Introduction to MPI Programming – Part 2

Center for Computation & Technology

Outline

- Collective communication
- Derived data types

Collective Communication

- Collective communications involves all processes in a communicator
  - One to all, all to one and all to all
- Three types of collective communications
  - Data movement
  - Collective computation
  - Synchronization

Collective vs. Point-to-point

- More concise program
  - One collective operation can replace multiple point-to-point operations
- Optimized collective communications usually are faster than the corresponding point-to-point communications

Data Movement: Broadcast

P0	A	B	C	D
P1				
P2				
P3				

Broadcast →

P0	A	B	C	D
P1	A	B	C	D
P2	A	B	C	D
P3	A	B	C	D

- Broadcast copies data from the memory of one processor to that of other processors
  - One to all operation
- Syntax: `MPI_Bcast ( send_buffer, send_count, send_type, rank, comm )`

Data Movement: Gather

P0	A			
P1	B			
P2	C			
P3	D			

Gather →

P0	A	B	C	D
P1	B			
P2	C			
P3	D			

- Gather copies data from each process to one process, where it is stored in rank order
  - One to all operation
- Syntax: `MPI_GATHER ( send_buffer, send_count, send_type, recv_buffer, recv_count, recv_type, recv_rank, comm )`

Example: MPI_Gather

```
…
integer,allocatable :: array(:),array_r(:)
! Initialize MPI
call mpi_init(ierr)
call mpi_comm_size(mpi_comm_world,nprocs,ierr)
call mpi_comm_rank(mpi_comm_world,myid,ierr)
! Initialize the array
allocate(array(2),array_r(2*nprocs))
array(0)=2*myid
array(1)=2*myid+1
! Gather data at the root process
call mpi_gather(array,2,mpi_integer, &
                array_r,2,mpi_integer, &
                0,mpi_comm_world)
if (myid.eq.0) then
  write(*,*) "The content of the array_r:"
  write(*,*) array_r
```

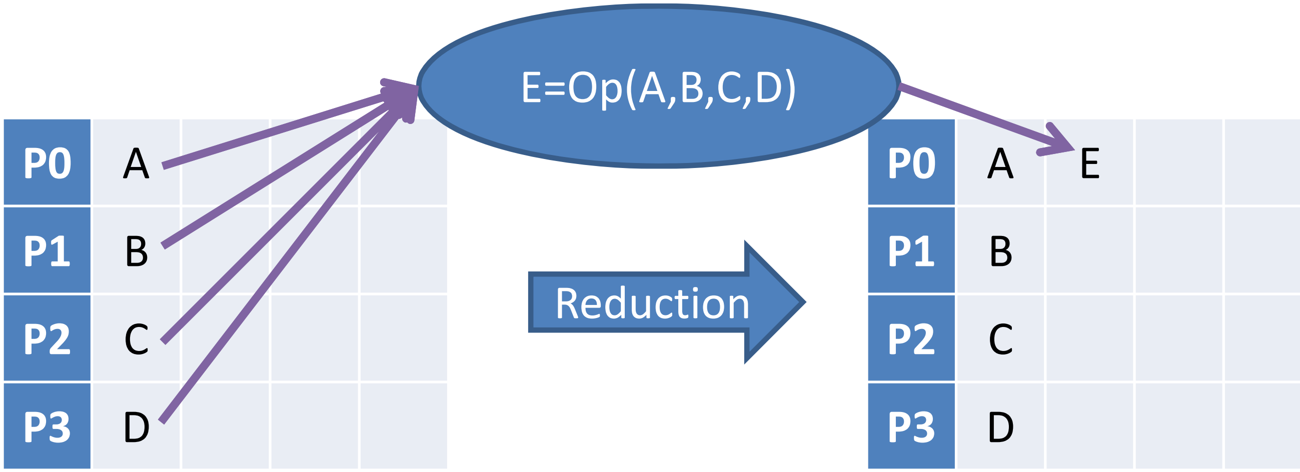
Example: MPI_Gather

```
…
integer,allocatable :: array(:),array_r(:)
! Initialize MPI
call mpi_init(ierr)
call mpi_comm_size(mpi_comm_world,nprocs,ierr)
call mpi_comm_rank(mpi_comm_world,myid,ierr)
! Initialize the array
```

```
[lyan1@qb563 ex]$ mpirun -np 4 ./a.out
 The content of the array:
           0           1           2           3           4           5
           6           7
```

```
                array_r,2,mpi_integer, &
                0,mpi_comm_world)
if (myid.eq.0) then
  write(*,*) "The content of the array_r:"
  write(*,*) array_r
```

