# What is MPI?

- A *message-passing library specification*
  - extended message-passing model
  - not a language or compiler specification
  - not a specific implementation or product
- For parallel computers, clusters, and heterogeneous networks
- Full-featured
- Designed to provide access to advanced parallel hardware for end users, library writers, and tool developers

- Credits for Slides: Rusty Lusk, Mathematics and Computer Science Division, Argonne National Laboratory



# Where Did MPI Come From?

- Early vendor systems (Intel's NX, IBM's EUI, TMC's CMMD) were not portable (or very capable)
- Early portable systems (PVM, p4, TCGMSG, Chameleon) were mainly research efforts
  - Did not address the full spectrum of issues
  - Lacked vendor support
  - Were not implemented at the most efficient level
- The MPI Forum organized in 1992 with broad participation by:
  - vendors: IBM, Intel, TMC, SGI, Convex, Meiko
  - portability library writers: PVM, p4
  - users: application scientists and library writers
  - finished in 18 months

# Novel Features of MPI

- Communicators encapsulate communication spaces for library safety
- Datatypes reduce copying costs and permit heterogeneity
- Multiple communication modes allow precise buffer management
- Extensive collective operations for scalable global communication
- Process topologies permit efficient process placement, user views of process layout
- Profiling interface encourages portable tools



# MPI References

- The Standard itself:
  - at `http://www.mpi-forum.org`
  - All MPI official releases, in both postscript and HTML
- Books:
  - *Using MPI: Portable Parallel Programming with the Message-Passing Interface*, 2nd Edition, by Gropp, Lusk, and Skjellum, MIT Press, 1999. Also *Using MPI-2*, w. R. Thakur
  - *MPI: The Complete Reference,* 2 vols, MIT Press, 1999.
  - *Designing and Building Parallel Programs*, by Ian Foster, Addison-Wesley, 1995.
  - *Parallel Programming with MPI*, by Peter Pacheco, Morgan-Kaufmann, 1997.
- Other information on Web:
  - at `http://www.mcs.anl.gov/mpi`
  - pointers to lots of stuff, including other talks and tutorials, a FAQ, other MPI pages

## Compiling and Running MPI Programs

- To compile and run MPI programs one uses special commands
  - mpicc compiles and includes the MPI libraries
  - mpirun sets up environment variables for running
    - mpirun –np # prog
- One can also configure the set of nodes to be used
- For details on this and on user level configuration of the 2 MPI versions MPICH and LAM see the references in http://discov.cs.kent.edu/resources/doc/mpiref.htm
- For examples from Pachero see http://nexus.cs.usfca.edu/mpi/



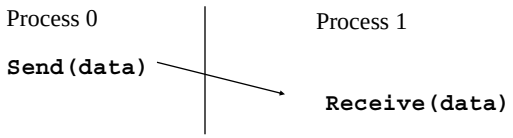
## Hello (C)

