Lecture 29: Collective Communication and Computation in MPI

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Collective Communication

- All communication in MPI is within a group of processes
- Collective communication is over *all* of the processes in that group
- MPI_COMM_WORLD defines all of the processes when the parallel job starts
- Can define other subsets
  - With MPI dynamic processes, can also create sets bigger than MPI_COMM_WORLD
  - Dynamic processes not supported on most massively parallel systems

Collective Communication as a Programming Model

- Programs using only collective communication can be easier to understand
  - Every program does roughly the same thing
  - No "strange" communication patterns
- Algorithms for collective communication are subtle, tricky
  - Encourages use of communication algorithms devised by experts

A Simple Example: Computing pi

```
MPI_Bcast(&n, 1, MPI_INT, 0,
          MPI_COMM_WORLD);
h   = 1.0 / (double) n;
sum = 0.0;
for (i = myid + 1; i <= n; i += numprocs) {
    x = h * ((double)i - 0.5);
    sum += f(x);
}
mypi = h * sum;
MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE,
          MPI_SUM, 0, MPI_COMM_WORLD);
```

Notes on Program

- MPI_Bcast is a "one-to-all" communication
  - Sends value of "n" to all processes
- MPI_Reduce is an "all-to-one" computation, with an operation (sum, represented as MPI_SUM) used to combine (reduce) the data
- Works with any number of processes, even one.
  - Avoids any specific communication pattern, selection of ranks, process topology

MPI Collective Communication

- Communication and computation is coordinated among a group of processes in a communicator.
- Groups and communicators can be constructed "by hand" or using topology routines.
- Non-blocking versions of collective operations added in MPI-3
- Three classes of operations: synchronization, data movement, collective computation.

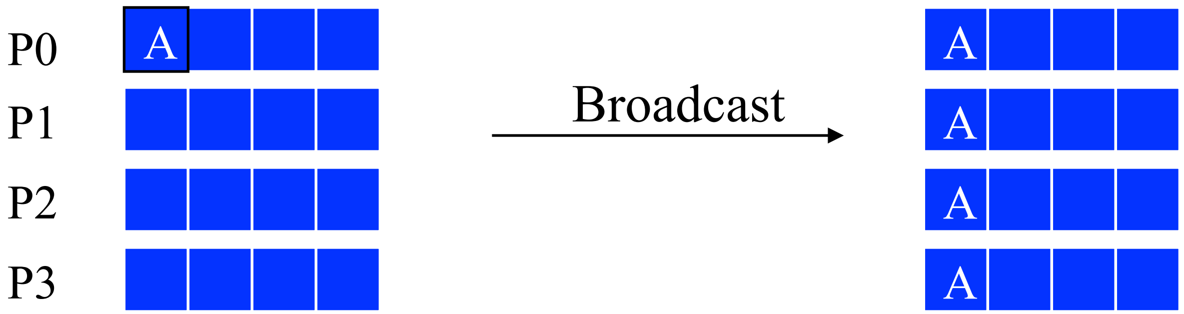
Synchronization

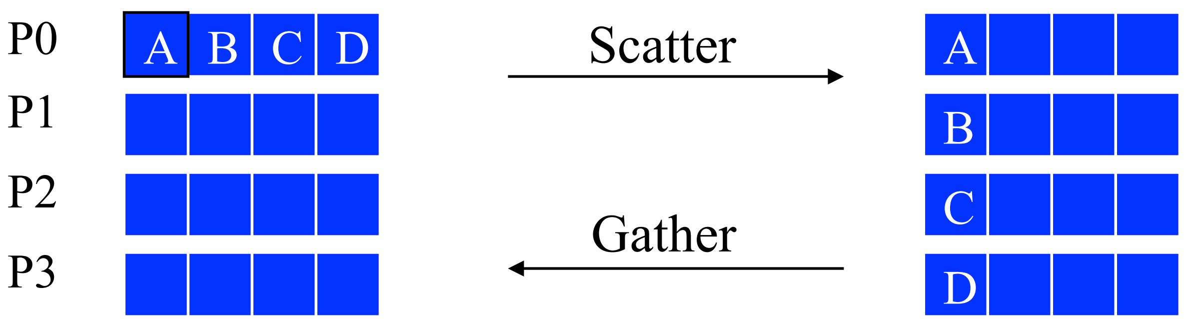
- **`MPI_Barrier( comm )`**
- Blocks until all processes in the group of the communicator **`comm`** call it.
- Almost never required in a parallel program
  - Occasionally useful in measuring performance and load balancing
  - In unusual cases, can increase performance by reducing network contention
  - Does *not* guarantee that processes exit at the same (or even close to the same) time