Collective Computation: Reduction

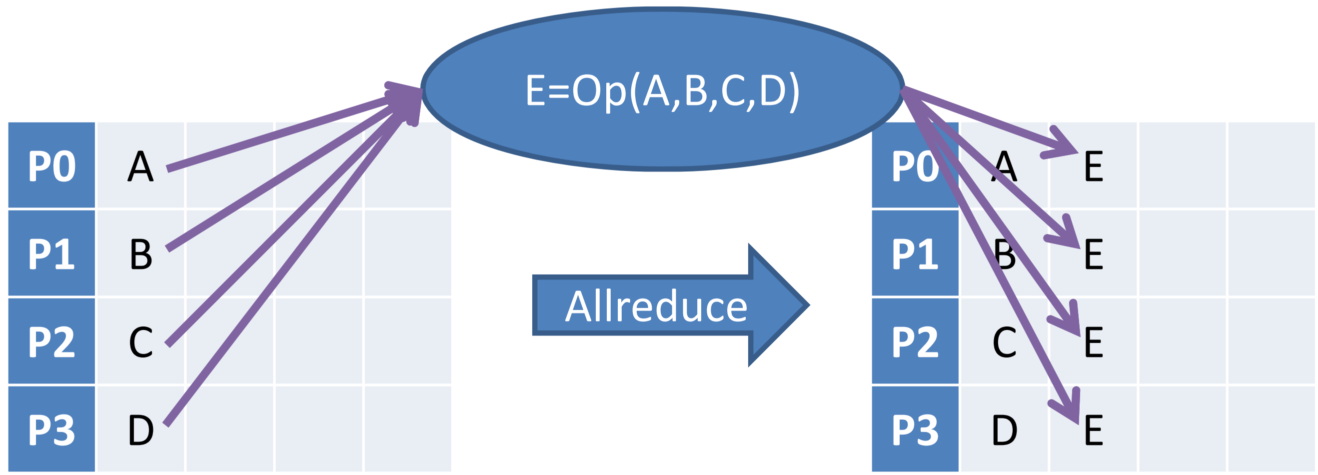


- MPI reduction collects data from each process, reduces them to a single value, and store it in the memory of one process
  - One to all operation
- Syntax: `MPI_Reduce( send_buffer, recv_buffer, count, data_type, reduction_operation, rank_of_receiving_process, communicator )`

Reduction Operation

- Summation and production
- Maximum and minimum
- Max and min location
- Logical
- Bitwise
- User defined

