Advanced Cluster Programming with MPI

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Thanks to

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Tutorial Outline

- Background
- Tuning for Performance on Clusters
- Parallel I/O in MPI-2
- Introduction to dynamic process management in MPI-2
- MPI and threads

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About This Tutorial

- Some of this material is taken from *Using MPI-2*, by Gropp, Lusk, and Thakur, MIT Press, 1999.
- Assumes familiarity with MPI but no deep knowledge.
- Most of the time is spent on those features most widely implemented at this time.
- Language-independent, but most examples are in C.
- Complete MPI-2 specification is on the web http://www.mpi-forum.org and in MPI: The Complete Reference, 2 volumes from MIT Press.

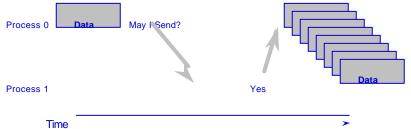
Contents of MPI-2

- Extensions to the message-passing model
 - Parallel I/O
 - One-sided operations
 - Dynamic process management
- Making MPI more robust and convenient
 - C++ and Fortran 90 bindings
 - External interfaces, handlers
 - Extended collective operations
 - Language interoperability
 - MPI interaction with threads

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What is message passing?

Data transfer plus synchronization



- Requires cooperation of sender and receiver
- Cooperation not always apparent in code

MPI Protocols

Quick review of MPI Message passing

- Basic terms
 - nonblocking Operation does not wait for completion
 - synchronous Completion of send requires initiation (but not completion) of receive
 - ready Correct send requires a matching receive
 - asynchronous communication and computation take place simultaneously, not an MPI concept (implementations may use asynchronous methods)

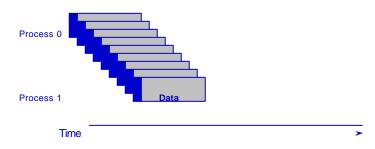
Message protocols

- Message consists of "envelope" and data
 - Envelope contains tag, communicator, length, source information, plus impl. private data
- Short
 - Message data (message for short) sent with envelope
- Eager
 - Message sent assuming destination can store
- Rendezvous
 - Message not sent until destination oks

Message Protocol Details

- Eager is not Rsend, rendezvous is not Ssend resp., but related
- User versus system buffer space
- Packetization
- Collective operations
- Datatypes, particularly non-contiguous
 - Handling of important special cases
 - Constant stride
 - Contiguous structures

Eager Protocol

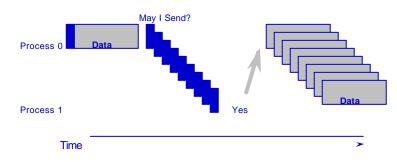


- Data delivered to process 1
 - No matching receive may exist; process 1 must then buffer and copy.

Eager Features

- Reduces synchronization delays
- Simplifies programming (just MPI_Send)
- Requires significant buffering
- May require active involvement of CPU to drain network at receiver's end
- May introduce additional copy (buffer to final destination)

Rendezvous Protocol



- Envelope delivered first
- Data delivered when user-buffer available
 - Only buffering of envelopes required

Rendezvous Features

- Robust and safe
 - (except for limit on the number of envelopes…)
- May remove copy (user to user direct)
- More complex programming (waits/tests)
- May introduce synchronization delays (waiting for receiver to ok send)

Short Protocol

- Data is part of the envelope
- Otherwise like eager protocol
- May be performance optimization in interconnection system for short messages, particularly for networks that send fixed-length packets (or cache lines)

User and System Buffering

- Where is data stored (or staged) while being sent?
 - User's memory
 - Allocated on the fly
 - Preallocated
 - System memory
 - · May be limited
 - · Special memory may be faster

Implementing MPI_Isend

- Simplest implementation is to always use rendezvous protocol:
 - MPI_Isend delivers a request-to-send control message to receiver
 - Receiving process responds with an ok-to-send
 - May or may not have matching MPI receive; only needs buffer space to store incoming message
 - Sending process transfers data
- Wait for MPI_Isend request
 - wait for ok-to-send message from receiver
 - wait for data transfer to be complete on sending side

Alternatives for MPI_Isend

- Use a short protocol for small messages
 - No need to exchange control messages
 - Need guaranteed (but small) buffer space on destination for short message envelope
 - Wait becomes a no-op
- Use eager protocol for modest sized messages
 - Still need guaranteed buffer space for both message envelope and eager data on destination
 - Avoids exchange of control messages

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Implementing MPI_Send

 Can't use eager always because this could overwhelm the receiving process

```
if (rank != 0) MPI_Send( 100 MB of data )
else receive 100 MB from each process
```

- Would like to exploit the blocking nature (can wait for receive)
- Would like to be fast
- Select protocol based on message size (and perhaps available buffer space at destination)
 - Short and/or eager for small messages
 - Rendezvous for longer messages

Implementing MPI_Rsend

- Just use MPI_Send; no advantage for users
- Use eager always (or short if small)
 - even for long messages

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Choosing MPI Alternatives

- MPI offers may ways to accomplish the same task
- Which is best?
 - Just like everything else, it depends on the vendor, system architecture
 - Like C and Fortran, MPI provides the programmer with the tools to achieve high performance without sacrificing portability
- The best choice depends on the use:
 - Consider choices based on system and MPI implementation
 - Example: Experiments with a Jacobi relaxation example

Tuning for MPI's Send/Receive Protocols

- Aggressive Eager
 - Performance problem: extra copies
 - Possible deadlock for inadequate eager buffering
 - Ensure that receives are posted before sends
 - MPI_Issend can be used to express "wait until receive is posted"
- Rendezvous with sender push
 - Extra latency
 - Possible delays while waiting for sender to begin
- Rendezvous with receiver pull
 - Possible delays while waiting for receiver to begin

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Rendezvous Blocking

- What happens once sender and receiver rendezvous?
 - Sender (push) or receiver (pull) may complete operation
 - May block other operations while completing
- Performance tradeoff
 - If operation does not block (by checking for other requests), it adds latency or reduces bandwidth.
- Can reduce performance if a receiver, having acknowledged a send, must wait for the sender to complete a separate operation that it has started.