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

int main( argc, argv )
int argc;
char *argv[];
{
    int rank, size;
    MPI_Init( &argc, &argv );
    MPI_Comm_rank( MPI_COMM_WORLD, &rank );
    MPI_Comm_size( MPI_COMM_WORLD, &size );
    printf( "I am %d of %d\n", rank, size );
    MPI_Finalize();
    return 0;
}
```

# MPI Basic Send/Receive

- We need to fill in the details in




- Things that need specifying:
  - How will "data" be described?
  - How will processes be identified?
  - How will the receiver recognize/screen messages?
  - What will it mean for these operations to complete?



# Some Basic Concepts

- Processes can be collected into groups
- Each message is sent in a context, and must be received in the same context
  - Provides necessary support for libraries
- A group and context together form a communicator
- A process is identified by its rank in the group associated with a communicator
- There is a default communicator whose group contains all initial processes, called **`MPI_COMM_WORLD`**

# MPI Datatypes

- The data in a message to send or receive is described by a triple (address, count, datatype), where
- An MPI *datatype* is recursively defined as:
  - predefined, corresponding to a data type from the language (e.g., MPI_INT, MPI_DOUBLE)
  - a contiguous array of MPI datatypes
  - a strided block of datatypes
  - an indexed array of blocks of datatypes
  - an arbitrary structure of datatypes
- There are MPI functions to construct custom datatypes, in particular ones for subarrays



# MPI Tags

- Messages are sent with an accompanying user-defined integer *tag*, to assist the receiving process in identifying the message
- Messages can be screened at the receiving end by specifying a specific tag, or not screened by specifying **`MPI_ANY_TAG`** as the tag in a receive
- Some non-MPI message-passing systems have called tags "message types". MPI calls them tags to avoid confusion with datatypes

# MPI Basic (Blocking) Send

MPI_SEND(start, count, datatype, dest, tag, comm)

- The message buffer is described by (**`start, count, datatype`**).
- The target process is specified by **`dest`**, which is the rank of the target process in the communicator specified by **`comm`**.
- When this function returns, the data has been delivered to the system and the buffer can be reused. The message may not have been received by the target process.



# MPI Basic (Blocking) Receive

MPI_RECV(start, count, datatype, source, tag, comm, status)

- Waits until a matching (both **`source`** and **`tag`**) message is received from the system, and the buffer can be used
- **`source`** is rank in communicator specified by **`comm`**, or **`MPI_ANY_SOURCE`**
- **`tag`** is a tag to be matched on or **`MPI_ANY_TAG`**
- receiving fewer than **`count`** occurrences of **`datatype`** is OK, but receiving more is an error
- **`status`** contains further information (e.g. size of message)

# MPI is Simple

- Many parallel programs can be written using just these six functions, only two of which are non-trivial:
  - **MPI_INIT**
  - **MPI_FINALIZE**
  - **MPI_COMM_SIZE**
  - **MPI_COMM_RANK**
  - **MPI_SEND**
  - **MPI_RECV**



# Collective Operations in MPI

- Collective operations are called by all processes in a communicator
- **MPI_BCAST** distributes data from one process (the root) to all others in a communicator
  - MPI_Bcast ( buffer, count, datatype, root, comm);
- **MPI_REDUCE** combines data from all processes in communicator and returns it to one process
  - MPI_Reduce( sendbuf, recvbuf, count, datatype, operation, root, comm);
- In many numerical algorithms, **SEND/RECEIVE** can be replaced by **BCAST/REDUCE**, improving both simplicity and efficiency

# Example: PI in C - 1

```
#include "mpi.h"
#include <math.h>
int main(int argc, char *argv[])
{
   int done = 0, n, myid, numprocs, i, rc;
   double PI25DT = 3.14159265358979323846264643;
   double mypi, pi, h, sum, x, a;
   MPI_Init(&argc,&argv);
   MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
   MPI_Comm_rank(MPI_COMM_WORLD,&myid);
   while (!done)  {
     if (myid == 0) {
       printf("Enter the number of intervals: (0 quits) ");
       scanf("%d",&n);
     }
     MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
     if (n == 0) break;
```



# Example: PI in C - 2

