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

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

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

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

Hello (C)

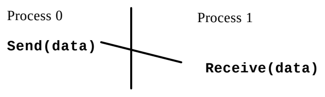
```
#include "mpi.h"
#include <stdio.h>

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;
}
```

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 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?

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) 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 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 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_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

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;
}
```

Example: PI in C - 1

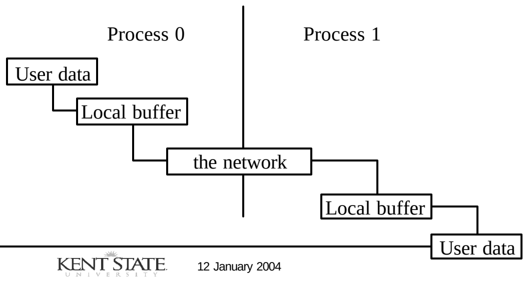
```
#include "mpi.h"
#include <math.h>
int main(int argc, char *argv[])
{
   int done = 0, n, myid, numprocs, i, rc;
   double PI25DT = 3.141592653589793238462643;
   double mypi, pi, h, sum, x, a;
   MPI_Init(&argc,&argv);
   MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
   MPI_Comm_rank(MPI_COMM_WORLD,&myid);
   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;
```

Alternative Set of 6 Functions

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

Buffers

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

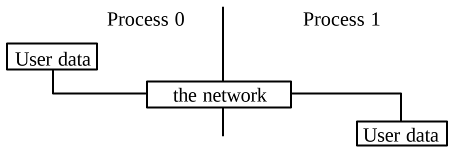


Blocking and Non-blocking Communication

- 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.

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.

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)**

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)
```

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**

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.

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)`**

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

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

Synchronization

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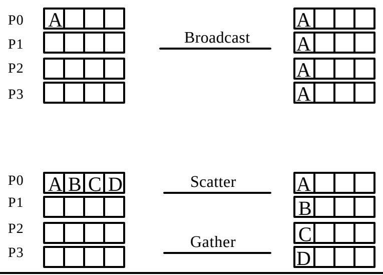
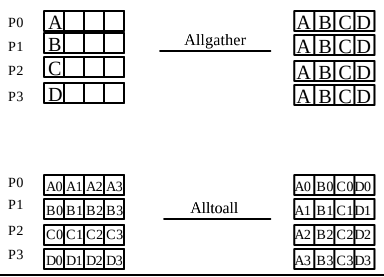
- Blocks until all processes in the group of the communicator **`comm`** call it.

Collective Data Movement



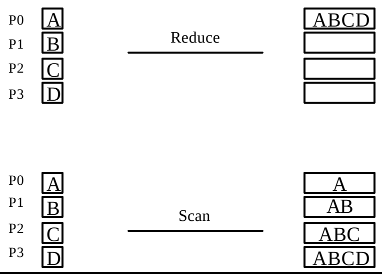
More Collective Data Movement



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.

Collective Computation



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

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

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.

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

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

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-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?

Higher Level I/O Libraries

- Scientific applications work with structured data and desire mor e 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

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

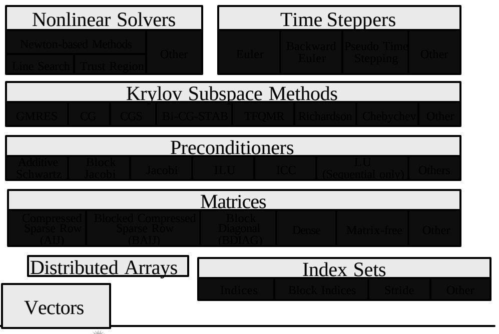
Exercise

- Jacobi problem in 2 dimensions with 1 -D decomposition
  - Explained in class
  - Simple version – fixed number of iterations
  - Fancy version – test for convergence

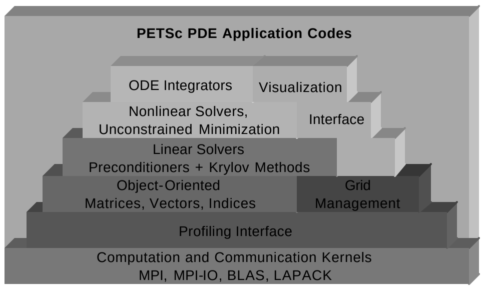
The PETSc Library

- 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)

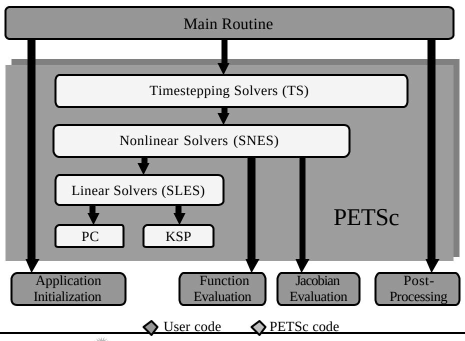
PETSc Numerical Components

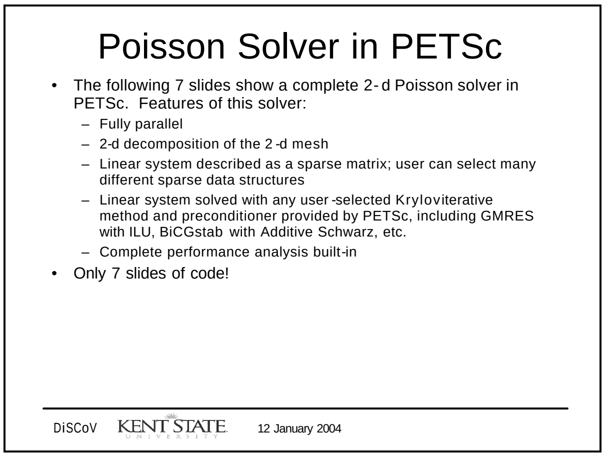


Structure of PETSc


PETSc PDE Application Codes
ODE Integrators
Visualization
Nonlinear Solvers, Unconstrained Minimization
Interface
Linear Solvers
Preconditioners + Krylov Methods
Object-Oriented Matrices, Vectors, Indices
Grid Management
Profiling Interface
Computation and Communication Kernels
MPI, MPI-IO, BLAS, LAPACK

Flow of Control for PDE Solution





Poisson Solver in PETSc

- The following 7 slides show a complete 2-d Poisson solver in PETSc. Features of this solver:
  - Fully parallel
  - 2-d decomposition of the 2-d mesh
  - Linear system described as a sparse matrix; user can select many different sparse data structures
  - Linear system solved with any user-selected Krylov iterative method and preconditioner provided by PETSc, including GMRES with ILU, BiCGstab with Additive Schwarz, etc.
  - Complete performance analysis built-in
- Only 7 slides of code!

DiSCoV KENT STATE UNIVERSITY 12 January 2004