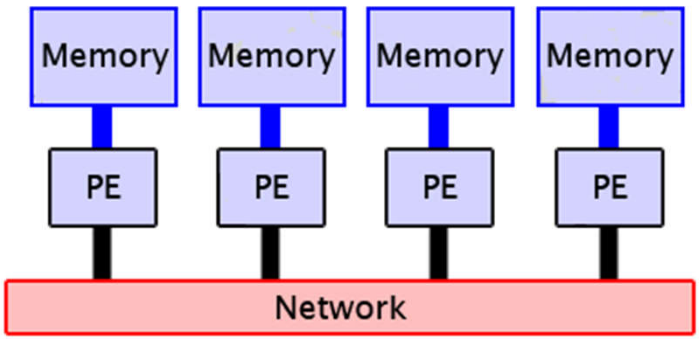
Distributed memory programming using MPI

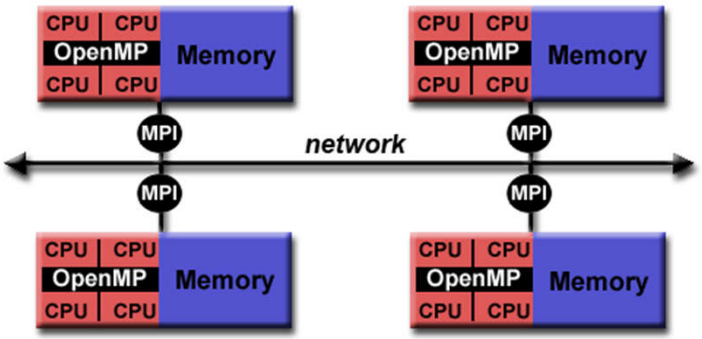
CS121 Parallel Computing

Fall 2024

Distributed memory programming

- Processes have local memory, and communicate by sending messages over network.
- Use standard C / C++ / Fortran. Call library for communication functions.
- Message Passing Interface (MPI)
  - Library developed by academics and industry in early 1990's.
    - Standardized clutter of existing HPC languages and tools.
  - Goals are portability, efficiency and flexibility.
  - Four versions
    - MPI 1.1-1.3, Jun 1995 – May 2008
    - MPI 2.1-2.2, Sep 2008 – Sep 2009
    - MPI 3.1, Jun 2015
    - MPI 4.0, Jun 2021
  - Defines an interface of message passing routines, but not implementation.
  - Vendors create own implementations optimized for their hardware.
  - MPICH (Argonne National Lab) and OpenMPI are most widely used implementations.
  - Also commercial implementations from Intel, Microsoft, etc.



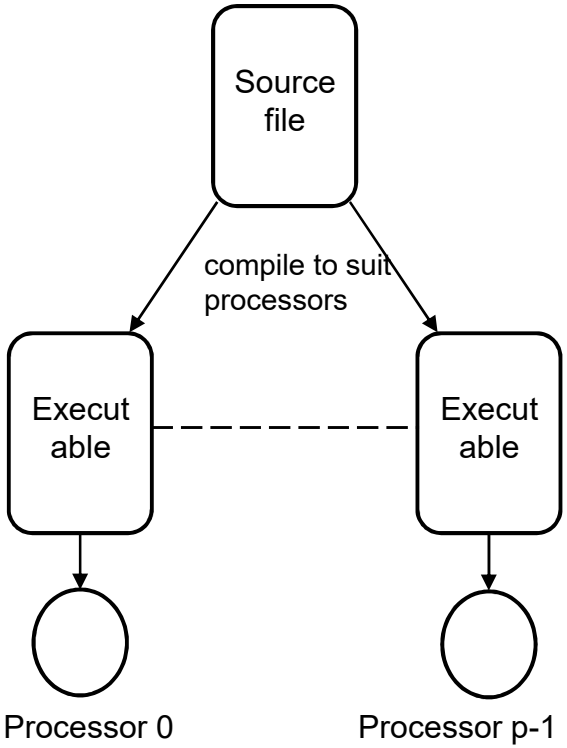


Structure of MPI

- MPI contains four main types of functions.
- Process creation
  - Divide the program into separate processes that can be executed on different processors.
- Sending and receiving messages
  - Point to point vs collective communication.
  - In contrast to shared memory programming where processes interact by reading and writing shared data in memory.
  - Newer versions of MPI also support shared memory style (one way) remote memory access.
- Defining new derived data types.
- Defining and structuring communication groups.
  - Communicators organize processes performing common task.
  - Define topologies for efficient communication.

Process model

- MPI based on SPMD (single program multiple data).
- Same program runs on different processors.
  - Processes do different things based on their ID.
  - Different from Single Instruction Multiple Data (SIMD)!
    - Processes aren't synchronized, and can execute different instructions or different branches of code.
- Process mapping
  - Typically map one process to each processor / core.
    - More processes can cause thrashing, though may also help reduce idling.
  - Programmer can't control the mapping.



Process creation example

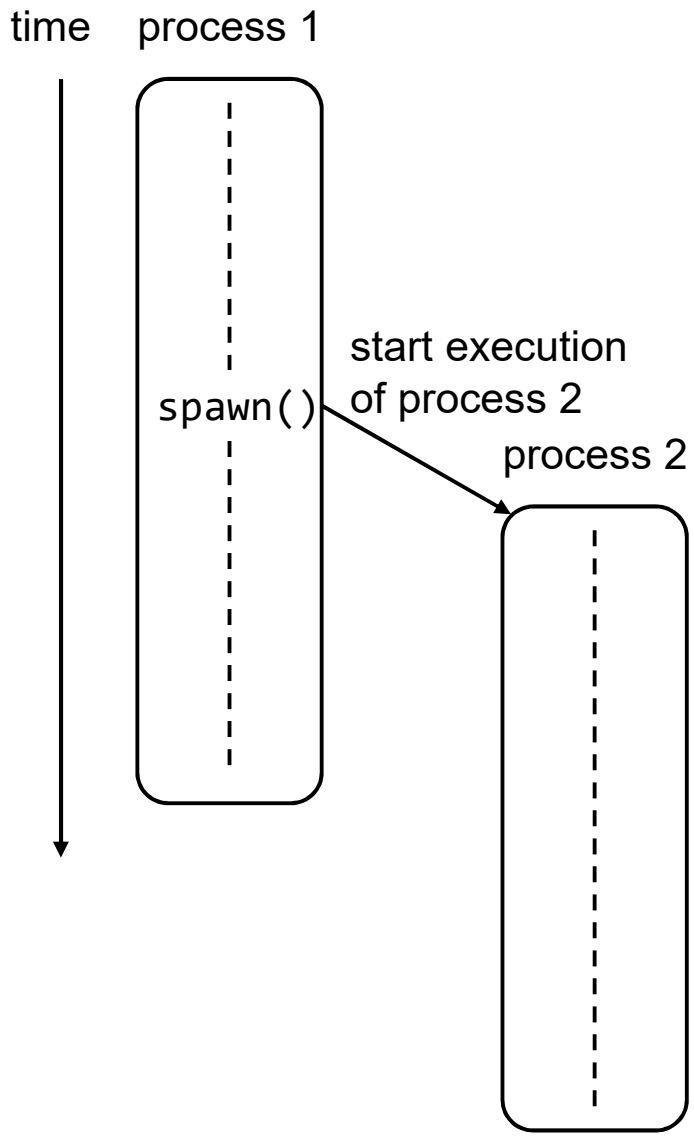
- Include `mpi.h`
- Must call `MPI_Init` and `MPI_Finalize` before and after using MPI functions.

```
#include <mpi.h>

main(int argc, char *argv[]) {
     int npes, myrank;

     MPI_Init(&argc, &argv);
     MPI_Comm_size(MPI_COMM_WORLD, &npes);
     MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
     printf("From process %d out of %d, Hello World!\n",
          myrank, npes);
     MPI_Finalize(); }
```

- Start program with `mpirun -hostfile hosts -np n myprog`
- Output appears on host starting `myprog`.
- Messages may get printed in arbitrary order, because processes run asynchronously.

MPMD model

- Separate programs for each processor.
  - Multi program multi data.
- Usually takes master-slave approach.
  - One processor executes master process, other processes started from within master process.
  - Dynamic process creation.
  - Higher overhead from starting processes, but sometimes easier to understand and program.
  - Used e.g. in Parallel Virtual Machine (PVM) programming system.



