelizing the Trapezoidal Rule

Apply Foster's approach

- Partition problem solution into tasks
- Identify communication channels between tasks
- Aggregate tasks into composite tasks
- Map composite tasks to cores

Parallel Pseudo-Code



Tasks and Communications for Trapezoidal Rule

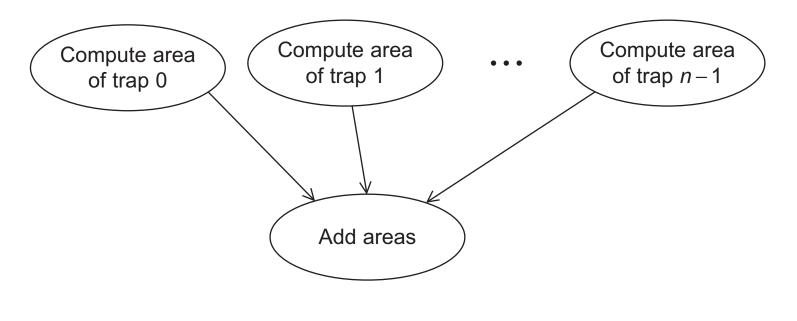


Figure 3.5

First Version (1)

```
int main(void) {
 1
 2
       int my_rank, comm_sz, n = 1024, local_n;
3
       double a = 0.0, b = 3.0, h, local_a, local_b;
4
      double local_int, total_int;
 5
       int source:
6
7
       MPI_Init(NULL. NULL):
8
       MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
       MPI_Comm_size(MPI_COMM_WORLD, &comm_sz);
9
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:
       local_int = Trap(local_a, local_b, local_n, h);
16
17
18
      if (my_rank != 0) {
          MPI_Send(&local_int, 1, MPI_DOUBLE, 0, 0,
19
                MPI_COMM_WORLD):
20
```

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);
             total_int += local_int:
26
27
          }
28
       }
29
30
       if (my_rank == 0) {
31
          printf("With n = \% d trapezoids, our estimate\n", n);
          printf("of the integral from %f to %f = \%.15e\n",
32
33
              a. b. total_int);
34
       }
       MPI_Finalize():
35
36
       return 0:
    } /* main */
37
```

First Version (3)

```
double Trap(
1
2
          double left_endpt /* in */,
          double right_endpt /* in */,
3
4
          int trap_count /* in */,
5
          double base_len /* in */) {
6
    double estimate, x;
7
      int i:
8
9
       estimate = (f(left_endpt) + f(right_endpt))/2.0;
       for (i = 1; i \leq trap_count-1; i++) {
10
          x = left_endpt + i*base_len;
11
          estimate += f(x):
12
13
       estimate = estimate*base_len:
14
15
16
      return estimate;
   } /* Trap */
17
```

Dealing with I/O

```
Each process just
#include <stdio.h>
#include <mpi.h>
                                   prints a message
int main(void) {
   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

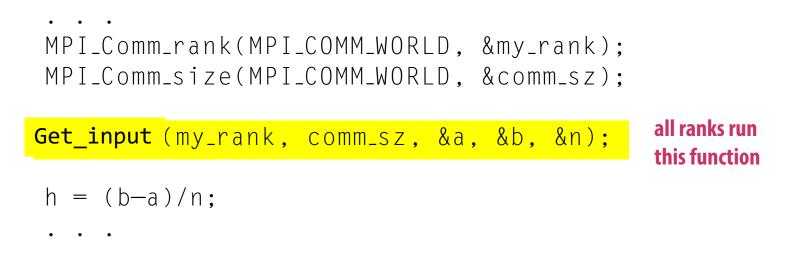
Proc 0 of 6 > Does anyone have a toothpick? Proc 1 of 6 > Does anyone have a toothpick? Proc 2 of 6 > Does anyone have a toothpick? Proc 4 of 6 > Does anyone have a toothpick? Proc 3 of 6 > Does anyone have a toothpick? Proc 5 of 6 > Does anyone have a toothpick?

Example output (could be any other permutation)

Non-deterministic 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



Example: passing the input data to all processes

Function for Reading User Input

```
void Get_input(
1
         int my_rank
                           /* in */.
2
3
         int comm_sz /* in */,
         double* a_p /* out */,
4
5
         double* b_p /* out */.
6
         int*
                n_p /* out */) {
7
      int dest;
8
      if (my_rank == 0) {
9
         printf("Enter a, b, and n \in);
10
         scanf("%lf %lf %d", a_p, b_p, n_p);
11
12
         for (dest = 1; dest < comm_sz; dest++) {</pre>
13
            MPI_Send(a_p, 1, MPI_DOUBLE, dest, 0, MPI_COMM_WORLD);
            MPI_Send(b_p, 1, MPI_DOUBLE, dest, 0, MPI_COMM_WORLD);
14
            MPI_Send(n_p, 1, MPI_INT, dest, 0, MPI_COMM_WORLD);
15
16
      } else { /* my_rank != 0 */
17
         MPI_Recv(a_p, 1, MPI_DOUBLE, 0, 0, MPI_COMM_WORLD.
18
19
               MPI_STATUS_IGNORE):
         MPI_Recv(b_p, 1, MPI_DOUBLE, 0, 0, MPI_COMM_WORLD,
20
               MPI_STATUS_IGNORE);
21
         MPI_Recv(n_p, 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
22
23
               MPI_STATUS_IGNORE):
24
25
      /* Get_input */
   }
```

This Could be the End

- Essentially, we could stop discussing MPI here
- Everything can be built on top of point-to-point send and receive functions
- What is missing
 - higher-level communication abstractions for convenience
 - efficient one-to-many, many-to-one, and many-to-many communication
 - functions for safe (deadlock free) operation
 - one-sided communication
 - efficient file I/0

MPI Collective Communication Routines

 MPI Collectives perform operations by involving all tasks available within one communicator

Type of collective operations

- synchronization: let all processes wait until all members of the group have reached a synchronization point (barrier)
- data movement: one-to-many and many-to-many communications (broadcast, scatter, gather, all to all)
- collective computation (reductions): one member of the group collects data from all other members and performs an operation on the data (min, max, add, multiply, ...)