Collective Data Movement

- One to all
  - Broadcast
  - Scatter (personalized)
- All to one
  - Gather
- All to all
  - Allgather
  - Alltoall (personalized)
- "Personalized" means each process gets *different* data

Collective Data Movement





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Comments on Broadcast

- All collective operations must be called by *all* processes in the communicator
- MPI_Bcast is called by both the sender (called the root process) and the processes that are to receive the broadcast
  - MPI_Bcast is not a "multi-send"
  - "root" argument is the rank of the sender; this tells MPI which process originates the broadcast and which receive
- Example of orthogonallity of the MPI design: MPI_Recv need not test for "multisend"

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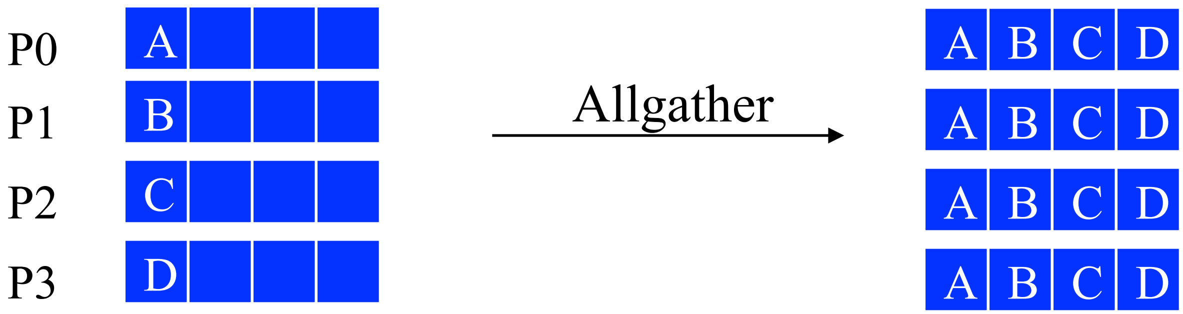
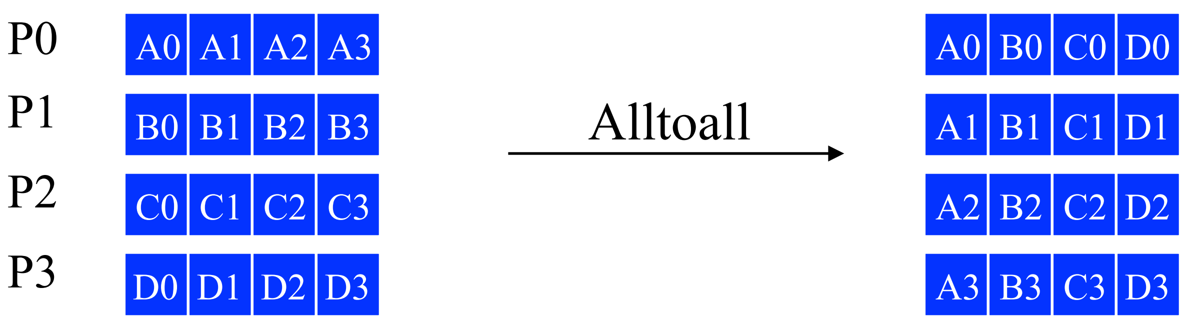
More Collective Data Movement





Notes on Collective Communication

- MPI_Allgather is equivalent to
  - MPI_Gather followed by MPI_Bcast
  - But algorithms for MPI_Allgather can be faster
- MPI_Alltoall performs a "transpose" of the data
  - Also called a personalized exchange
  - Tricky to implement efficiently and in general
    - For example, does *not* require O(p) communication, especially when only a small amount of data is sent to each process

Special Variants

- The basic routines send the same amount of data from each process
  - E.g., MPI_Scatter(&v,1,MPI_INT,…) sends 1 int to each process
- What if you want to send a different number of items to each process?
  - Use MPI_Scatterv
- The “v” (for vector) routines allow the programmer to specify a different number of elements for each destination (one to all routines) or source (all to one routines).
- Efficient algorithms exist for these cases, though not as fast as the simpler, basic routines

