# 并行计算

(Parallel Computing)

# 分布式内存编程 - MPI

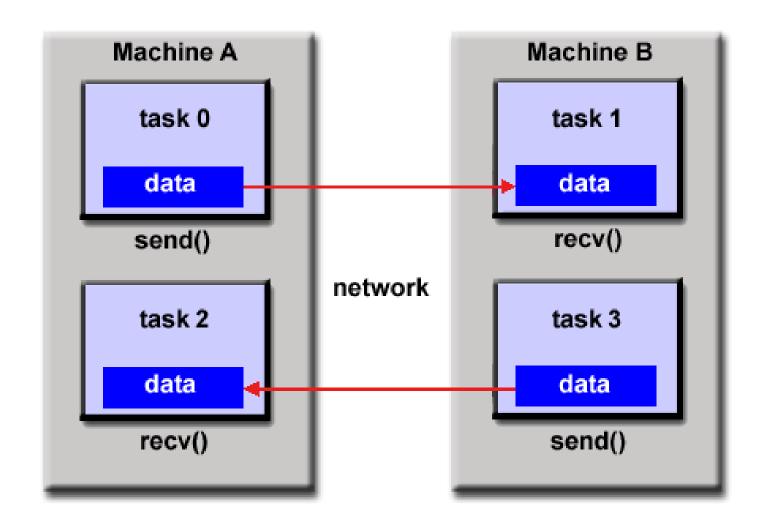
# 学习内容:

- 第一个 MPI 程序
- 梯形法则(Trapezoidal Rule)求面积
- 集体通信(Collective communication)

# 分布式内存编程 - MPI

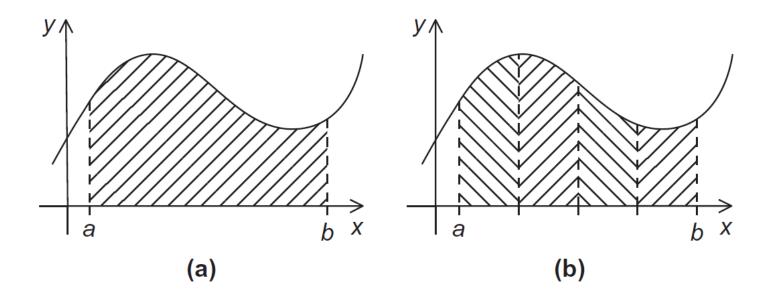
# 学习内容:

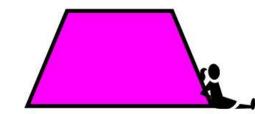
- MPI 中的派生数据类型(derived datatypes)
- MPI 程序的性能评价
- 并行排序
- MPI 程序的安全性



```
MPI include file
    Declarations, prototypes, etc.
          Program Begins
                          Serial code
      Initialize MPI environment
                                 Parallel code begins
Do work & make message passing calls
     Terminate MPI environment Parallel code ends
                          Serial code
           Program Ends
```

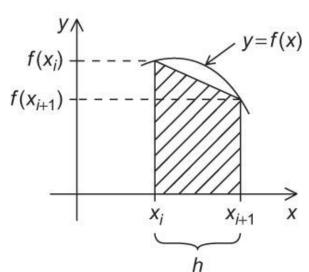
```
#include "mpi.h"
#include <stdio.h>
#include <stdlib.h>
int main (int argc, char *argv[])
int numtasks, rank, dest, source, rc, count, tag=1;
char inmsq, outmsq='x';
MPI Status Stat;
MPI Init(&argc,&argv);
MPI Comm size(MPI COMM WORLD, &numtasks);
MPI Comm rank (MPI COMM WORLD, &rank);
if (rank == 0) {
  dest = 1;
  source = 1;
  rc = MPI Send(&outmsq, 1, MPI CHAR, dest, taq, MPI COMM WORLD);
  rc = MPI Recv(&inmsg, 1, MPI CHAR, source, tag, MPI COMM WORLD, &Stat);
else if (rank == 1) {
  dest = 0;
  source = 0;
  rc = MPI Recv(&inmsg, 1, MPI CHAR, source, tag, MPI COMM WORLD, &Stat);
  rc = MPI Send(&outmsg, 1, MPI CHAR, dest, tag, MPI COMM WORLD);
MPI Finalize();
```