```
    h   = 1.0 / (double) n;
     sum = 0.0;
     for (i = myid + 1; i <= n; i += numprocs) {
       x = h * ((double)i - 0.5);
       sum += 4.0 / (1.0 + x*x);
     }
     mypi = h * sum;
     MPI_Reduce(&mypi, &pi, 1, MPI_DOUBLE, MPI_SUM, 0,
                MPI_COMM_WORLD);
     if (myid == 0)
       printf("pi is approximately %.16f, Error is .16f\n",
              pi, fabs(pi - PI25DT));
   }
   MPI_Finalize();
  return 0;
}
```

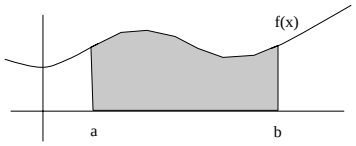
# Alternative Set of 6 Functions

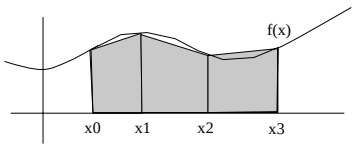
- Using collectives:
  - **`MPI_INIT`**
  - **`MPI_FINALIZE`**
  - **`MPI_COMM_SIZE`**
  - **`MPI_COMM_RANK`**
  - **`MPI_BCAST`**
  - **`MPI_REDUCE`**



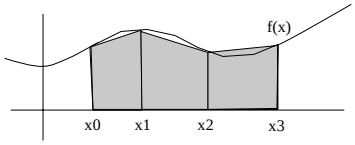
# Trapezoid Rule

- Numerical Integration (Quadrature)
  - approximate the area under the curve by calculating the area of rectangles (the Rectangle Rule) or trapezoids (the Trapezoidal Rule) that fit close to the curve.



## Trapezoid Rule




- The base of each trapezoid is h = x1-x0 = x2-x1 etc.
- The area formed by one trapezoid is
  - area of one trapezoid = ½ * h * (f(left) + f(right))
- The area under the curve is:

  Area = ½ * h * (f(x0) + f(x1)) + ½ * h * (f(x1) + f(x2)) + ½ * h * (f(x2) + f(x3))
- which simplifies to

  Area = h * { ½f(x0) + f(x1) + f(x2) + ½f(x3) }



## Parallelizing Trapezoid Rule

- Divide interval [a,b] into np parts, one for each processor.
- Each processor performs the trapezoidal rule on its part.

## Serial and Parallel Versions

- Serial
- Parallel

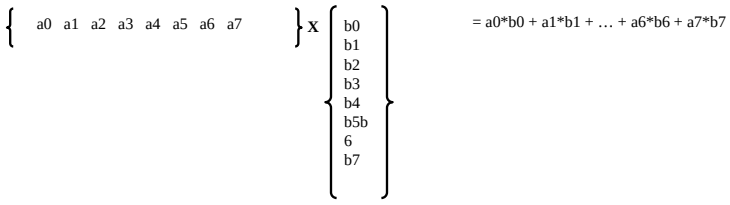


## Adaptive Quadrature

- Adaptive quadrature allows the program to calculate the new value for the integral with a different number of trapezoids each time.
- The program terminates when the final result is "close enough".
- Pseudocode for a sequential program:

```
new = 1;
diff = 100000;
numtraps = 1;
limit = 0.001;
while (( diff > limit) && (numtraps < 2048)  ) {
  old = new;
  numtraps = numtraps*2;
  calculate (new) ;
  diff = abs( (new-old) ) / new;
}
print(new);
```

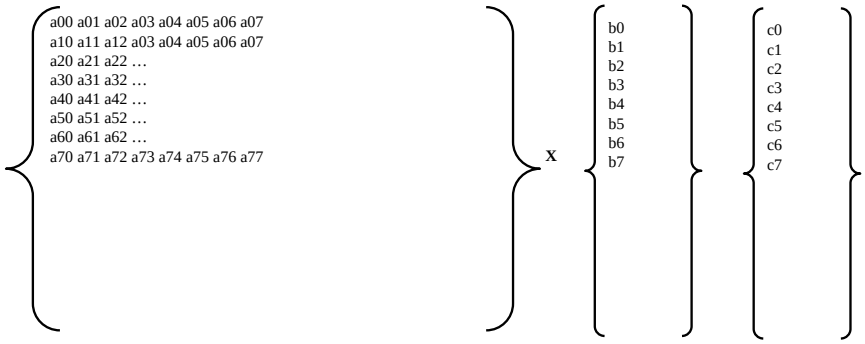
## Dot products – Block Decomposition




- Serial
- Parallel
- Parallel with Allreduce



## Matrix- Vector Multiplication – version 1




- Block-row distribution of the matrix
- Copy of vector on every process
- Each process calculates its corresponding portion of the result vector

## How to get the data to where needed

- If the matrix is located in a single process at the start, can use MPI_Scatter to send the rows to all processes.
- (Watch out for how the matrix is stored – in C it is row-major!)
  - MPI_Scatter(
  - void* send_data,
  - int send_count,
  - MPI_Datatype send_type,
  - void* recv_data,
  - int recv_count,
  - MPI_Datatype recv_type,
  - int root,
  - MPI_Comm comm);

Vector Example:

