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Programming with MPI: Advanced Topics

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Goals

- To gain an awareness of specialized features in MPI that you may want to use right away in writing parallel applications
- To create a little mental catalog of MPI's more advanced capabilities for future reference

As we go through each section, we'll want to consider:

- Why was this set of routines included? What might they be good for?
- Can we think of an example where they would be useful?



Introduction and Outline

- 1. Advanced point-to-point communication
- 2. Persistent communication
 - LAB -
- 3. Communicators and groups
- 4. Collective communication with non-contiguous data
- 5. Derived datatypes
- 6. Parallel I/O (MPI-2)
- 7. Status of MPI-2



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1. Advanced Point-to-Point Communication



Types of Parallel Overhead in Point-to-Point Calls

- **System overhead** time spent in sending packets across the network, copying to internal MPI buffers, etc.
- Synchronization overhead time spent in waiting for other processes to participate in a communication event
- Memory overhead buffers set aside for handling communication, whether by the user or internally to MPI



Standard Send, Receive

- Standard-Mode Blocking Calls: MPI_Send, MPI_Recv
- MPI_Send returns only when the buffer is safe to reuse:
 - the small message has been copied elsewhere, or
 - the large message has actually been transferred;
 - the small/large threshold is implementation dependent
- Rule of thumb: a send only completes if a matching receive is posted/executed





Synchronous and Buffered Modes

Synchronous Mode: MPI_Ssend

- Transfer is not initiated until matching receive is posted
- Non-local: handshake needed
- Returns after message is sent Buffered Mode: MPI_Bsend
- Completes as soon as the message is copied into the user-provided buffer
- Buffer must be provided using MPI_Buffer_attach
- One buffer per process





Ready Mode and Deadlock

Ready Mode: MPI_Rsend

- Initiates transfer immediately
- Assumes that a matching receive has already been posted
- Error if receiver isn't ready Deadlock
- All tasks are waiting for events that yet haven't been initiated
- Can be avoided by reordering calls, by using non-blocking or buffered (e.g., "eager") calls, or with MPI_Sendrecv





Discussion of Send Modes

- Synchronous mode is portable and "safe"
 - does not depend on order (ready mode) or buffer space (buffered mode)
 - incurs substantial overhead
- Ready mode has least total overhead, but how can error be avoided?
 - sometimes the logic of the code implies the receiver must be ready
- Buffered mode decouples sender and receiver
 - sender doesn't have to sync; receiver doesn't have to be ready
 - system and memory overheads are incurred by copying to the buffer
 - sender can control size of message buffers and total amount of space
- Standard mode tries to strike a balance
 - small messages are buffered on receiver's side (avoiding sync overhead)
 - large messages are sent synchronously (avoiding big buffer space)



MPI_Sendrecv and MPI_Sendrecv_replace

- MPI_Sendrecv (blocking)
 - send message A from one buffer; receive message B in another buffer
 - destination of A, source of B can be same or different
- MPI_Sendrecv_replace (blocking)
 - send message A from one buffer; receive message B in SAME buffer
 - again, destination of A, source of B can be same or different
 - system takes care of the extra internal buffering
- Illustration 1: data swap between processors
 - destination and source are identical
- Illustration 2: chain of processors
 - send result to myrank+1, receive next input from myrank-1



Non-Blocking Calls

- Calls return immediately
- System handles buffering
- Not "safe" to access message contents until action is known to be completed
- With MPI_Isend, message buffer is reusable right away if tag or receiver is different; otherwise, check status
- With MPI_Irecv, user must always check for data; only small messages are buffered





Use of Non-Blocking Communication

- Non-blocking calls permit overlap of computation and communication
- All send modes are available: MPI_Irsend, MPI_Ibsend, MPI_Issend
- Non-blocking calls must normally be resolved through a second call
 - main options: MPI_Wait, MPI_Test, MPI_Request_free
 - variants like MPI_Waitany help to resolve calls in arbitrary order
 - reason for doing this: avoid running out of request handles
- Outline for typical code:

for (i=0;i<M;i++) MPI_Irecv(<declare receive buffers>);
for (i=0;i<N;i++) MPI_Isend(<mark data for sending>);
 /* Do local operations */
MPI_Waitall(<make sure all receives finish>)

/* Operate on received data */
MPI_Waitall(<clear request handles for all sends>)



Sandwich Shop Analogy

The request handle is like your order number.