Collections Visual Overview

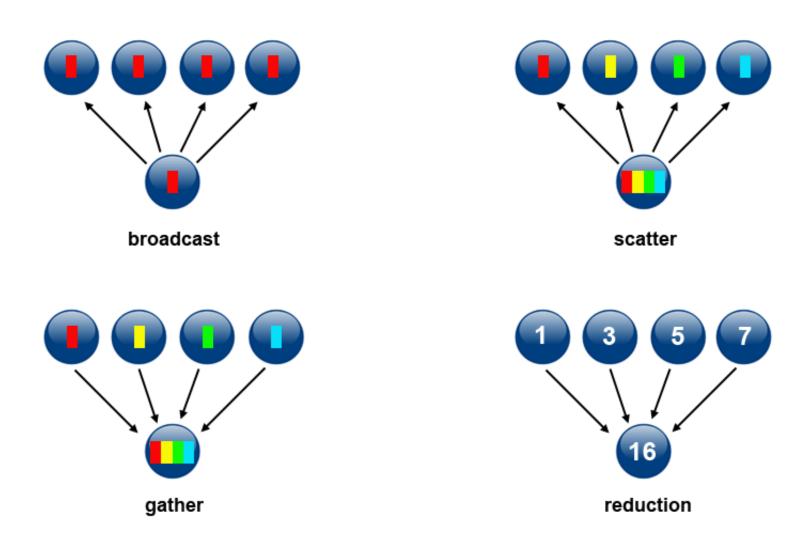


image: LLNL MPI tutorial

Reduction: Tree-Structured Global Sum

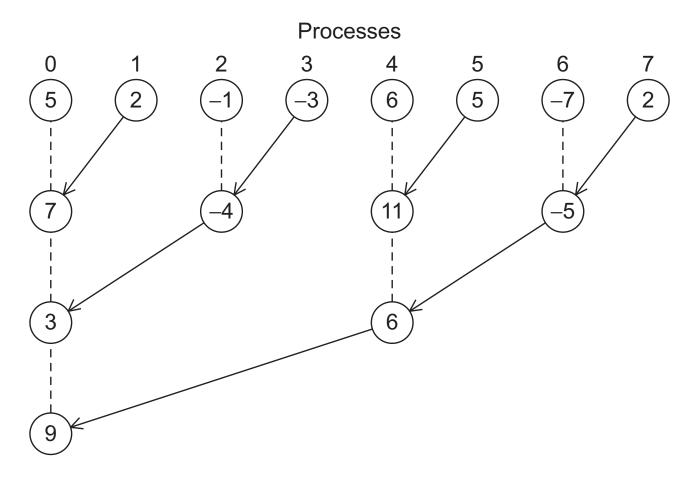


Figure 3.6

An Alternative Tree-Structured Global Sum

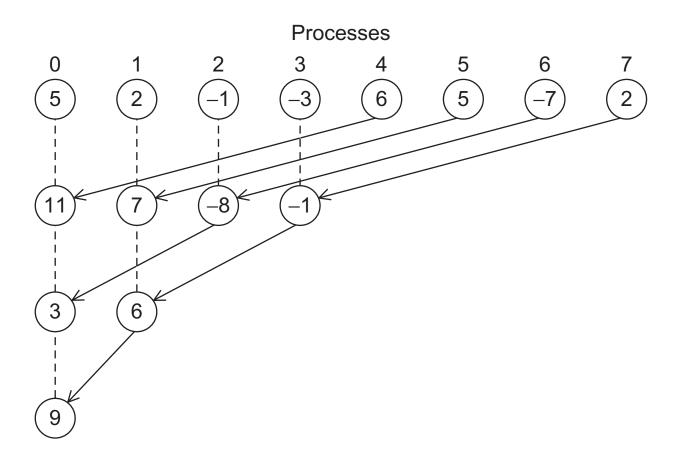


Figure 3.7

MPI_Reduce

_					
	<pre>int MPI_Reduce(</pre>				
	void*	input_data_p	/*	in	*/,
	void*	output_data_p	/*	out	*/,
	int	count	/*	in	*/,
	MPI_Datatype	datatype	/*	in	*/,
	MPI_Op	operator	/*	in	*/,
	int	dest_process	/*	in	*/,
	MPI_Comm	COMM	/*	in	*/);

MPI_Reduce function signature

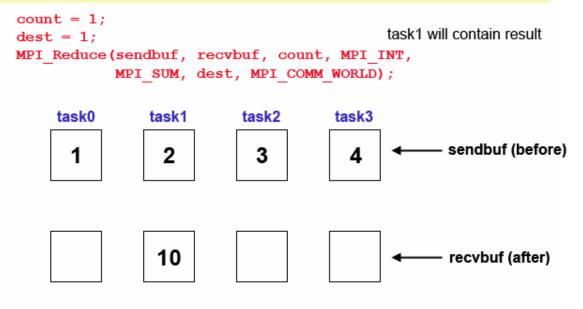
example: sum scalar value (local_int) from each rank

example: element-wise summation of arrays from each rank

MPI_Reduce Illustration

MPI_Reduce

Perform reduction across all tasks in communicator and store result in 1 task



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 vs. Point-to-Point Communications

