Lecture 10

int MPI_Cart_shift (MPI_Comm comm, int direction, int displ, int *source, int *dest)

comm - communicator with Cartesian structure

direction - coordinate dimension of shift, in range [0,n-1] for an n-dimensional Cartesian grid

displ - displacement (> 0: upwards shift, < 0: downwards shift), with periodic wraparound possible if communicator created with periodic boundary conditions turned on

Outputs are possible inputs to MPI_Sendrecv :

source - rank of process to receive data from, obtained by subtracting displ from coordinate determined by direction

dest - rank of process to send data to, obtained by adding displ to coordinate determined by direction

These may be undefined (i.e. = MPI_PROC_NULL) if shift points outside grid structure and the periodic boundary conditions off

MPI_Cart_shift(comm, 1, 1, &source, &dest);

0	1	2
(0,0)	(0,1)	(0,2)
2,1	0,2	1,0
3	4	5
(1,0)	(1,1)	(1,2)
5,4	3,5	4,3
6	7	8
(2,0)	(2,1)	(2,2)
8,7	6,8	7,6

Communicator defined with periodic boundary conditions

MPI_Cart_shift(comm, 1, 1, &source, &dest);

0	1	2
(0,0)	(0,1)	(0,2)
-1,1	0,2	1,-1
3	4	5
(1,0)	(1,1)	(1,2)
-1,4	3,5	4,-1
6	7	8
(2,0)	(2,1)	(2,2)
-1,7	6,8	7,-1

Communicator NOT defined with periodic boundary conditions

MPI_Cart_shift(comm, 0, -1, &source, &dest);

0	1	2
(0,0)	(0,1)	(0,2)
3,-1	4,-1	5,-1
3	4	5
(1,0)	(1,1)	(1,2)
6,0	7,1	8,2
6	7	8
(2,0)	(2,1)	(2,2)
-1,3	-1,4	-1,5

Communicator NOT defined with periodic boundary conditions

Graph topology

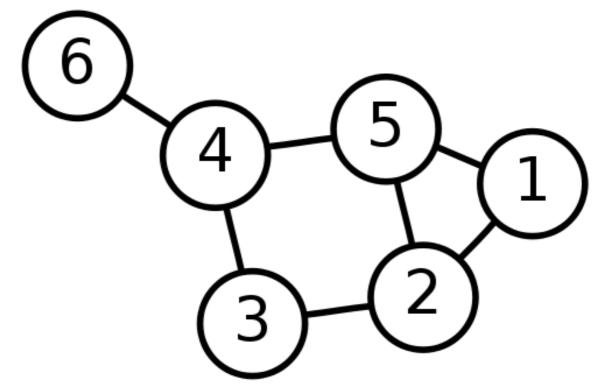
Graph - abstract representation of a set of objects (vertices, nodes, points) where some pairs are connected by links (edges)

The degree of a vertex is the number of edges that connect to it

In MPI topology, vertices usually stand for processes and edges for communications links

However, it is still possible to send a message between any two vertices, they do not have to be connected

Edges may represent optimal (fast) communications links



MPI_Graph_create

int MPI_Graph_create (MPI_Comm comm_old, int nnodes, int *index , int *edges , int reorder , MPI_Comm *comm_graph)

Creates a communicator with a graph topology attached
comm_old - input communicator without topology

nnodes - number of nodes in graph

index - array of integers describing node degrees

edges - array of integers describing graph edges

reorder - ranking may be reordered (true) or not (false) (logical)

comm graph - communicator with graph topology added

The *i*-th entry of *index* stores the total number of neighbours of the first *i* graph nodes (i.e. *index* is cumulative)

The list of neighbours of nodes 0, 1, . . . , *nnodes*-1 are stored in consecutive locations in array edges (each edge counted twice since bi-directional communication assumed)

Example:

Assume 4 processes such that

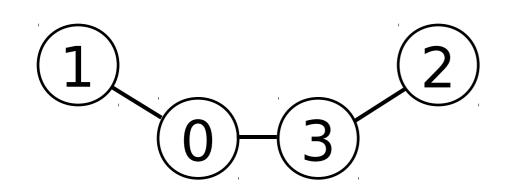
The input should be

nnodes = 4

index = (2,3,4,6)

edges = (1,3,0,3,0,2)

process	neighbours		
0	1,3		
1	0		
2	3		
3	0,2		



Some graph topology functions

MPI_Graphdims_get - returns number of nodes and edges in a graph

MPI_Graph_get - returns index and edges as supplied to MPI_Graph_create

MPI_Graph_neighbours_count - returns the number of neighbours of a given process

MPI_Graph_neighbours - returns the edges associated with given process

MPI Graph map - returns a graph topology recommended by the MPI system

Overall, graph topology is more general that Cartesian, but not widely used as it is less convenient for many problems

If the computational problem cannot be represented in a Cartesian grid topology, then most likely load balancing becomes a serious issue to be addressed

Communicators and Topologies: Matrix Multiplication Example

Fox's algorithm

A and B are n x n matrices

Compute C = AB in parallel

Let $q = \operatorname{sqrt}(p)$ be an integer such that it divides n, where p is the number of processes

Create a Cartesian topology with processes (i,j), i,j=0,...,q-1

Denote nb = n/q

Distribute A and B by blocks on p processes such that $A_{i,j}$ and $B_{i,j}$ are nb x nb blocks stored on process (i,j)

Algorithm goal

Perform the operation with as few communications as possible

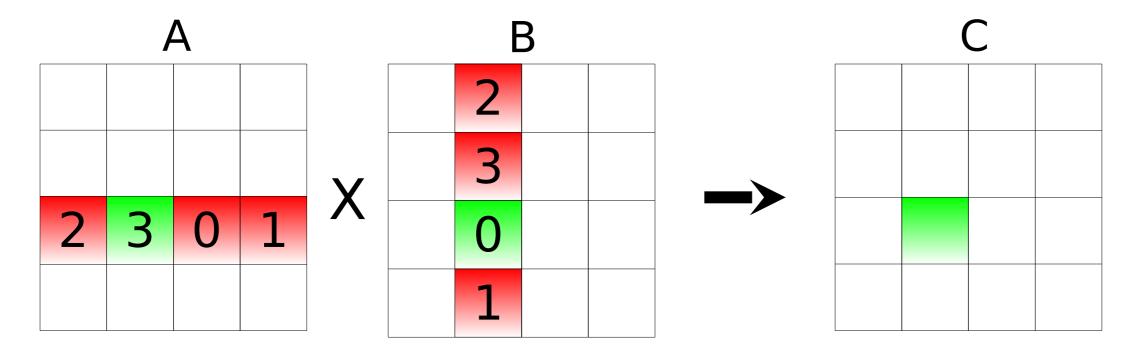
Have a clear communication scheme that results in effective code

On process (i,j), we want to compute

$$C_{i,j} = A_{i,0}B_{0,j} + A_{i,1}B_{1,j} + ... + A_{i,n-1}B_{n-1,j}$$

Rewrite this as

Example: 4 x 4 block matrix



Highlighted blocks need to compute result block for process



Available to process at start



Has to be received from other processors

Numbers indicate order in which operations are done

```
Initially, assume C_{i,j} = 0, the zero block, on each (i,j)

Process (i,j) at stage 0:

- (i,j) has B_{i,j}

- (i,j) needs A_{i,i} which it has to get from process (i,i)

- (i,i) broadcasts A_{i,i} across processor row i

- C_{i,j} = C_{i,j} + A_{i,i}B_{i,j}
```

Process (i,j) at stage 1:

- (i,j) has $B_{i,j}$, but needs $B_{i+1,j}$ Shift the j-th block column of B by one block up Block 0 goes to block q-1
- (i,j) needs $A_{i,i+1}$ which it has to get from process (i,i+1)
- (i,i+1) broadcasts A_{i,i+1} across processor row i
- $C_{i,j} = C_{i,j} + A_{i,i+1}B_{i+1,j}$

Similarly on next stages

Algorithm outline

```
On process (i,j)
q = sqrt(p)
for s=0 to q-1
 k = (i+s) \mod q
 broadcast A<sub>i,k</sub> across row i
 C_{i,i} = C_{i,i} + A_{i,k}B_{k,i}
 send B_{k,j} to ((i-1) mod q, j)
 receive B_{k+1,i} from ((i+1) mod q,j)
```