MPI in a nutshell

- Many functions, but most programs require only a few functions.
- Initialization.
- Point-to-point communication.
  - Send, receive.
- Collective communication.
  - Broadcast, scatter / gather, all to all, reduce, scan, barrier.
- Derived data types.
  - Contiguous, indexed, struct.
- Communicators, virtual topologies.
- More info at `http://www.mpi-forum.org/docs/`

Communicators

- Communication domain, aka communicator, is a set of processes that can communicate with each other.
  - A program can define multiple communicators.
  - Processes can belong to multiple communication domains.
  - Used to isolate and organize communication.
- Communicators have type `MPI_Comm`.
- All communication must specify a communicator.
- MPI_COMM_WORLD default communicator created automatically.
- Communicator has a size (number of processes in communicator).
  - `int MPI_Comm_size(MPI_Comm comm, int *size)`
- Each process in communicator has a rank (ID).
  - `int MPI_Comm_rank(MPI_Comm comm, int *rank)`
  - Used to allow different processors to do different things.

Sending messages

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

- `buf` is the data to send, i.e. a program variable.
- There are `count` items in `buf`, e.g. the size of the array.
- Buffer items must have type `MPI_Datatype`.
  - `MPI_CHAR, MPI_SHORT, MPI_INT, MPI_FLOAT, MPI_BYTE, MPI_PACKED`
  - Can also send user defined (derived) types.
- Message sent to process in communicator `comm` with rank `dest`.
- `tag` used to differentiate multiple messages between source and destination.
- Messages between pair of processes sent / received in FIFO order.

Receiving messages

```
int MPI_Recv(void *buf, int count, MPI_Datatype type, int source,
int tag, MPI_Comm comm, MPI_Status *status)
```

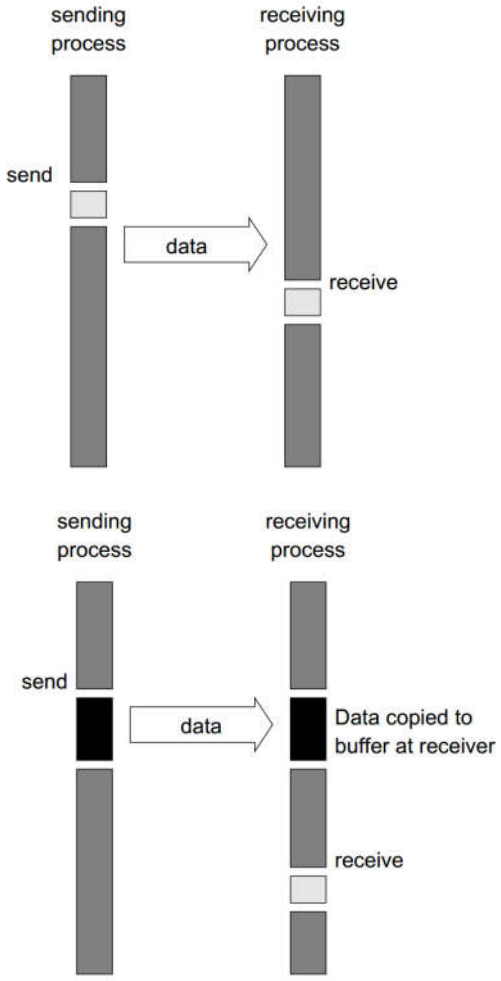
- `buf` gives location to store received messge.
- `count` must be at least number of items to receive.
  - If message too large, MPI_ERROR_TRUNCATE will occur.
- Message received from process with rank `source` in communicator `comm`.
  - Source can also be set to `MPI_ANY_SOURCE` to receive from any process.
- Will only receive message with tag `tag`.
  - Tag can also be set to `MPI_ANY_TAG`.
- `status` useful when receiving using wildcards.
  - `MPI_Status` is a struct with fields `MPI_SOURCE`, `MPI_TAG`, `MPI_ERROR` to get info on wildcard message.
- Fairness not guaranteed. If two sends match a receive, only one send completes.

```c
#include "mpi.h"
#include <stdio.h>

main(int argc, char *argv[])  {
int numtasks, rank, dest, source, rc, count, tag=1;
char inmsg, outmsg='x';
MPI_Status Stat;   // required variable for receive routines

MPI_Init(&argc,&argv);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);

// task 0 sends to task 1 and waits to receive a return message
if (rank == 0) {
  dest = 1;
  source = 1;
  MPI_Send(&outmsg, 1, MPI_CHAR, dest, tag, MPI_COMM_WORLD);
  MPI_Recv(&inmsg, 1, MPI_CHAR, source, tag, MPI_COMM_WORLD, &Stat);
  }

// task 1 waits for task 0 message then returns a message
else if (rank == 1) {
  dest = 0;
  source = 0;
  MPI_Recv(&inmsg, 1, MPI_CHAR, source, tag, MPI_COMM_WORLD, &Stat);
  MPI_Send(&outmsg, 1, MPI_CHAR, dest, tag, MPI_COMM_WORLD);
  }

// query recieve Stat variable and print message details
MPI_Get_count(&Stat, MPI_CHAR, &count);
printf("Task %d: Received %d char(s) from task %d with tag %d \n",
       rank, count, Stat.MPI_SOURCE, Stat.MPI_TAG);

MPI_Finalize();
}
```

Source: https://computing.llnl.gov/tutorials/mpi/

Blocking communication

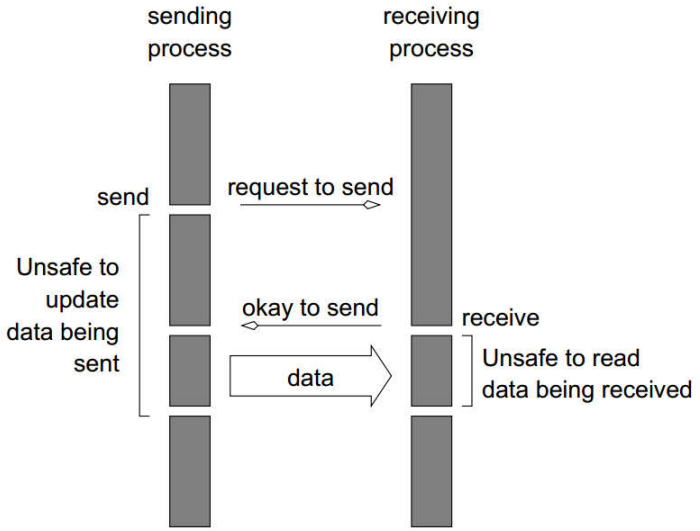
- MPI_Send is blocking: the function won't return immediately after being called.
- Blocking ensures the data is correctly sent.
  - Sender and receiver aren't synchronized, so sender must wait until receiver is ready.
- Waiting time depends on if an MPI implementation uses a system send buffer.
  - If there's a buffer, MPI_Send returns after data copied from application buffer to system buffer.
    - Data is later transferred to system buffer of receiver.
  - With no buffer, sender waits until matching receive occurred.
    - At this point, the data is either in the receiver's hardware or application buffer.
- `MPI_Recv` always causes process to block until data is received into its store buffer.



Source: Introduction to Parallel Computing. Grama et al.

Nonblocking communication

- Would be more efficient if process can immediately resume execution after calling send or receive.
- Data to be transferred is stored in memory buffer.
  - Process continues with computation while data is being transferred.
  - But must not modify buffer until transfer complete.
- Need functions to detect when transfer complete.



Source: Introduction to Parallel Computing. Grama et al.

Nonblocking communication

```
int MPI_Isend(void *buf, int count, MPI_Datatype type, int
dest, int tag, MPI_Comm comm, MPI_Request *req);

int MPI_Irecv(void *buf, int count, MPI_Datatype type, int
source, int tag, MPI_Comm comm, MPI_Request *req);

int MPI_Test(MPI_Request *req, int *flag, MPI_Status *status);

int MPI_Wait(MPI_Request *req, MPI_Status *status);
```

- `MPI_Isend` and `MPI_Irecv` return immediately after being called.
- But must still know when operations complete.
- Use a request object to identify the operation.
  - This object used later to test completion.
  - Can also use to make process wait (block) until operation completes.