- MPI_Test You go to the counter ask the guy if your order number is ready. (If it isn't, then you can go back to your table and talk some more with your friends.)
- MPI_Wait You hang around the counter until your order number is definitely ready. (Maybe your friends won't talk to you until you bring them some food!)
- MPI_Request_free You turn in your order number without learning the status of your food. (Perhaps you've canceled your order; or perhaps the order is obviously ready, and you already know what's in it.)
 The number can be reused *after* you turn in your ticket.





MPI_Wait and MPI_Test

- **MPI_Wait** halts progress until a *specific* non-blocking request (send or receive) is satisfied; the related message buffer is then safe to use
 - MPI_Waitall does the same thing for a *whole array* of requests
 - MPI_Waitany waits for any one request from an array
 - MPI_Waitsome waits for one or more requests from an array
- **MPI_Test** immediately returns the status (no waiting!) of a specific non-blocking operation, again identified by a request handle
 - returns flag = true only if the operation is complete
 - allows alternative instructions to be carried out if operation isn't complete
 - has the same variants: MPI_Testall, MPI_Testany, MPI_Testsome



Other Ways to Gain Flexibility in Communication

- MPI_ANY_SOURCE, MPI_ANY_TAG are "wildcards" that may be used by receives (blocking and non-blocking) in situations where the source or tag of a message does not need to be known in advance
 - the status argument returns source, tag, and error status
 - a separate call to MPI_Get_count determines the size of the message
 - but... what if you need to know a message's size before receiving it?
- **MPI_Iprobe** returns the properties of any message that has arrived without receiving it into a buffer (maybe you need to do a big malloc!)

• **MPI_Probe** blocks until such a message arrives (no flag)



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2. Persistent Communication



How Persistent Communication Works

- Motivation: we'd like to save the argument list of an MPI call to reduce overhead for subsequent calls with the same arguments
- INIT takes the original argument list of a send or receive call and creates a persistent *communication request* from it
 - MPI_Send_init (for nonblocking send)
 - MPI_Bsend_init (for buffered send can do Rsend or Ssend as well)
 - MPI_Recv_init (for nonblocking receive)
- START starts an operation based on the *communication request*
 - MPI_Start
 - MPI_Startall
- REQUEST_FREE frees the persistent communication request
 - MPI_Request_free



Typical Situation Where Persistence Might Be Used

```
MPI_Recv_init(buf1,count,type,src,tag,comm,&req[0]);
MPI_Send_init(buf2,count,type,src,tag,comm,&req[1]);
```

```
for (i=1; i < BIGNUM; i++)
{
     MPI_Start(&req[0]);
     MPI_Start(&req[1]);
     MPI_Waitall(2,req,status);
     do_work(buf1,buf2);
}</pre>
```

```
MPI_Request_free(&req[0]);
MPI_Request_free(&req[1]);
```



Performance Benefits from Using Persistence

Improvement in Wallclock Time (IBM SP2) Persistent vs. Conventional Communication

size, bytes	mode	improvement	mode	improvement
8	async	19 %	sync	15 %
4096	async	11 %	sync	4.7 %
8192	async	5.9 %	sync	2.9 %
800,000	-	-	sync	0 %
8,000,000	-	-	sync	0 %

• **Takeaway**: it's most effective when applied to lots of small messages



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3. Communicators and Groups



Communicators and Groups: Definitions

 All MPI communication is relative to a *communicator* which contains a *context* and a *group*. The group is just a set of processes.



 Processes may have different ranks in different communicators.





Subdividing Communicators: Approach #1

• To subdivide a communicator into multiple non-overlapping communicators, one approach is to use MPI_Comm_split

MPI_Comm_rank(MPI_COMM_WORLD,&rank);
myrow = (int)(rank/ncol); //yields 0, 1,... nrows-1
MPI_Comm_split(MPI_COMM_WORLD,myrow,rank,row_comm);





Arguments to MPI_Comm_split

```
MPI_Comm_rank(MPI_COMM_WORLD,&rank);
myrow = (int)(rank/ncol); //yields 0, 1,... rows-1
MPI_Comm_split(MPI_COMM_WORLD,myrow,rank,row_comm);
```

- 1. Communicator to split
- 2. Key all processes with the same key go in the same communicator
- 3. Value to determine ordering in the result communicator (optional)
- 4. Result communicator



Subdividing Communicators: Approach #2

- The same goal can be accomplished using groups
- MPI_Comm_group extract the group defined by a communicator
- MPI_Group_incl make a new group from selected members of the existing group (e.g., members in the same row of a 2D layout)
- **MPI_Comm_create** form a communicator based on this group





Code for Approach #2

MPI_Group base_grp,grp; MPI_Comm row_comm,temp_comm; int row_list[NCOL], irow, myrank_in_world;