Implementation (just essential parts)

```
/* setupgrid.c */
void Setup grid(GRID INFO_T* grid)
 int old rank;
 int dimensions[2];
 int wrap around[2];
 int coordinates[2];
 int free coords[2];
 /* Set up Global Grid Information */
 MPI Comm size(MPI COMM WORLD, &(grid->p));
 MPI Comm rank(MPI COMM WORLD, &old rank);
 /* We assume p is a perfect square */
 grid > q = (int) sqrt((double) grid > p);
 dimensions[0] = dimensions[1] = grid->q;
 /* We want a circular shift in second dimension. */
 /* Don't care about first
 wrap around[0] = wrap around[1] = 1;
```

```
MPI Cart create(MPI COMM WORLD, 2, dimensions,
         wrap around, 1, &(grid->comm));
MPI Comm rank(grid->comm, &(grid->my rank));
MPI Cart coords(grid->comm, grid->my rank, 2,
         coordinates);
grid->my row = coordinates[0];
grid->my col = coordinates[1];
/* Set up row communicators */
free coords[0] = 0;
free coords[1] = 1;
MPI Cart sub(grid->comm, free coords, &(grid->row comm));
/* Set up column communicators */
free coords[0] = 1;
free coords[1] = 0;
MPI Cart sub(grid->comm, free coords, &(grid->col comm));}
```

```
void Fox(int n,GRID INFO T* grid,
     LOCAL MATRIX T* local A, LOCAL MATRIX T* local B,
     LOCAL MATRIX T* local C)
 LOCAL MATRIX T* temp A;
 int
           stage;
           bcast root;
 int
           n bar; /* n/sqrt(p)
 int
 int
           source;
 int dest;
 MPI Status status;
 n bar = n/grid > q;
 Set to zero(local C);
 /* Calculate addresses for circular shift of B */
 MPI Cart shift (grid->col comm, 0, -1, &source, &dest);
 /* Set aside storage for the broadcast block of A */
 temp A = Local matrix allocate(n bar);
```



```
for (stage = 0; stage < qrid > q; stage++)
  bcast root = (grid->my row + stage) % grid->q;
  if (bcast root == grid->my col)
     MPI Bcast(local A, 1, local matrix mpi t,
           bcast root, grid->row comm);
     Local matrix multiply(local A, local B,
                   local C);
  else
     MPI Bcast(temp A, 1, local matrix mpi t,
           bcast root, grid->row comm);
     Local matrix multiply(temp A, local B,
                   local C);
  MPI_Sendrecv_replace(local_B, 1, local_matrix_mpi_t,
               dest, 0, source, 0,
               grid->col comm, &status);
```

Grouping Data for Communication

Introduction

In general, sending a message may be an expensive operation

Rule of thumb: the fewer messages send, the better the performance of the program

MPI provides three mechanisms for grouping individual data items into a single message:

- count parameter, which we have already seen before
- derived datatypes
- MPI Pack/MPI Unpack routines

Consider send and receive

Their execution can be divided into two phases:

- startup
- communication

Their cost varies among systems

Denote the runtime of the startup phase by t_s , and the communication phase by t_c

The cost of sending a message of k units is

$$t_s + k * t_c$$

Usually t_s is much larger than t_c

Their values vary among systems

It generally pays to group data before sending/receiving, in order to reduce the number of times that communication needs to be started.

This will be especially important for messages of small size (i.e. small k)

Simplest grouping

Use *count* parameter, as discussed in previous lectures.

```
int MPI_Send (void *buf, int count, MPI_Datatype datatype, int dest, int tag, MPI_Comm comm)
```

```
int MPI_Bcast ( void *buffer, int count, MPI_Datatype datatype,
    int root, MPI_Comm comm )
```

Derived Types

Say we want to send in one communication real numbers a and b, and integer n.

```
Suppose we try:

typedef struct {
  float a;
  float b;
  int n;
} INDATA_T

/* ... */
INDATA_T indata;

/* ... */
MPI_Bcast(&indata, 1, INDATA_T,0,MPI_COMM_WORLD);
```

Will not work. Arguments to functions must be variables, not defined types.

Need a method of defining a type that can be used as a function argument, i.e. a type that can be stored in a variable.