Tuning for Rendezvous with Sender Push

- Ensure receives posted before sends
 - better, ensure receives match sends before computation starts; may be better to do sends before receives
- Ensure that sends have time to start transfers
- Can use short control messages
- Beware of the cost of extra messages
 - Intel i860 encouraged use of control messages with ready send (force type)

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Tuning for Rendezvous with Receiver Pull

- Place MPI_Isends before receives
- Use short control messages to ensure matches
- Beware of the cost of extra messages

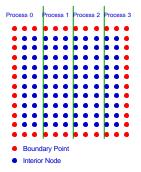
Experiments with MPI Implementations

- Multiparty data exchange
- Jacobi iteration in 2 dimensions
 - Model for PDEs, Sparse matrix-vector products, and algorithms with surface/volume behavior
 - Issues are similar to unstructured grid problems (but harder to illustrate)
- Others at http://www.mcs.anl.gov/mpi/tutorials/perf

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Jacobi Iteration (Fortran Ordering)

Simple parallel data structure



- Processes exchange columns with neighbors
- Local part declared as xlocal(m,0:n+1)

Background to Tests

- Goals
 - Identify better performing idioms for the same communication operation
 - Understand these by understanding the underlying MPI process
 - Provide a starting point for evaluating additional options (there are many ways to write even simple codes)

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Some Send/Receive Approaches

- Based on operation hypothesis. Most of these are for polling mode. Each of the following is a hypothesis that the experiments test
 - Better to start receives first
 - Ensure recvs posted before sends
 - Ordered (no overlap)
- More details at http://www.mcs.anl.gov/mpi/tutorial/perf/mpiexmpl/src3/runs.html

Send and Recv

 Simplest use of send and recv integer status(MPI_STATUS_SIZE)

```
call MPI_Send( xlocal(1,1), m, MPI_DOUBLE_PRECISION, & left_nbr, 0, ring_comm, ierr )
call MPI_Recv( xlocal(1,0), m, MPI_DOUBLE_PRECISION, & right_nbr, 0, ring_comm, status, ierr )
call MPI_Send( xlocal(1,n), m, MPI_DOUBLE_PRECISION, & right_nbr, 0, ring_comm, ierr )
call MPI_Recv( xlocal(1,n+1), m, MPI_DOUBLE_PRECISION, & left_nbr, 0, ring_comm, status, ierr )
```

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Performance of Simplest Code

- Very poor performance for large m
 - Rendezvous sequentializes sends/receives
- Good to OK performance for modest m
 - -eager operations

Better to start sends first

 Irecv, Isend, Waitall - ok performance integer statuses(MPI_STATUS_SIZE,4), requests(4)

```
call MPI_Isend( xlocal(1,n), m, MPI_DOUBLE_PRECISION, & right_nbr, ring_comm, requests(1), ierr )
call MPI_Isend( xlocal(1,1), m, MPI_DOUBLE_PRECISION, & left_nbr, ring_comm, requests(3), ierr )
call MPI_Irecv( xlocal(1,0), m, MPI_DOUBLE_PRECISION,& left_nbr, ring_comm, requests(2), ierr )
call MPI_Irecv( xlocal(1,n+1), m, MPI_DOUBLE_PRECISION,& right_nbr, ring_comm, requests(4), ierr )
call MPI_Waitall( 4, requests, statuses, ierr )
```

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Summary of Results

- Better to start sends before receives
 - Most implementations use rendezvous protocols for long messages (Cray, IBM, SGI, MPICH, LAM)
 - Sending the envelope immediately is the best way to improve performance
- Short messages even better
 - Eager messages have lowest latency

MPI I/O

- Goals of this part
 - introduce the important features of MPI I/O in the form of example programs, following the outline of the Parallel I/O chapter in *Using MPI-2*
 - focus on how to achieve high performance
- What can you expect from this session?
 - learn how to use MPI I/O and, hopefully, like it
 - be able to go back home and immediately use MPI I/O in your applications
 - get much higher I/O performance than what you have been getting so far using other techniques

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MPI I/O

- Why do I/O in MPI?
 - Why not just Posix?
 - Performance
 - Single file output (instead of one file / process)
- Example of MPI I/O: Non-parallel I/O from an MPI program
 - Emphasizes similarities with conventional I/O
 - High performance parallel I/O later

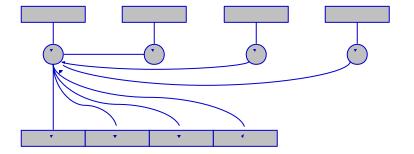
Why MPI is a Good Setting for Parallel I/O

- 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

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Introduction to Parallel I/O

 First example: non-parallel I/O from an MPI program



Next few examples have:

```
#include "mpi.h"
#include <stdio.h>
#define BUFSIZE 1000

int main(int argc, char *argv[])
{
    int i, myrank, numprocs, buf[BUFSIZE];

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
    MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
    ....
    MPI_Finalize();
    return 0;
}
```

Non-Parallel I/O from MPI Program

```
MPI Status status;
FILE *myfile;
for (i=0; i<BUFSIZE; i++)</pre>
    buf[i] = myrank * BUFSIZE + i;
if (myrank != 0)
    MPI_Send(buf, BUFSIZE, MPI_INT, 0, 99,
             MPI_COMM_WORLD);
else {
    myfile = fopen("testfile", "w");
    fwrite(buf, sizeof(int), BUFSIZE, myfile);
    for (i=1; i<numprocs; i++) {</pre>
        MPI_Recv(buf, BUFSIZE, MPI_INT, i, 99,
                 MPI_COMM_WORLD, &status);
        fwrite(buf, sizeof(int), BUFSIZE, myfile);
    fclose(myfile);
}
                                                         40
```

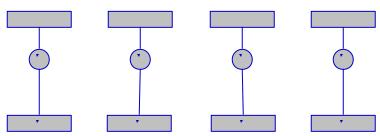
Pros and Cons of Sequential I/O

- Pros:
 - parallel machine may support I/O from only one process
 - I/O libraries (e.g. HDF-4, SILO, etc.) not parallel
 - resulting single file is handy for ftp, mv
 - big blocks improve performance
 - short distance from original, serial code
- Cons:
 - lack of parallelism limits scalability, performance

