Today's agenda

- Homework discussion
- Collective Communications: All-with-All
- Derived Datatypes
- Groups, Contexts and Communicators
- Topologies
- Language Binding issues
- The Runtime and Environment Management
- The MPI profiling interface and tracing
Reduce-Scatter

- \texttt{MPI\_Reduce\_scatter(void *sendbuf, void *recvbuff, int *recv\_cnt, MPI\_Datatype type, MPI\_Op op, MPI\_Comm comm)}

- \texttt{MPI\_REDUCE\_SCATTER(sendbuf, recvbuf, recv\_cnt, type, op, comm, ier)}

- Can be considered as a

  \begin{verbatim}
  MPI\_Reduce(sendbuf, tmpbuf, cnt, type, op, root, comm);
  MPI\_Scatterv(tmpbuf, recv\_cnt, displs, type, recvbuf, recv\_cnt[myid], type, root, comm);
  \end{verbatim}

  where \texttt{cnt} is the total sum of the \texttt{recv\_cnt} values and \texttt{displs[k]} is the sum of the \texttt{recv\_cnt} for up to processor \texttt{k-1}.

- Implementations may use a more optimal approach
How it would work for matvec

Parallel Programming for Multicore Machines Using OpenMP and MPI
3DFFT

Parallel Programming for Multicore Machines Using OpenMP and MPI
Alternative decomposition
Why Derived Datatypes?

- So far all MPI operations seen operate on 1D arrays of predefined datatypes.
  
  - Multidimensional arrays (linearly stored in memory) can be sent as the equivalent 1D array
  
  - Contiguous sections of arrays need to be copied (implicitly in Fortran 90/95) to one big chunk to sent over
  
  - Edges, vertices etc. of 2D/3D arrays need to be sent separately or packed to a sent buffer on the sent side and unpacked from the receive buffer on the receive side, at the programmer's effort
  
  - Strided data needs to be packed/sent/received/unpacked as above.
  
- Message aggregation: int & double in same message
What is a Derived Datatype?

- A general datatype is an opaque object specifying:
  - A sequence of basic datatypes
  - A sequence of integer (byte) displacements

- Type signature:
  - \{type1, type2, ..., typeN\}

- Type map:
  - \{(type1,disp1), (type2,disp2)\}

- The displacements are not required to be positive, distinct, or in increasing order. Therefore, the order of items need not coincide with their order in store, and an item may appear more than once.
A derived datatype describes the memory layout of, e.g., structures, common blocks, subarrays, some variables in the memory.
More details

- Basic (predefined) MPI datatypes are in fact defined in the same way, based on base language datatypes.

- (User) derived datatypes can be defined in terms of basic as well as other defined datatypes.
  - This level of recursive definition can be repeated to construct very complicated datatypes.

- Just like basic datatypes, defined datatypes can be used as arguments to communication routines.

- An efficient implementation of communication events when working with such complicated datatypes is left to the implementation.
  - May use optimizations known to work on architecture.
Size and Extent

- Size: length of "useful" part == data to be transferred
- Extent: the span from the first byte to the last byte occupied by entries in this datatype, rounded up to satisfy alignment requirements.
- Alignment is architecture/language/compiler specific

```plaintext
oldtype

newtype

size : = 6* size(oldtype)

extent : = 8* extent(oldtype)

better visualization of newtype:
```

Figure by MIT OpenCourseWare.
Datatype construction: Contiguous

- **MPI_Type_contiguous**(int count, MPI_Datatype oldtype, MPI_Datatype *newtype)

- The simplest possible derived datatype

- Concatenation of `count` copies of oldtype variables

- Call with 2, MPI_DOUBLE_PRECISION to get your own MPI_DOUBLE_COMPLEX in Fortran if absent.

![Diagram of datatype construction](image-url)
Datatype construction: Vector

- **MPI_Type_vector**(int count, int blocklength, int stride, MPI_Datatype oldtype, MPI_Datatype *newtype)

- Concatenation of *count* copies of blocks of oldtype variables of size *blocklength* positioned *stride* blocks apart. **Strides** (displacements) can be negative.