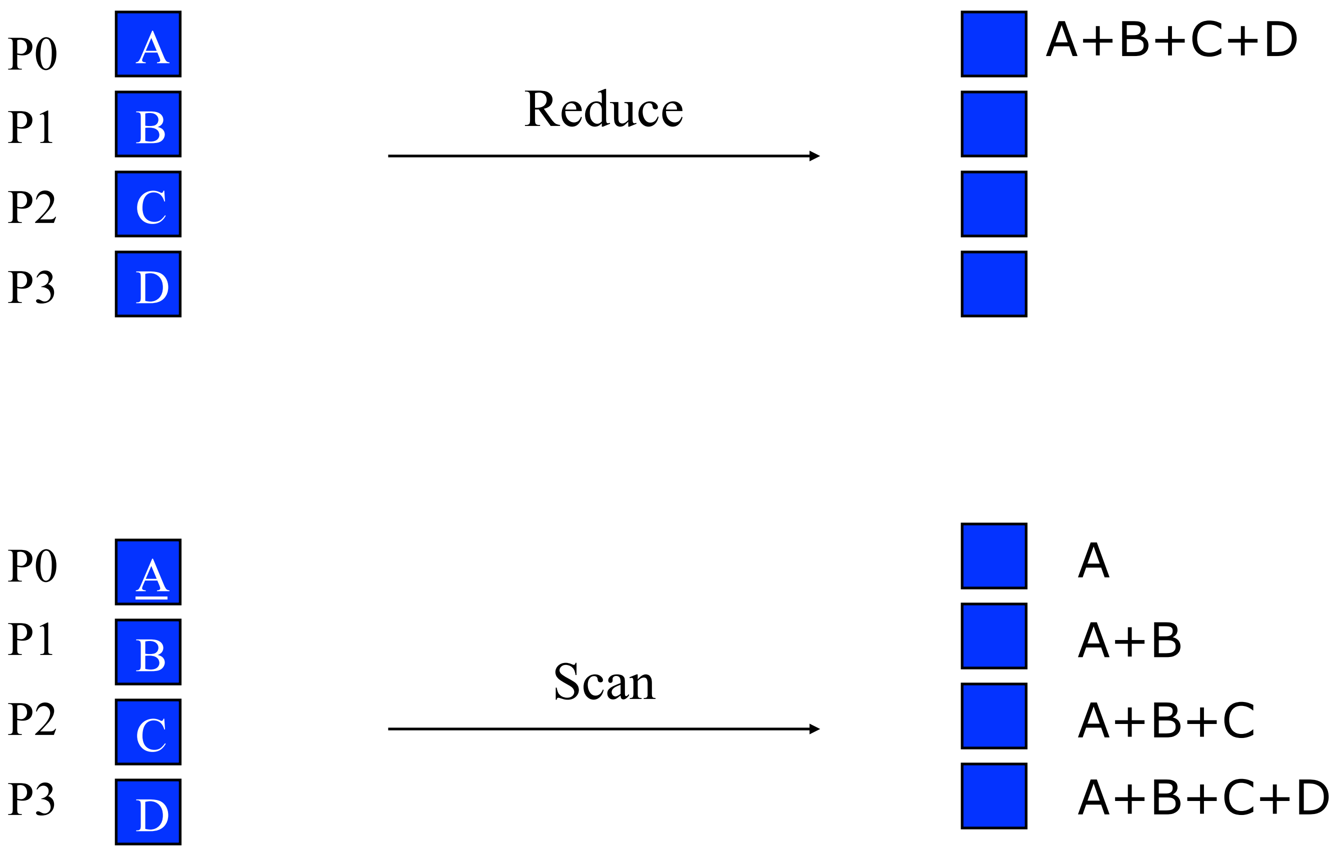
Special Variants (Alltoall)

- In one case (MPI_Alltoallw), there are two "vector" routines, to allow more general specification of MPI datatypes for each source
  - Recall that only the type *signature* needs to match; this allows different layouts in memory for each data being sent