```
/* data starts at process 0 */
float vector[8], local_vector[2];
…
MPI_Scatter( vector, 2, MPI_FLOAT,
             local_vector, 2, MPI_FLOAT,
             0, MPI_COMM_WORLD);
```

would send 2 elements to each process and store them into local_vector;



- If the vector is initially distributed in block fashion among all processes, can use MPI_Gather to get a copy of the whole vector into the root process.
  - MPI_Gather(
  - void* send_data,
  - int send_count,
  - MPI_Datatype send_type,
  - void* recv_data,
  - int recv_count,
  - MPI_Datatype recv_type,
  - int root,
  - MPI_Comm comm);

- If the vector is initially distributed in block fashion among all processes, can use MPI_Allgather to get a copy of the whole vector into the **every** process.
  - MPI_Allgather(
  - void* send_data,
  - int send_count,
  - MPI_Datatype send_type,
  - void* recv_data,
  - int recv_count,
  - MPI_Datatype recv_type,
  - MPI_Comm comm);

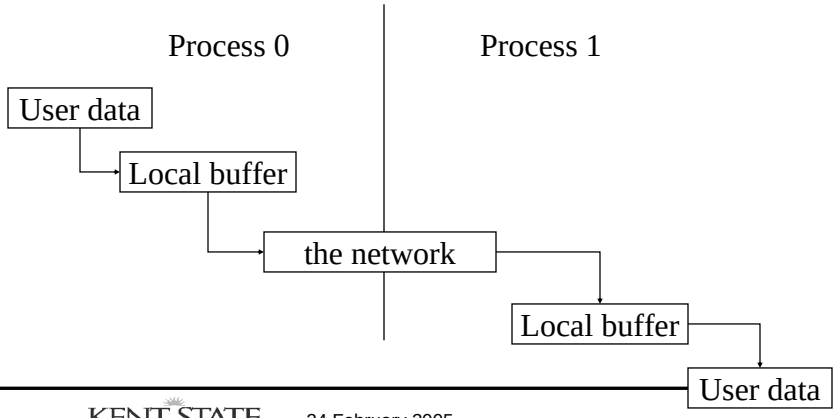


## C Versions of Matrix-Vector Multiply

- Serial
- Parallel

# Buffers

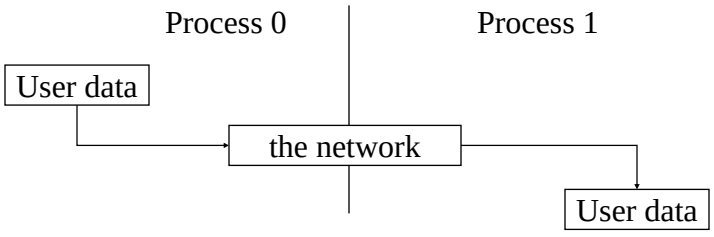
- When you send data, where does it go? One possibility is:






# Avoiding Buffering

- It is better to avoid copies:




This requires that **`MPI_Send`** wait on delivery, or that **`MPI_Send`** return before transfer is complete, and we wait later.

# Blocking and Non-blocking Communication

- So far we have been using *blocking* communication:
  - `MPI_Recv` does not complete until the buffer is full (available for use).
  - `MPI_Send` does not complete until the buffer is empty (available for use).
- Completion depends on size of message and amount of system buffering.



# Sources of Deadlocks

- Send a large message from process 0 to process 1
  - If there is insufficient storage at the destination, the send must wait for the user to provide the memory space (through a receive)
- What happens with this code?

| Process 0 | Process 1 |
|---|---|
| **Send(1)** | **Send(0)** |
| **Recv(1)** | **Recv(0)** |

- This is called “unsafe” because it depends on the availability of system buffers

## Some Solutions to the “unsafe” Problem

- Order the operations more carefully:

| Process 0 | Process 1 |
|---|---|
| **Send(1)** | **Recv(0)** |
| **Recv(1)** | **Send(0)** |

Supply receive buffer at same time as send:

| Process 0 | Process 1 |
|---|---|
| **Sendrecv(1)** | **Sendrecv(0)** |



## More Solutions to the “unsafe” Problem

- Supply own space as buffer for send

| Process 0 | Process 1 |
|---|---|
| **Bsend(1)** | **Bsend(0)** |
| **Recv(1)** | **Recv(0)** |

Use non-blocking operations:

| Process 0 | Process 1 |
|---|---|
| **Isend(1)** | **Isend(0)** |
| **Irecv(1)** | **Irecv(0)** |
| **Waitall** | **Waitall** |

# MPI's Non-blocking Operations

- Non-blocking operations return (immediately) "request handles" that can be tested and waited on.