Deadlock example 1

- Must be careful about ordering of sends or receives. Otherwise processes can deadlock, i.e. wait forever.

```
int a[10], b[10], myrank;
MPI_Status status;
...
      MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
      MPI_Send(a, 10, MPI_INT, 1, 1,
            MPI_COMM_WORLD);
      MPI_Send(b, 10, MPI_INT, 1, 2,
            MPI_COMM_WORLD);
}
else if (myrank == 1) {
      MPI_Recv(b, 10, MPI_INT, 0, 2,
            MPI_COMM_WORLD);
      MPI_Recv(a, 10, MPI_INT, 0, 1,
            MPI_COMM_WORLD);}
```

- If buffering, then probably no deadlock.
- If no buffering, processes will deadlock waiting to receive from each other.
- Cause is that tags are sent and received in different orders

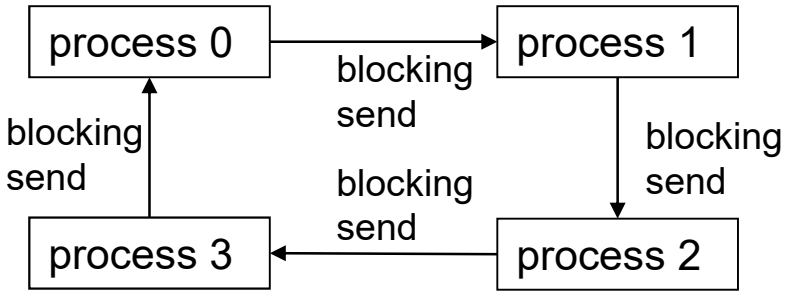
```
int a[10], b[10], myrank;
MPI_Status status;
...
      MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
      MPI_Send(a, 10, MPI_INT, 1, 1,
            MPI_COMM_WORLD);
      MPI_Send(b, 10, MPI_INT, 1, 2,
            MPI_COMM_WORLD);
}
else if (myrank == 1) {
      MPI_Recv(b, 10, MPI_INT, 0, 1,
            MPI_COMM_WORLD);
      MPI_Recv(a, 10, MPI_INT, 0, 2,
            MPI_COMM_WORLD);}
```

- Resolve the deadlock by using same tag order for send and recv.

Deadlock example 2

```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Send(a, 10, MPI_INT, (myrank+1)%npes,
      1, MPI_COMM_WORLD);
MPI_Recv(b, 10, MPI_INT, (myrank-1)%npes,
      1, MPI_COMM_WORLD);
```

- Here, npes processes in a ring. Process i sends to i+1, receives from i-1.
- No deadlock with buffering, since MPI_Send returns and MPI_Recv can occur.
- Without buffering, processes deadlock blocking for matching receive.




```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank%2 == 0) {
      MPI_Send(a, 10, MPI_INT, (myrank+1)%npes,
            1, MPI_COMM_WORLD);
      MPI_Recv(b, 10, MPI_INT, (myrank-1)%npes,
            1, MPI_COMM_WORLD);
}
else {
      MPI_Recv(b, 10, MPI_INT, (myrank-1)%npes,
            1, MPI_COMM_WORLD);
      MPI_Send(a, 10, MPI_INT, (myrank+1)%npes,
            1, MPI_COMM_WORLD); }
```

- Solution is to first let even numbered processes send and odd processes recv, then let odd processes send and even processes recv.
- This is cumbersome. It would be nice to have built-in way to avoid deadlock.

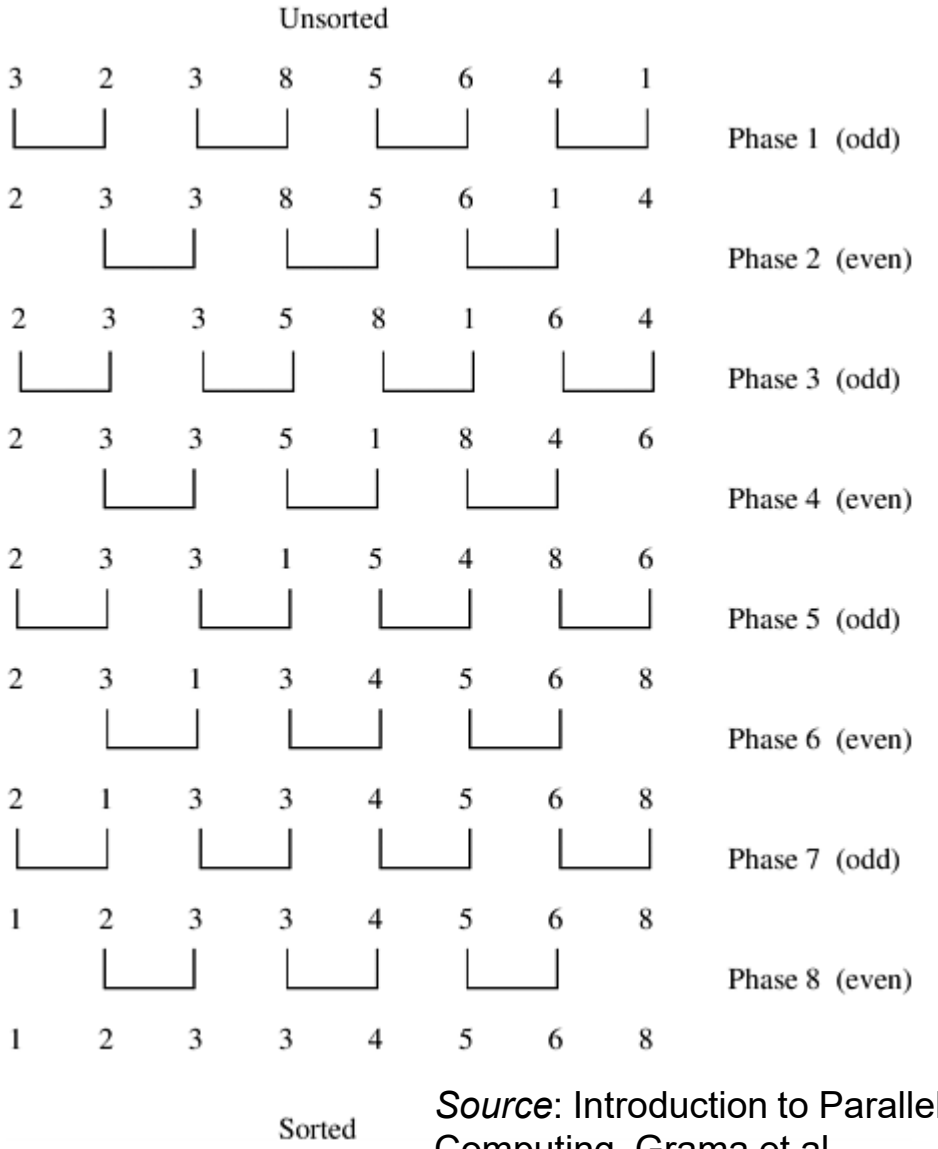
Send and receive simultaneously

- `int MPI_Sendrecv(void *sendbuf, int sendcount, MPI_Datatype senddatatype, int dest, int sendtag, void *recvbuf, int recvcount, MPI_Datatype recvdatatype, int source, int recvtag, MPI_Comm comm, MPI_Status *status)`

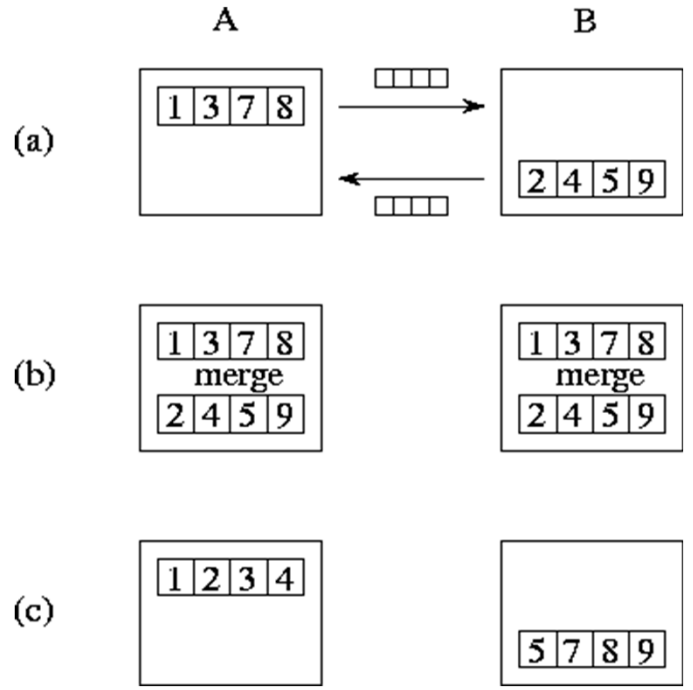
```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Sendrecv(a, 10, MPI_INT, (myrank+1)%npes, 1, b, 10, MPI_INT,
     (myrank-1)%npes, 1, MPI_COMM_WORLD, &status);
```

- MPI_Sendrecv sends a message and starts a receive before blocking.
- Will block until send completes and receiving application buffer receives message.
  - No deadlock on ring.