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

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



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

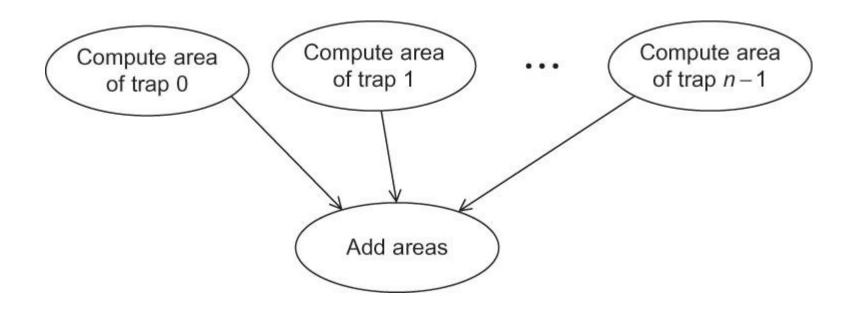
Sum of trapezoid areas = 
$$h[f(x_0)/2 + f(x_1) + f(x_2) + \dots + f(x_{n-1}) + f(x_n)/2]$$

●串行程序的伪代码

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

```
/* Input: a, b, n */
h = (b-a)/n;
approx = (f(a) + f(b))/2.0;
for (i = 1; i <= n-1; i++) {
    x_i = a + i*h;
    approx += f(x_i);
}
approx = h*approx;</pre>
```

- > 将问题解决方案划分为任务
- ▶ 确认任务之间的通信
- > 聚合任务为组合任务
- ➤ 将确定的任务映射到 core



```
●并行化
```

```
Get a, b, n;
      h = (b-a)/n;
      local_n = n/comm_sz;
      local a = a + my rank*local n*h;
4
5
      local_b = local_a + local_n*h;
6
      local integral = Trap(local_a, local_b, local_n, h);
      if (my_rank != 0)
         Send local integral to process 0;
      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;
```

```
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;
      int source:
6
      MPI Init(NULL, NULL);
8
      MPI Comm rank (MPI COMM WORLD, &my rank);
9
      MPI Comm size (MPI COMM WORLD, &comm sz);
10
11
      h = (b-a)/n; /* h is the same for all processes */
      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);
```

```
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 (my_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 */
```

```
double Trap(
 2
         double left_endpt /* in */,
         double right_endpt /* in */,
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;
10
      for (i = 1; i \le trap_count - 1; i++) {
11
         x = left endpt + i*base len;
12
         estimate += f(x);
13
14
      estimate = estimate * base len;
15
16
      return estimate;
17
         Trap */
```

# 3.处理 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 */
```

# 3.处理 I/O

```
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



#### 3.处理 I/O

#### ●输入

- ▶大多数 MPI 的实现仅允许 MPI\_COMM\_WORLD 中的进程 0 访问 stdin
- ▶进程 0 必须读取数据 (scanf) 并发送给其他进程

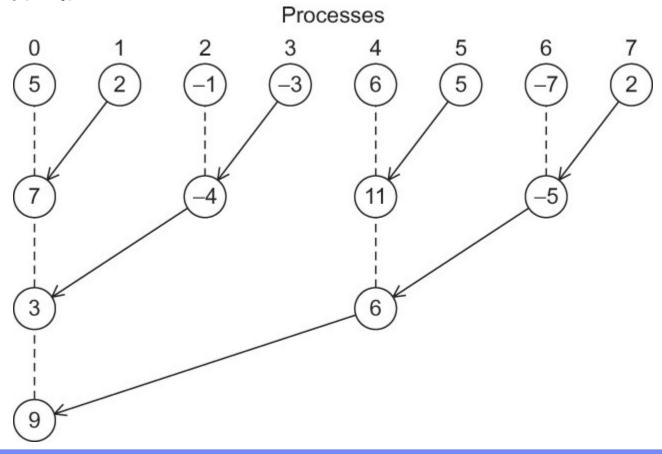
```
MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
MPI_Comm_size(MPI_COMM_WORLD, &comm_sz);
Get_input(my_rank, comm_sz, &a, &b, &n);
h = (b - a)/n;
...
```

### 3.处理 I/O void Get\_input(

●输入

```
int my_rank /* in */,
  int comm_sz /* in */,
  double * a_p /* out */,
  double* b_p /* out */,
  int*
       n_p /* 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 */
```