```
MPI_Isend(start, count, datatype,
     dest, tag, comm, request)
MPI_Irecv(start, count, datatype,
     dest, tag, comm, request)
MPI_Wait(&request, &status)
```

- One can also test without waiting:

```
MPI_Test(&request, &flag, status)
```



# Multiple Completions

- It is sometimes desirable to wait on multiple requests:

```
MPI_Waitall(count, array_of_requests,
   array_of_statuses)
MPI_Waitany(count, array_of_requests,
   &index, &status)
MPI_Waitsome(count, array_of_requests,
   array_of indices, array_of_statuses)
```

- There are corresponding versions of **`test`** for each of these.

# Communication Modes

- MPI provides multiple *modes* for sending messages:
  - Synchronous mode (**`MPI_Ssend`**): the send does not complete until a matching receive has begun. (Unsafe programs deadlock.)
  - Buffered mode (**`MPI_Bsend`**): the user supplies a buffer to the system for its use. (User allocates enough memory to make an unsafe program safe.
  - Ready mode (**`MPI_Rsend`**): user guarantees that a matching receive has been posted.
    - Allows access to fast protocols
    - undefined behavior if matching receive not posted
- Non-blocking versions (**`MPI_Issend`**, etc.)
- **`MPI_Recv`** receives messages sent in any mode.



# Other Point-to Point Features

- **`MPI_Sendrecv`**
- **`MPI_Sendrecv_replace`**
- **`MPI_Cancel`**
  - Useful for multibuffering
- Persistent requests
  - Useful for repeated communication patterns
  - Some systems can exploit to reduce latency and increase performance

# MPI_Sendrecv

- Allows simultaneous send and receive
- Everything else is general.
  - Send and receive datatypes (even type signatures) may be different
  - Can use Sendrecv with plain Send or Recv (or Irecv or Ssend_init, …)
  - More general than “send left”

| Process 0 | Process 1 |
|---|---|
| **`SendRecv(1)`** | **`SendRecv(0)`** |



# Collective Operations in MPI

- Collective operations must be called by all processes in a communicator.
- **`MPI_BCAST`** distributes data from one process (the root) to all others in a communicator.
- **`MPI_REDUCE`** combines data from all processes in communicator and returns it to one process.
- In many numerical algorithms, **`SEND/RECEIVE`** can be replaced by **`BCAST/REDUCE`**, improving both simplicity and efficiency.

# 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.
- Tags are not used; different communicators deliver similar functionality.
- No non-blocking collective operations.
- Three classes of operations: synchronization, data movement, collective computation.



# Synchronization

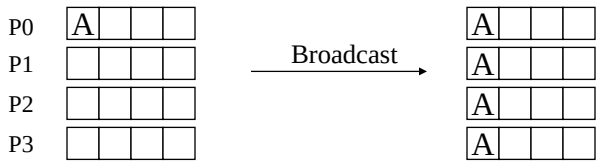
- **`MPI_Barrier( comm )`**
- Blocks until all processes in the group of the communicator **`comm`** call it.

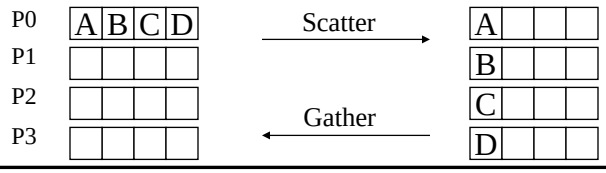
# Synchronization

- **`MPI_Barrier( comm, ierr )`**
- Blocks until all processes in the group of the communicator **`comm`** call it.

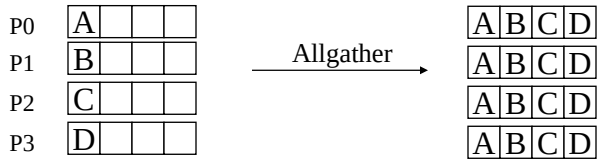


# Collective Data Movement



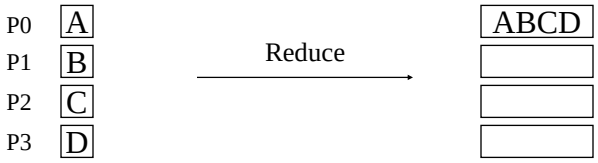
# More Collective Data Movement

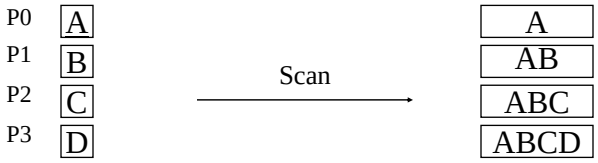






# Collective Computation



# MPI Collective Routines

- Many Routines: **`Allgather, Allgatherv, Allreduce, Alltoall, Alltoallv, Bcast, 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`**, **`Reduce`**, **`Reduce_scatter`**, and **`Scan`** take both built-in and user-defined combiner functions.



# 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`** | Binary and |
| • **`MPI_Bor`** | Binary or |
| • **`MPI_Bxor`** | Binary 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
  - 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 can use "deferred synchronization" ideas to provide better performance



# 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.

## Blocking and Non-blocking

- Blocking
  - `MPI_Recv` does not complete until the buffer is full (available for use).
  - `MPI_Send` does not complete until the buffer is empty (available for use).
- Non-blocking operations return (immediately) "request handles" that can be tested and waited on.