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Non-MPI Parallel I/O

Each process writes to a separate file



Pro: parallelism

Con: lots of small files to manage

Non-MPI Parallel I/O

```
char filename[128];
FILE *myfile;

for (i=0; i<BUFSIZE; i++)
    buf[i] = myrank * BUFSIZE + i;
sprintf(filename, "testfile.%d", myrank);
myfile = fopen(filename, "w");
fwrite(buf, sizeof(int), BUFSIZE, myfile);
fclose(myfile);</pre>
```

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MPI I/O to Separate Files

- · Same pattern as previous example
- MPI I/O replaces Unix I/O in a straightforward way
- Easy way to start with MPI I/O
- Does not exploit advantages of MPI I/O
 - in producing single file
 - in allowing collective operations
- Note files cannot be read conveniently by a different number of processes

MPI I/O to Separate Files

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MPI Versions of Unix I/O

```
Unix
                    MPI
  FILE myfile;
                       MPI_File myfile;
  myfile =
                       MPI_File_open(...)
    fopen(...)
                         takes info, comm
                         args
                       MPI_File_read/write(.
  fread(...)
                         ..) take (addr,
  fwrite(...)
                         count, datatype)
  fclose
                       MPI_File_close
```

Parallel I/O in MPI

- MPI provides effective ways to describe and perform high-performance parallel I/O
 - Requires specifying all data to move
 - Natural once you get used to it

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Beyond POSIX I/O with MPI

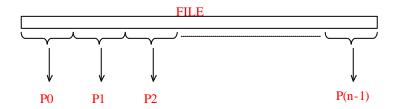
- Why do I/O in MPI?
- non-parallel I/O from an MPI program
- non-MPI parallel I/O to separate files
- parallel I/O to shared file with MPI I/O
- Fortran-90 version
- Reading a file with a different number of processes
- C++ version
- Survey of advanced features in MPI I/O

Parallel I/O with MPI

- Nonparallel I/O shown earlier
 - Simple but
 - Poor performance (single process writes to one file) or
 - Awkward and not interoperable with other tools (each process writes a separate file)
- Parallel I/O
 - Provides high performance
 - Can provide a single file that can be used with other tools (such as visualization programs)

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Using MPI for Simple I/O



Each process needs to read a chunk of data from a common file

Using Individual File Pointers

Using Explicit Offsets

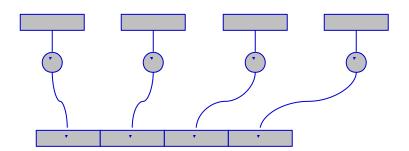
Writing to a File

- Use MPI_File_write or MPI_File_write_at
- Use MPI_MODE_WRONLY or MPI_MODE_RDWR as the flags to MPI_File_open
- If the file doesn't exist previously, the flag
 MPI_MODE_CREATE must also be passed to
 MPI_File_open
- We can pass multiple flags by using bitwise-or '|'
 in C, or addition '+" in Fortran

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MPI Parallel I/O to Single File

Processes write to shared file



 MPI_File_set_view assigns regions of the file to separate processes

File Views

- Specified by a triplet (displacement, etype, and filetype) passed to MPI_File_set_view
- displacement = number of bytes to be skipped from the start of the file
- etype = basic unit of data access (can be any basic or derived datatype)
- filetype = specifies which portion of the file is visible to the process

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MPI Parallel I/O to Single File

MPI_File_set_view

- Describes that part of the file accessed by a single MPI process.
- Arguments to MPI_File_set_view:
 - -MPI_File file
 - MP_Offset disp
 - MPI_Datatype etype
 - MPI_Datatype filetype
 - char *datarep
 - MPI_Info info

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MPI I/O in Fortran

```
PROGRAM main

use mpi

integer ierr, i, myrank, BUFSIZE, thefile
parameter (BUFSIZE=100)
integer buf(BUFSIZE)
integer(kind=MPI_OFFSET_KIND) disp

call MPI_INIT(ierr)
call MPI_COMM_RANK(MPI_COMM_WORLD, myrank, ierr)
do i = 0, BUFSIZE
    buf(i) = myrank * BUFSIZE + i
enddo

* in F77, see implementation notes (might be integer*8)
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```

MPI I/O in Fortran contd.

C++ Version

C++ Version, Part 2

```
MPI::Offset filesize = thefile.Get_size();
                = filesize / sizeof(int);
    bufsize
                = filesize / numprocs + 1;
    buf = new int[bufsize];
    thefile.Set_view(myrank * bufsize * sizeof(int),
                     MPI_INT, MPI_INT, "native",
                     MPI::INFO_NULL);
    thefile.Read(buf, bufsize, MPI_INT, &status);
    count = status.Get_count(MPI_INT);
    cout << "process " << myrank << " read " << count</pre>
         << " ints" << endl;
    thefile.Close();
    delete [] buf;
    MPI::Finalize();
    return 0;
}
                                                         61
```

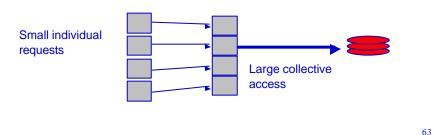
Other Ways to Write to a Shared File