All the processes in the communicator must call the same collective function

- e.g. 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 will cause the program to hang or crash
- arguments passed by each process to an MPI collective must be "compatible", e.g. 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 will cause the program 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

Send and receive matching

- point-to-point communication: matched on the basis of tags and communicators
- collective communications: don't use tags, matching on the basis of the communicator and the order in which they're called

Example

- Collectives are matched by order in which they are called (not tags)

- example: MPI_ADD reduction, with rank 0 as destination
- after executing these statements value of b=1+2+1 and d=2+1+2

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, <mark>&d</mark> ,)	MPI_Reduce(&a, <mark>&b</mark> ,)		
2	MPI_Reduce(&c, &d,)	MPI_Reduce(&a, <mark>&b</mark> ,)	MPI_Reduce(&c, <mark>&d</mark> ,)		

memory location of destination used by senders is irrelevant

 Using the same buffer for both input and output is illegal and may result in invalid results (aliasing)

MPI_Reduce(&x, &x, 1, MPI_DOUBLE, MPI_SUM, 0, comm);

 MPI has special functions for sending and receiving using a single buffer (e.g. MPI_Sendrecv_replace)

MPI_Allreduce

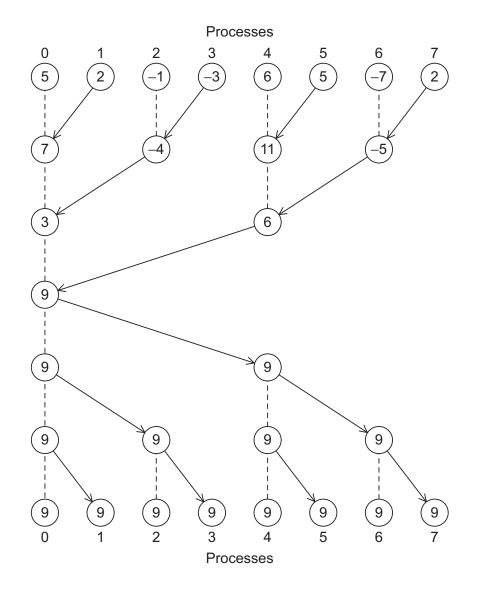
 Useful in a situation in which all of the processes need the result of a global sum in order to complete some larger computation

int MPI_Allreduce(
void*	input_data_p	/*	in	*/,
void*	output_data_p	/*	out	*/,
int	count	/*	in	*/,
MPI_Datatype	datatype	/*	in	*/,
MPI_Op	operator	/*	in	*/,
MPI_Comm	COMM	/*	in	*/);

MPI_Allreduce function signature

 Essentially the same function as MPI_Reduce but without dest_process argument, because all process shall receive the result

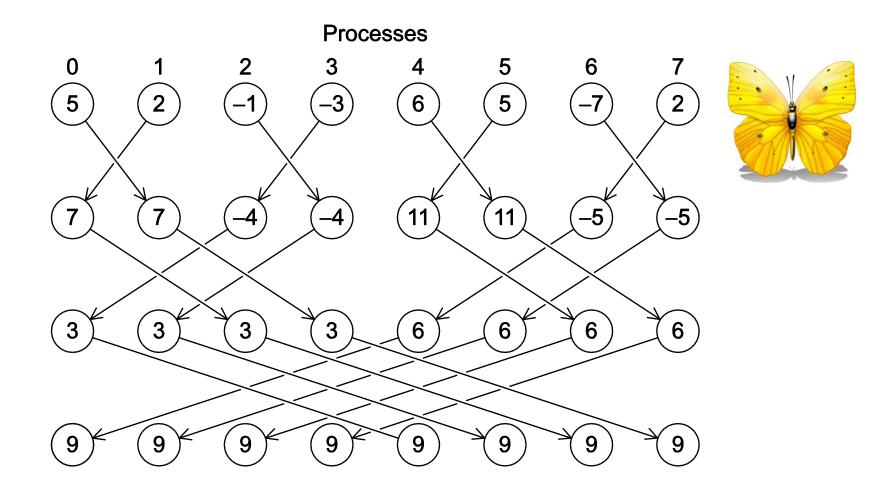
Naïve implementation of MPI_Allreduce



A global sum followed by distribution of the result.

Figure 3.8

Efficient Implementation of MPI_Allreduce



A butterfly-structured global sum

Figure 3.9

Broadcast

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

<pre>int MPI_Bcast(</pre>							
void*	data_p	/*	in/out	*/,			
int	count	/*	in	*/,			
MPI_Datatype	datatype	/*	in	*/,			
int	source_proc	/*	in	*/,			
MPI_Comm	COMM	/*	in	*/);			