MPI_Comm_group(MPI_COMM_WORLD,&base_grp); //get base MPI_Comm_rank(MPI_COMM_WORLD,&myrank_in_world);

```
irow = (myrank_in_world/NCOL);
for (i=0; i <NCOL; i++) row_list[i] = i;
for (i=0; i <NROW; i++){
    MPI_Group_incl(base_grp,NCOL,row_list,&grp);
    MPI_Comm_create(MPI_COMM_WORLD,grp,&temp_comm);
    if (irow == i) *row_comm=temp_comm; //toss others
    for (j=0;j<NCOL;j++) row_list[j] += NCOL;
}
```



Communicators and Groups: Summary

- In Approach #1, we used MPI_Comm_split to split one communicator into multiple non-overlapping communicators.
- This approach is relatively compact and is suitable for regular decompositions.
- In Approach #2, we broke the communicator into (sub)groups and made these into new communicators to suit our needs.
- We did this using MPI_Comm_group, MPI_Group_incl, and MPI_Comm_create.
- This approach is quite flexible and is more generally applicable.
- Many other group functions are available: union, intersection, difference, include, exclude, range-include, range-exclude.



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4. Collective Communication with Non-Contiguous Data



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Review: Scatter and Gather





Introducing Scatterv, Gatherv

- MPI_{Scatter,Gather,Allgather}v
- What does **v** stand for?
 - varying size and relative location of messages
- Advantages
 - more flexibility
 - less need to copy data into temporary buffers
 - more compact
- Disadvantage
 - harder to program



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Scatter vs. Scatterv



• DISPLS(J) is the displacement from SENDBUF to the beginning of the J-th message, in units of SENDTYPE. Defined on ROOT.



Allgatherv Example

```
MPI Comm size(comm,&ntids);
sizes = (int*)malloc(ntids*sizeof(int));
MPI Allgather(&n,1,MPI INT, sizes,1,MPI INT, comm);
offsets = (int*)malloc(ntids*sizeof(int));
s=0;
for (i=0; i<ntids; i++)</pre>
  {offsets[i]=s; s+=sizes[i];}
N = S;
result_array = (int*)malloc(N*sizeof(int));
MPI Allgatherv
   ((void*)local_array,n,MPI_INT,(void*)result_array,
    sizes,offsets,MPI INT,comm);
free(sizes); free(offsets);
```



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5. Derived Datatypes



Derived Datatypes: Motivation

- MPI basic datatypes are predefined for contiguous data of single type
- What if an application needs to communicate data of mixed type or in non-contiguous locations?
 - solutions that involve making multiple MPI calls, copying data into a buffer and packing, etc., are slow, clumsy and wasteful of memory
 - better to create/derive datatypes for these special needs from the existing datatypes
 - called "derived" because you build them up from more fundamental types
- Here are several of their advantages :
 - 1. They can be created recursively
 - 2. They can be created conditionally, at runtime
 - 3. Packing and unpacking are done automatically



General Datatypes

- **Contiguous**: Vector with "stride" of one
- Vector: Fixed-size blocks separated by constant stride
- **Hvector**: Like vector, but with stride in bytes
- Indexed: Arrays of block sizes and indices (like scatterv/gatherv)
- Hindexed: Indexed, with indices in bytes
- Struct: General mixed types (for C structs etc.)



Picturing Some Derived Datatypes





Using MPI's Vector Type

• Function MPI_TYPE_VECTOR allows creating non-contiguous vectors with constant stride. Where might one use it?

mpi_type_vector(count,blocklen,stride,oldtype,vtype,ierr)

	1	6	11	16	
ncols = 4	2	7	12	17	
nrows = 5	3	8	13	18	
	4	9	14	19	
	5	10	15	20	

Array A

```
call MPI_Type_commit(vtype,ierr)
```

```
call MPI_Send(A(nrows,1),1,vtype...)
```



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6. Parallel I/O (MPI-2)



Parallel I/O with MPI-IO

- Why parallel I/O?
 - I/O was lacking from the MPI-1 specification
 - Due to need, it was defined independently, then subsumed into MPI-2
- What is parallel I/O? It occurs when:
 - multiple MPI tasks can read or write simultaneously,
 - from or to a single file,
 - in a parallel file system,
 - through the MPI-IO interface.
- A parallel file system works by:
 - appearing as a normal Unix file system, while
 - employing multiple I/O servers (usually) for high sustained throughput.