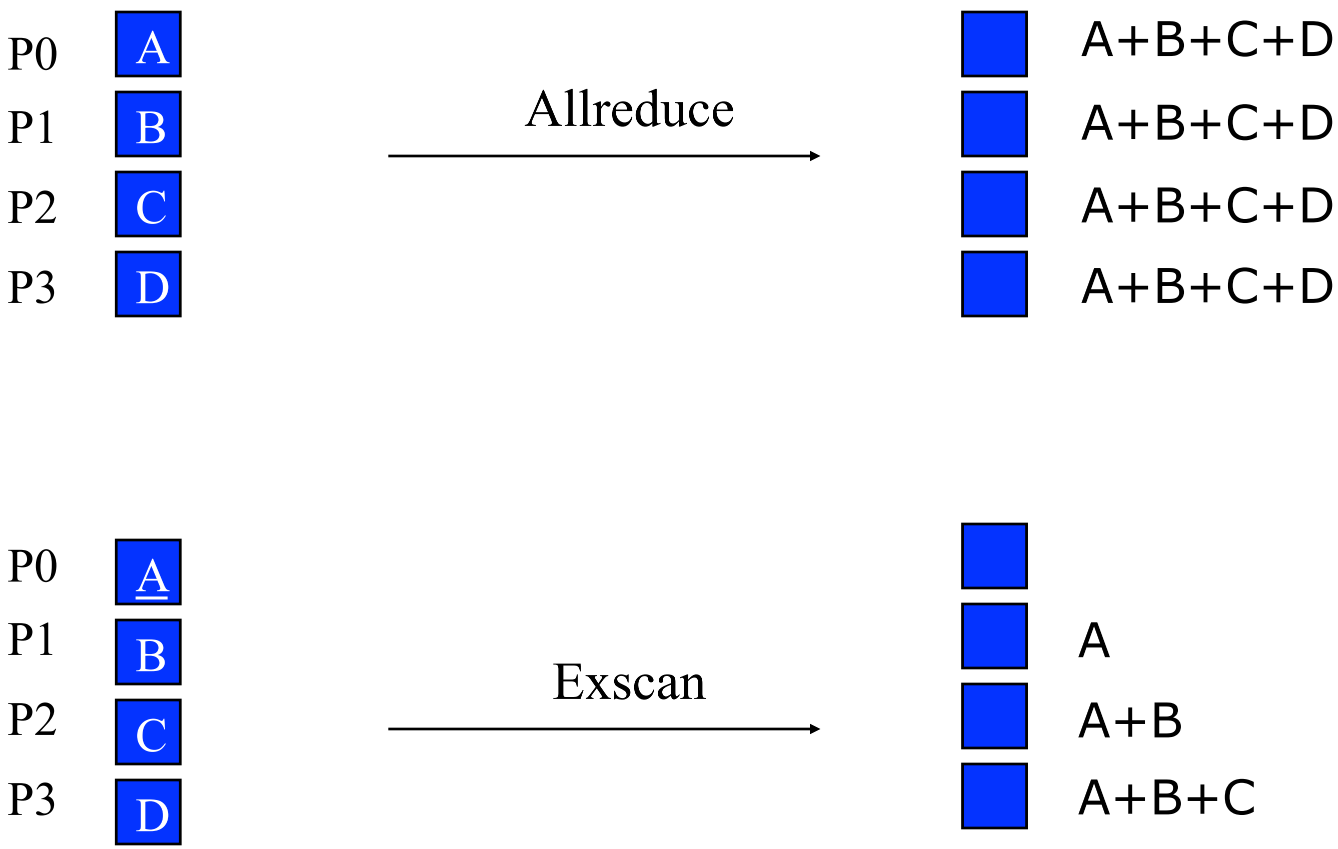
Collective Computation

- Combines communication with computation
  - ♦ Reduce
    - All to one, with an operation to combine
  - ♦ Scan, Exscan
    - All prior ranks to all, with combination
  - ♦ Reduce_scatter
    - All to all, with combination
- Combination operations either
  - ♦ Predefined operations
  - ♦ User defined operations

Collective Computation



Collective Computation



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MPI Collective Routines: Summary

- Many Routines, including: **`Allgather`, `Allgatherv`, `Allreduce`, `Alltoall`, `Alltoallv`, `Alltoallw`, `Bcast`, `Exscan`, `Gather`, `Gatherv`, `Reduce`, `Reduce_scatter`, `Scan`, `Scatter`, `Scatterv`**
- **`All`** versions deliver results to all participating processes.
- V versions allow the hunks to have different sizes.
- **`Allreduce`**, **`Exscan`**, **`Reduce`**, **`Reduce_scatter`**, and **`Scan`** take both built-in and user-defined combiner functions.
- Most routines accept both intra- and inter-communicators
  - Intercommunicator versions are collective between ***two*** groups of processes

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MPI Built-in Collective Computation Operations

• **`MPI_MAX`**	Maximum
• **`MPI_MIN`**	Minimum
• **`MPI_PROD`**	Product
• **`MPI_SUM`**	Sum
• **`MPI_LAND`**	Logical and
• **`MPI_LOR`**	Logical or
• **`MPI_LXOR`**	Logical exclusive or
• **`MPI_BAND`**	Bitwise and
• **`MPI_BOR`**	Bitwise or
• **`MPI_BXOR`**	Bitwise exclusive or
• **`MPI_MAXLOC`**	Maximum and location
• **`MPI_MINLOC`**	Minimum and location

How Deterministic are Collective Computations?