Collective Computation: Allreduce

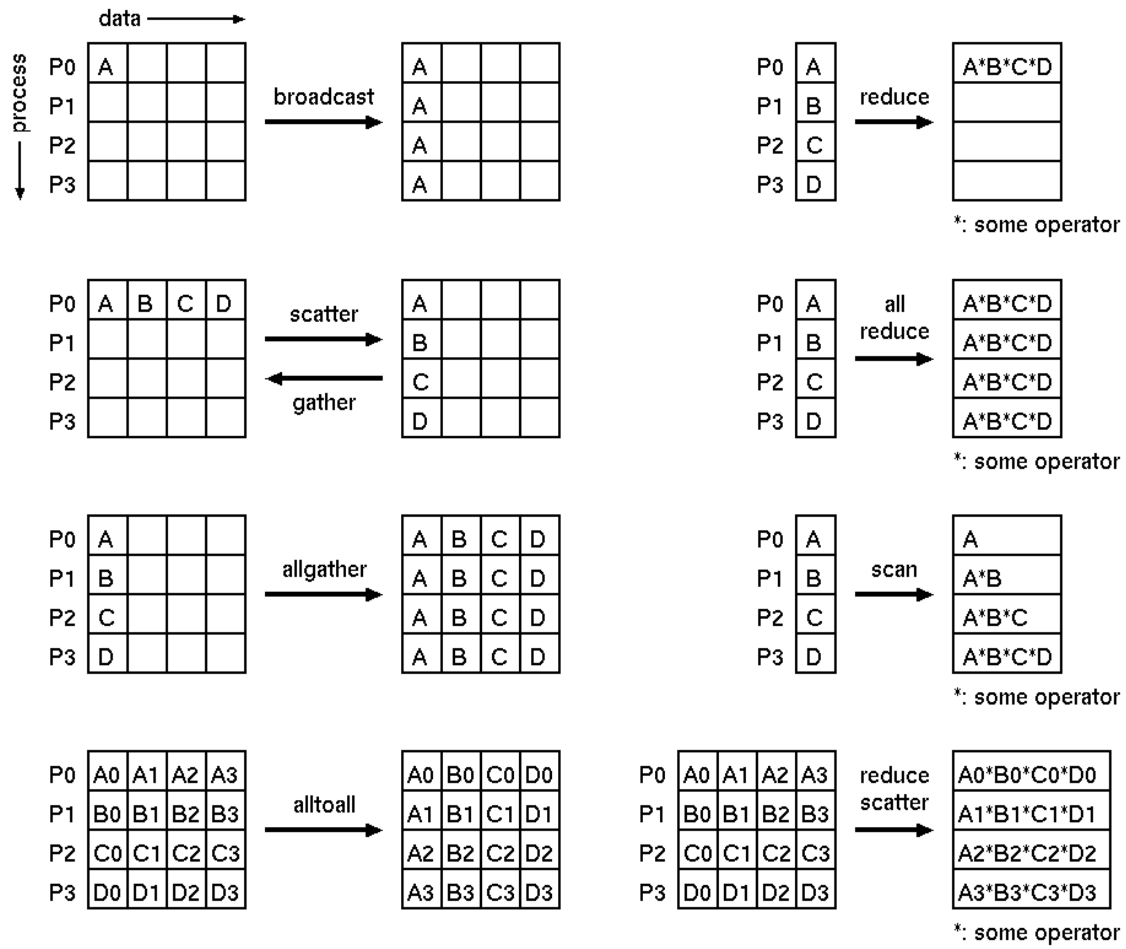


- MPI allreduce collects data from each process, reduces them to a single value, and store it in the memory of EVERY process
  - All to all operation
- Syntax: `MPI_Allreduce( send_buffer, recv_buffer, count, data_type, reduction_operation, communicator )`

Synchronization

- MPI_Barrier (Communicator)
  - Blocks processes in a group until all processes have reached the same synchronization point
  - Synchronization is collective since all processes are involved
  - Could cause significant overhead, so do NOT use it unless absolutely necessary

Other Collective Communications



Source: Practical MPI Programming, IBM Redbook

Exercise 3a: Find Global Maximum

- Goal: repeat Exercise 2a with appropriate collective communication function(s)

Exercise 3b: Matrix Multiplication version 3

- Goal: Replace the part in version 2 that sends the result to the root process with appropriate collective operation(s)

Exercise 3c: Laplace Solver version 2

- Goal: Replace the part in version 1 that finds the global maximum convergence and distributes it to all processes with appropriate collective operation(s)