MPI-IO Advantages

- Two common alternatives to parallel MPI-IO are:
 - 1. Rank 0 accesses a file; it gathers/scatters file data from/to other ranks.
 - 2. Each rank opens a separate file and does I/O to it independently.
- Alternative I/O schemes are simple enough to code, but have either
 - 1. Poor scalability (e.g., the single task is a bottleneck) or
 - 2. ile management challenges (e.g., files must be collected from local disk).
- MPI-IO provides
 - mechanisms for performing synchronization,
 - syntax for data movement, and
 - means for defining noncontiguous data layout in a file (MPI datatypes).



Noncontiguous Accesses

- Parallel applications commonly need to write distributed arrays to disk
 - Better to do this to a single file, instead of multiple
- A big advantage of MPI I/O over Unix I/O is the ability to specify noncontiguous accesses in both a file **and** a memory buffer.
 - Read or write such a file in parallel by using derived datatypes within a single MPI function call
 - Let the MPI implementation to optimize the access
- Collective I/O combined with noncontiguous accesses generally yields the highest performance
- HPC parallel I/O requires some extra work, but it
 - potentially provides high throughput and
 - offers a single (unified) file for viz and pre/post processing



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Simple MPI-IO

Each MPI task reads/writes a single block:





File Pointers and Offsets

- In simple MPI-IO, each MPI process reads or writes a single block.
- I/O functions must be preceded by a call to MPI_File_open, which defines both an *individual* file pointer for the process, and a *shared* file pointer for the communicator.
- We have three means of positioning where the read or write takes place for each process:
 - 1. Use individual file pointers, call MPI_File_seek/read
 - 2. Calculate byte offsets, call MPI_File_read_at
 - 3. Access a shared file pointer, call MPI_File_seek/read_shared
- Techniques 1 and 2 are naturally associated with C and Fortran, respectively. In any case, the goal is roughly indicated by the previous figure.



Reading by Using Individual File Pointers – C Code

```
MPI_File fh;
MPI_Status status;
```

```
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &nprocs);
```

```
bufsize = FILESIZE/nprocs;
nints = bufsize/sizeof(int);
```



Reading by Using Explicit Offsets – F90 Code

```
include 'mpif.h'
integer status(MPI_STATUS_SIZE)
integer (kind=MPI OFFSET KIND) offset
```

nints = FILESIZE/(nprocs*INTSIZE)
offset = rank * nints * INTSIZE



Operations with Pointers, Offsets, Shared Pointers

- MPI_File_open flags:
 - MPI_MODE_RDONLY (read only)
 - MPI_MODE_WRONLY (write only)
 - MPI_MODE_RDWR (read and write)
 - MPI_MODE_CREATE (create file if it doesn't exist)
 - Use bitwise-or '|' in C, or addition '+" in Fortran, to combine multiple flags
- To write into a file, use MPI_File_write or MPI_File_write_at, or...
- The following operations reference the implicitly-maintained shared pointer defined by MPI_File_open
 - MPI_File_read_shared
 - MPI_File_write_shared
 - MPI_File_seek_shared



File Views

- A view is a triplet of arguments (displacement, etype, filetype) that is passed to MPI_File_set_view.
 - *displacement* = number of bytes to be skipped from the start of the file
 - *etype* = unit of data access (can be any basic or derived datatype)
 - *filetype* = specifies layout of etypes within file
- Note that etype is considered to be the elementary type, but since it can be a derived datatype, there's really nothing elementary about it.
- In the file view depicted on the next slide, etype is double precision, filetype is a vector type, and displacement is used to stagger the starting positions by MPI rank.



Example #1: File Views for a Four-Task Job





File View Examples

- In Example 1, we write contiguous data into a contiguous block defined by a file view.
 - We give each process a different file view so that together, the processes lay out a series of blocks in the file, one block per process.
- In Example 2, we write contiguous data into two separate blocks defined by a different file view.
 - Each block is a contiguous type in memory, but the pair of blocks is a vector type in the file view.
 - We again use displacements to lay out a series of blocks in the file, one block per process, in a repeating fashion.