Even-odd sort



Source: Introduction to Parallel Computing. Grama et al.



- If each processor has multiple values, then instead of simply swapping them, do compare-split step.
- This combines the values from two processes, and puts the smaller half in left process, larger half in right process.

Even-odd sort in MPI

```
#include <stdlib.h>
#include <mpi.h> /* Include MPI's header file */

main(int argc, char *argv[])
{
int n; /* The total number of elements to be sorted */
int npes; /* The total number of processes */
int myrank; /* The rank of the calling process */
int nlocal; /* The local number of elements, and the
            array that stores them */
int *elmnts; /* The array that stores the local
            elements */
int *relmnts; /* The array that stores the received
            elements */
int oddrank; /* The rank of the process during odd-
            phase communication */
int evenrank; /* The rank of the process during even-
            phase communication */
int *wspace; /* Working space during the compare-split
            operation */
int i;
MPI_Status status;

/* Initialize MPI and get system information */
MPI_Init(&argc, &argv);
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

n = atoi(argv[1]);
nlocal = n/npes; /* Compute the number of elements to
            be stored locally. */
```

```
/* Allocate memory for the various arrays */
elmnts = (int *)malloc(nlocal*sizeof(int));
relmnts = (int *)malloc(nlocal*sizeof(int));
wspace = (int *)malloc(nlocal*sizeof(int));

/* Fill-in the elmnts array with random elements */
srandom(myrank);
for (i=0; i<nlocal; i++)
      elmnts[i] = random();

/* Sort the local elements using the built-in
quicksort routine */
qsort(elmnts, nlocal, sizeof(int), IncOrder);

/* Determine the rank of the processors that myrank
needs to communicate with during the */
/* odd and even phases of the algorithm */
if (myrank%2 == 1) {
      oddrank = myrank-1;
      evenrank = myrank+1;
}
else {
      oddrank = myrank+1;
      evenrank = myrank-1;
}
```

Source: Introduction to Parallel Computing. Grama et al.

Even-odd sort in MPI

```
/* Set first processor's communication ranks */
if (oddrank == -1 || oddrank == npes)
      oddrank = MPI_PROC_NULL;
if (evenrank == -1 || evenrank == npes)
      evenrank = MPI_PROC_NULL;

/* Main loop of the odd-even sorting algorithm */
for (i=0; i<npes-1; i++) {
      if (i%2 == 1) /* Odd phase */
            MPI_Sendrecv(elmnts, nlocal, MPI_INT,
            oddrank, 1, relmnts, nlocal, MPI_INT,
            oddrank, 1, MPI_COMM_WORLD, &status);
      else /* Even phase */
            MPI_Sendrecv(elmnts, nlocal, MPI_INT,
            evenrank, 1, relmnts, nlocal, MPI_INT,
            evenrank, 1, MPI_COMM_WORLD, &status);

      CompareSplit(nlocal, elmnts, relmnts, wspace,
            myrank < status.MPI_SOURCE);
      }

free(elmnts); free(relmnts); free(wspace);
MPI_Finalize();
}
```

```
CompareSplit(int nlocal, int *elmnts, int *relmnts,
int *wspace, int keepsmall) {
   int i, j, k;

   for (i=0; i<nlocal; i++)
      wspace[i] = elmnts[i];
/* Copy the elmnts array into the wspace array */

   if (keepsmall) { /* Keep nlocal smaller elts */
      for (i=j=k=0; k<nlocal; k++) {
         if (j == nlocal || (i < nlocal &&
            wspace[i] < relmnts[j]))
            elmnts[k] = wspace[i++];
         else
            elmnts[k] = relmnts[j++];
      }}
   else { /* Keep the nlocal larger elements */
      for (i=k=nlocal-1, j=nlocal-1; k>=0; k--) {
         if (j == 0 || (i >= 0 && wspace[i] >=
            relmnts[j]))
            elmnts[k] = wspace[i--];
         else
            elmnts[k] = relmnts[j--];
}}}

int IncOrder(const void *e1, const void *e2) {
   return (*((int *)e1) - *((int *)e2));
}
```

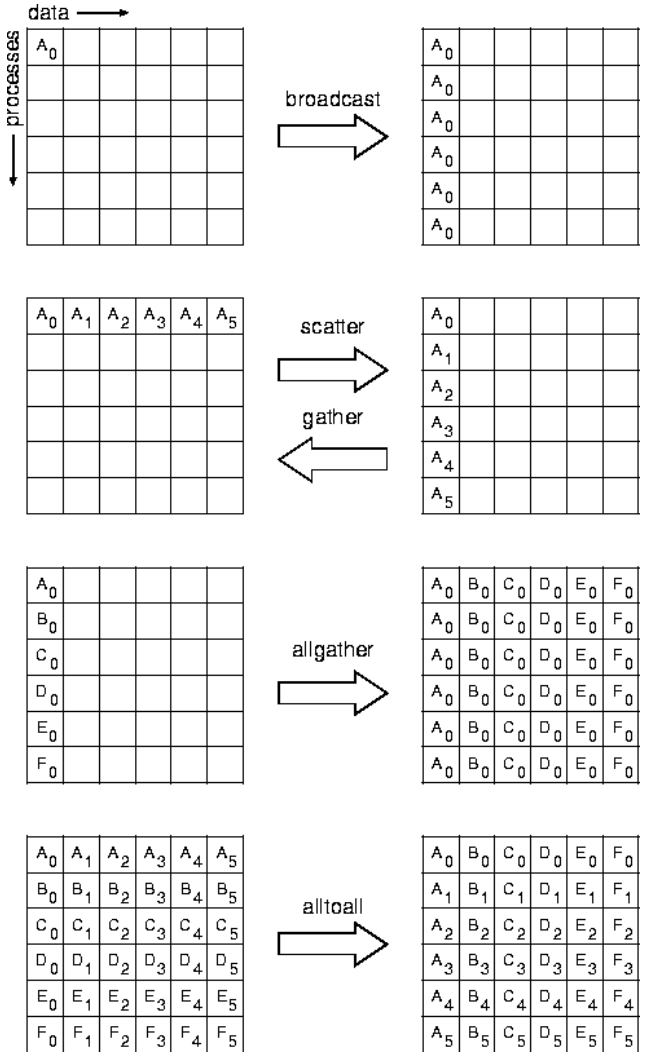
Collective communication

- Collective communication are routines that provide message passing between a group of processes.
  - One-to-many, e.g. broadcast, scatter
  - Many-to-one, e.g. gather, reduce
  - Many-to-many, e.g. All-to-all
- Collective communication may be implemented using point-to-point routines.
- Specialized implementation of collective communication is likely to be more efficient.
- Collectives are blocking in MPI 1 and 2, but MPI 3 includes nonblocking collectives.

Collective communication

- As with point to point communication, need to specify the communicator.

  - `MPI_Bcast()`
  - `MPI_Reduce()`
    - `MPI_Allreduce()`
  - `MPI_Scan()`
  - `MPI_Gather()`
  - `MPI_Scatter()`
    - `MPI_Scatterv()`
  - `MPI_Alltoall()`
    - `MPI_Alltoallv()`
  - `MPI_Barrier()`

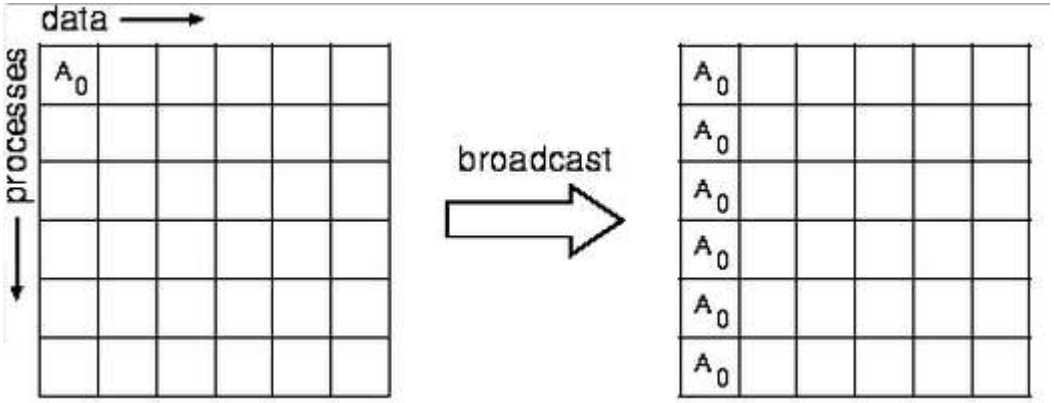


Source: http://www.mpi-forum.org/docs/mpi-1.1/mpi-11-html/coll-fig1.gif

Broadcast

```
int MPI_Bcast(void *buf, int count, MPI_Datatype type, int
source, MPI_Comm comm)
```

- Send the data in `buf` at the `source` process to all processes (including `source`) in `comm`.
  - Non-`source` nodes store the incoming data in their `buf`.
- Note that even though the message is coming from `source`, all processes, including the receiving ones, call `MPI_Bcast()`.
  - See the example on the next slide.