Basic Data Types

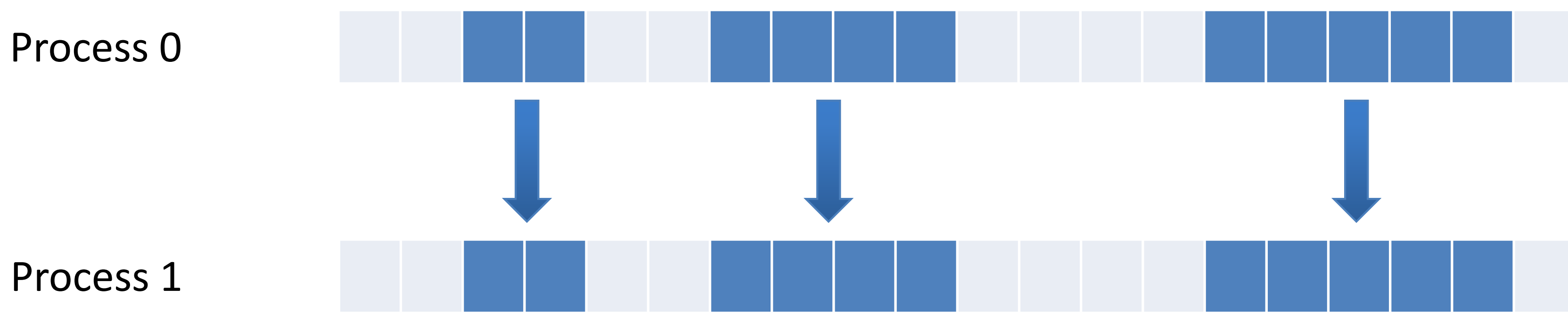
MPI Data Type	C Data Type
MPI_CHAR	Signed char
MPI_SHORT	Signed short int
MPI_INT	Signed int
MPI_LONG	Signed long int
MPI_UNSIGNED_CHAR	Unsigned char
MPI_UNSIGNED_SHORT	Unsigned short
MPI_UNSIGNED	Unsigned int
MPI_UNSIGNED_LONG	Unsigned long int
MPI_FLOAT	Float
MPI_DOUBLE	Double
MPI_LONG_DOUBLE	Long double
MPI_BYTE	
MPI_PACKED	

MPI Data Type	Fortran Data Type
MPI_INTEGER	INTEGER
MPI_REAL	REAL
MPI_REAL8	REAL*8
MPI_DOUBLE_PRECISION	DOUBLE PRECISION
MPI_COMPLEX	COMPLEX
MPI_LOGICAL	LOGICAL
MPI_CHARACTER	CHARACTER(1)
MPI_BYTE	
MPI_PACKED	

Why Derived Data Types?

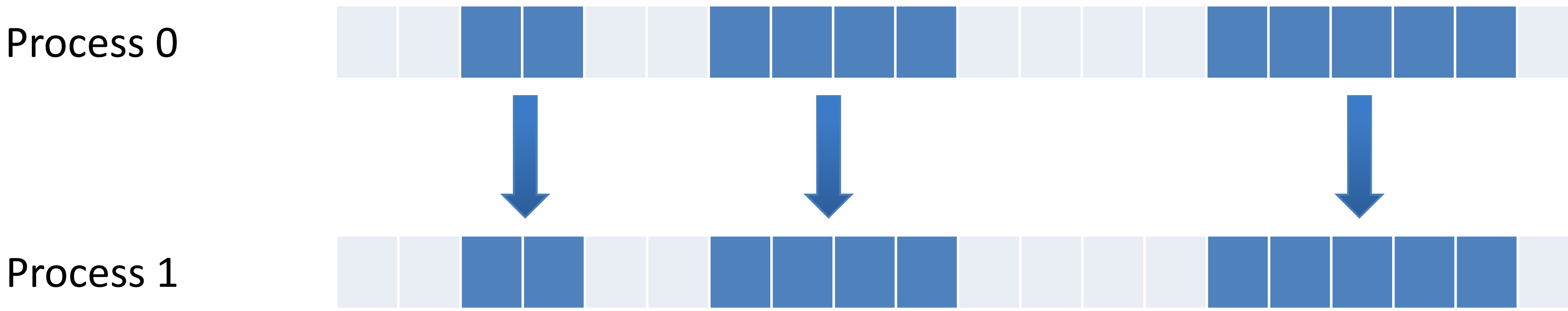
- The communication functions we have seen so far deal with contiguous data of the same type
- What if the data to be transferred is
  - Not contiguous?
  - Not of the same type?