MPI_Bcast function signature

 For the sending process data_p is an input, for all other processes an output

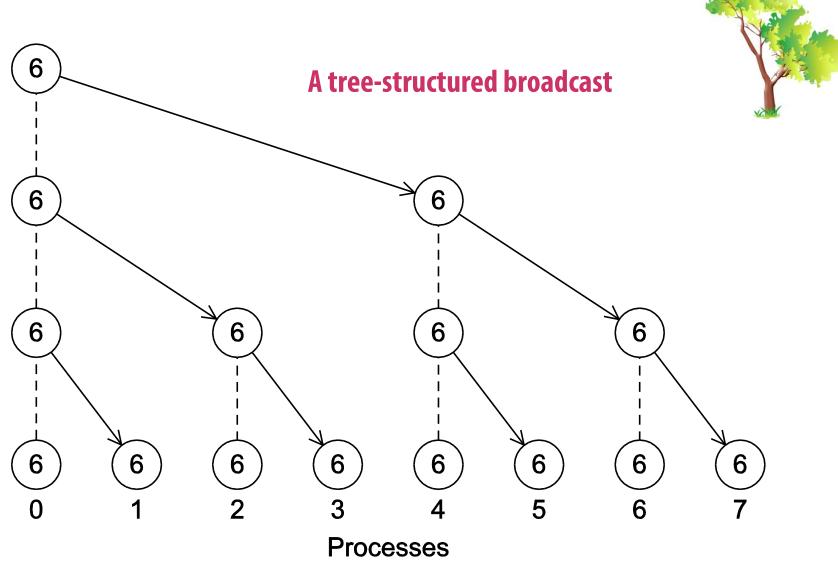


Figure 3.10

MPI_Bcast Illustration

MPI_Bcast

Broadcasts a message from one task to all other tasks in communicator

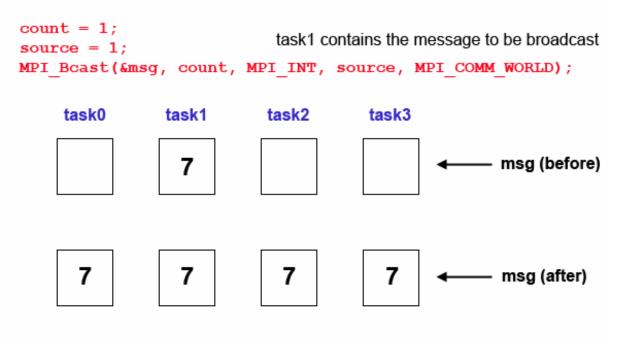


image: LLNL MPI tutorial

Recap: Function for Reading User Input

```
void Get_input(
 1
                  my_rank /* in */.
2
         int
             comm_sz /* in */.
         int
3
         double* a_p /* out */,
4
5
         double* b_p /* out */,
6
         int*
                            /* out */) {
                  n_p
7
      int dest;
8
      if (my_rank == 0) {
9
10
         printf("Enter a, b, and n\n");
         scanf("%lf %lf %d", a_p, b_p, n_p);
11
12
         for (dest = 1; dest < comm_sz; dest++) {</pre>
            MPI_Send(a_p, 1, MPI_DOUBLE, dest, 0, MPI_COMM_WORLD);
13
            MPI_Send(b_p, 1, MPI_DOUBLE, dest, 0, MPI_COMM_WORLD);
14
            MPI_Send(n_p, 1, MPI_INT, dest, 0, MPI_COMM_WORLD);
15
16
      } else { /* my_rank != 0 */
17
         MPI_Recv(a_p, 1, MPI_DOUBLE, 0, 0, MPI_COMM_WORLD,
18
19
               MPI_STATUS_IGNORE):
         MPI_Recv(b_p, 1, MPI_DOUBLE, 0, 0, MPI_COMM_WORLD,
20
21
               MPI_STATUS_IGNORE);
         MPI_Recv(n_p, 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
22
               MPI_STATUS_IGNORE):
23
24
25
      /* Get_input */
```

point-to-point communication

Implementation of Get_input using MPI_Bcast

```
void Get_input(
1
2
         int
            my_rank /* in */,
3
         int comm_sz /* in */,
        double* a_p /* out */,
4
5
        double* b_p /* out */,
              6
         int*
7
      if (my_rank == 0) {
8
9
         printf("Enter a, b, and n n);
         scanf("%lf %lf %d", a_p, b_p, n_p);
10
11
12
      MPI_Bcast(a_p, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
      MPI_Bcast(b_p, 1, MPI_DOUBLE, 0, MPI_COMM_WORLD);
13
      MPI_Bcast(n_p, 1, MPI_INT, 0, MPI_COMM_WORLD);
14
      /* Get_input */
15
```

broadcast: simpler, more efficient

Data Distributions

- Goal: We want to efficiently execute operations on matrices or vectors in a distributed memory machine
- Example: vector summation

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

= $(x_0 + y_0, x_1 + y_1, \dots, x_{n-1} + y_{n-1})$
= $(z_0, z_1, \dots, z_{n-1})$
= \mathbf{z}

Serial implementation

```
1 void Vector_sum(double x[], double y[], double z[], int n) {
2     int i;
3     4     for (i = 0; i < n; i++)
5         z[i] = x[i] + y[i];
6     } /* Vector_sum */</pre>
```

Distribution of Data to Processes

- How to partition and distribute data to processes
- Example: partitioning a 12 component vector to 3 processes

					С	om	pon	ents				
									Blo	ock-	Cycl	ic
Process		B	ock			Су	clic		Blo	ocks	ize =	2
0	0	1	2	3	0	3	6	9	0	1	6	7
1	4	5	6	7	1	4	7	10	2 '	З	8	9
2	8	9	10	11	2	5	8	11	4	5	10	11

- 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

 Once the data is distributed, the implementation of the parallel code is straight forward

```
void Parallel vector sum(
1
2
         double local_x[] /* in */.
3
         double local_y[] /* in */,
         double local_z[] /* out */,
4
5
         int local_n /* in */) {
     int local_i:
6
7
      for (local_i = 0; local_i < local_n; local_i++)</pre>
8
9
         local_z[local_i] = local_x[local_i] + local_y[local_i];
      /* Parallel_vector_sum */
10
```

A 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

int	MPI_Scatter(
	void*	send_buf_p	/*	in	*/,
	int	send_count	/*	in	*/,
	MPI_Datatype	send_type	/*	in	*/,
	void*	recv_buf_p	/*	out	*/,
	int	recv_count	/*	in	*/,
	MPI_Datatype	recv_type	/*	in	*/,
	int	src_proc	/*	in	*/,
	MPI_Comm	COMM	/*	in	*/);