```
MPI_File_seek
MPI_File_read_at
MPI_File_write_at
MPI_File_read_shared
MPI_File_write_shared
```

Collective operations

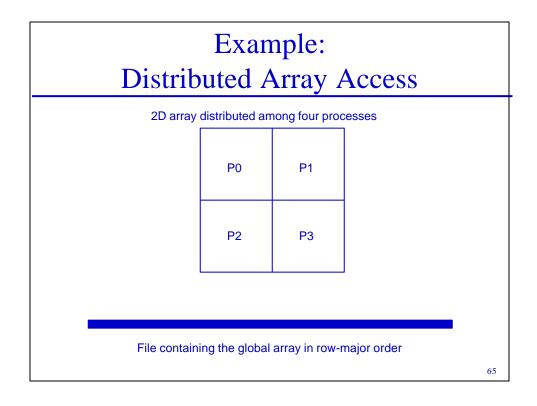
Collective I/O in MPI

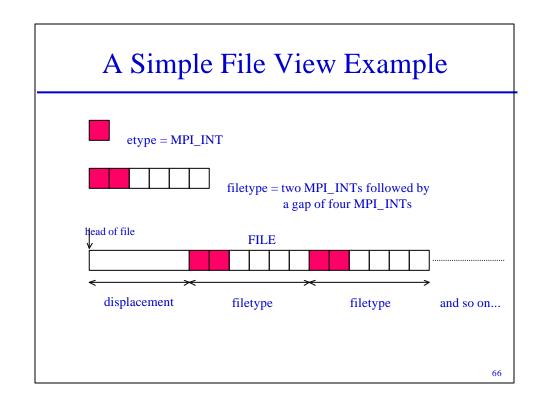
- A critical optimization in parallel I/O
- Allows communication of "big picture" to file system
- Framework for 2-phase I/O, in which communication precedes I/O (can use MPI machinery)
- Basic idea: build large blocks, so that reads/writes in I/O system will be large



Noncontiguous Accesses

- · Common in parallel applications
- Example: distributed arrays stored in files
- A big advantage of MPI I/O over Unix I/O is the ability to specify noncontiguous accesses in memory and file within a single function call by using derived datatypes
- Allows implementation to optimize the access
- Collective IO combined with noncontiguous accesses yields the highest performance.





File View Code

Collective I/O

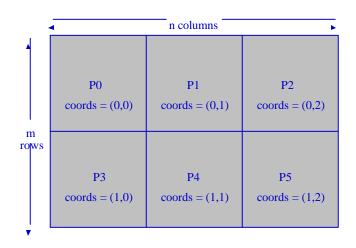
- MPI_File_read_all,MPI_File_read_at_all, etc
- _all indicates that all processes in the group specified by the communicator passed to MPI_File_open will call this function
- Each process specifies only its own access information -- the argument list is the same as for the non-collective functions

Collective I/O

- By calling the collective I/O functions, the user allows an implementation to optimize the request based on the combined request of all processes
- The implementation can merge the requests of different processes and service the merged request efficiently
- Particularly effective when the accesses of different processes are noncontiguous and interleaved

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Accessing Arrays Stored in Files



nproc(1) = 2, nproc(2) = 3

Using the "Distributed Array" (Darray) Datatype

Darray Continued

A Word of Warning about Darray

- The darray datatype assumes a very specific definition of data distribution -- the exact definition as in HPF
- For example, if the array size is not divisible by the number of processes, darray calculates the block size using a *ceiling* division (20 / 6 = 4)
- darray assumes a row-major ordering of processes in the logical grid, as assumed by cartesian process topologies in MPI-1
- If your application uses a different definition for data distribution or logical grid ordering, you cannot use darray. Use subarray instead.

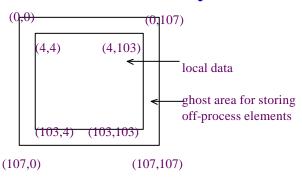
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Using the Subarray Datatype

```
gsizes[0] = m;  /* no. of rows in global array */
gsizes[1] = n;  /* no. of columns in global array*/
psizes[0] = 2;  /* no. of procs. in vertical dimension */
psizes[1] = 3;  /* no. of procs. in horizontal dimension */
lsizes[0] = m/psizes[0];  /* no. of rows in local array */
lsizes[1] = n/psizes[1];  /* no. of columns in local array */
dims[0] = 2; dims[1] = 3;
periods[0] = periods[1] = 1;
MPI_Cart_create(MPI_COMM_WORLD, 2, dims, periods, 0, &comm);
MPI_Comm_rank(comm, &rank);
MPI_Cart_coords(comm, rank, 2, coords);
```

Subarray Datatype contd.

Local Array with Ghost Area in Memory



- Use a subarray datatype to describe the noncontiguous layout in memory
- Pass this datatype as argument to MPI_File_write_all

Local Array with Ghost Area

Accessing Irregularly <u>Distributed Arrays</u>



The map array describes the location of each element of the data array in the common file

Accessing Irregularly Distributed Arrays

Nonblocking I/O

Split Collective I/O

- A restricted form of nonblocking collective I/O
- Only one active nonblocking collective operation allowed at a time on a file handle
- Therefore, no request object necessary

```
MPI_File_write_all_begin(fh, buf, count, datatype);
for (i=0; i<1000; i++) {
    /* perform computation */
}
MPI_File_write_all_end(fh, buf, &status);</pre>
```

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Shared File Pointers

Passing Hints to the **Implementation**

```
MPI_Info info;
MPI_Info_create(&info);
/* no. of I/O devices to be used for file striping */
MPI_Info_set(info, "striping_factor", "4");
/* the striping unit in bytes */
MPI Info set(info, "striping unit", "65536");
MPI_File_open(MPI_COMM_WORLD, "/pfs/datafile",
              MPI_MODE_CREATE | MPI_MODE_RDWR, info, &fh);
MPI_Info_free(&info);
                                                        83
```

Examples of Hints

(used in ROMIO) • striping_unit striping_factor MPI-2 predefined hints • cb_buffer_size cb_nodes • ind rd buffer size New Algorithm **Parameters** • ind_wr_buffer_size start_iodevice pfs_svr_buf Platform-specific hints direct read direct_write 84

I/O Consistency Semantics

- The consistency semantics specify the results when multiple processes access a common file and one or more processes write to the file
- MPI guarantees stronger consistency semantics if the communicator used to open the file accurately specifies all the processes that are accessing the file, and weaker semantics if not
- The user can take steps to ensure consistency when MPI does not automatically do so
- Warning: NFS (Network File System) does not support access from multiple processes. Clusters should use PVFS (Parallel Virtual File System) instead.

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File Interoperability

- Users can optionally create files with a portable binary data representation
- "datarep" parameter to MPI_File_set_view
- native default, same as in memory, not portable
- internal impl. defined representation providing an impl. defined level of portability
- external32 a specific representation defined in MPI, (basically 32-bit big-endian IEEE format), portable across machines and MPI implementations

General Guidelines for Achieving High I/O Performance

- Buy sufficient I/O hardware for the machine
- Use fast file systems (such as PVFS), not NFS-mounted home directories
- Do not perform I/O from one process only
- Make large requests wherever possible
- For noncontiguous requests, use derived datatypes and a single collective I/O call

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Achieving High I/O Performance with MPI

- Any application as a particular "I/O access pattern" based on its I/O needs
- The same access pattern can be presented to the I/O system in different ways depending on what I/O functions are used and how
- See the SC98 paper in which we classify the different ways of expressing I/O access patterns in MPI-IO into four *levels*: level 0 level 3

http://www.supercomp.org/sc98/TechPapers/sc98 FullAbstracts/Thakur447

 We demonstrate how the user's choice of level affects performance

Example: Distributed Array Access

Large array distributed among 16 processes

P0	P1	P2	Р3
P4	P5	P6	P7
P8	P9	P10	P11
P12	P13	P14	P15

Each square represents a subarray in the memory of a single process

Level-0 Access (C)

 Each process makes one independent read request for each row in the local array (as in Unix)