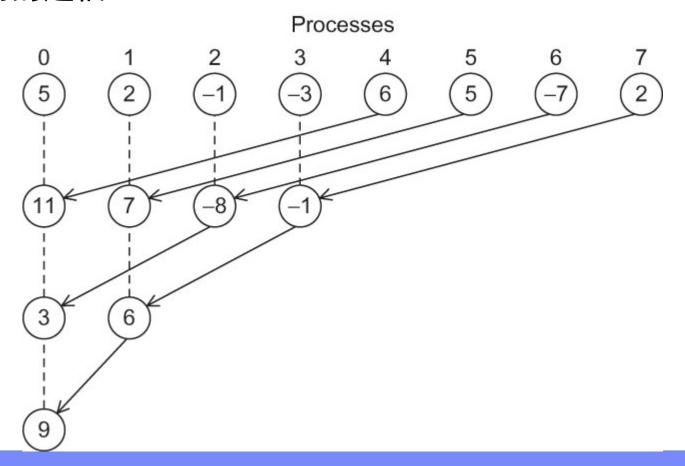
●树结构的通信



#### ●树结构的通信

- a. 进程 1, 3, 5, 7 分别发送数据给进程 0, 2, 4, 6
- b. 进程 0, 2, 4, 6 累加接收到的值
- c. 进程2和6分别发送累加后的值给进程0和4
- d. 进程 0 和 4 累加接收到的值
- e. 进程 4 发送新的累加值给进程 0
- f. 进程 0 累加接收到的值

●树结构的通信

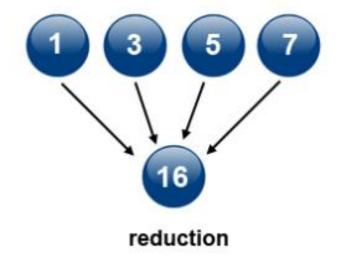


#### MPI\_Reduce

- ▶实现 global\_sum 的方法有很多,如何比较它们哪个最优?
- ➤ MPI 提供了 global sum 函数,由 MPI 的实现来完成优化工作
- ▶不同于 MPI\_Send MPI\_Recv, global sum 函数需要多于两个进程之间进行 通信,在梯形法则求面积的例子中,包含了 MPI\_COMM\_WORLD 中所有的 进程
- ➤ 这种通信称为 collective commnunication
- ➤ MPI\_Send MPI\_Recv 称为点对点通信

MPI\_Reduce

MPI\_Reduce



●MPI\_Reduce

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

- ●集体通信 vs. 点对点通信
  - ➤ 通信器中的所有进程必须调用同一 collective 通信函数
    - 例如: 一个进程中调用 MPI\_Reduce, 另一个进程中调用 MPI\_Recv, 将 会产生错误
  - ▶每个进程传递给集体通信的参数必须"兼容"
    - 例如:如果一个进程传递 0 作为 dest\_process 而另一个进程传递 1,则 MPI\_Reduce 的结果是错误的
  - ➤ output\_data\_p 参数只在 dest\_process 中使用。其他进程也需传递实参给 output\_data\_p, 即使只传递 NULL

- ●集体通信 vs. 点对点通信
  - ▶点对点通信通过 tag 和通信器匹配
  - ▶集体通信不使用 tag
  - ▶ 它们仅通过通信器和调用的顺序来匹配

●集体通信 vs. 点对点通信

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,)

Multiple calls to MPI\_Reduce

- ●集体通信 vs. 点对点通信
  - ➤每个进程以运算符 MPI\_SUM 调用 MPI\_Reduce, 目的进程为进程 0

$$> b = 3, d = 6?$$

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,)

- ●集体通信 vs. 点对点通信
  - ▶内存位置的名称与匹配 MPI\_Reduce 调用无关
  - ➤调用的顺序决定了 MPI\_Reduce 的匹配
  - ➤ 因此,b=1+2+1=4, d=2+1+2=5

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,)

- ●集体通信 vs. 点对点通信
  - ▶输入和输出使用同一缓冲区,为非法调用,结果不可预测

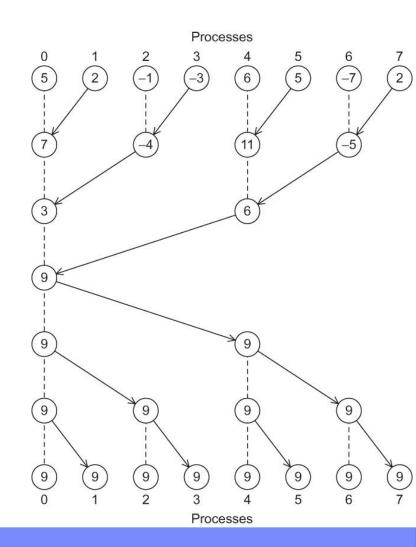
```
MPI_Reduce(&x, &x, 1, MPI_DOUBLE, MPI_SUM, 0, comm);
```