Why Derived Data Types



Solution 1
Call MPI_SEND/MPI_RECEIVE multiple times (once for each contiguous segment)

Why Derived Data Types



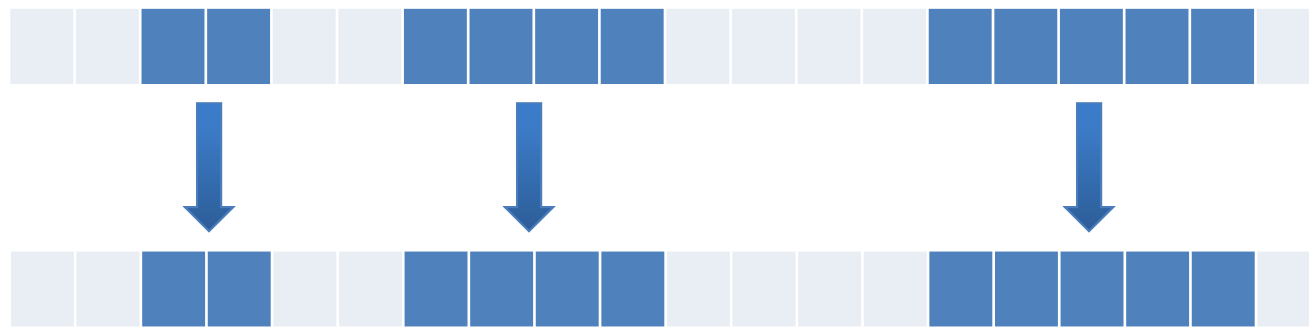
<u>Solution 2</u>

Process 0: copy data into contiguous buffer, then call MPI_SEND

Process 1: call MPI_RECEIVE, then copy data to destination

Why Derived Data Types

Process 0



Process 1

<u>Solution 3</u>
Define a new data type to describe the data to be transferred, then call MPI_SEND/MPI_RECV
- Most efficient

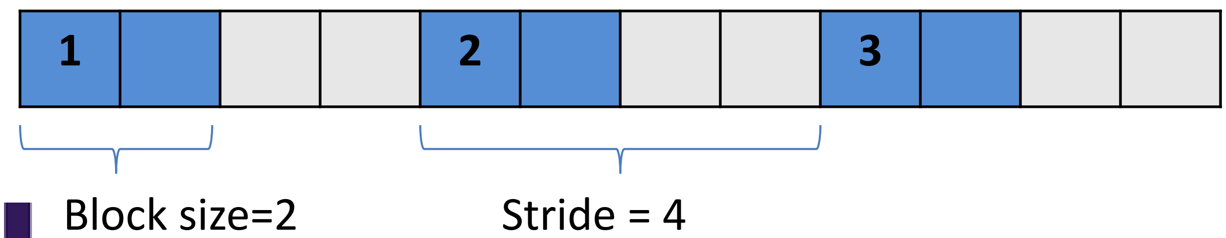
Derived Data Type: Contiguous

- Allows replication of one data type into contiguous locations
- Syntax: `MPI_Type_Contiguous(count, old_type, new_type)`
- The new data type must be commited before being used for communication:
  - `MPI_Type_Commit(new_type)`