Example #1: File Views for a Four-Task Job

• 1 block from each task, written in task order



MPI_File_set_view assigns regions of the file to separate processes



Code for Example #1

#define N 100
MPI_Datatype arraytype;
MPI_Offset disp;

disp = rank*sizeof(int)*N; etype = MPI_INT; MPI_Type_contiguous(N, MPI_INT, &arraytype); MPI_Type_commit(&arraytype);

MPI_File_write(fh, buf, N, etype, MPI_STATUS_IGNORE);



Example #2: File Views for a Four-Task Job

• 2 blocks from each task, written in round-robin fashion to a file



MPI_File_set_view assigns regions of the file to separate processes



Code for Example #2

/* processor writes 2 'ablk', each with NW ints */
 MPI_Type_contiguous(NW, MPI_INT, &ablk);
 MPI_Type_commit(&ablk);
 MPI_File_write(fh, (void *)buf, 2, ablk, &status);



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
- Preliminary communication can use MPI machinery to aggregate data
- Basic idea: build large blocks, so that reads/writes in I/O system will be more efficient





MPI Routines for Collective I/O

- Typical routine names:
 - MPI_File_read_all
 - MPI_File_read_at_all, etc.
- The _all indicates that all processes in the group specified by the communicator passed to MPI_File_open will call this function
- Each process provides nothing beyond its own access information, including its individual pointer
 - The argument list is therefore the same as for the non-collective functions
- Collective I/O operations work with shared pointers, too
 - The general rule is to replace _shared with _ordered in the routine name
 - Thus, the collective equivalent of MPI_File_read_shared is MPI_File_read_ordered



Advantages of Collective I/O

- By calling the collective I/O functions, the user allows an implementation to optimize the request based on the combined requests 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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Collective Choreography





Asynchronous Operations

Asynchronous operations give the system even more opportunities to optimize I/O.

For each *noncollective* I/O routine, there is an *nonblocking* variant.

- MPI_File_iwrite and MPI_File_iread, e.g., are nonblocking calls.
- The general naming convention is to replace "read" with "iread", or "write" with "iwrite".
- These nonblocking routines are analogous to the nonblocking sends and receives in MPI point-to-point communication.
- Accordingly, these types of calls should be terminated with MPI_Wait.



Collective Asynchronous Operations

For each *collective* I/O routine, there is a *split* variant.

- A collective I/O operation can *begin* at some point and *end* at some later point.
- When using file pointers: MPI_File_read_all_begin/end; MPI_File_write_all_begin/end
- When using explicit offsets: MPI_File_read_at_all_begin/end; MPI_File_write_at_all_begin/end
- When using shared pointers: MPI_File_read_ordered_begin/end; MPI_File_write_ordered_begin/end



Passing Along Hints to MPI-IO

```
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_Info_free(&info);



Examples of Hints (also used in ROMIO)

striping_unit striping factor • MPI-2 predefined hints cb buffer size cb nodes New algorithm ind_rd_buffer_size parameters ind_wr_buffer_size ٠ start iodevice pfs_svr_buf Platform-specific hints direct read • direct write



MPI-IO Summary

- MPI-IO 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
 - the ability to pass hints to the implementation
- In particular, when accesses are noncontiguous, users must:
 - Create derived datatypes
 - Define file views
 - Use the collective I/O functions
- Use of these features is encouraged, because I/O is expensive! It's best to let the system make tuning decisions on your behalf.



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7. Status of MPI-2



Features of MPI-2

- Parallel I/O (MPI-IO) probably the most popular
- One-sided communication (put / get)
- Dynamic process management (spawn)
- Expanded collective communication operations (e.g., non-blocking)
- Support for multithreading
- Additional support for programming languages
 - C++ interface
 - limited F90 support
 - interfaces for debuggers, profilers



MPI-2 Status Assessment

- Virtually all vendors offer MPI-1
 - Well-established free implementations (MPICH, OpenMPI) support networks of heterogeneous workstations, e.g.
 - The functionality of MPI-1 (or even a subset) is sufficient for most applications
- Reasonable MPI-2 implementations are available from most vendors
- MPI-2 implementations have tended to appear in stages with I/O first
 - MPI-IO now available in most MPI implementations
 - One-sided communication available in some where hardware supports it
 - OpenMPI (aka LAM) and MPICH2 now becoming complete
 - Dynamic process management may not mesh well with batch systems



References

- William Gropp, Ewing Lusk, and Anthony Skjellum, Using MPI, Second Edition (MIT Press, 1999)
- William Gropp, Ewing Lusk, and Rajeev Thakur, <u>Using MPI-2</u> (MIT Press, 1999)

http://www.scribd.com/doc/28220855/Using-MPI-2-Advanced-Features

Index to the MPI 1.1 standard

http://www.mpi-forum.org/docs/mpi-11-html/node182.html

Index to the MPI 2 standard

http://www.mpi-forum.org/docs/mpi-20-html/node306.htm

The I/O Stress Benchmark Codes

https://asc.llnl.gov/computing_resources/purple/archive/benchmarks/ior/