- MPI\_Allreduce
  - ▶当所有的进程都需要计算结

果(如: sum)以进行后续的

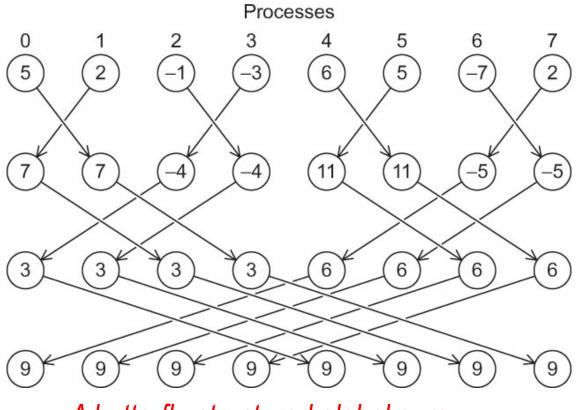
计算

A global sum followed by distribution of the result.





MPI\_Allreduce



A butterfly-structured global sum.

- MPI\_Allreduce
  - ▶ 同样的,我们不希望去决定使用哪种通信结构,如何去优化代码
  - ➤ MPI 提供了 MPI Reduce 的变种, 在所有进程中存放结果

- ●广播 (Broadcast)
  - > 将属于一个进程的数据发送到通信器中的所有进程

> source\_proc 进程将 data\_p 指向的内容发送给 comm 通信器中的所有进程

●广播(Broadcast)

```
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 */
```

#### ●数据分布

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

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

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

$$= \mathbf{z}$$

Compute a vector sum.

●数据分布

```
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>
```

- ●数据分布
  - ▶并行化
    - 对应元素相加
    - 任务之间不需要通信
    - 映射到核心(core): 如何划分?
      - 块划分(block partition)
      - 循环划分(cyclic partition)
      - 块-循环划分(block-cyclic partition)

- ●数据分布
  - ▶并行化
    - 将12维向量映射到3个进程的不同划分

	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

#### ●数据分布

▶并行化

```
void Parallel_vector_sum(
double local_x[] /* in */,
double local_y[] /* in */,
double local_z[] /* out */,
int local_n /* in */) {
int local_i;

for (local_i = 0; local_i < local_n; local_i++)
    local_z[local_i] = local_x[local_i] + local_y[local_i];
} /* Parallel_vector_sum */</pre>
```

- ●分发 (Scatter)
  - ▶进程0读入向量x和y,广播给其他进程?
    - 如果10个进程,向量为10000维
    - 每个进程为向量分配10000维空间,仅操作其中的1000维
    - 如果采用块划分,我们希望进程0仅发送1000-1999维给进程1,2000-2999
       给进程2,.....

#### ●分发 (Scatter)

➤MPI\_Scatter 可以用来在进程 0 读入整个向量,向其他进程发送它们所需的数据

- ●分发 (Scatter)
  - ▶如果通信器 comm 包含 comm\_sz 个进程,则 MPI\_Scatter 将 send\_buf\_p 指向的数据分成 comm\_sz 份,第一份发给进程 0,第二份发给进程 1,以此类推
  - ▶ 其他进程将本地向量作为 rece\_buf\_p 参数,将 local\_n 作为 recv\_count 参数

#### ●分发 (Scatter)

- ▶假设使用块划分,进程0读入向量的所有n维数据到send\_buf\_p中
- ▶进程 0 获得第一块 local\_n = n / comm\_sz 维数据,进程1获得下一块 local\_n
- ▶每个进程传递本地向量作为 recv\_buf\_p 参数, recv\_count 应为 local\_n
- ▶ send\_count 应为发送给每个进程的数据量,即: local\_n