MPI provides just such a type: MPI_Datatype

We do not assume that a,b,n are contiguous in memory. For example, consider the case when they are defined and stored on process 0 as:

	Variable	A	ddress	Conte	ents	
	a		24	0.0	0	
	b		40	1.0	0	
	n		48	102	24	
	 a			<u> </u>	<u>n</u>	
Memory						
	24	16	40	4	8	
	←	2	4	>	•	

We would like to send this data in a single message while preserving the relative arrangement in memory, i.e. displacement between *a* and *b* should remain 16 bytes, and between *a* and *n* remain 24 bytes.

Information needed to send the a,b,n data from the example

- 1. There are three elements to be transmitted
- 2.a. 1st element is a float
 - b. 2nd element is a float
 - c. 3rd is an int
- 3.a. 1st is displaced 0 bytes from the beginning of message
 - b. 2nd element is displaced 16 bytes from beginning of message
 - c. 3rd element is displaced 24 bytes from beginning of message
- 4. The beginning of the message has address &a

New datatype will store information from section 1, 2 and 3.

Each of the receiving processes can determine exactly where the data should be received.

The principle behind MPI's derived types is to provide all the information except the address of the beginning of message in a new MPI datatype.

Then when program calls MPI_Send, MPI_Recv etc, it simply provides the address of the first element and the communications system can determine exactly what needs to be sent and received.

MPI Type struct

count - number of elements (or blocks, each containing an array of contiguous elements)

blocklens[] - number of elements in each block

indices[] - byte displacement of each block.MPI_Aint is a special type for storing addresses, can handle addresses longer than can be stored in int

old_types[] - type of elements in each block. These can be datatypes created by previous MPI_Type_struct calls

newtype - new datatype

In our previous example, all *blocklens* entries would be 1, even though the first two had the same type, since all three elements were not contiguous in memory.

To be able to use the newly created datatype in communications, must call MPI_Type_commit

Example from P. Pacheco, PP with MPI

```
void Build derived type(
     float* a_ptr /* in */,
     float* b_ptr /* in */,
     int* n ptr /* in */,
     /* pointer to new MPI type */
     MPI Datatype* mesg mpi t ptr /* out */) {
  /* The number of elements in each "block" of the */
    new type. For us, 1 each.
  int block lengths[3];
  /* Displacement of each element from start of new */
     type. The "d i's."
  /* MPI Aint ("address int") is an MPI defined C */
  /* type. Usually an int.
  MPI Aint displacements[3];
  /* MPI types of the elements. The "t i's."
                                              */
 MPI Datatype typelist[3];
  /* Use for calculating displacements
                                             */
  MPI Aint start address;
  MPI Aint address;
  block lengths[0] = block lengths[1] = block lengths[2] = 1;
```

```
/* Build a derived datatype consisting of */
/* two floats and an int
typelist[0] = MPI_FLOAT;
typelist[1] = MPI FLOAT;
typelist[2] = MPI INT;
/* First element, a, is at displacement 0
                                           */
displacements[0] = 0;
/* Calculate other displacements relative to a */
MPI_Address(a ptr, &start address);
/* Find address of b and displacement from a */
MPI Address(b ptr, &address);
displacements[1] = address - start address;
/* Find address of n and displacement from a */
MPI Address(n ptr, &address);
displacements[2] = address - start address;
/* Build the derived datatype */
MPI_Type_struct(3, block_lengths, displacements,
  typelist, mesg mpi t ptr);
/* Commit it -- tell system we'll be using it for communication*/
MPI_Type_commit(mesg_mpi_t_ptr);}
```

```
void Get data3(
     float* a_ptr /* out */,
     float* b ptr /* out */,
     int* n ptr /* out */,
     int my rank /* in */) {
  MPI Datatype mesg mpi_t; /* MPI type corresponding */
                  /* to 2 floats and an int */
 if (my rank == 0){
     printf("Enter a, b, and n\n");
     scanf("%f %f %d", a ptr, b ptr, n ptr);
  }
  Build_derived_type(a_ptr, b_ptr, n_ptr, &mesg_mpi_t);
  MPI Bcast(a ptr, 1, mesg mpi t, 0, MPI COMM WORLD);
```

Other Derived Datatype Constructors

MPI_Type_struct is the most general datatype constructor in MPI

The user must provide a complete description of each element of the type.

If we have a special case where the data to be transmitted consists of a subset of the entries in an array, we should not need to provide such detailed information since all elements have the same basic type.