![Diagram](image-url)

Figure by MIT OpenCourseWare.
More about vector types

- Type before described as
  - `MPI_Type_vector(2, 3, 5, oldtype, newtype)`
- `MPI_Type_contiguous(n, oldtype, newtype)` same as:
  - `MPI_Type_vector(n, 1, 1, oldtype, newtype)`
  - `MPI_Type_vector(1, n, k, oldtype, newtype)` for any k
- `MPI_Type_hvector()` requires stride to be in bytes, instead of `oldtype` units. Type is `MPI_Aint`.
- `MPI_Type_indexed(int count, int *array_of_blocklen, int *array_of_displacements, MPI_Datatype oldtype, MPI_Datatype *newtype); MPI_Type_hindexed()`
  - For vectors with variably sized blocks, variable strides
Datatype construction: Structure

```c
Struct buff_layout
{
    int i_val[3];
    double d_val[5];
}
buffer;

array_of_types[0]=MPI_INT;
array_of_blocklengths[0]=3;
array_of_displacements[0]=0;
array_of_types[1]=MPI_DOUBLE;
array_of_blocklengths[1]=5;
array_of_displacements[1]=...;
MPI_Type_struct(2, array_of_blocklengths,
               array_of_displacements, array_of_types,
               &buff_datatype);
MPI_Type_commit(&buff_datatype);

buffer = the start address of the data

MPI_Send(&buffer, 1, buff_datatype, ...)

the datatype handle describes the data layout

```

Figure by MIT OpenCourseWare.
Alignment, gaps and addresses

- MPI_Type_struct(int count, int *array_of_blocklengths, MPI_Aint *array_of_displacements, MPI_Datatype *array_of_oldtypes, MPI_Datatype *newtype);

- Alignment restrictions may require the presence of gaps in your structure.

- count=2, array_of_blocklengths=[3,5], array_of_types=[MPI_INT,MPI_DOUBLE]

- What about array_of_displacements? [0,addr1-addr0]
Address, size and extent

- **MPI_Address(void* location, MPI_Aint *address)**
- **MPI_BOTTOM** for the start of the address space
  - Use MPI_Address to get absolute addresses for your constituent parts and calculate the correct displacement, with the gaps the compiler requires
  - **MPI_Type_lb/ub() & MPI_LB/UB** for endbounds
- **MPI_Type_extent(MPI_Datatype datatype, MPI_Aint *extent)**
  - Will calculate the proper extent in bytes of the datatype
- **MPI_Type_size(MPI_Datatype datatype, int *size)**
  - Will calculate the proper size in bytes ("useful" part that gets communicated) of the datatype.
Correct usage of addresses (std)

- Successively declared variables in C or Fortran are not necessarily stored at contiguous locations. Thus, care must be exercised that displacements do not cross from one variable to another. Also, in machines with a segmented address space, pointers arithmetic has some peculiar properties. Thus, the use of pointer addresses should instead be replaced by the use of absolute addresses, i.e. displacements relative to the start address MPI_BOTTOM.

- Variables belong to the same sequential storage if they belong to the same array, to the same COMMON block in Fortran, or to the same structure in C. Beware of unions! Look up the rules in the standard!
Creating & destroying datatypes

- **MPI_Type_commit(MPI_Datatype *datatype)**
  - You can now go ahead and use the datatype in any communication operation that makes sense.
  - A datatype may specify overlapping entries. The use of such a datatype in a receive operation is erroneous. (This is erroneous even if the actual message received is short enough not to write any entry more than once.)

- **MPI_Type_free(MPI_Datatype *datatype)**
  - Freeing a datatype does not affect any other datatype that was built from the freed datatype. The system behaves as if input datatype arguments to derived datatype constructors are passed by value. Any communication operations using this datatype that are still pending will complete fine.
Creating equivalent types

- Create types:
  - CALL MPI_TYPE_CONTIGUOUS( 2, MPI_REAL, type2, ...)
  - CALL MPI_TYPE_CONTIGUOUS( 4, MPI_REAL, type4, ...)
  - CALL MPI_TYPE_CONTIGUOUS( 2, type2, type22, ...)

- With proper care, any of the above can be used to accomplish the same end. Which is to be used is a matter of programming clarity and performance. While in principle complex types composed of complex types should not be slower, implementations may not really manage the indirection well.
Matching sends & receives

- Sends:
  - CALL MPI_SEND( a, 4, MPI_REAL, ...)
  - CALL MPI_SEND( a, 2, type2, ...)
  - CALL MPI_SEND( a, 1, type22, ...)
  - CALL MPI_SEND( a, 1, type4, ...)

- Receives:
  - CALL MPI_RECV( a, 4, MPI_REAL, ...)
  - CALL MPI_RECV( a, 2, type2, ...)
  - CALL MPI_RECV( a, 1, type22, ...)
  - CALL MPI_RECV( a, 1, type4, ...)