```
MPI_Isend(start, count, datatype, dest, tag, comm, request)
MPI_Irecv(start, count, datatype, dest, tag, comm, request)
MPI_Wait(&request, &status)
```

  - One can also test without waiting:

```
MPI_Test(&request, &flag, status)
```



## Persistent Requests

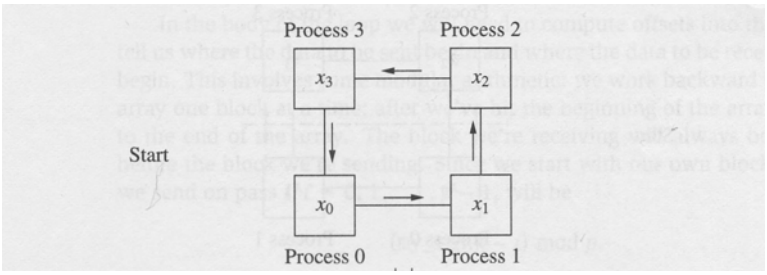
- Persistent requests
  - Useful for repeated communication patterns
  - Some systems can exploit to reduce latency and increase performance

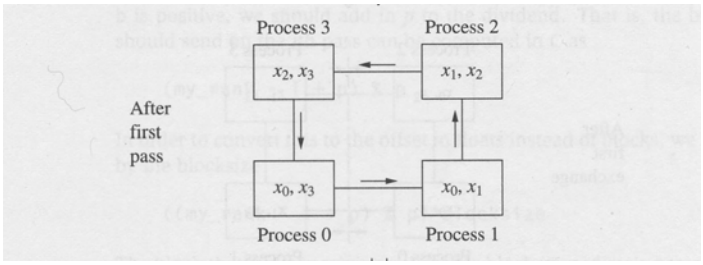
# Communication Modes

- MPI provides multiple *modes* for sending messages:
  - Synchronous mode (**`MPI_Ssend`**): the send does not complete until a matching receive has begun. (Unsafe programs deadlock.)
  - Buffered mode (**`MPI_Bsend`**): the user supplies a buffer to the system for its use. (User allocates enough memory to make an unsafe program safe.
  - Ready mode (**`MPI_Rsend`**): user guarantees that a matching receive has been posted.
    - Allows access to fast protocols
    - undefined behavior if matching receive not posted
- Non-blocking versions (**`MPI_Issend`**, etc.)
- **`MPI_Recv`** receives messages sent in any mode.

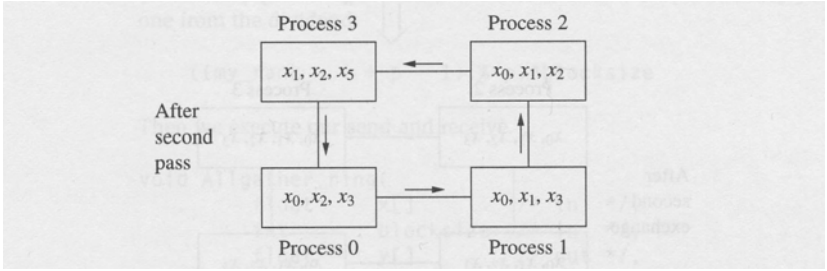


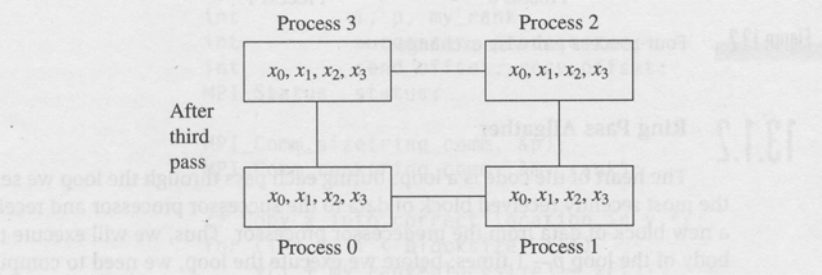
# Ring Based Allgather




Process 3
Process 2
$x_2, x_3$
$x_1, x_2$
After
first
pass
$x_0, x_3$
$x_0, x_1$
Process 0
Process 1




Process 3
Process 2
$x_1, x_2, x_5$
$x_0, x_1, x_2$
After
second
pass
$x_0, x_2, x_3$
$x_0, x_1, x_3$
Process 0
Process 1






## Advanced Communication Examples

- All_gather Ring
  - Blocking
  - Nonblocking
  - Persistent
  - Synchronous
  - Ready
  - Buffered
- Examples

# MPICH Goals

- Complete MPI implementation