Broadcast example

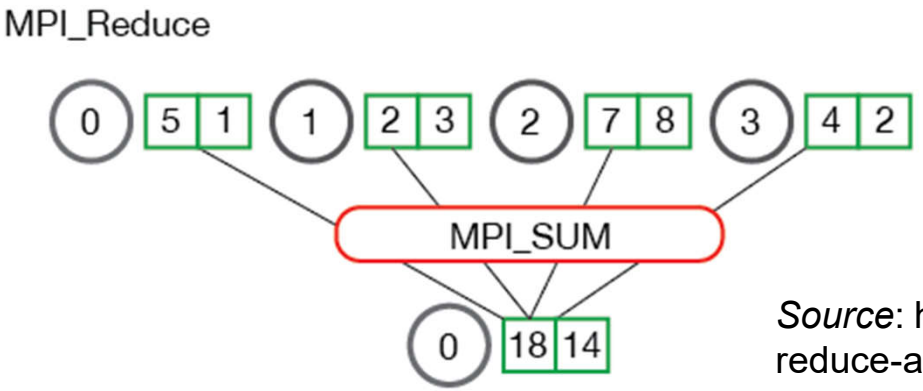
```
#include <mpi.h>

int main(int argc, char** argv) {
   int myrank;
   int buf;
   const int root=0;

   MPI_Init(&argc, &argv);
   MPI_Comm_rank(MPI_COMM_WORLD, &myrank);

   if (myrank == root) {
      buf = 1; }

   /* All procs call bcast.  buf is sent from
   root to all procs */
   MPI_Bcast(&buf, 1, MPI_INT, root,
      MPI_COMM_WORLD);

   MPI_Finalize();
   return 0;
}
```

- This code causes process `root` to send `buf` (i.e. the value 1) to all the processes.
- Since MPI uses an SPMD model, all processes run the same code.
- So even the non-root processes do `MPI_Bcast(&buf, 1, MPI_INT, root, MPI_COMM_WORLD)`
- However, since their `myrank != root`, then instead of sending, the `MPI_Bcast()` will cause them to receive.
- Think of `MPI_Bcast()` as saying "participate in a broadcast", with the type of participation depending on the process's rank.
- The other collective operations work similarly, i.e. all procs run the same code, but do different things depending on their rank.

Reduce

```
int MPI_Reduce(void *sendbuf, void *recvbuf, int count,
MPI_Datatype type, MPI_Op op, int target, MPI_Comm comm)
```

- Combine the elements stored in the buffer `sendbuf` of each process in `comm` using the operation `op`, and store the combined values in `recvbuf` of process `target`.
- Ex Add the values from all the processes.
- Operations include `MPI_MAX, MPI_MIN, MPI_SUM, MPI_PROD, MPI_LAND, MPI_MAXLOC.`
  - `MPI_MAXLOC` p returns a pair of values (v,l) in `recvbuf`, where v is the max value, and l is the smallest ranked process with the value.

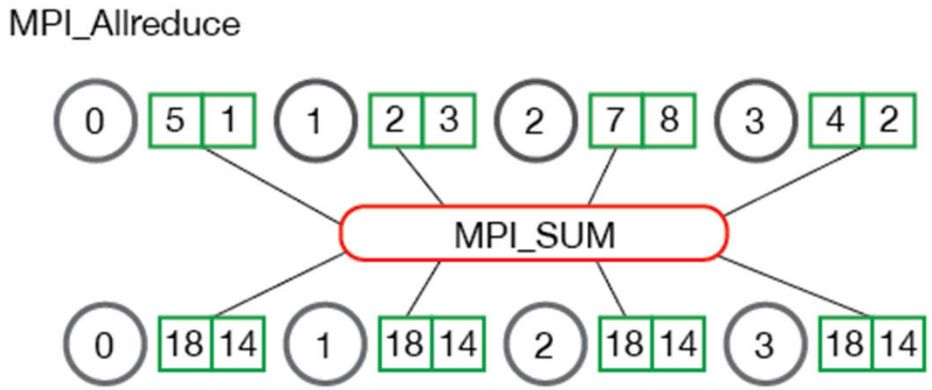


Source: http://mpitutorial.com/tutorials/mpi-reduce-and-allreduce/

Allreduce

```
int MPI_Allreduce(void *sendbuf, void *recvbuf, int count,
MPI_Datatype type, MPI_Op op, MPI_Comm comm)
```

- Same as reduce, but store the result at all the processes.

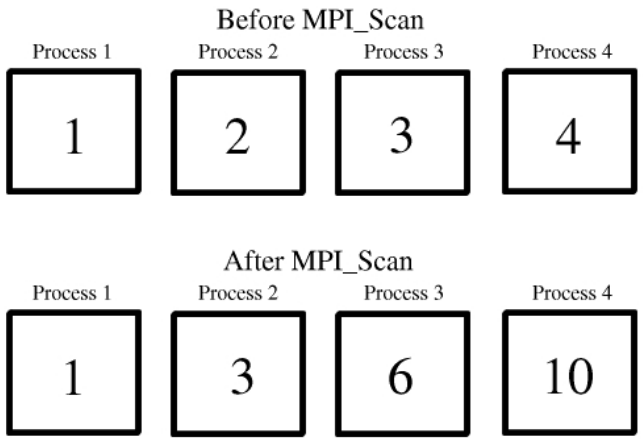


Source: http://mpitutorial.com/tutorials/mpi-reduce-and-allreduce/

Scan

```
int MPI_Scan(void *sendbuf, void *recvbuf, int count,
MPI_Datatype type, MPI_Op op, MPI_Comm comm)
```

- List the data in the `sendbuf`'s of all the processes by process rank.
- Process i applies `op` (elementwise) to the first i `sendbuf`'s and stores the result in its `recvbuf`.
- Ex Add values from the processes.
- This operation is also called prefix sum.
  - Can apply other operators besides sum, as in reduce.

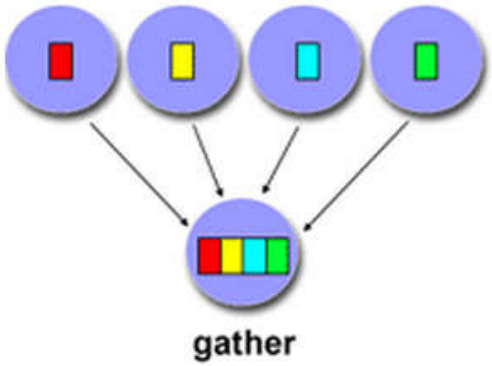


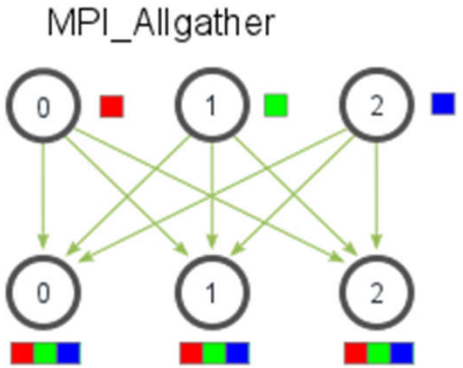
Source: http://www.rc.usf.edu/tutorials/classes/tutorial/mpi/images/scan_ex.jpg

Gather

```
int MPI_Gather(void *sendbuf, int sendcount, MPI_Datatype sendtype, void
*recvbuf, int recvcount, MPI_Datatype recvtype, int target, MPI_Comm comm)

int MPI_Allgather(void *sendbuf, int sendcount, MPI_Datatype sendtype, void
*recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)
```

- Gather collects the `sendbuf`'s from all the processes in `comm` into the `recvbuf` of process `target`.
  - If k processes in `comm` each with `sendbuf` of size t, then `target` will receive k*t items.
  - Allgather collects this data at all the processes.

