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# Introduction to MPI Programming – Part 2

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# 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
- All collective communications are blocking
  - Non-blocking collective communications are being worked into the MPI 3.0 standard

# 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 )`

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# Example: MPI_Gather

```fortran
…
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
```

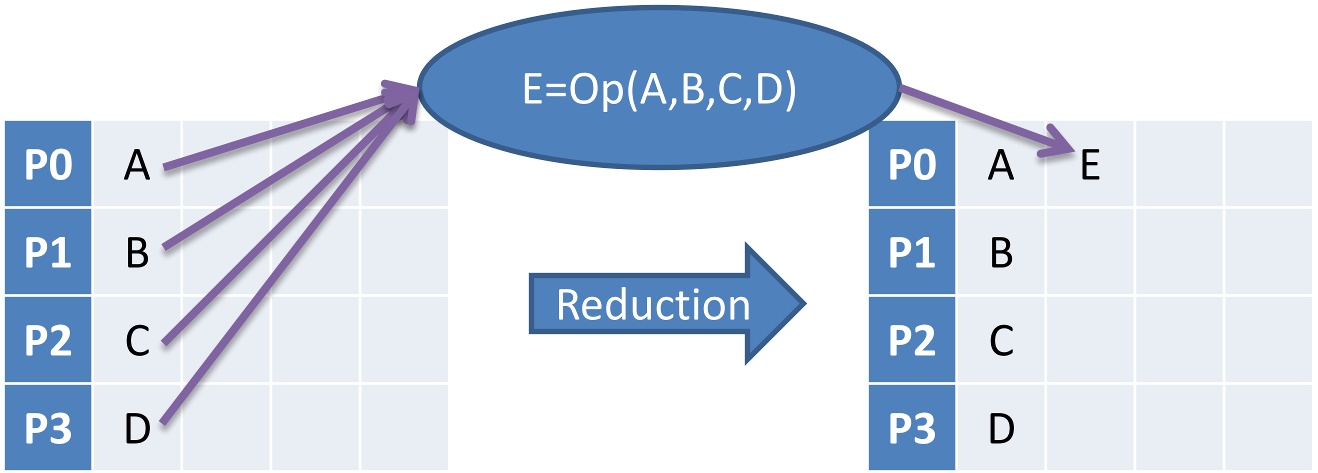
# Example: MPI_Gather

```
…
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

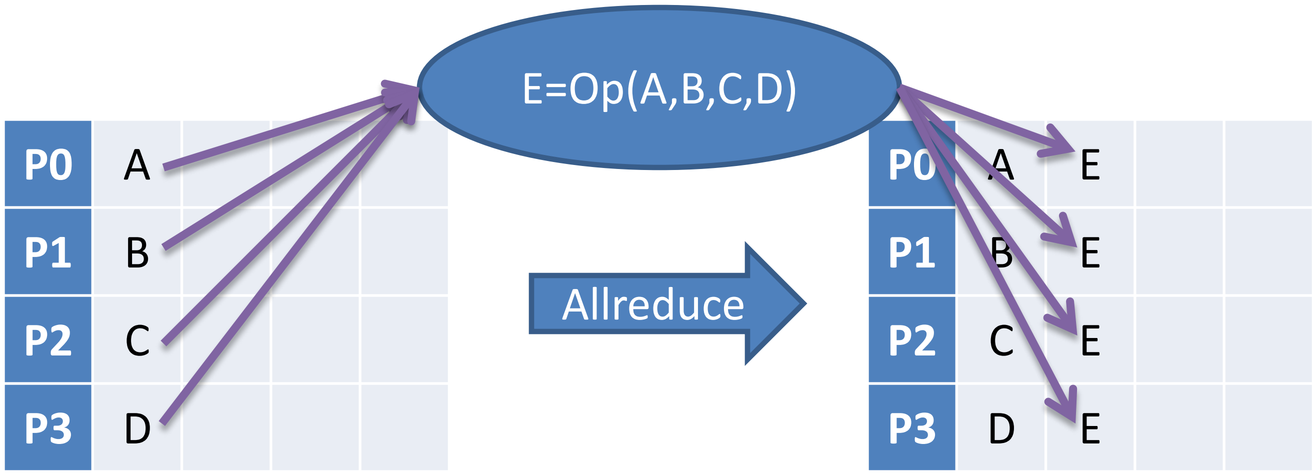



- MPI reduction collects data from each process, reduces them to a single value, and store it in the memory of one process
  - One to all operation
- Syntax: `MPI_Reduce( send_buffer, recv_buffer, count, data_type, reduction_operation, rank_of_receiving_process, communicator )`

# Reduction Operation

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