- Each of the sends matches any of the receives.
Counting

- MPI_Get_elements(MPI_Status *status, MPI_Datatype datatype, int *count)
- MPI_Get_count(MPI_Status *status, MPI_Datatype datatype, int *count)
- Define a derived datatype

CALL MPI_TYPE_CONTIGUOUS(2, MPI_REAL, Type2, ierr)
CALL MPI_TYPE_COMMIT(Type2, ierr)

- One processors sends consecutively:

CALL MPI_SEND(a, 2, MPI_REAL, 1, 0, comm, ierr)
CALL MPI_SEND(a, 3, MPI_REAL, 1, 0, comm, ierr)
Counting example

- The other process receives

```fortran
CALL MPI_RECV(a, 2, Type2, 0, 0, comm, stat, ierr)
CALL MPI_GET_COUNT(stat, Type2, i, ierr)  !i=1
CALL MPI_GET_ELEMENTS(stat, Type2, i, ierr) !i=2
CALL MPI_RECV(a, 2, Type2, 0, 0, comm, stat, ierr)
CALL MPI_GET_COUNT(stat, Type2, i, ierr)  ! returns i=MPI_UNDEFINED
CALL MPI_GET_ELEMENTS(stat, Type2, i, ierr) !i=3
```

Parallel Programming for Multicore Machines Using OpenMP and MPI
Datatyping array sections

REAL a(100,100,100), e(9,9,9) ! e=a(1:17:2, 3:11, 2:10)

CALL MPI_TYPE_VECTOR( 9, 1, 2, MPI_REAL, oneslice, ierr)

CALL MPI_TYPE_HVECTOR(9, 1, 100*sizeofreal, oneslice, twoslice, ierr)

CALL MPI_TYPE_HVECTOR( 9, 1, 100*100*sizeofreal, twoslice, 1, threeslice, ierr)

CALL MPI_TYPE_COMMIT( threeslice, ierr)

CALL MPI_SENDRECV(a(1,3,2), 1, threeslice, myrank, 0, e, 9*9*9, MPI_REAL, myrank, 0, MPI_COMM_WORLD, status, ierr)
Groups, Contexts, Communicators

- **Group**: An ordered set of processes, each associated with a rank (within a continuous range). Part of a communicator.
  - Predefined: MPI_GROUP_EMPTY, MPI_GROUP_NULL

- **Context**: A property of a communicator that partitions the communication space. Not externally visible.
  - Contexts allow Pt2Pt and collective calls not to interfere with each other; same with calls belonging to different communicators.

- **Communicator**: Group+Context+cached info
  - Predefined: MPI_COMM_WORLD, MPI_COMM_SELF
  - Intra- and Inter-communicators
Group Constructors

- MPI_Comm_group(MPI_Comm comm, MPI_Group *group)
- MPI_Group_union(MPI_Group group1, MPI_Group group2, MPI_Group *newgroup)
- MPI_Group_intersection(MPI_Group group1, MPI_Group group2, MPI_Group *newgroup)
- MPI_Group_difference(MPI_Group group1, MPI_Group group2, MPI_Group *newgroup)
- MPI_Group_incl(MPI_Group group, int n, int *ranks, MPI_Group *newgroup)
- MPI_Group_excl(MPI_Group group, int n, int *ranks, MPI_Group *newgroup)
- MPI_Group_range_incl(MPI_Group group, int n, int ranges[][3], MPI_Group *newgroup)
- MPI_Group_range_excl(MPI_Group group, int n, int ranges[][3], MPI_Group *newgroup)
More group functions

- `MPI_Group_free(MPI_Group *group)`
- `MPI_Group_size(MPI_Group group, int *size)`
- `MPI_Group_rank(MPI_Group group, int *rank)`
- `MPI_Group_translate_ranks (MPI_Group group1, int n, int *ranks1, MPI_Group group2, int *ranks2)`
- `MPI_Group_compare(MPI_Group group1, MPI_Group group2, int *result)`

- `MPI_IDENT` results if the group members and group order is exactly the same in both groups. This happens for instance if `group1` and `group2` are the same handle. `MPI_SIMILAR` results if the group members are the same but the order is different. `MPI_UNEQUAL` results otherwise.
Communicator Functions

- MPI_Comm_dup(MPI_Comm comm, MPI_Comm *newcomm)
- MPI_Comm_create(MPI_Comm comm, MPI_Group group, MPI_Comm *newcomm)
- MPI_Comm_split(MPI_Comm comm, int color, int key, MPI_Comm *newcomm)
- MPI_Comm_compare(MPI_Comm comm1, MPI_Comm comm2, int *result)
- MPI_Comm_free(MPI_Comm *comm)
- And the MPI_Comm_size, MPI_Comm_rank we have already met.
Inter-Communicators

- So far all communications have been between processes belonging to the same communicator.