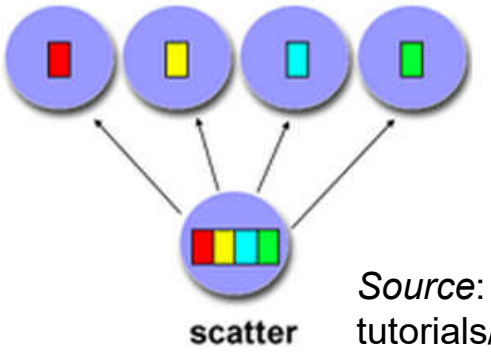




Scatter

```
int MPI_Scatter(void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf,
int recvcount, MPI_Datatype recvtype, int source, MPI_Comm comm)

int MPI_Scatterv(void *sendbuf, int *sendcounts, int *displs, MPI_Datatype sendtype,
void *recvbuf, int recvcount, MPI_Datatype recvtype, int source, MPI_Comm comm)
```

- Scatter sends the data at location i*`recvcount` in `sendbuf` to the `recvbuf` of i'th process in `comm`.
  - All scattered data have the same size.
- Scatterv sends data of different sizes to different processes.
  - Sizes of data specified in `sendcounts`.
  - Data to send to process i starts at location `displs`[i] in `sendbuf`.
  - For the receiving processes (i.e. all processes other than `source`), the first 4 arguments don't matter.
  - Each receiving process sets `recvcount` to the number of items it expects to get.

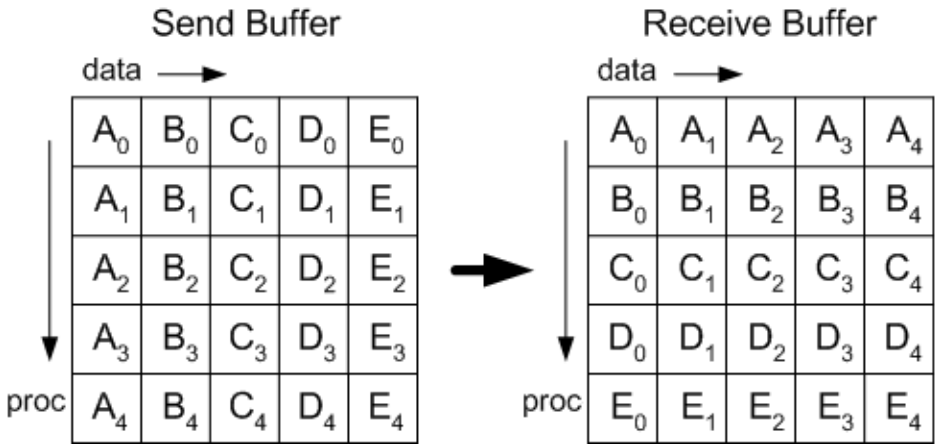


Source: https://computing.llnl.gov/tutorials/mpi/

Alltoall

```
int MPI_Alltoall(void *sendbuf, int sendcount, MPI_Datatype sendtype, void
*recvbuf, int recvcount, MPI_Datatype recvtype, MPI_Comm comm)

int MPI_Alltoallv(void *sendbuf, int *sendcounts, int *sdispls,
MPI_Datatype sendtype, void *recvbuf, int *recvcounts, int *rdispls,
MPI_Datatype recvtype, MPI_Comm comm)
```

- Alltoall sends to process i `sendcount` elements from `sendbuf` starting from location i*`sendcount` of `sendbuf`.
- Alltoallv is similar, but allows sending different size data to each process.

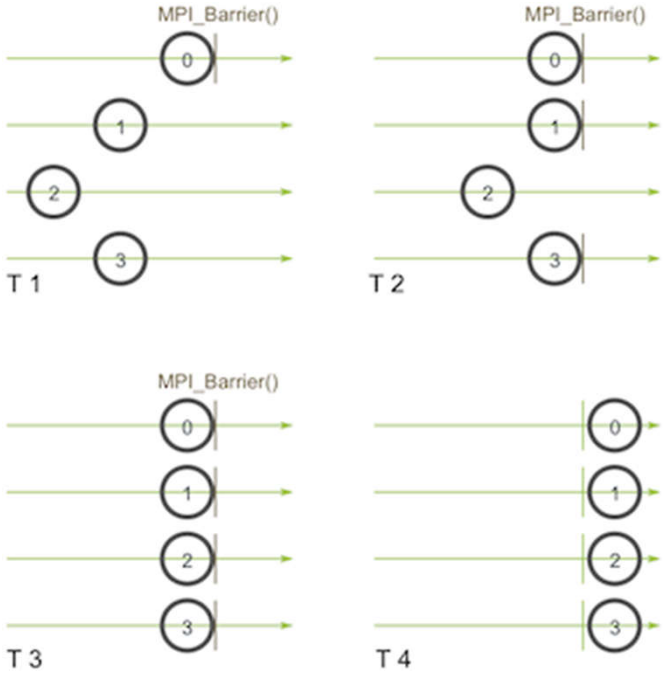


Source: https://cvw.cac.cornell.edu/MPIcc/alltoall

Barrier

```
int MPI_Barrier(MPI_Comm comm)
```

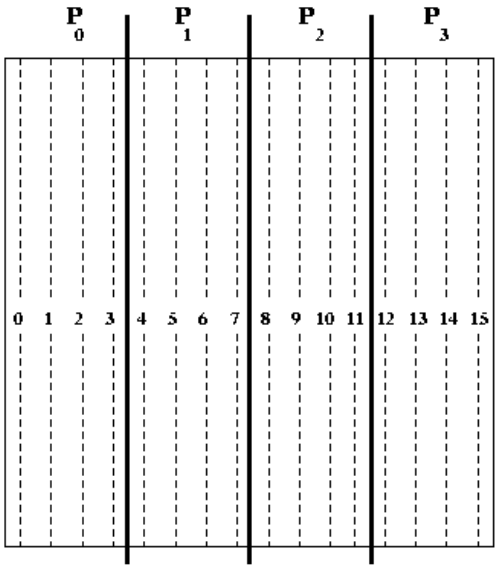
- Used to synchronize all the processes in `comm` at a certain point in the code before any of them can proceed.
  - All processes in comm must reach the barrier. Otherwise, all processes will block forever.
- Can use multiple barriers.
  - All processes must reach the b'th barrier before proceeding to barrier b+1.



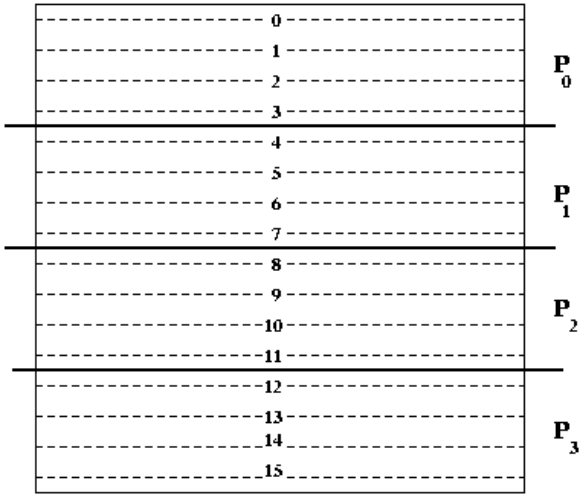
Source: http://mpitutorial.com/tutorials/mpi-broadcast-and-collective-communication/barrier.png

Storing a matrix

- Linear algebra one of the main applications for parallel computing.
- A large matrix can be stored in a distributed fashion on the parallel processors using row or column striping.
- Even with columnwise block stripping, we store columns in row-major format.



(a) Columnwise block stripping

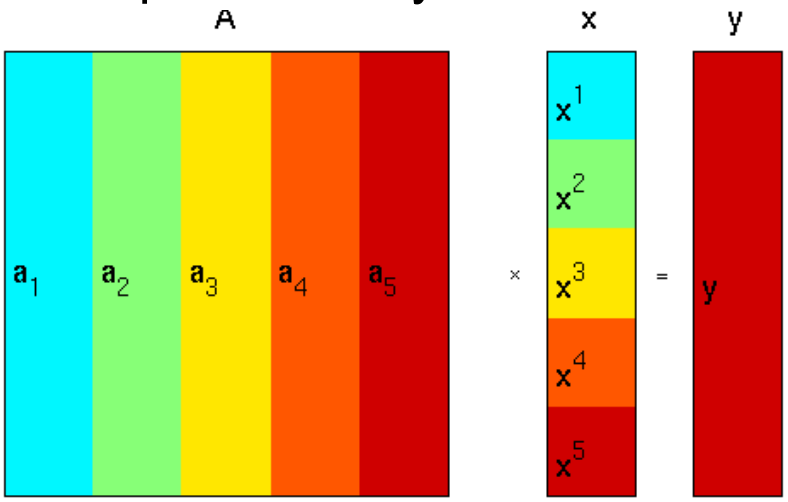


(b) Rowwise block stripping

Source: http://www.cse.iitd.ernet.in/~dheerajb/MPI/Document/onedblk.gif

Column-wise matrix vector mult

- Compute y = A*x using p processes.
  - A is an $n \times n$ matrix, x and y are $n \times 1$ vectors.
  - Each process holds n/p columns from A and n/p values from x.
- Each process does dot product on its columns with its portions of x.
  - Process ends up with n (partial) dot products.
- y[i] = sum of the p partial dot products for the i'th row held at the different processes.
  - Do a sum reduce for each row of y.
- Finally, distribute n/p values of y to each of the processes.