# Collective Computation: Allreduce

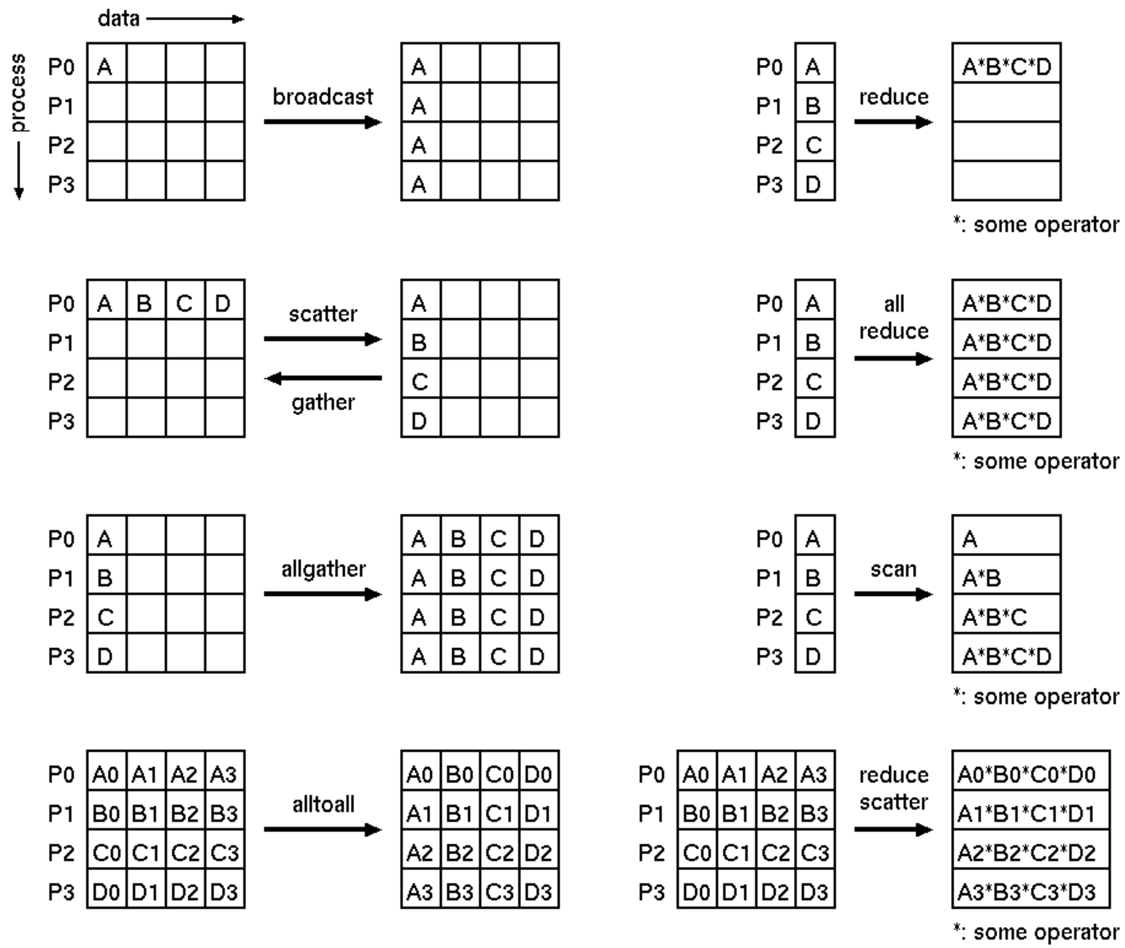



- MPI allreduce collects data from each process, reduces them to a single value, and store it in the memory of EVERY process
  - All to all operation
- Syntax: `MPI_Allreduce( send_buffer, recv_buffer, count, data_type, reduction_operation, communicator )`

# 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
    - Usually for external event, i.e. I/O

# 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: 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?

# Solutions for Non-contiguous Data

- Make multiple communication calls
  - One for each contiguous segment
- Pack data into contiguous buffer, transfer, and unpack at the receiving end
- Use MPI derived data types
  - Tell the library what is desired and let it decide how the communication is done
  - Most efficient

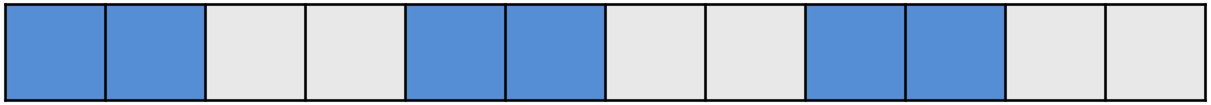
# Derived Data Type: Contiguous

- 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)`

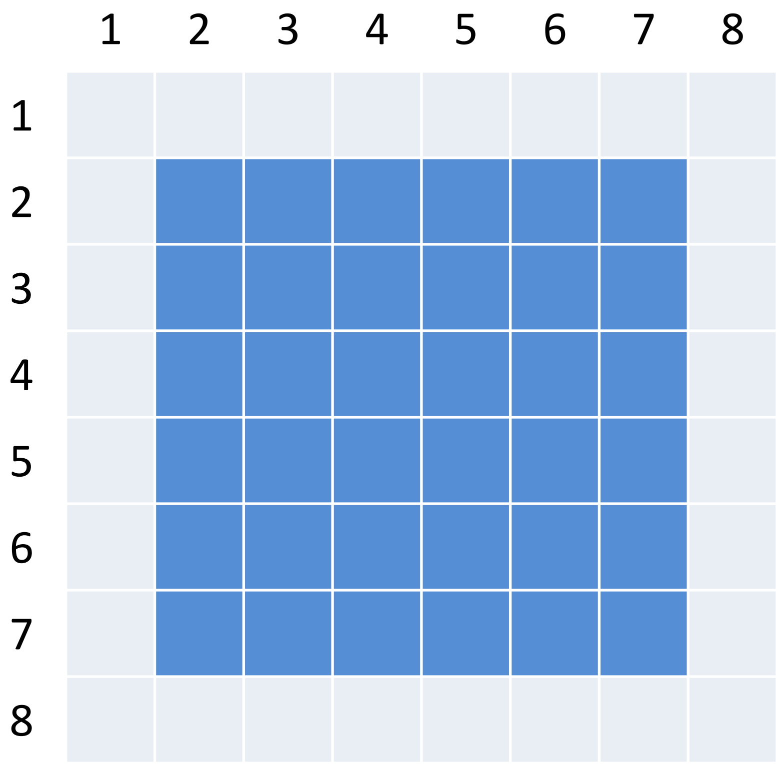
# Derived Data Type: Vector

- 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)
```