```
MPI_File_open(..., file, ..., &fh)
for (i=0; i<n_local_rows; i++) {
    MPI_File_seek(fh, ...);
    MPI_File_read(fh, &(A[i][0]), ...);
}
MPI_File_close(&fh);</pre>
```

Level-0 Access (Fortran)

 Each process makes one independent read request for each column in the local array (as in Unix)

```
call MPI_File_open(..., file, ..., fh, ierr)
do i=1, n_local_cols
    call MPI_File_seek(fh, ..., ierr)
    call MPI_File_read(fh, A(1,i), ..., ierr)
enddo
call MPI_File_close(fh, ierr)
```

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Level-1 Access (C)

 Similar to level 0, but each process uses collective I/O functions

```
MPI_File_open(MPI_COMM_WORLD, file, ...,
&fh);
for (i=0; i<n_local_rows; i++) {
    MPI_File_seek(fh, ...);
    MPI_File_read_all(fh, &(A[i][0]), ...);
}
MPI_File_close(&fh);</pre>
```

Level-1 Access (Fortran)

 Similar to level 0, but each process uses collective I/O functions

```
call MPI_File_open(MPI_COMM_WORLD, file,
..., fh, ierr)
do i=1, n_local_cols
    call MPI_File_seek(fh, ..., ierr)
    call MPI_File_read_all(fh, A(1,i), ...,
ierr)
enddo
call MPI_File_close(fh, ierr)
```

Level-2 Access (C)

 Each process creates a derived datatype to describe the noncontiguous access pattern, defines a file view, and calls independent I/O functions

```
MPI_Type_create_subarray(..., &subarray,
...);

MPI_Type_commit(&subarray);

MPI_File_open(..., file, ..., &fh);

MPI_File_set_view(fh, ..., subarray, ...);

MPI_File_read(fh, A, ...);

MPI_File_close(&fh);
```

Level-2 Access (Fortran)

 Each process creates a derived datatype to describe the noncontiguous access pattern, defines a file view, and calls independent I/O functions

```
call MPI_Type_create_subarray(..., subarray,
..., ierr)
call MPI_Type_commit(subarray, ierr)
call MPI_File_open(..., file, ..., fh, ierr)
call MPI_File_set_view(fh, ..., subarray,
..., ierr)
call MPI_File_read(fh, A, ..., ierr)
call MPI_File_close(fh, ierr)
```

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Level-3 Access (C)

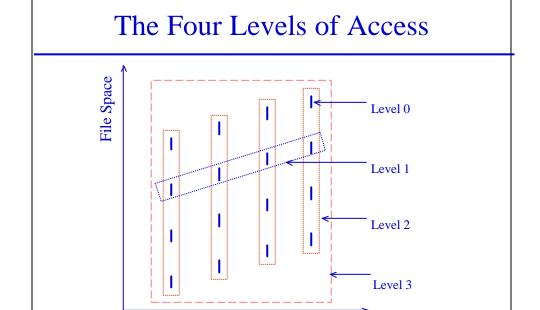
 Similar to level 2, except that each process uses collective I/O functions

```
MPI_Type_create_subarray(...,
&subarray, ...);
MPI_Type_commit(&subarray);
MPI_File_open(MPI_COMM_WORLD, file,
..., &fh);
MPI_File_set_view(fh, ..., subarray,
...);
MPI_File_read_all(fh, A, ...);
MPI_File_close(&fh);
```

Level-3 Access (Fortran)

 Similar to level 2, except that each process uses collective I/O functions