MPI provides three derived datatype constructors for this situation:

MPI_Type_contiguous - builds a derived datatype whose elements are contiguous entries in an array

MPI_Type_vector - does this for equally spaced entries in an array

MPI_Type_indexed - does this for arbitrary entries of an array

MPI_Type_contiguous

count - number of elements

old_type - old datatype

new_type - new datatype

Matrix Example

float A[10][10]; /* define 10 by 10 matrix */

C language stores two-dimensional arrays in row-major order. This means A[2][3] is preceded by A[2][2] and followed by A[2][4].

If we want to send, for example, third row of A from process 0 to process 1, this is easy

```
if (myrank == 0) {
    MPI_Send(&(A[2][0]),10, MPI_FLOAT,1,0,MPI_COMM_WORLD
    } else { /*my_rank = 1 */
    MPI_Recv(&(A[2][0]),10,MPI_FLOAT,0,0,MPI_COMM_WORLD, &status);
}
```

We could have defined a new datatype to handle the row of the matrix with MPI_Type_Contiguous, but clearly in this case there is little need since using just MPI_Send and MPI_Recv is so easy (and more efficient).

If we want to send the third column of A, then those entries no longer form a continuous block in memory, hence a single MPI_Send and MPI_Recv pair is no longer sufficient.

MPI_Type_vector

int MPI_Type_vector (int count, int blocklen, int stride, MPI_Datatype old_type, MPI_Datatype *newtype)

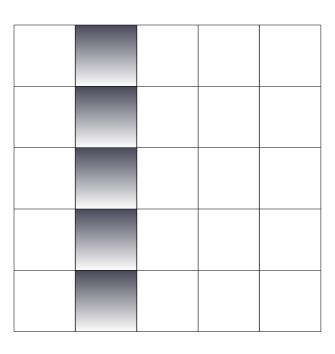
count - number of blocks

blocklen - number of elements in each block

stride - number of elements between start of each block

old_type - old datatype

new_type - new datatype



Example continued

```
/* column_mpi_t is declared to have type MPI_Datatype */

MPI_Type_vector(10,1,10,MPI_FLOAT, &column_mpi_t);

MPI_Type_commit(&column_mpi_t);

if (my_rank==0)
    MPI_Send(&(A[0][2]),1,column_mpi_t,1,0,MPI_COMM_WORLD)

else
    MPI_Recv(&(A[0][2]),1,column_mpi_1,0,0,MPI_COMM_WORLD, &status);

/* column_mpi_t can be used to send any column in any 10 by 10 matrix of floats */
```

MPI_Type_indexed

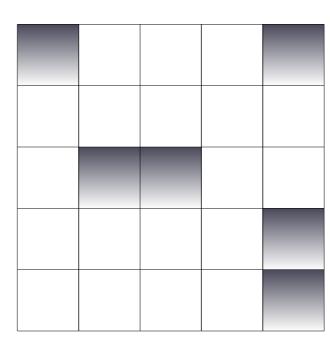
count - number of blocks, also number of entries in blocklens[] and in indices[]

blocklens[] - number of elements in each block

indices[] - displacement of each block in multiples of old_type

old_type - old type

newtype - new type



Can a pair of MPI_Send/MPI_Recv have different types?

Yes, as long as they are compatible.

For example, a type containing N floats will be compatible with type containing N floats, even if displacements between elements are different.

For example:

```
float A[10][10]; if (my_rank == 0 )  MPI\_Send(\&(A[0][0]),1,column\_mpi\_t,1,0,MPI\_COMM\_WORLD); \\ else if (my_rank == 1) \\ MPI\_Recv(\&(A[0][0],10,MPI\_FLOAT,0,0,MPI\_COMM\_WORLD,&status);
```

This will send the first column of the matrix A on process 0 to the first row of matrix A on process 1

In contrast, collective communications (eg. MPI_Bcast) must use the same datatype across all processes when called

Alternative: pack/unpack

MPI_Pack - allows one to explicitly store noncontiguous data in contiguous memory locations.

MPI_Unpack - can be used to copy data from a contiguous buffer into noncontiguous memory locations.