Source: https://www.informatik.uni-konstanz.de/fileadmin/informatik/ag-saupe/Webpages/lehre/na_08/Lab1/1_Preliminaries/html/matrixVectorProduct.html

Column-wise matrix vector mult

```
ColMatrixVectorMultiply(int n, double *a,
     double *x, double *y, MPI_Comm comm)
{
     int i, j;
     int nlocal;
     double *py;
     double *fy;
     int npes, myrank;
     MPI_Status status;

/* Get communicator information */
     MPI_Comm_size(comm, &npes);
     MPI_Comm_rank(comm, &myrank);
     nlocal = n/npes;

/* Allocate memory for arrays storing
intermediate results. */
     py = (double *)
          malloc(n*sizeof(double));
     fy = (double *)
          malloc(n*sizeof(double));
```

```
/* Compute partial-dot products that
correspond to local columns of A*/
     for (i=0; i<n; i++) {
          py[i] = 0.0;
          for (j=0; j<nlocal; j++)
               py[i] += a[i*nlocal+j]*x[j];
     }

/* Sum-up results by performing an
element-wise reduction operation */
     MPI_Reduce(py, fy, n, MPI_DOUBLE,
          MPI_SUM, 0, comm);

/* Redistribute fy in a fashion similar to
vector x */
     MPI_Scatter(fy, nlocal, MPI_DOUBLE,
          y, nlocal, MPI_DOUBLE, 0, comm);

     free(py); free(fy);
}
```

Source: Introduction to Parallel Computing. Grama et al.

Derived data types

- MPI comes with a number of standard built in types.
- To send more complicated data structures, programmer defines derived types.
- Four main types, contiguous, vector, indexed and struct.
- `MPI_Type_commit(&datatype)` commits defined datatype.
- `MPI_Type_extent(&datatype)` returns size in bytes of the datatype.
- `MPI_Type_free(&datatype)` Deallocates a datatype, prevent memory exhaustion.

Defining new datatypes

- `MPI_Type_contiguous(count, oldtype, &newtype)`
  - Place `count` copies of `oldtype` contiguously.
- `MPI_Type_vector(count, blocklength, stride, oldtype, &newtype)`
  - Similar to contiguous, use `count` copies of `oldtype` each of `blocklength`, with `stride` bytes in between.
- `MPI_Type_indexed (count, blocklens[], offsets[], old_type, &newtype)`
  - Similar to vector, except `blocklens` and `offsets` vectors (of size count) specify size and offset of each element in the datatype.
- `MPI_Type_struct (count,blocklens[], offsets[], old_types, &newtype)`
  - Form a datatype according to a completely defined map of the component data types.

```c
#include "mpi.h"
#include <stdio.h>
#define SIZE 4

main(int argc, char *argv[])  {
int numtasks, rank, source=0, dest, tag=1, i;
float a[SIZE][SIZE] =
  {1.0, 2.0, 3.0, 4.0,
   5.0, 6.0, 7.0, 8.0,
   9.0, 10.0, 11.0, 12.0,
  13.0, 14.0, 15.0, 16.0};
float b[SIZE];

MPI_Status stat;
MPI_Datatype columntype;   // required variable


MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

// create vector derived data type
MPI_Type_vector(SIZE, 1, SIZE, MPI_FLOAT, &columntype);
MPI_Type_commit(&columntype);

if (numtasks == SIZE) {
   // task 0 sends one element of columntype to all tasks
   if (rank == 0) {
      for (i=0; i<numtasks; i++)
         MPI_Send(&a[0][i], 1, columntype, i, tag, MPI_COMM_WORLD);
      }

   // all tasks receive columntype data from task 0
   MPI_Recv(b, SIZE, MPI_FLOAT, source, tag, MPI_COMM_WORLD, &stat);
   printf("rank= %d  b= %3.1f %3.1f %3.1f %3.1f\n",
          rank,b[0],b[1],b[2],b[3]);
   }
else
   printf("Must specify %d processors. Terminating.\n",SIZE);

// free datatype when done using it
MPI_Type_free(&columntype);
MPI_Finalize();
}
```

MPI_ Type_vector

count = 4; blocklength = 1; stride = 4;
MPI_Type_vector(count, blocklength, stride, MPI_FLOAT, &columntype);

1.0	2.0	3.0	4.0
5.0	6.0	7.0	8.0
9.0	10.0	11.0	12.0
13.0	14.0	15.0	16.0

a[4][4]

MPI_Send(&a[0][1], 1, columntype, dest, tag, comm);

2.0	6.0	10.0	14.0

1 element of columntype

```
rank= 0  b= 1.0 5.0 9.0 13.0
rank= 1  b= 2.0 6.0 10.0 14.0
rank= 2  b= 3.0 7.0 11.0 15.0
rank= 3  b= 4.0 8.0 12.0 16.0
```

Source: https://computing.llnl.gov/tutorials/mpi

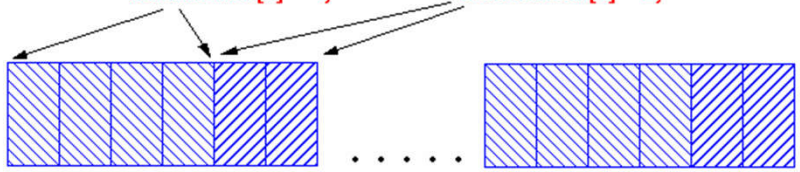
```c
#include "mpi.h"
#include <stdio.h>
#define NELEM 25

main(int argc, char *argv[])  {
int numtasks, rank, source=0, dest, tag=1, i;

typedef struct {
  float x, y, z;
  float velocity;
  int  n, type;
  }          Particle;
Particle     p[NELEM], particles[NELEM];
MPI_Datatype particletype, oldtypes[2];   // required variables
int          blockcounts[2];

// MPI_Aint type used to be consistent with syntax of
// MPI_Type_extent routine
MPI_Aint    offsets[2], extent;

MPI_Status stat;

MPI_Init(&argc,&argv);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

// setup description of the 4 MPI_FLOAT fields x, y, z, velocity
offsets[0] = 0;
oldtypes[0] = MPI_FLOAT;
blockcounts[0] = 4;

// setup description of the 2 MPI_INT fields n, type
// need to first figure offset by getting size of MPI_FLOAT
MPI_Type_extent(MPI_FLOAT, &extent);
offsets[1] = 4 * extent;
oldtypes[1] = MPI_INT;
blockcounts[1] = 2;

// define structured type and commit it
MPI_Type_struct(2, blockcounts, offsets, oldtypes, &particletype);
MPI_Type_commit(&particletype);

// task 0 initializes the particle array and then sends it to each task
if (rank == 0) {
  for (i=0; i<NELEM; i++) {
     particles[i].x = i * 1.0;
     particles[i].y = i * -1.0;
     particles[i].z = i * 1.0;
     particles[i].velocity = 0.25;
     particles[i].n = i;
     particles[i].type = i % 2;
     }
  for (i=0; i<numtasks; i++)
     MPI_Send(particles, NELEM, particletype, i, tag, MPI_COMM_WORLD);
  }

// all tasks receive particletype data
MPI_Recv(p, NELEM, particletype, source, tag, MPI_COMM_WORLD, &stat);

printf("rank= %d   %3.2f %3.2f %3.2f %3.2f %d %d\n", rank,p[3].x,
     p[3].y,p[3].z,p[3].velocity,p[3].n,p[3].type);

// free datatype when done using it
MPI_Type_free(&particletype);
MPI_Finalize();
}
```

MPI_ Type_struct

typedef struct { float x, y, z, velocity; int n, type; } Particle;
Particle particles[NELEM];

MPI_Type_extent(MPI_FLOAT, &extent);

count = 2; oldtypes[0] = MPI_FLOAT; oldtypes[1] = MPI_INT
offsets[0] = 0; offsets[1] = 4 * extent;
blockcounts[0] = 4; blockcounts[1] = 2;



particles[NELEM]