```
call MPI_Type_create_subarray(...,
subarray, ..., ierr)
call MPI_Type_commit(subarray, ierr)
call MPI_File_open(MPI_COMM_WORLD, file,
..., fh, ierr)
call MPI_File_set_view(fh, ..., subarray,
..., ierr)
call MPI_File_read_all(fh, A, ..., ierr)
call MPI_File_close(fh, ierr)
```



2

3

Processes

0

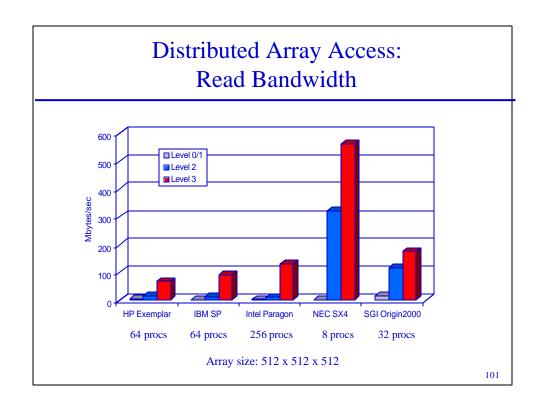
Optimizations

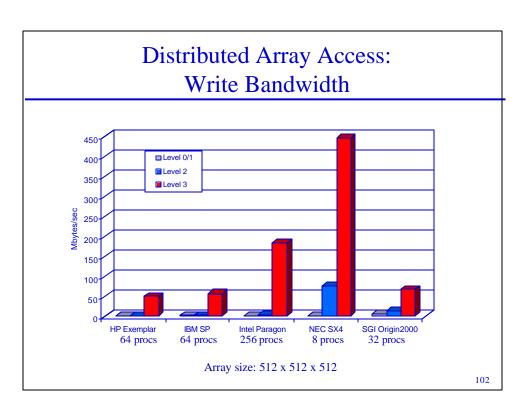
- Given complete access information, an implementation can perform optimizations such as:
 - Data Sieving: Read large chunks and extract what is really needed
 - Collective I/O: Merge requests of different processes into larger requests
 - Improved prefetching and caching

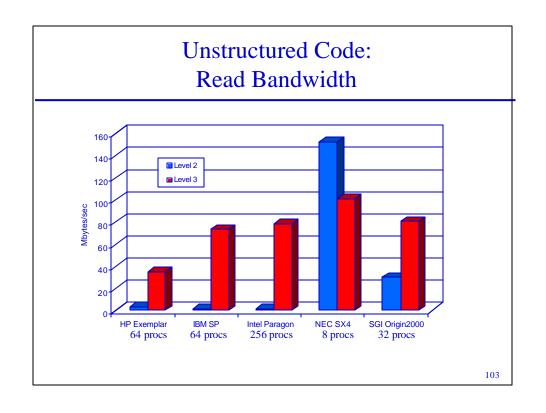
99

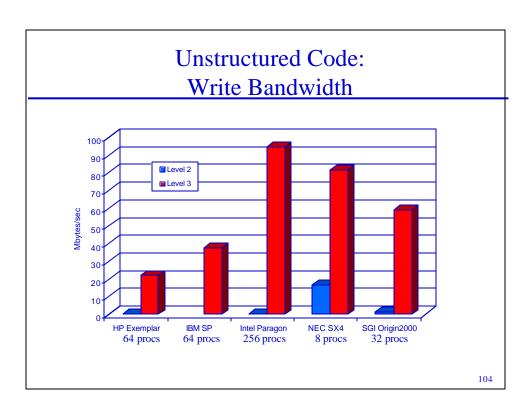
Performance Results

- Distributed array access
- Unstructured code from Sandia
- On five different parallel machines:
 - HP Exemplar
 - IBM SP
 - Intel Paragon
 - NEC SX-4
 - SGI Origin2000









Independent Writes

- On Paragon
- Lots of seeks and small writes
- Time shown = 130 seconds



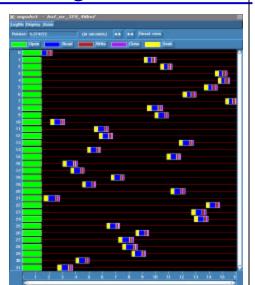
Collective Write

- On Paragon
- Computation and communication precede seek and write
- Time shown =2.75 seconds



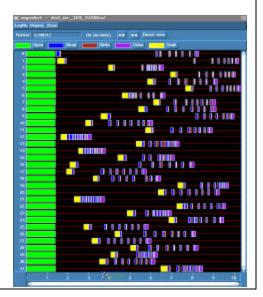
Independent Writes with Data Sieving

- On Paragon
- Access data in large "blocks" and extract needed data
- Requires lock, read, modify, write, unlock for writes
- 4 MB blocks
- Time = 16 sec.



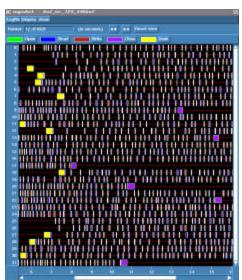
Changing the Block Size

- Smaller blocks mean less contention, therefore more parallelism
- 512 KB blocks
- Time = 10.2 seconds



Data Sieving with Small Blocks

- If the block size is too small, however, the increased parallelism doesn't make up for the many small writes
- 64 KB blocks
- Time = 21.5 seconds



Common Errors

- Not defining file offsets as MPI_Offset in C and integer (kind=MPI_OFFSET_KIND) in Fortran (or perhaps integer *8 in Fortran 77)
- In Fortran, passing the offset or displacement directly as a constant (e.g., 0) in the absence of function prototypes (F90 mpi module)
- Using darray datatype for a block distribution other than the one defined in darray (e.g., floor division)
- filetype defined using offsets that are not monotonically nondecreasing, e.g., 0, 3, 8, 4, 6. (happens in irregular applications)

Summary

- MPI I/O has many features that can help users achieve high performance
- The most important of these features are the ability to specify noncontiguous accesses, the collective I/O functions, and the ability to pass hints to the implementation
- · Users must use the above features!
- In particular, when accesses are noncontiguous, users must create derived datatypes, define file views, and use the collective I/O functions

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Dynamic Process Management in MPI

- Standard way of starting processes in PVM
- Not so necessary in MPI
- Useful in assembling complex distributed applications
- Issues
 - maintaining simplicity, flexibility, and correctness
 - interaction with operating system, resource manager, and process manager
 - connecting independently started processes

Starting New MPI Processes

- MPI_Comm_spawn
 - Starts n new processes
 - Collective over communicator
 - Necessary for scalability
 - Returns an intercommunicator
 - Does not change MPI COMM WORLD
 - "SPMD" (Single Program Multiple Data)
- MPI_Comm_spawn_multiple
 - Link MPI_Comm_spawn
 - "MPMD" (Multiple Program Multiple Data)

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The MPI Environment

- MPI does not specify a particular process management environment
 - You can use whatever you have (Condor, LoadLeveler, PBS, etc.)
 - No particular system is defined
 - MPI Forum attempted to define an abstract interface to third-party process managers, but could no consensus reached
- Still need to pass information to process management system
 - Led to MPI_Info

Communicating Data to (and through) MPI

- MPI-2 defines a new object, MPI_Info
- Provides an extensible list of key=value pairs
- Used in I/O, One-sided, and Dynamic to package variable, optional types of arguments that may not be standard

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Using MPI_Info in Fortran

Example use for MPI_Comm_spawn:

Using MPI_Info in C

Example use for MPI_Comm_spawn:

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Other Process Management Features

- MPI_Comm_connect and MPI_Comm_accept allow two running MPI programs to connect and interoperate
 - Not intended for client/server applications
 - Useful in assembling complex distributed applications
- MPI_Join allows the use of a TCP socket to connect two applications

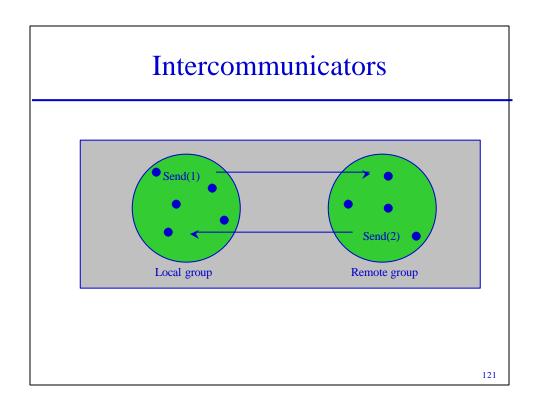
Dynamic Process Management

- Spawning new processes is collective, returning an intercommunicator.
 - Local group is group of spawning processes.
 - Remote group is group of new processes.
 - New processes have own MPI_COMM_WORLD.
 - MPI_Comm_get_parent lets new processes find parent communicator.

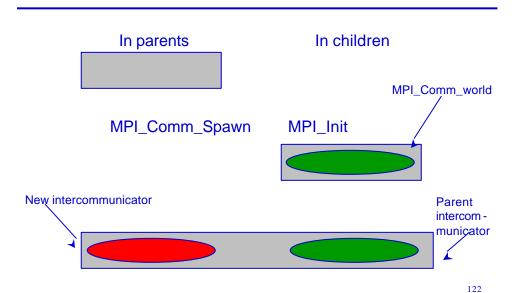
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Intercommunicators

- Contain a local group and a remote group
- Point-to-point communication is between a process in one group and a process in the other.
- Can be merged into a normal (intra) communicator.
- Created by MPI_Intercomm_create in MPI-1.
- Play a more important role in MPI-2, created in multiple ways.



Spawning New Processes



Spawning Processes

MPI_Comm_spawn(command, argv, numprocs, info, root, comm, intercomm, errcodes)

- Tries to start numprocs process running command, passing them command-line arguments argv.
- The operation is collective over comm.
- Spawnees are in remote group of intercomm.
- Errors are reported on a per-process basis in errcodes.
- Info used to optionally specify hostname, archname, wdir, path, file, softness.

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Spawning Multiple Executables

- MPI_Comm_spawn_multiple(...)
- Arguments command, argv, numprocs, info all become arrays.
- Still collective

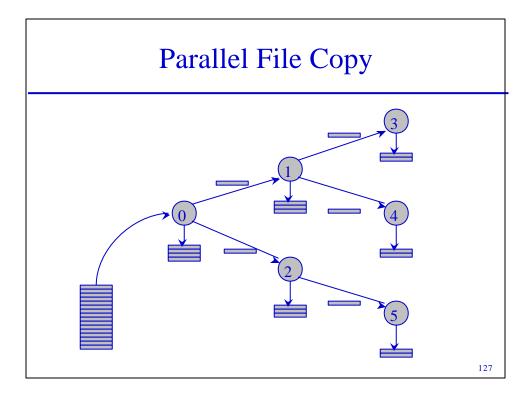
In the Children

- MPI_Init (only MPI programs can be spawned)
- MPI_COMM_WORLD is processes spawned with one call to MPI_Comm_spawn.
- MPI_Comm_get_parent obtains parent intercommunicator.
 - Same as intracommunicator returned by MPI_Comm_spawn in parents.
 - Remote group is spawners.
 - Local group is those spawned.

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Manager-Worker Example

- Single manager process decides how many workers to create and which executable they should run.
- Manager spawns n workers, and addresses them as 0, 1, 2, ..., n-1 in new intercomm.
- Workers address each other as 0, 1, ... n-1 in MPI_COMM_WORLD, address manager as 0 in parent intercomm.
- One can find out how many processes can usefully be spawned (MPI_UNIVERSE_SIZE attribute of MPI_COMM_WORLD).



Parallelism in Distributing Files

- All processes writing in parallel
- Message-passing in parallel (assume scalable implementation of MPI_Bcast)
- Pipeline parallelism with blocks from the file
- Use syntax adopted from cp:

pcp 0-63 /home/progs/cpi /tmp/cpi

Code for pcp Master -1