MPI_Pack

```
int MPI Pack (void *inbuf, int incount, MPI Datatype datatype,
       void *outbuf, int outcount, int *position, MPI Comm comm)
inbuf - input buffer start (what needs to be packed)
incount - number of input data items
datatype - datatype of each input data item
outbuf - output buffer start (packed message)
outcount - output buffer size, in bytes (size of container for message)
position - current position in buffer, in bytes (integer)
```

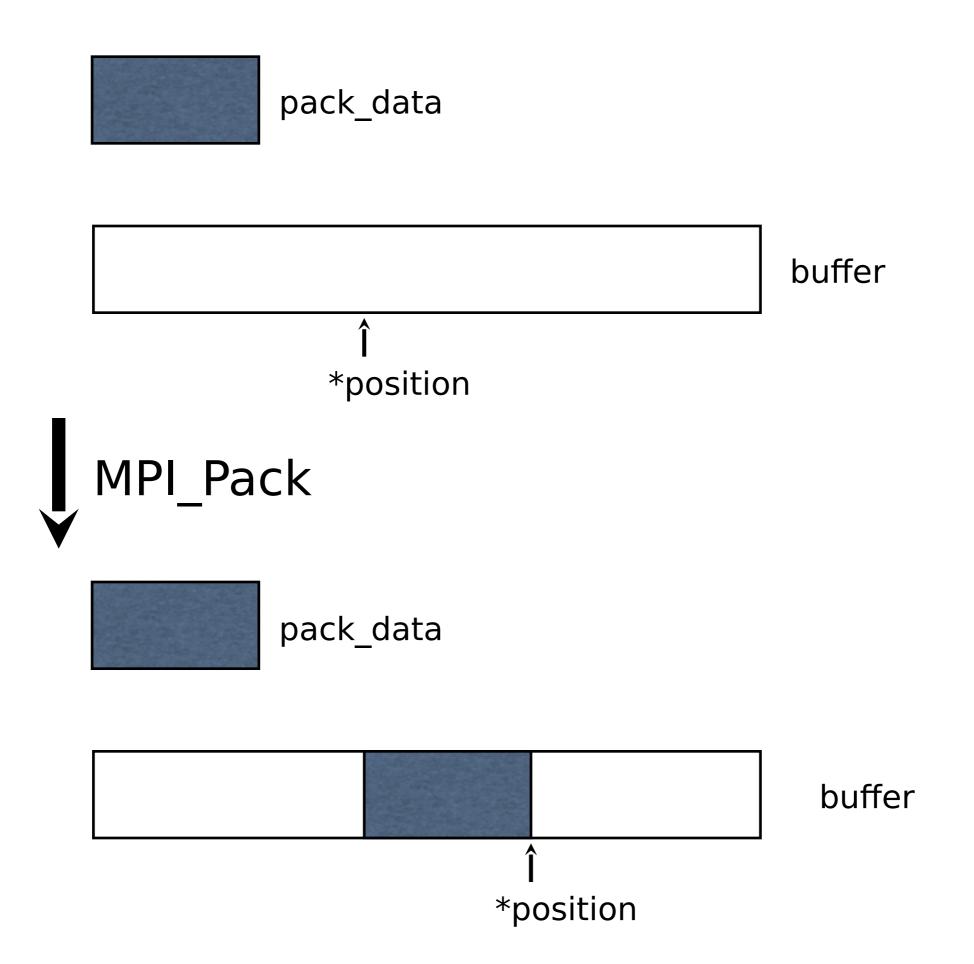
In a typical MPI_Pack call, position references the first free location in buffer (in that case position=0 for first call)