MPI_Type_struct(count, blockcounts, offsets, oldtypes, &particletype);

MPI_Send(particles, NELEM, particletype, dest, tag, comm);

Sends entire (NELEM) array of particles, each particle being comprised four floats and two integers.

```
rank= 0   3.00 -3.00 3.00 0.25 3 1
rank= 2   3.00 -3.00 3.00 0.25 3 1
rank= 1   3.00 -3.00 3.00 0.25 3 1
rank= 3   3.00 -3.00 3.00 0.25 3 1
```

More on communicators

```
1  #include "mpi.h"
2  #include <stdio.h>
3  #define NPROCS 8
4
5  main(int argc, char *argv[])  {
6  int         rank, new_rank, sendbuf, recvbuf, numtasks,
7              ranks1[4]={0,1,2,3}, ranks2[4]={4,5,6,7};
8  MPI_Group  orig_group, new_group;   // required variables
9  MPI_Comm   new_comm;   // required variable
10
11 MPI_Init(&argc,&argv);
12 MPI_Comm_rank(MPI_COMM_WORLD, &rank);
13 MPI_Comm_size(MPI_COMM_WORLD, &numtasks);
14
15 if (numtasks != NPROCS) {
16   printf("Must specify MP_PROCS= %d. Terminating.\n",NPROCS);
17   MPI_Finalize();
18   exit(0);
19   }
20
21 sendbuf = rank;
22
23 // extract the original group handle
24 MPI_Comm_group(MPI_COMM_WORLD, &orig_group);
25
26 //  divide tasks into two distinct groups based upon rank
27 if (rank < NPROCS/2) {
28   MPI_Group_incl(orig_group, NPROCS/2, ranks1, &new_group);
29   }
30 else {
31   MPI_Group_incl(orig_group, NPROCS/2, ranks2, &new_group);
32   }
33
34 // create new new communicator and then perform collective communicat
35 MPI_Comm_create(MPI_COMM_WORLD, new_group, &new_comm);
36 MPI_Allreduce(&sendbuf, &recvbuf, 1, MPI_INT, MPI_SUM, new_comm);
37
38 // get rank in new group
39 MPI_Group_rank (new_group, &new_rank);
40 printf("rank= %d newrank= %d recvbuf= %d\n",rank,new_rank,recvbuf);
41
42 MPI_Finalize();
43 }
```

- Communicators are a programming aid to group processes that perform a common task.
- Collective computations are done within a communicator.
  - MPI 2 allows collectives between communicators.
- Processes have a unique rank in each communicator they belong to.

```
rank= 7 newrank= 3 recvbuf= 22
rank= 0 newrank= 0 recvbuf= 6
rank= 1 newrank= 1 recvbuf= 6
rank= 2 newrank= 2 recvbuf= 6
rank= 6 newrank= 2 recvbuf= 22
rank= 3 newrank= 3 recvbuf= 6
rank= 4 newrank= 0 recvbuf= 22
rank= 5 newrank= 1 recvbuf= 22
```

Virtual topologies

- Map a communicator of processes to a virtual topology.
- Virtual topology may not correspond to the physical topology of underlying hardware.
- Nevertheless, allows MPI implementation to try to optimize mapping of virtual to physical topology, e.g. mapping a virtual mesh to a physical hypercube.
- Also a programming convenience, to match topology of application communications to virtual topology.
  - A 3D physics code can use a virtual 3D mesh topology.
- Main topologies are regular torus and graph.
  - `MPI_Cart_create(MPI_Comm oldcomm, int ndim, int dims[], int qperiodic[], int qreorder, MPI_Comm *newcomm)`
  - `MPI_Dist_graph_create_adjacent(MPI_Comm oldcomm, int indegree, int sources[], int sourceweights[], int outdegree, int dests[], int destweights[], MPI_Info info, int qreorder, MPI_Comm *newcomm)`

```c
#include "mpi.h"
#include <stdio.h>
#define SIZE 16
#define UP    0
#define DOWN  1
#define LEFT  2
#define RIGHT 3

main(int argc, char *argv[])  {
int numtasks, rank, source, dest, outbuf, i, tag=1,
   inbuf[4]={MPI_PROC_NULL,MPI_PROC_NULL,MPI_PROC_NULL,MPI_PROC_NULL,},
   nbrs[4], dims[2]={4,4},
   periods[2]={0,0}, reorder=0, coords[2];

MPI_Request reqs[8];
MPI_Status stats[8];
MPI_Comm cartcomm;   // required variable

MPI_Init(&argc,&argv);
MPI_Comm_size(MPI_COMM_WORLD, &numtasks);

if (numtasks == SIZE) {
   // create cartesian virtual topology, get rank, coordinates, neighbor ranks
   MPI_Cart_create(MPI_COMM_WORLD, 2, dims, periods, reorder, &cartcomm);
   MPI_Comm_rank(cartcomm, &rank);
   MPI_Cart_coords(cartcomm, rank, 2, coords);
   MPI_Cart_shift(cartcomm, 0, 1, &nbrs[UP], &nbrs[DOWN]);
   MPI_Cart_shift(cartcomm, 1, 1, &nbrs[LEFT], &nbrs[RIGHT]);

   printf("rank= %d coords= %d %d  neighbors(u,d,l,r)= %d %d %d %d\n"
          rank,coords[0],coords[1],nbrs[UP],nbrs[DOWN],nbrs[LEFT],
          nbrs[RIGHT]);

   outbuf = rank;

   // exchange data (rank) with 4 neighbors
   for (i=0; i<4; i++) {
      dest = nbrs[i];
      source = nbrs[i];
      MPI_Isend(&outbuf, 1, MPI_INT, dest, tag,
                MPI_COMM_WORLD, &reqs[i]);
      MPI_Irecv(&inbuf[i], 1, MPI_INT, source, tag,
                MPI_COMM_WORLD, &reqs[i+4]);
      }

   MPI_Waitall(8, reqs, stats);

   printf("rank= %d                  inbuf(u,d,l,r)= %d %d %d %d\n",
          rank,inbuf[UP],inbuf[DOWN],inbuf[LEFT],inbuf[RIGHT]);  }
else
   printf("Must specify %d processors. Terminating.\n",SIZE);

MPI_Finalize();
}
```

0 (0,0)	1 (0,1)	2 (0,2)	3 (0,3)
4 (1,0)	5 (1,1)	6 (1,2)	7 (1,3)
8 (2,0)	9 (2,1)	10 (2,2)	11 (2,3)
12 (3,0)	13 (3,1)	14 (3,2)	15 (3,3)

```
rank=   0 coords=  0 0 neighbors(u,d,l,r)=  -1  4 -1  1
rank=   0                  inbuf(u,d,l,r)=  -1  4 -1  1
rank=   8 coords=  2 0 neighbors(u,d,l,r)=   4 12 -1  9
rank=   8                  inbuf(u,d,l,r)=   4 12 -1  9
rank=   1 coords=  0 1 neighbors(u,d,l,r)=  -1  5  0  2
rank=   1                  inbuf(u,d,l,r)=  -1  5  0  2
rank=  13 coords=  3 1 neighbors(u,d,l,r)=   9 -1 12 14
rank=  13                  inbuf(u,d,l,r)=   9 -1 12 14
...
...
rank=   3 coords=  0 3 neighbors(u,d,l,r)=  -1  7  2 -1
rank=   3                  inbuf(u,d,l,r)=  -1  7  2 -1
rank=  11 coords=  2 3 neighbors(u,d,l,r)=   7 15 10 -1
rank=  11                  inbuf(u,d,l,r)=   7 15 10 -1
rank=  10 coords=  2 2 neighbors(u,d,l,r)=   6 14  9 11
rank=  10                  inbuf(u,d,l,r)=   6 14  9 11
rank=   9 coords=  2 1 neighbors(u,d,l,r)=   5 13  8 10
rank=   9                  inbuf(u,d,l,r)=   5 13  8 10
```

MPI 2, 3 and 4

- MPI 2 added
  - Dynamic process creation.
  - Improved collectives.
  - Thread-safe.
  - Parallel I/O.
  - One sided (~ shared memory) communication.
- MPI 3 added
  - Nonblocking collectives.
  - Better support for multi-threading.
  - Improved shared memory parallelism.
  - User-defined collectives.
  - Large counts for large datasets.
- MPI 4 added
  - More fault tolerant.
  - Hybrid programming (MPI + OpenMP / CUDA).