```
#include <sys/types.h>
#include <sys/stat.h>
#include <fcntl.h>
#define BUFSIZE
                   256*1024
#define CMDSIZE
                   80
int main( int argc, char *argv[] )
    int
             num_hosts, mystatus, allstatus, done, numread;
    int
             infd, outfd;
    char
             outfilename[MAXPATHLEN], controlmsg[CMDSIZE];
    char
             buf[BUFSIZE];
             soft_limit[20];
    char
    MPI_Info hostinfo;
    MPI_Comm pcpslaves, all_procs;
    MPI_Init( &argc, &argv );
                                                         129
```

pcp Master - 2

pcp master - 3

pcp Master - 4

```
MPI_Bcast( outfilename, MAXPATHLEN, MPI_CHAR, 0,
           all_procs );
if ( (outfd = open( outfilename,
      O_CREAT | O_WRONLY | O_TRUNC, S_IRWXU ) ) == -1 )
    mystatus = -1;
else
    mystatus = 0;
MPI_Allreduce( &mystatus, &allstatus, 1, MPI_INT,
               MPI_MIN, all_procs );
if ( allstatus == -1 ) {
    fprintf( stderr, "Output file %s not opened\n",
             outfilename );
    MPI_Finalize();
    return 1;
}
                                                     132
```

pcp Master - 5

```
done = 0;
while (!done) {
  numread = read( infd, buf, BUFSIZE );
  MPI_Bcast( &numread, 1, MPI_INT, 0, all_procs );
  if ( numread > 0 ) {
      MPI_Bcast( buf, numread, MPI_BYTE, 0, all_procs);
      write( outfd, buf, numread );
  }
  else {
    close( outfd );
    done = 1;
  }
}
MPI_Comm_free( &pcpslaves );
MPI_Comm_free( &all_processes );
MPI_Finalize();
return 0;
```

pcp Slave - 1