- Portable to all platforms supporting the message-passing model
- High performance on high-performance hardware
- As a research project:
  - exploring tradeoff between portability and performance
  - removal of performance gap between user level (MPI) and hardware capabilities
- As a software project:
  - a useful free implementation for most machines
  - a starting point for vendor proprietary implementations



# MPICH Architecture

- Most code is completely portable
- An “Abstract Device” defines the communication layer
- The abstract device can have widely varying instantiations, using:
  - sockets
  - shared memory
  - other special interfaces
    - e.g. Myrinet, Quadrics, InfiniBand, Grid protocols

## Getting MPICH for your cluster

- http://www.mcs.anl.gov/mpi/mpich
- Either MPICH-1 or
- MPICH-2



## What's in MPI-2

- Extensions to the message-passing model
  - Dynamic process management
  - One-sided operations (remote memory access)
  - Parallel I/O
  - Thread support
- Making MPI more robust and convenient
  - C++ and Fortran 90 bindings
  - External interfaces, handlers
  - Extended collective operations
  - Language interoperability

## MPI as a Setting for Parallel I/O

- Writing is like sending and reading is like receiving
- Any parallel I/O system will need:
  - collective operations
  - user-defined datatypes to describe both memory and file layout
  - communicators to separate application-level message passing from I/O-related message passing
  - non-blocking operations
- I.e., lots of MPI-like machinery



## MPI-2 Status

- Many vendors have partial implementations, especially I/O