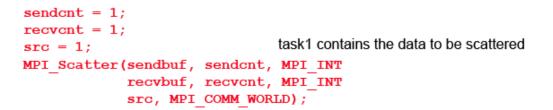
MPI_Scatter function signature

- Performs only block distribution, works only if number of elements is evenly divisible by number of processes
- Note: send_count and recv_count is size of elements being sent to each process, not total size of data

MPI_Scatter Illustration

MPI_Scatter

Sends data from one task to all other tasks in communicator



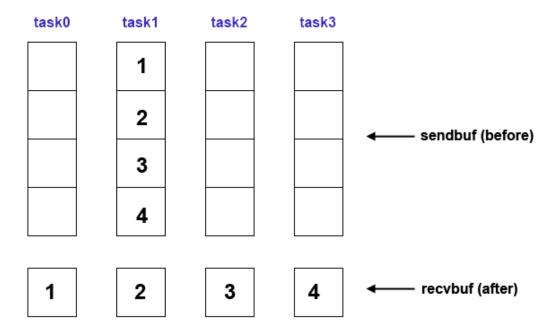


image: LLNL MPI tutorial

Reading and Distributing a Vector

```
void Read_vector(
1
         double local_a[] /* out */,
2
3
         int local_n /* in */,
         int n /* in */,
4
         char vec_name[] /* in */,
5
6
        int my_rank /* in */,
7
         MPI_Comm comm /* in */) {
8
9
      double* a = NULL:
      int i:
10
11
12
      if (my_rank == 0) {
         a = malloc(n*sizeof(double)):
13
14
         printf("Enter the vector %s\n", vec_name);
         for (i = 0; i < n; i++)
15
16
            scanf("%]f". &a[i]):
         MPI_Scatter(a, local_n, MPI_DOUBLE, local_a, local_n,
17
              MPI_DOUBLE, 0, comm);
18
19
         free(a):
20
      } else {
21
         MPI_Scatter(a, local_n, MPI_DOUBLE, local_a, local_n,
22
              MPI_DOUBLE, 0, comm);
23
      }
      /* Read_vector */
24
```

Gather

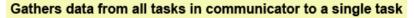
 Collect all of the components of the vector onto process 0, and then process 0 can process all of the components.

int	MPI_Gather(
	void*	send_buf_p	/*	in	*/,
	int	send_count	/*	in	*/,
	MPI_Datatype	send_type	/*	in	*/,
	void*	recv_buf_p	/*	out	*/,
	int	recv_count	/*	in	*/,
	MPI_Datatype	recv_type	/*	in	*/,
	int	dest_proc	/*	in	*/,
	MPI_Comm	comm	/*	in	*/);

MPI_Gather function signature

MPI_Gather Illustration

MPI_Gather



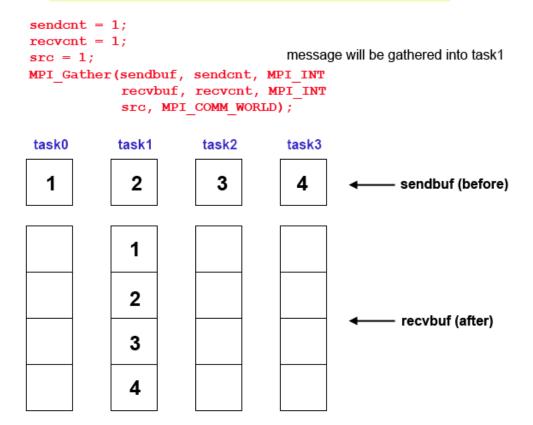


image: LLNL MPI tutorial

Print a Distributed Vector

```
void Print vector(
1
2
         double local_b[] /* in */.
3
         int local_n /* in */,
         int n /* in */,
4
5
         char title[] /* in */,
6
      int my_rank /* in */,
                       /* in */) {
      MPI_Comm comm
7
8
9
      double* b = NULL:
      int i:
10
11
      if (my_rank == 0) {
12
         b = malloc(n*sizeof(double));
13
         MPI_Gather(local_b, local_n, MPI_DOUBLE, b, local_n,
14
15
               MPI_DOUBLE, 0, comm);
         printf("%s\n", title);
16
         for (i = 0; i < n; i++)
17
            printf("%f ", b[i]);
18
         printf("\n");
19
         free(b):
20
21
      } else {
         MPI_Gather(local_b, local_n, MPI_DOUBLE, b, local_n,
22
23
               MPI_DOUBLE. 0. comm):
24
      /* Print_vector */
25
   }
```

Allgather

i

- 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

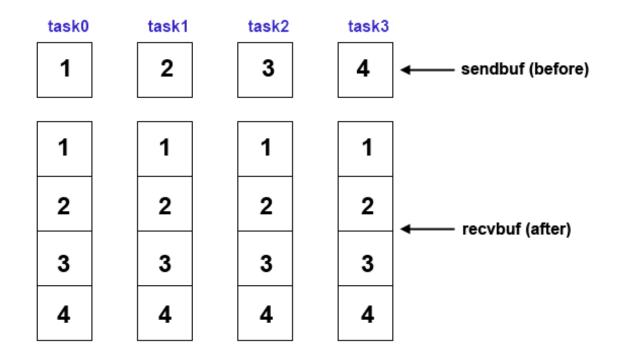
nt	MPI_Allgather(
	void*	send_buf_p	/*	in *	k/,
	int	send_count	/*	in	*/,
	MPI_Datatype	send_type		in	-
	void*	recv_buf_p	/*	out	*/,
	int	recv_count	/*	in	*/,
	MPI_Datatype	recv_type	/*	in	*/,
	MPI_Comm	comm	/*	in	*/);

MPI_Allgather function signature

MPI_Allgather Illustration

MPI_Allgather

Gathers data from all tasks and then distributes to all tasks in communicator



Example: Vector Addition

See source code

- vector_add.c (serial code)
- mpi_vector_add.c (MPI code)