- MPI allows for communications between different communicators.
  - They can only be Pt2Pt and not collective
  - They require the generation of inter-communicator objects.
  - For more look at the material on the Web and the standard.
Virtual Topologies

- Employing the information cached in communicators we can map an (intra-)communicator's processes to an underlying topology (cartesian or graph) that better reflects the communication requirements of our algorithm.

- This has possible performance advantages: The process to hardware mapping could be thus more optimal. In practice this is rare.

- The notational power of this approach however allows code to be far more readable and maintainable.
A cartesian topology

Ranks and Cartesian process coordinates

Figure by MIT OpenCourseWare.

Parallel Programming for Multicore Machines Using OpenMP and MPI
Cartesian topology calls

- `MPI_Cart_create(MPI_Comm comm_old, int ndims, int *dims, int *periods, int reorder, MPI_Comm *comm_cart)`
  - Extra processes get MPI_COMM_NULL for `comm_cart`
- `MPI_Dims_create(int nnodes, int ndims, int *dims)`
  - If `ndims(k)` is set, this is a constraint
- For graphs, `MPI_Graph_create()`, same rules
- `MPI_Topo_test(MPI_Comm comm, int *status)`
  - Returns MPI_CART, MPI_GRAPH, MPI_UNDEFINED
- `MPI_Cartdim_get, MPI_Cart_get` etc. for cartesian topologies
- `MPI_Graphdim_get, MPI_Graph_get` etc. for graphs
Ranks in cartesian communicators

- Ranks and Cartesian process coordinates in `comm_cart`

- Ranks in `comm` and `comm_cart` may differ, if `recorder = 1` or `.TRUE.`.
- This reordering can allow MPI to optimize communications

Figure by MIT OpenCourseWare.
Cartesian rank/coordinate functions

- **MPI_Cart_rank(MPI_Comm comm, int *coords, int *rank);** out of range values get shifted (periodic topos)

- **MPI_Cart_coords(MPI_Comm comm, int rank, int maxdims, int *coords)**
Cartesian shift

- `MPI_Cart_shift(MPI_Comm comm, int direction, int disp, int *rank_source, int *rank_dest)`

- `MPI_PROC_NULL` for shifts at non-periodic boundaries

---

Parallel Programming for Multicore Machines Using OpenMP and MPI
Cartesian subspaces

- Rank and Cartesian process coordinates in `comm_sub`

- `MPI_Cart_sub(comm_cart, remain_dims, comm_sub, ierror)`

Figure by MIT OpenCourseWare.

Parallel Programming for Multicore Machines Using OpenMP and MPI
More functions

- `MPI_Graph_neighbors_count(MPI_Comm comm, int rank, int *nneighbors)`
- `MPI_Graph_neighbors(MPI_Comm comm, int rank, int maxneighbors, int *neighbors)`
- Used in that order to get the neighbors of a process in a graph.
Fortran binding issues

call MPI_GET_ADDRESS(buf,bufaddr,ierror) ditto...
call MPI_TYPE_CREATE_STRUCT(1,1,bufaddr,MPI_REAL,type,ierror) ditto...
call MPI_TYPE_COMMIT(type,ierror) ditto...
val_old = buf register = buf

val_old = register

call MPI_RECV(MPI_BOTTOM,1,type,...) ditto...
val_new = buf val_new = register

call MPI_IRECV(buf,..req) call MPI_IRECV(buf,..req) call MPI_IRECV(buf,..req) register = buf b1 = buf

call MPI_WAIT(req,..) call MPI_WAIT(req,..) call MPI_WAIT(req,..) b1 = buf b1 = register
Further Fortran issues

Basic vs. Extended Fortran Support
Strong typing in F90 a problem with choice args
A scalar should not be passed instead of a vector.
Extra work to code with KIND numerical types
MPI_IRecv(buf(a:b:c), ...)
Fortran derived datatypes require MPI equivalents
Problems with input arguments that are copied...
e.g. MPI_Recv with a buffer that was passed to the parent subroutine as a section or an assumed shape array argument that is associated with such a section.
The MPI runtime

- Provides for process placement, execution & handling
- Handles signals (SIGKILL, SIGSUSP, SIGUSR1/2)
- Usually collects stdout and stderr, may propagate stdin
- May propagate environment variables
- May provide support for debugging, profiling, tracing
- May interface with a queuing system for better process placement
- MPI-2 specifies *(but doesn't require)* standardized mpirun clone: mpiexec. Others: poe, mpprun, prun...
- Command line arguments and/or environment variables allow for different behavior/performance
MPI environment

