## 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**

•MPI\_Reduce\_scatter(void \*sendbuf, void \*recvbuff, int \*revcnt, MPI\_Datatype type, MPI\_Op op, MPI\_Comm comm)

•MPI\_REDUCE\_SCATTER(sendbuf, recvbuf, recvcnt, type, op, comm, ier)

•Can be considered as a

MPI\_Reduce(sendbuf, tmpbuf, cnt, type, op, root, comm);

MPI\_Scatterv(tmpbuf, recvcnt, displs, type, recvbuff, recvcnt[myid], type, root, comm);

where cnt is the total sum of the recvcnt values and displs[k] is the sum of the recvcnt for up to processor k-1.

•Implementations may use a more optimal approach

### How it would work for matvec



Figure by MIT OpenCourseWare.

### **3DFFT**



Figure by MIT OpenCourseWare.

### Alternative decomposition



Figure by MIT OpenCourseWare.

### 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.

basic datatype 0	displacement of datatype 0
basic datatype 1	displacement of datatype 1
basic datatype n-1	displacement of datatype n-1

Figure by MIT OpenCourseWare.

### A derived datatype



Figure by MIT OpenCourseWare.

### 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



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.



Figure by MIT OpenCourseWare.

### 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. <u>Strides</u> (displacements) can be negative.



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



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\_blocklenghts=[3,5], array\_of\_types=[MPI\_INT,MPI\_DOUBLE]
- What about array\_of\_displacements ? [0,addr1-addr0]

oldtypes MPI_INT MPI_DOUBLE						
addr_0	addr_1					
newtype						
block 0 holes, if <u>double</u> needs an block 1 8 byte alignment						
in_buf_datatype						
out huf datature						
out_out_adadype       out_i_val						

Figure by MIT OpenCourseWare.

## • 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 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, ie. 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.

# • 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 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 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



Figure by MIT OpenCourseWare.

### 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



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)



Figure by MIT OpenCourseWare.

### 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



Figure by MIT OpenCourseWare.

### Cartesian subspaces



Figure by MIT OpenCourseWare.

### 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) d					
call MPI_TYPE_CREATE_STRUCT(1,1, bufaddr,MPI_REAL,type,ierror) dit					
call MPI_TYPE_COMMIT(type,ierror) d					
val_old = buf					
		val_old = register			
call MPI_RECV(MPI_BOTTOM,1,type,) ditte					
val_new = buf		val_new = register			
call MPI_IRECV(buf,req) MPI_IRECV(buf,req)	call MPI_IRECV(buf,req)	call			
	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 has minimum overhead and high flexibility.
- All MPI calls have a shifted name of PMPI\_... instead of MPI\_...
- A profiling library can write it's 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)
    - <u>MPE/Jumpshot (ANL)</u>
    - 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.
- <u>Uses the slower "daemon" mode</u> 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



### 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



### More Jumpshot



Paralle

### Even more Jumpshot



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