Use Case: Matrix-Vector Multiplication

<i>a</i> ₀₀	<i>a</i> ₀₁	•••	$a_{0,n-1}$		
<i>a</i> ₁₀	<i>a</i> ₁₁	•••	<i>a</i> _{1,<i>n</i>-1}	<i>x</i> ₀	Y1
•	•		•	<i>x</i> ₁	•
a_{i0}	<i>a</i> _{<i>i</i>1}	•••	$a_{i,n-1}$	=	$y_i = a_{i0}x_0 + a_{i1}x_1 + \cdots + a_{i,n-1}x_{n-1}$
•	•		•	x_{n-1}	:
$a_{m-1,0}$	$a_{m-1,1}$	• • •	$a_{m-1,n-1}$		<u>Ут-1</u>

Figure 3.11

Serial Pseudo-Code for Matrix-Vector Multiplication

Use Case: Matrix-Vector Multiplication (2)

The C programming langue

- tedious idiosyncrasies with handling multi-dimensional arrays
- not possible to write generic functions that accept multi-dimensional arrays of varying size
- Hence, programmers typically express two (or higher)-dimensional arrays as one-dimensional arrays (linearized storage)

$$\begin{pmatrix} 0 & 1 & 2 & 3 \\ 4 & 5 & 6 & 7 \\ 8 & 9 & 10 & 11 \end{pmatrix}$$
 stored as $0 \ 1 \ 2 \ 3 \ 4 \ 5 \ 6 \ 7 \ 8 \ 9 \ 10 \ 11.$

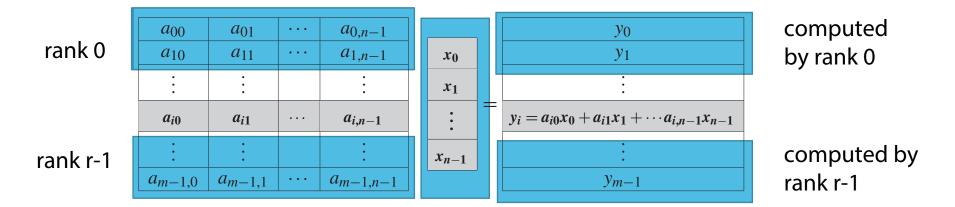
 Requires explicit mapping from higher-dimensions to single dimension in the code

Use Case: Matrix-Vector Multiplication (3)

```
void Mat vect mult(
1
                                        A[],x[],y[] are linear
          double A[] /* in */,
2
          double x[] /* in */,
                                        1D arrays
3
          double y[] /* out */,
4
5
          int _____ /* in */.
                                        matrix dimensions
6
          int n /* in */) {
                                        explicitly passed to
7
       int i, j;
                                        function
8
9
       for (i = 0; i < m; i++) {
          y[i] = 0.0;
10
                                        explicit mapping
          for (j = 0; j < n; j++)
11
                                        from higher dimensions
             y[i] += A[i*n+j]*x[j];
12
                                        to 1D array index
13
       }
       /* Mat_vect_mult */
14
```

Serial Pseudo-Code for Matrix-Vector Multiplication with linearized arrays

Use Case: Matrix-Vector Multiplication (4)



rows of matrix A will be	
block-distributed to all	
ranks	

x will be copied to all ranks

Example: Matrix-Vector Multiplication

See source code

- mat_vect_mult.c (serial code)
- mpi_mat_vect_mult.c (MPI code)

MPI matrix-vector multiplication function

```
void Mat_vect_mult(
 1
2
         double local_A[] /* in */.
 3
         double local_x[] /* in */,
4
         double local_y[] /* out */,
        int local_m /* in */,
5
6
        int n /* in */.
        int local_n /* in */,
7
8
         MPI_Comm comm /* in */) {
9
      double* x;
      int local_i, j;
10
      int local_ok = 1:
11
12
13
      x = malloc(n*sizeof(double));
                                                    code shows only
      MPI_Allgather(local_x, local_n, MPI_DOUBLE,
14
                                                    distribution of vector x
            x, local_n, MPI_DOUBLE, comm);
15
                                                    (but not A)
16
      for (local_i = 0; local_i < local_m; local_i++) {</pre>
17
         local_y[local_i] = 0.0;
18
         for (j = 0; j < n; j++)
19
            local_y[local_i] += local_A[local_i*n+j]*x[j];
20
21
22
      free(x):
23 }
     /* Mat_vect_mult */
```

MPI 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

Allow efficient data handling

- function that sends data knows this information about a collection of data items, allowing it to collect the items from memory before they are sent
- function that receives data can distribute the items into their correct destinations in memory when they're received
- Consists of a sequence of basic MPI data types together with a displacement for each of the data types
- Trapezoidal Rule example:

Address
24
40
48

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

Creating Derived Datatypes

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

int	MPI_Type_create_	struct(
	int	count	/*	in	
	int	array_of_blocklengths[]	/*	in	
	MPI_Aint	array_of_displacements[]	/*	in	
	MPI_Datatype	array_of_types[]	/*	in	

MPI_Datatype array_of_types[] MPI_Datatype* new_type_p

/*	п	*/,
/*	in	*/,
/*	out	*/);