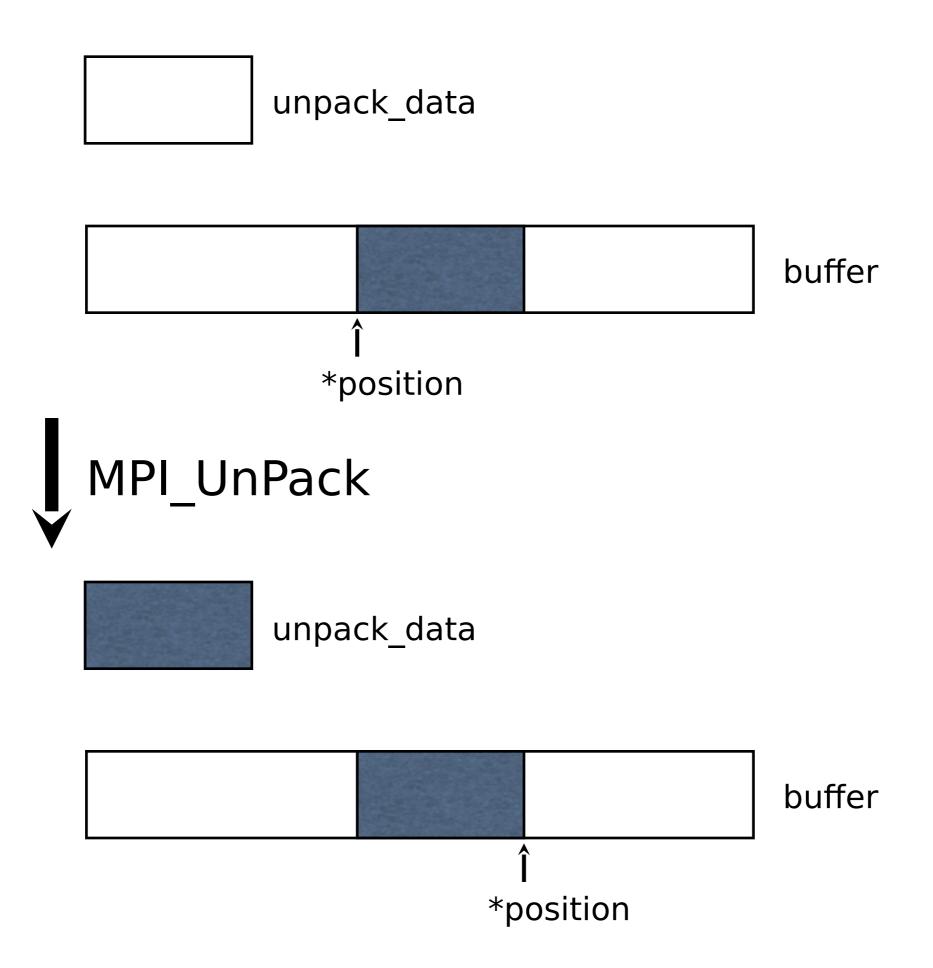
MPI_Pack then returns incremented position indicating the first free location in buffer after data has been packed Convenient since position is automatically calculated for user

comm - communicator that will be using outbuf

MPI Unpack

```
int MPI Unpack (void *inbuf, int insize, int *position,
          void *outbuf, int outcount, MPI Datatype datatype,
          MPI Comm comm )
inbuf - input buffer, contains packed message made by MPI Pack
insize - size of input buffer, in bytes
position - current position in buffer, in bytes (integer)
     Data unpacked in same order as it was packed
     Position incremented when MPI Unpack returns
     Convenient since position is automatically calculated for user
outbuf - output buffer start (where you want to unpack the data to)
outcount - number of items to be unpacked
datatype - datatype of each output item
comm - communicator that will be using inbuf
```





MPI_Pack/MPI_Unpack example

from P. Pacheco, Parallel Programming with MPI

```
/* read real a and b, integer n, pack data, MPI Bcast, then unpack */
void Get data4(
     float* a ptr /* out */,
     float* b ptr /* out */,
     int* n_ptr /* out */,
     int my rank /* in */) {
  char buffer[100]; /* Store data in buffer
  int position; /* Keep track of where data is */
               /* in the buffer
  if (my rank == 0){
     printf("Enter a, b, and n\n");
     scanf("%f %f %d", a ptr, b ptr, n ptr);
```

```
/* Now pack the data into buffer. Position = 0 * / 
/* says start at beginning of buffer.
position = 0;
/* Position is in/out */
MPI_Pack(a_ptr, 1, MPI FLOAT, buffer, 100,
  &position, MPI COMM_WORLD);
/* Position has been incremented: it now
/* references the first free location in buffer. */
MPI Pack(b ptr, 1, MPI FLOAT, buffer, 100,
  &position, MPI COMM WORLD);
/* Position has been incremented again. */
MPI Pack(n ptr, 1, MPI INT, buffer, 100,
  &position, MPI COMM WORLD);
/* Position has been incremented again. */
/* Now broadcast contents of buffer */
MPI Bcast(buffer, 100, MPI PACKED, 0,
  MPI COMM WORLD);
```

```
else {
     MPI Bcast(buffer, 100, MPI PACKED, 0,
       MPI COMM WORLD);
    /* Now unpack the contents of buffer */
    position = 0;
     MPI Unpack(buffer, 100, &position, a ptr, 1,
       MPI FLOAT, MPI COMM WORLD);
    /* Once again position has been incremented: */
    /* it now references the beginning of b.
     MPI Unpack(buffer, 100, &position, b ptr, 1,
       MPI FLOAT, MPI COMM WORLD);
     MPI Unpack(buffer, 100, &position, n ptr, 1,
       MPI INT, MPI COMM WORLD);
} /* Get data4 */
```