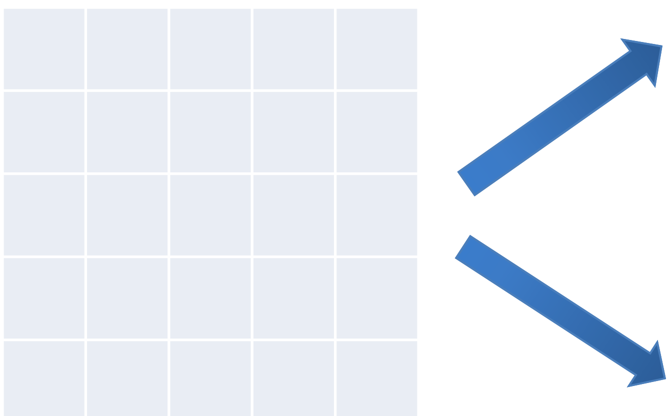
Derived Data Type: Vector

- Allows replication of a data type into locations that consist of equally spaced blocks
- Syntax: `MPI_Type_Vector(count, block size, stride, old_type, new_type)`

```
Call mpi_type_vector(3,2,4,mpi_real8,my_vector_type,ierr)
Call mpi_type_commit(my_vector_type,ierr)
```



Data Ordering: C vs. Fortran



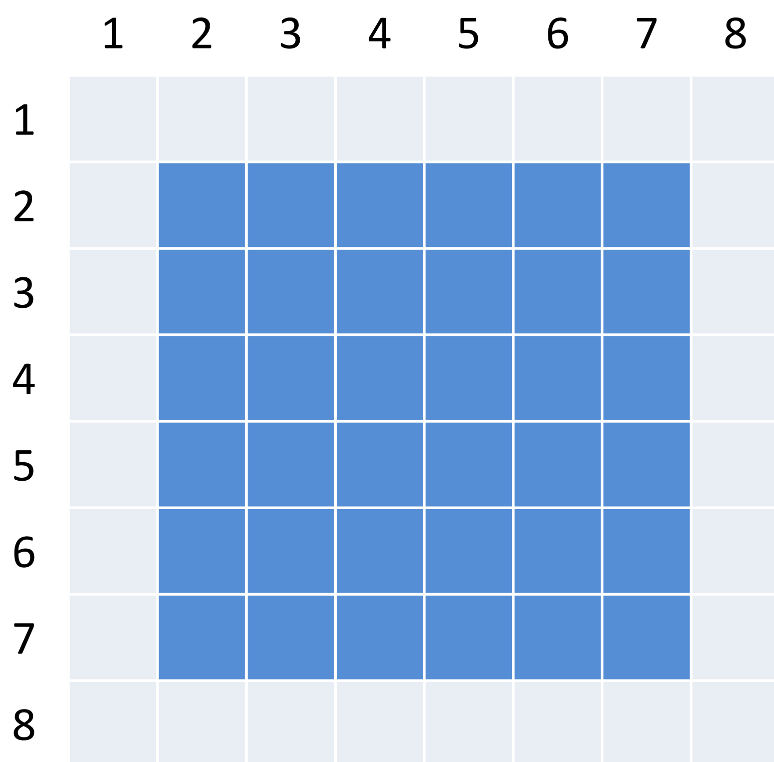
0,0	0,1	0,2	…	1,0	1,1	1,2	…	4,3	4,4

C

0,0	1,0	2,0	…	0,1	1,1	2,1	…	3,4	4,4

Fortran

Example: Broadcasting Submatrix



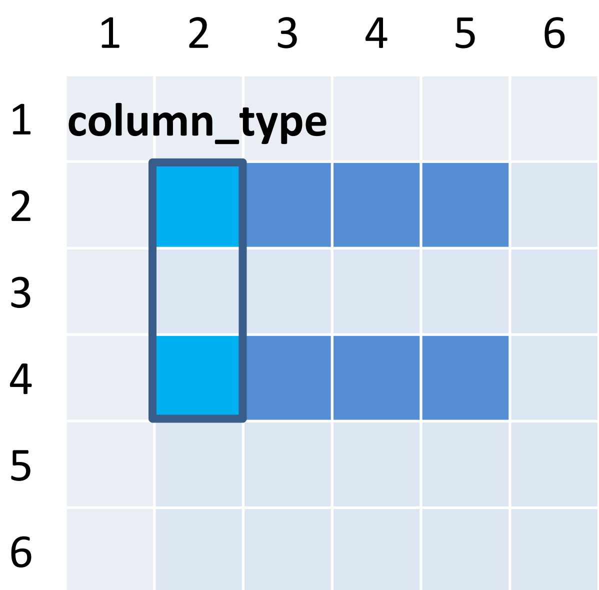

```
!Number of blocks
nblocks=6
!Block length
blocklen=6
!Stride
stride=8

!Define the new data type
CALL MPI_TYPE_VECTOR(NBLCK,BLCKLEN,STRD, &
  MPI_INTEGER,submat_type,IERR)
CALL MPI_TYPE_COMMIT(submat_type,IERR)

!Call broadcast
CALL MPI_BCAST(AMAT(2,2),1,submat_type,0, &
  MPI_COMM_WORLD,IERR)
```

Derived Data Type: HVector

- The same with `MPI_Type_Vector`, except that the unit of the `stride` is byte instead of `old_type`
  - More flexible than the vector type
  - We can use `MPI_Type_Extent(datatype,extent)` to decide the extent (in bytes) of an MPI data type

Nested Derived Data Type

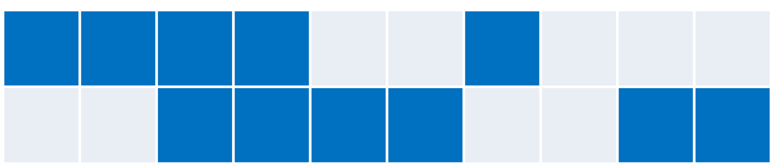
- New data types can be created out of user-defined data types




```
Call mpi_type_extent(mpi_integer, &
         size_of_int, ierr)
call mpi_type_vector(2,1,2,mpi_integer, &
         column_type,ierr)
call mpi_type_hvector(4,1,6*size_of_int, &
         column_type,new_type,ierr)
```

Derived Data Type: Indexed