*/, */,

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 Using Derived Datatype (1)

```
void Build_mpi_type(
     double* a_p /* in */,
                          /* in */,
/* in */,
     double* b_p
     int*
                   n_p
     MPI_Datatype* input_mpi_t_p /* out */) {
  int array_of_blocklengths[3] = \{1, 1, 1\};
  MPI_Datatype array_of_types[3] = {MPI_DOUBLE, MPI_DOUBLE, MPI_INT}
  MPI_Aint a_addr, b_addr, n_addr;
  MPI_Aint array_of_displacements[3] = {0};
  MPI_Get_address(a_p, &a_addr);
  MPI_Get_address(b_p, &b_addr);
  MPI_Get_address(n_p, &n_addr);
   array_of_displacements[1] = b_addr-a_addr;
   array_of_displacements[2] = n_addr-a_addr;
  MPI_Type_create_struct(3, array_of_blocklengths,
        array_of_displacements, array_of_types,
        input_mpi_t_p);
  MPI_Type_commit(input_mpi_t_p);
  /* Build_mpi_type */
```

Get Input Function Using Derived Datatype (2)



PERFORMANCE EVALUATION

Elapsed Parallel Time

- Returns the number of seconds that have elapsed since some time in the past
 - MPI_Wtime available as part of MPI library

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
- "timer.h" may not be part of default include path
 - you may have to inform the compiler about the directory containing timer.h
 - in gcc add option: -I/path/to/timer_h

```
#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

int MPI_Barrier(MPI_Comm comm /* in */);

MPI_Barrier function signature



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, O, 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		

(milliseconds)

Reminder: Speedup and Efficiency

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

Speedups and Efficiency of Parallel Matrix-Vector Multiplication

speedup

efficiency

	Order of Matrix					Orc	ler of N	latrix			
comm_sz	1024	2048	4096	8192	16,384	comm_sz	1024	2048	4096	8192	16,384
1	1.0	1.0	1.0	1.0	1.0	1	1.00	1.00	1.00	1.00	1.00
2	1.8	1.9	1.9	1.9	2.0	2	0.89	0.94	0.97	0.96	0.98
4	2.1	3.1	3.6	3.9	3.9	4	0.51	0.78	0.89	0.96	0.98
8	2.4	4.8	6.5	7.5	7.9	8	0.30	0.61	0.82	0.94	0.98
16	2.4	6.2	10.8	14.2	15.5	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 processes increase
 - strongly scalable: programs can maintain a constant efficiency without increasing the problem size
 - weakly scalable: program maintain a constant efficiency if the problem size increases at the same rate as the number of processes



Parallelizing a Sorting Algorithm

- n keys and p = comm sz 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

```
1
   void Bubble_sort(
2
         int a[] /* in/out */,
3
         int n /* in */) {
4
      int list_length, i, temp;
5
6
      for (list_length = n; list_length >= 2; list_length---)
7
          for (i = 0; i < list_length-1; i++)
8
             if (a[i] > a[i+1]) {
                temp = a[i];
9
10
                a[i] = a[i+1];
11
                a[i+1] = temp;
12
             }
13
      /* Bubble_sort */
14 }
```

Odd-Even Transposition Sort

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

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

Odd phases, compare swaps:

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

Example

Start: 5, 9, 4, 3

Even phase

- compare-swap (5,9) and (4,3)
- result: 5, 9, 3, 4

Odd phase

- compare-swap (9,3)
- result: 5, 3, 9, 4

Even phase

- compare-swap (5,3) and (9,4)
- result: 3, 5, 4, 9

Odd phase

- compare-swap (5,4)
- result: 3, 4, 5, 9

Serial Odd-Even Transposition Sort

```
void Odd_even_sort(
1
2
          int a[] /* in/out */.
3
          int n /* in */) {
       int phase, i, temp;
4
5
       for (phase = 0; phase < n; phase++)</pre>
6
          if (phase % 2 == 0) { /* Even phase */
7
             for (i = 1; i < n; i += 2)
8
9
                if (a[i-1] > a[i]) {
10
                   temp = a[i];
                    a[i] = a[i-1]:
11
                    a[i-1] = temp:
12
13
14
          } else { /* Odd phase */
             for (i = 1; i < n-1; i += 2)
15
16
                if (a[i] > a[i+1]) {
                   temp = a[i];
17
                    a[i] = a[i+1]:
18
                    a[i+1] = temp;
19
20
                 }
21
       /* Odd_even_sort */
22 }
```

Communications Among Tasks in Odd-Even Sort

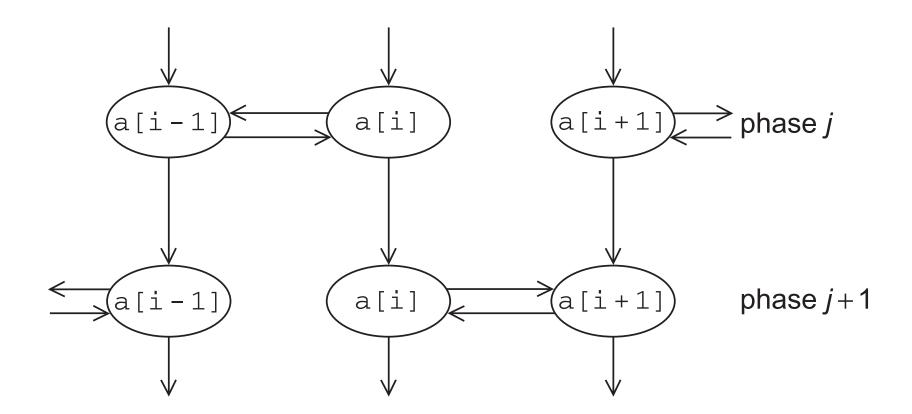


Figure 3.11

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

Parallel Odd-Even Transposition Sort

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

Theorem: If parallel odd-even transposition sort is run with p processes, then after p phases the list will be sorted.

Pseudo-Code