MPI_Pack_size

int MPI_Pack_size (int incount, MPI_Datatype datatype, MPI_Comm comm,
 int *size)

incount - count argument to packing call (i.e. number of elements to be packed)

datatype - datatype of elements to be packed

comm - communicator for packing call

size - upper bound on size of packed message, in bytes

Useful for determining the size of the buffer which needs to be allocated for packed message

Which method to use?

If data stored as consecutive entries of array, always use the *count* and *datatype* parameters in communications functions. Involves no additional overhead.

If there are a large number of elements not in contiguous memory locations, building a derived type will probably involve less overhead than a large number of calls to MPI_Pack/MPI_Unpack

If the data all have the same type and are stored at regular intervals in memory (e.g. column of matrix), then it will almost certainly be much easier and faster to use a derived datatype rather than MPI_Pack/MPI_Unpack

Typically, overhead of creating datatype is incurred only once, while the overhead of calling MPI_Pack/MPI_Unpack must be incurred every time data is communicated.

Using MPI_Pack/MPI_Unpack may be appropriate if only sending heterogenous data only a few times

Ultimately, choice will depend on particular MPI implementation and network hardware

Design and Coding of Parallel Programs

Example: Sorting

Writing parallel code

Use various strategies you learned for writing serial code.

It's hard to write a code in one go, so proceed in stages.

First, decide how your data and computational work will be distributed between processes.

Once that is clear, use a mixture of "top down" and "bottom up" approach to gradually build the code.

Proceeding "top down", write the main function first. In the first rough draft, use dummy type definitions and define subprograms as stubs initially.

When the main program is done, start working on subprograms ("bottom up").

Delay defining data structures as long as possible, to maintain flexibility.

If something looks hard, procrastinate i.e. leave writing it until later if possible, replace it with a stub function.

Test your code frequently as you proceed along the writing stages.

Test with various numbers of processors. Code which works on 1 or 2 may fail on 3 or more etc.

Use a "driver" to test your subprogram i.e. a highly simplified main function that has only sufficient data to correctly launch the subprogram.

Add informative output statements to your code so you can see what is happening. Put those in #DEBUG sections if you like.

Since I/O can be troublesome, you can use hardwired input values initially.

Take advantage of a debugger (DDT on SHARCNET) as much as possible.

If compiling on SHARCNET, keep all your files there and use a graphical editor to edit your files remotely.

Example: Sorting

Let's write a program which sorts a list of keys (e.g. numbers or words) into process-ascending order: keys on process q are to be sorted into increasing order, with all keys on q being greater than all keys on q-1 and less then all keys on q+1.

In other words, you can think of a linear array distributed in block fashion across processes, and we want to sort the elements of the array in increasing order.

General sorting on parallel processors is a difficult problem and an active area of research.

We will consider the simplifying case where the keys are distributed randomly and uniformly. This will allow for easily dividing the keys almost uniformly between processes.

In this example, will assume keys are non-negative integers uniformly distributed in some range. This allows for easy data distribution.

For example, assume range is 1 and 100, and assume there are 4 processes. In that case, process 0 should receive keys 1 to 25, process 1 keys 26 to 50 etc.

Initial state before sort

Process	Keys (in range 1 to 100)
0	71,4,63,42,64,82
1	27,96,38,7,47,76
2	53,75,10,13,2,58
3	49,79,22,85,33,99

Final state after sort

Process	Keys (in range 1 to 100)
0	2,4,7,10,13,22
1	27,33,38,42,47,49
2	53,58,63,64,71,75
3	76,79,82,85,96,99

Algorithm

- 1. Get local keys set up initial state
- 2. Use the uniform distribution to determine which process should get each key.
- 3. Send keys to appropriate processes. Receive keys from processes.
- 4. Sort local keys.
- 5. Print results.