- Allows replication of a data type into locations that consist of unequally spaced blocks with varying length
- Syntax: `MPI_Type_indexed (count, blocklens[], offsets[], old_type, new_type)`
  - `blocklens` and `offsets` are array of size `count` that specify the length and displacement of each block, respectively



```
Count=4
blocklens=[4,1,4,2]
Offsets=[0,6,12,18]
```

Derived Data Type: Struct

- Most general data type constructor
- Allows a new data type that represents arrays of types, each of which has a different block length, displacement (in bytes) and type
- Syntax: `MPI_Type_struct (count, blocklens[], offsets[], old_types[], new_type)`

Exercise 4a: Matrix Transposition

- Goal: write a MPI program that transposes a matrix in parallel
  - 2-d process grid
  - Each process initializes its own sub-matrix
  - Do we really need the local transposition?

Exercise 4b: Matrix Multiplication Version 4

- Goal: change the matrix multiplication to two-dimensional decomposition
  - Arrange the processes into a 2-d grid
  - Each process should only owns a sub-matrix of A, B and C
  - Assemble the matrix C at the root process using the partial result from each process

Exercise 4c: Laplace Solver Version 3

- Goal: change our Laplace solver to two-dimensional decomposition
- Hints
  - Change how the size of sub-domain is calculated
  - Change how the boundary condition is set
  - Data transfer along two more directions
    - Those data are not contiguous
      - Fortran: use derived data types
      - C: need to pack it into a contiguous buffer