- Initialize, Finalize and Abort functionality
- Error (exception) handling
- Other inquiry functions:
  - double MPI_Wtime(void), double MPI_Wtick(void)
  - MPI_WTIME_IS_GLOBAL
  - MPI_Get_processor_name(char *name, int *resultlen)
- MPI communicator inquiry (size, rank) for MPI_COMM_WORLD
Exceptions

- Use exceptions and MPI return codes!
- Default error handler: MPI_ERRORS_ARE_FATAL
  - The handler, when called, causes the program to abort on all executing processes. This has the same effect as if MPI_ABORT was called by the process that invoked the handler.
- Alternative: MPI_ERRORS_RETURN
  - The handler has no effect other than returning the error code to the user. Put checks for the error codes in your source!
- MPICH provides two more:
  - MPE_Errors_call_dbx_in_xterm, MPE_Signals_call_debugger
Error Handling

- Environment Error handling routines:
  - MPI_Errhandler_create(MPI_Handler_function *function, MPI_Errhandler *errhandler)
  - MPI_Errhandler_set(MPI_Comm comm, MPI_Errhandler errhandler)
  - MPI_Errhandler_get(MPI_Comm comm, MPI_Errhandler *errhandler)
  - MPI_Errhandler_free(MPI_Errhandler *errhandler)
  - MPI_Error_string(int errorcode, char *string, int *resultlen)
  - MPI_Error_class(int errorcode, int *errorclass)
The MPI Profiling Interface

- The MPI standard takes great pains to offer a specification for a useful profiling interface that does have minimum overhead and high flexibility.

- All MPI calls have a shifted name of PMPI_... instead of MPI_...

- A profiling library can write its own MPI_... call, calling the corresponding PMPI_... call to actually do the message passing.

- This provides a way to trace as well as profile in terms of cost in time a parallel program's execution for performance or debugging reasons.
MPI Profiling & Performance Tools

- An extremely wide choice of tools:

  - Research codes:
    - AIMS (NASA Ames)
    - (sv)Pablo (UIUC)
    - Paradyn/Dyninst (University of Wisconsin)
    - TAU (University of Oregon)
    - XMPI (Indiana University)
    - MPE/Jumpshot (ANL)
    - Paragraph/MPICL
    - FPMPI
    - Also lightweight statistics tools: mpiP, ipm

  - Commercial tools (VT, speedshop, Intel Trace A/C, VAMPIR)
XMPI

- Works with LAM/MPI, could work with other implementations.
- A GUI for launching MPI parallel programs, monitoring them in real time and also do post-mortem analysis on them.
- Uses the slower "daemon" mode of LAM, provides individual message detail and has multiple views. The daemon mode allows cmdline tracing tools mpimsg and mpitask to be more informative.
- Very easy to use but non-daemon mode is required for performance tuning. Launch with `-ton` and collect tracefile with `lamtrace`.
XMPI in action

Green: Represents the length of time a process runs outside of MPI.

Red: Represents the length of time a process is blocked, waiting for communication to finish before the process resumes execution.

Yellow: Represents a process's overhead time inside MPI (for example, time spent doing message packing).
MPE (from MPICH/MPICH2)

- Set of utility routines, including graphics
- Graphical viewing of traces with (n)upshot, jumpshot
- Compile with -mpe=mpitrace to enable basic tracing
  - A message printed to stdout at every entry and exit
- Compile with -mpe=mpilog to enable logging
  - ALOG, CLOG, CLOG2, UTE, SLOG and SLOG2 format
  - Converters between formats (eg. Clog2slog2)
- SLOG2 is the newest and most scalable
- Jumpshot-4 is needed for looking at SLOG2 files
Jumpshot

Event Count vs Time

Time: 17.50243

Connectivity Options
- Disconnected States
- Connected States

View Options
- MPI-Process
- Thread
- Processor

Frame Information
- Number of Frames = 3
- Current Frame = 2

Frame Operations
- Previous
- Display
- Next
More Jumpshot

The diagram shows a file statistics viewer with various types of operations and their associated durations. The operations include:

- Running
- User_Marker_Interval
- MPI_Finalize
- MPI_Comm_size
- MPI_Comm_rank
- MPI_Allreduce
- MPI_Wait
- MPI_Isend
- MPI_Irecv

The horizontal axis represents time in seconds, ranging from 0 to 150.
Parallel Programming for Multicore Machines Using OpenMP and MPI