- MPICH2 is nearly complete, not completely tested
- Expect completion by Thanksgiving

## Some Research Areas

- MPI-2 RMA interface
  - Can we get high performance?
- Fault Tolerance and MPI
  - Are intercommunicators enough?
- MPI on 64K processors
  - Umm…how do we make this work :)?
  - Reinterpreting the MPI “process”
- MPI as system software infrastructure
  - With dynamic processes and fault tolerance, can we build services on MPI?



## High-Level Programming With MPI

- MPI was designed from the beginning to support libraries
- Many libraries exist, both open source and commercial
- Sophisticated numerical programs can be built using libraries
  - Solve a PDE (e.g., PETSc)
  - Scalable I/O of data to a community standard file format

# Higher Level I/O Libraries

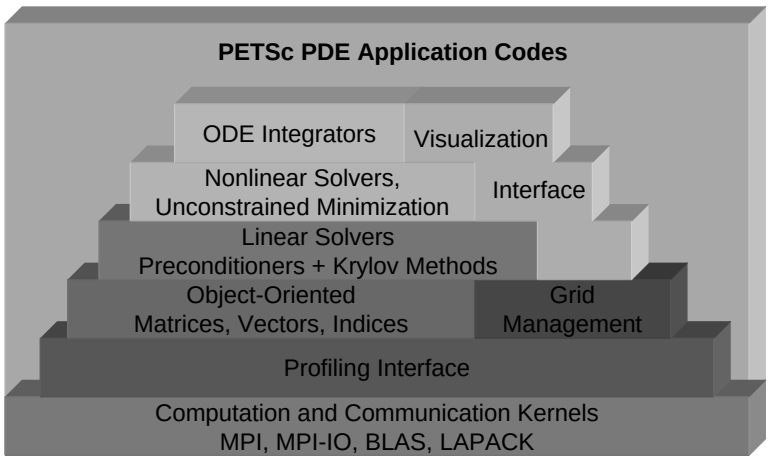
- Scientific applications work with structured data and desire more self-describing file formats
- netCDF and HDF5 are two popular “higher level” I/O libraries
  - Abstract away details of file layout
  - Provide standard, portable file formats
  - Include metadata describing contents
- For parallel machines, these should be built on top of MPI-IO



# The PETSc Library

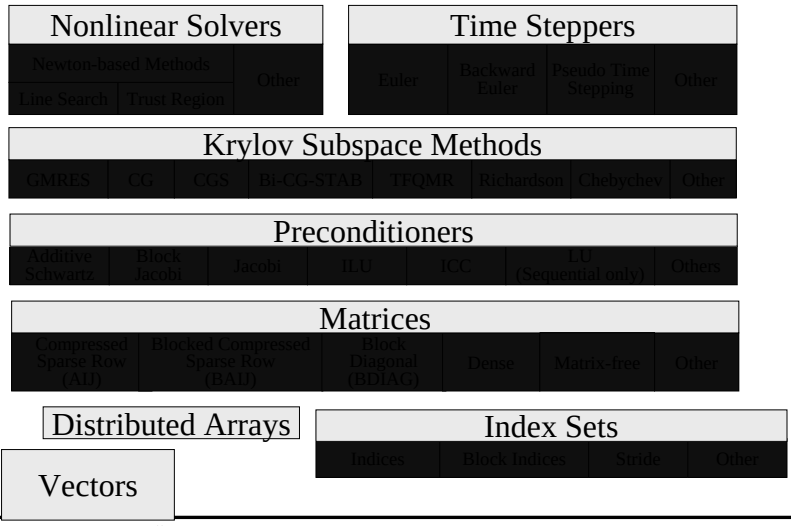
- PETSc provides routines for the parallel solution of systems of equations that arise from the discretization of PDEs
  - Linear systems
  - Nonlinear systems
  - Time evolution
- PETSc also provides routines for
  - Sparse matrix assembly
  - Distributed arrays
  - General scatter/gather (e.g., for unstructured grids)

# Structure of PETSc






# PETSc Numerical Components



# Flow of Control for PDE Solution