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

- ●收集(Gather)
  - ▶进程0收集向量的所有分量进行后续处理

- ●收集(Gather)
  - ▶进程 0 中由 send\_buf\_p 引用的数据存放在 recv\_buf\_p 中第一块位置,进程 1 中由 send\_buf\_p 引用的数据存放在 recv\_buf\_p 中第二块位置,以此类推
  - ➤ recv\_count 为从每个进程接收到的数据量

```
int MPI Gather(
     void*
                   send_buf_p /* in
                                     */,
     int
                   send_count /* in
                                     */,
                   send_type /* in
                                     */,
     MPI_Datatype
            recv_buf_p /* out
     void*
                                     */,
     int
                   recv_count /* in
                                     */,
                  recv_type /* in
                                     */,
     MPI_Datatype
     int
                              /* in
                   dest_proc
                                     */,
                                     */);
     MPI Comm
                              /* in
                   comm
```

●收集(Gather)

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

●全收集(Allgather): 矩阵与向量相乘

$$A = (a_{ij})$$
 is an  $m \times n$  matrix

 $\mathbf{x}$  is a vector with n components

y = Ax is a vector with m components

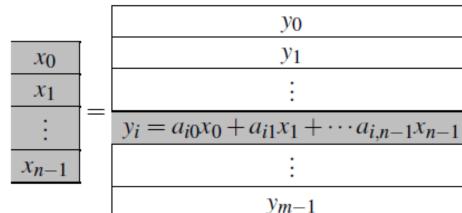
$$y_i = a_{i0}x_0 + a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{i,n-1}x_{n-1}$$

i-th component of y

Dot product of the i-th row of A with x.

●全收集(Allgather): 矩阵与向量相乘

<i>a</i> <sub>00</sub>	<i>a</i> <sub>01</sub>	• • •	$a_{0,n-1}$
$a_{10}$	$a_{11}$	:	$a_{1,n-1}$
:	•••		
$a_{i0}$	a.		<i>a</i> : _ 1
410	$a_{i1}$		$a_{i,n-1}$
:	:		:



●全收集(Allgather): 矩阵与向量相乘

```
/* For each row of A */
for (i = 0; i < m; i++) {
    /* Form dot product of ith row with x */
    y[i] = 0.0;

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

Serial pseudo-code

●全收集(Allgather): 矩阵与向量相乘

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

●全收集(Allgather): 矩阵与向量相乘

```
void Mat_vect_mult(
       double A[] /* in */,
        double x[] /* in */,
  double y[] /* out */,
  int m /* in */,
     int n /* in */) {
   int i, j;
9
     for (i = 0; i < m; i++) {
        y[i] = 0.0;
10
        for (j = 0; j < n; j++)
11
           y[i] += A[i*n+j]*x[j];
12
13
    /* Mat_vect_mult */
14
```

- ●全收集(Allgather): 矩阵与向量相乘
  - ▶并行化
    - y[i] += A[i \* n + j] \* x[j];
    - 将 A 按行划分
    - y[i] 的计算包含了 A 中第 i 行的所有元素和 x 中的所有元素

- ●全收集(Allgather): 矩阵与向量相乘
  - ▶并行化
    - 为减少通信,将 x 中的所有元素分配给每个进程
    - 实际应用中,矩阵与向量相乘的结果 y 可能是下一次相乘的输入
    - 如何使得每个进程获得相乘的结果?
    - MPI\_Gather + MPI\_Bcast ?

- ●全收集(Allgather): 矩阵与向量相乘
  - ▶并行化
    - 将每个进程的 send\_buf\_p 的内容拼接起来存放到每个进程的 recv\_buf\_p
    - recv\_count 为从每个进程接收到的数据量

●全收集(Allgather): 矩阵与向量相乘

▶并行化

```
void Mat_vect_mult(
         double local_A[] /* in */,
         double local_x[] /* in */,
         double local_y[] /* out */,
4
         int local_m /* in */, int n /* in */,
5
6
7
         int local_n /* in */,
         MPI_Comm comm /* in */) {
8
      double* x:
9
      int local_i, j;
10
11
      int local_ok = 1:
12
      x = malloc(n*sizeof(double));
13
      MPI_Allgather(local_x, local_n, MPI_DOUBLE,
14
            x. local_n, MPI_DOUBLE, comm);
15
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
20
             local_y[local_i] += local_A[local_i*n+j]*x[j];
21
      free(x):
22
      /* Mat_vect_mult */
23
```

- ●集体操作的类型
  - ▶同步(Synchronization): 进程等待组内其他进程到达同步点
  - ➤数据移动(Data Movement): broadcast, scatter/gather
  - ▶集体计算(Collective Computation): 一个进程收集其他进程的数据,并对该数据进行操作(min, max, add, multiply 等)