```
#include "mpi.h"
#include <stdio.h>
#include <sys/types.h>
#include <sys/stat.h>
#include <fcntl.h>
#define BUFSIZE
                   256*1024
#define CMDSIZE
int main( int argc, char *argv[] )
             mystatus, allstatus, done, numread;
    int
    char
             outfilename[MAXPATHLEN], controlmsg[CMDSIZE];
    int
             outfd;
             buf[BUFSIZE];
   MPI_Comm slavecomm, all_processes;
   MPI_Init( &argc, &argv );
   MPI_Comm_get_parent( &slavecomm );
                                                                134
```

psp Slave - 2

```
MPI_Intercomm_merge( slavecomm, 1, &all_procs );
MPI_Bcast( controlmsg, CMDSIZE, MPI_CHAR, 0,
           all_procs );
if ( strcmp( controlmsg, "exit" ) == 0 ) {
    MPI_Finalize();
    return 1;
MPI_Bcast( outfilename, MAXPATHLEN, MPI_CHAR, 0,
           all_procs );
if ( (outfd = open( outfilename, O_CREAT|O_WRONLY|O_TRUNC,
                S_IRWXU ) ) == -1 )
    mystatus = -1;
else
    mystatus = 0;
MPI_Allreduce( &mystatus, &allstatus, 1, MPI_INT, MPI_MIN,
            all procs );
if ( allstatus == -1 ) {
  MPI_Finalize();
  return -1;
                                                            135
```

pcp Slave - 3

```
/* at this point all files have been successfully opened */
   done = 0;
   while ( !done ) {
      MPI_Bcast( &numread, 1, MPI_INT, 0, all_processes );
      if ( numread > 0 ) {
          MPI_Bcast( buf, numread, MPI_BYTE, 0, all_procs );
          write( outfd, buf, numread );
      else {
          close( outfd );
          done = 1;
      }
   MPI_Comm_free( &slavecomm );
   MPI_Comm_free( &all_processes );
   MPI_Finalize();
   return 0;
                                                               136
```

Establishing Connections

- Two sets of MPI processes may wish to establish connections, e.g.,
 - Two parts of an application started separately.
 - A visualization tool wishes to attach to an application.
 - A server wishes to accept connections from multiple clients. Both server and client may be parallel programs.
- Establishing connections is collective but asymmetric ("Client"/"Server").
- Connection results in an intercommunicator.

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Establishing Connections Between Parallel Programs In server In client MPI_Accept MPI_Connect New intercommunicator

Connecting Processes

- Server:
 - MPI_Open_port(info, port_name)
 - system supplies port_name (output argument)
 - might be host:num; might be low-level switch #, etc.
 - MPI_Comm_accept(port_name, info, root, comm, &intercomm)
 - · collective over comm
 - returns intercomm; remote group is clients
- Client:
 - MPI_Comm_connect(port_name, info, root, comm, &intercomm)
 - · remote group is server

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Optional Name Service

 allow connection between service_name known to users and system-supplied port_name

port_name)

- MPI implementations are allowed to ignore this service.
 - But most implementations could use openLDAP

Bootstrapping

MPI_Join(fd, intercomm)

- collective over two processes connected by a socket.
- The fd is a file descriptor for an open, quiescent socket.
- The intercomm is a new intercommunicator.
- Can be used to build up full MPI communication.
- The fd fd is not used for MPI communication.

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MPI and Threads

- MPI describes parallelism between processes
- Thread parallelism provides a sharedmemory model within a process
- OpenMP and pthreads are common
 - OpenMP provides convenient features for loop-level parallelism

Threads and MPI in MPI-2

- MPI-2 specifies four levels of thread safety
 - MPI_THREAD_SINGLE: only one thread
 - MPI_THREAD_FUNNELED : only one thread that makes MPI calls
 - MPI_THREAD_SERIALIZED : only one thread at a time makes MPI calls
 - MPI_THREAD_MULTIPLE : any thread can make MPI calls at any time
- MPI_Init_thread(..., required, &provided) can be used instead of MPI_Init

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MPI and OpenMP

- Loop-level parallelism
 - Requires only MPI_THREAD_FUNNELLED
- Task-parallelism
 - Requires MPI_THREAD_MULTIPLE

Using OpenMP with MPI

- The famous cpi program, using OpenMP for loop-level
- Worker/manager

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cpi with Bcast/Reduce and OpenMP

```
<get n to use>
MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
    = 1.0 / (double) n;
sum = 0.0;
#pragma omp parallel for private(x) reduction(+:sum)
for (i = myid + 1; i <= n; i += numprocs) {</pre>
    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);
if (myid == 0) {
    printf("pi is %.16f, Error is %.16f\n",
            pi, fabs(pi - PI25DT));
}
                                                      146
```

Task Parallelism with MPI and OpenMP

```
#pragma omp sections
{
    # pragma omp section
    {
        while (not_done) {
            MPI_Recv(...);
            if (status.MPI_TAG == ALL_DONE) break;
            <handle message>
            }
        }
    # pragma omp section
    {
        <compute thread>
        }
}
```

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MPI Thread Levels and OpenMP

- MPI THREAD SINGLE
 - OpenMP not permitted
- MPI_THREAD_FUNNELED
 - All MPI calls in the "main" thread
 - MPI calls outside of any OpenMP sections
 - Most if not all MPI implementations support this level
- MPI THREAD SERIALIZED
 - #pragma omp parallel...#pragma omp single{MPI calls allowed here as well
- MPI_THREAD_MULTIPLE
 - Any MPI call anywhere
 - But be careful of races
 - Some MPI implementations support this level

Conclusions

- MPI is a proven, effective, portable parallel programming model
- MPI has succeeded because
 - features are orthogonal (complexity is the product of the number of *features*, not routines)
 - programmer can control memory motion (critical in high-performance computing)
 - complex programs are no harder than easy ones
 - open process for defining MPI led to a solid design
- MPI I/O is widely available and efficient
- Dynamic process management becoming available

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Tutorial Material on MPI, MPI-2





http://www.mcs.anl.gov/mpi/{usingmpi,usingmpi2}