```
Sort local keys;
for (phase = 0; phase < comm_sz; phase++) {</pre>
   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;
                              /* Even rank */
   else
      partner = my_rank + 1;
else
                       /* Odd phase */
  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;
```

MPI_PROC_NULL is a constant defined by MPI. If used as source or destination, no communication will take place and the communication call will simply return

Watch Out for Deadlocks

A straight-forward implementation would communicate as follows

MPI_Send(msg, size, MPI_INT, (my_rank+1) % comm_sz, 0, comm); MPI_Recv(new_msg, size, MPI_INT, (my_rank+comm_sz-1) % comm_sz, 0, comm, MPI_STATUS_IGNORE).

Problem

MPI rank 1

MPI rank 2

MPI_Send(... dest=2, ...)

may block until received by rank 2

MPI_Send(... dest=1, ...)

may block until received by rank 1

Safety in MPI programs

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

Hence, if MPI_Send executed by each process blocks, no process will be able to start executing a call to MPI_Recv

- the program will hang or deadlock
- each process is blocked waiting for an event that will never happen.

Safety in MPI programs

- 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.

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

int	MPI_Ssend(
	void*	msg_buf_p	/*	in	*/,
	int	msg_size	/*	in	*/,
	MPI_Datatype	msg_type	/*	in	*/,
	int	dest	/*	in	*/,
	int	tag	/*	in	*/,
	MPI_Comm	communicator	/*	in	*/);

MPI_Ssend function signature

 We can experimentally check whether a program is safe by replacing all MPI_Send calls with MPI_Ssend and check for crashes or deadlocks

Restructuring Communication

MPI_Send(msg, size, MPI_INT, (my_rank+1) % comm_sz, 0, comm); MPI_Recv(new_msg, size, MPI_INT, (my_rank+comm_sz-1) % comm_sz,

O, comm, MPI_STATUS_IGNORE).



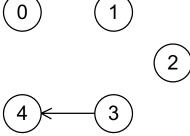
Manual communication scheduling: change order of send and receive for every other process

```
if (my_rank % 2 == 0) {
    MPI_Send(msg, size, MPI_INT, (my_rank+1) % comm_sz, 0, comm);
    MPI_Recv(new_msg, size, MPI_INT, (my_rank+comm_sz-1) % comm_sz,
        0, comm, MPI_STATUS_IGNORE).
} else {
    MPI_Recv(new_msg, size, MPI_INT, (my_rank+comm_sz-1) % comm_sz,
        0, comm, MPI_STATUS_IGNORE).
    MPI_Send(msg, size, MPI_INT, (my_rank+1) % comm_sz, 0, comm);
}
```

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



•		\bigcirc \bigcirc			
int	MPI_Sendrecv(Time 2			
	void*	send_buf_p	/*	in	*/,
	int	send_buf_size	/*	in	*/,
	MPI_Datatype	send_buf_type	/*	in	*/,
	int	dest	/*	in	*/,
	int	send_tag	/*	in	*/,
	void*	recv_buf_p	/*	out	*/,
	int	recv_buf_size	/*	in	*/,
	MPI_Datatype	recv_buf_type	/*	in	*/,
	int	source	/*	in	*/,
	int	recv_tag	/*	in	*/,
	MPI_Comm	communicator	/*	in	*/,
	MPI_Status*	status_p	/*	in	*/);

MPI_Sendrecv function signature

MPI_Sendrecv_replace

int	<pre>int MPI_Sendrecv_replace(</pre>						
	void*	buf_p	/*	in/out	*/,		
	int	buf_size	/*	in	*/,		
	MPI_Datatype	buf_type	/*	in	*/,		
	int	dest	/*	in	*/,		
	int	send_tag	/*	in	*/,		
	int	source	/*	in	*/,		
	int	recv_tag	/*	in	*/,		
	MPI_Comm	communicator	/*	in	*/,		
	MPI_Status*	status_p	/*	in	*/);		

MPI_Sendrecv_replace function signature

same functionality as MPI_Sendrecv but replaces data in send buffer with received data

Parallel Odd-Even Transposition Sort

Further optimization, sort local lists only once

```
void Merge_low(
     int my_keys[], /* in/out */
      int recv_keys[], /* in */
      int temp_keys[], /* scratch */
      int local_n /* = n/p, in */ {
   int m_i, r_i, t_i;
  m_i = r_i = t_i = 0:
  while (t_i < local_n) {</pre>
     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++)</pre>
     my_keys[m_i] = temp_keys[m_i];
  /* Merge_low */
}
```

merging avoids sorting lists that are already sorted

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)

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
- 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 (strongly) scalable
- An MPI program is unsafe if its correct behavior depends on the fact that MPI_Send is buffering its input

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- Illustrations for MPI collectives taken from the excellent MPI tutorial published by Lawrence Livermore National Lab
 - <u>https://computing.llnl.gov/tutorials/mpi/</u>

Change log

1.2.3 (2017-11-20)

- add slide 102 to clarify deadlock situation
- clarify slides 108, 109

1.2.2 (2017-11-06)

- clarify slides 49, 72
- remove slide 102 (safe communication with 5 processes)

1.2.1 (2017-10-24)

- extend table of contents (teaser for Advanced MPI section)
- clarify slide 20, 22
- fix error on slide 38 (also in book) Get_input instead of Get_data
- correction of spelling and grammatical errors

1.2.0 (2017-10-23)

- updated for winter term 2017/18
- clarify slide 16
- add information on wildcards slide 21
- cosmetics (title case)

Change log

1.1.0 (2017-07-13)

- fix typos on slide 40

1.0.3 (2016-12-01)

- add slide 71 for clarification of matrix / vector distribution
- cosmetics and correction of minor typos

1.0.2 (2016-11-29)

- slide 49, clarify kind of reduction and receiver in example
- add slide numbers everywhere

1.0.1 (2016-11-24)

- cosmetic changes to part 1, initial version of remaining slides

1.0.0 (2016-11-24)

- initial version of slides (part 1)