# Example: Broadcasting Submatrix



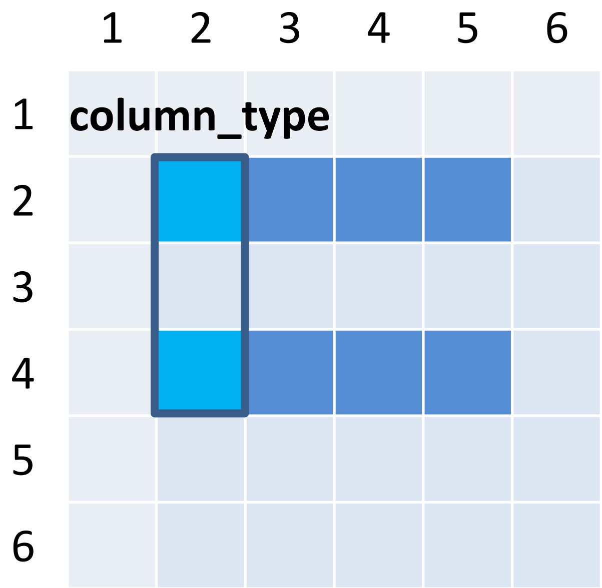

```
!Number of blocks
nblocks=6
!Block length
blocklen=6
!Stride
stride=8

!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

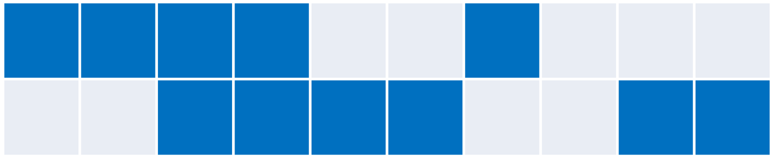
- New data types can be created out of user-defined data types




```
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: 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