- In exact arithmetic, you always get the same results
  - but roundoff error, truncation can happen
- MPI does *not* require that the same input give the same output every time
  - Implementations are **encouraged** but **not required** to provide *exactly* the same output given the same input
  - Round-off error may cause slight differences
- Allreduce ***does*** guarantee that the *same* value is received by **all** processes for each call
- Why didn't MPI mandate determinism?
  - Not all applications need it
  - Implementations of collective algorithms can use "deferred synchronization" ideas to provide better performance

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Defining your own Collective Operations

- Create your own collective computations with:
  ```
  MPI_Op_create( user_fcn, commutes, &op );
  MPI_Op_free( &op );

  user_fcn( invec, inoutvec, len, datatype );
  ```
- The user function should perform:
  ```
  inoutvec[i] = invec[i] op inoutvec[i];
  ```
  for i from 0 to len-1.
- The user function can be non-commutative.

Understanding the Definition of User Operations

- The declaration is
```
void user_op(void *invec, void *inoutvec,
             int *len, MPI_Datatype *dtype)
```
  - Why pointers to len, dtype?
    - An attempt to make the C and Fortran-77 versions compatible (Fortran effectively passes most arguments as pointers)
  - Why a void return?
    - No error cases expected
- Both assumptions turned out to be poor choices
- Why the “commutes” flag?
  - Not all operations are commutative. Can you think of one that is not?

An Example of a Non-Commutative Operation

- Matrix multiplication is not commutative
- Consider using MPI_Scan to compute the product of 3x3 matrices from each process
  - MPI implementation is free to use both associativity and commutivity in the algorithms ***unless*** the operation is marked as non commutative
- Try it yourself – write the operation and try it using simple rotation matrices

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Define the Groups

- MPI_Comm_split(MPI_Comm oldcomm, int color, int key, MPI_Comm *newcomm)
  - ♦ Collective over input communicator
  - ♦ Partitions based on "color"
  - ♦ Orders rank in new communicator based on key
  - ♦ Usually the best routine for creating a new communicator over a proper subset of processes
    - Don't use MPI_Comm_create
  - ♦ Can also be used to reorder ranks
    - Question: How would you do that?

Define the Groups

- MPI_Comm_create_group(
  MPI_Comm oldcomm,
  MPI_Group group, int tag,
  MPI_Comm *newcomm)
  - ♦ New in MPI-3
    - Collective only over input group, *not* oldcomm
  - ♦ Requires formation of group using MPI group creation routines
    - MPI_Comm_group to get an initial group
    - MPI_Group_incl, MPI_Group_range_incl, MPI_Group_union, etc.

Collective Communication Semantics

- Collective routines *on the same communicator* must be called in the same order on all participating processes
- If multi-threaded processes are used (MPI_THREAD_MULTIPLE), it is the *users* responsibility to ensure that the collective routines follow the above rule
- Message tags are not used
  - ♦ Use different communicators if necessary to separate collective operations on the same process

NonBlocking Collective Operations

- MPI-3 introduced nonblocking versions of collective operations
  - All return an MPI_Request, use the usual MPI_Wait, MPI_Test, etc. to complete.
  - May be mixed with point-to-point and other MPI_Requests
  - Few implementations are fast or offer much concurrency (as of 2015)
  - Follow same ordering rules as blocking operations
- Even MPI_Ibarrier
  - Useful for distributed termination detection

Neighborhood Collectives

- Collective operation on an MPI communicator with a defined topology
  - ♦ For Cartesian (MPI_CART), immediate neighbors in coordinate directions
    - Cooresponds to using MPI_Cart_shift with disp=1 in each coordinate
  - ♦ For Graph (MPI_DIST_GRAPH), immediate neighbors (as returned by MPI_Dist_graph_neighbors)
- MPI_Neighbor_alltoall
  - ♦ Sends distinct messages to each neighbor
  - ♦ Receives distinct messages from each neighbor
- MPI_Ineighbor_alltoall for nonblocking version
- Provides an alternative for halo exchanges