Presentation

Introduction

MPI

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October 20, 2005

http://www.chpc.utah.edu
Overview

• **Quick introduction** (in case you slept/missed last time)
• MPI concepts, initialization.
• Point-to-point communication.
• Collective communication.
• Grouping data for communication.
• **Quick glance at advanced topics.**
Distributed memory

- Process has access only to its local memory
- Data between processes must be communicated
- More complex programming
- Cheap commodity hardware
- CHPC: Linux clusters (Arches, Icebox), Sierra

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MPI Basics

- Standardized message-passing library
  - uniform API
  - guaranteed behavior
  - source code portability
- Complex set of operations
  - various point-to-point communication
  - collective communication
  - process groups
  - processor topologies
  - software library development functions
Example 1

```fortran
program hello
integer i, n, ierr, my_rank, nodes
include "mpif.h"

call MPI_Init(ierr)
call MPI_Comm_size(MPI_COMM_WORLD,nproc,ierr)
call MPI_Comm_rank(MPI_COMM_WORLD,my_rank,ierr)
if (my_rank .eq. 0) then
  do i=1,nproc-1
    call MPI_Recv(n,1,MPI_INTEGER,i,0,MPI_COMM_WORLD,
&      status,ierr)
    print*, 'Hello from process', n
  enddo
else
  call MPI_Send(my_rank,1,MPI_INTEGER,0,0,MPI_COMM_WORLD,ierr)
endif
call MPI_Finalize(ierr)
return
```

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Program output

da1:~> %
    /uufs/delicatearch.arches/sys/bin/mpif77 ex1.f -o ex1

da1:~> % qsub -I -l nodes=2:ppn=2,walltime=1:00:00

da001:~> %
    /uufs/delicatearch.arches/sys/bin/mpirun.ch_gm
        -np 4 -machinefile $PBS_NODEFILE ex1

Hello from process  1
Hello from process  2
Hello from process  3
• must be included in subroutines and functions that use MPI calls
• provide required declarations and definitions
• Fortran – mpif.h
  ▪ declarations of MPI-defined datatypes
  ▪ error codes
• C – mpi.h
  ▪ also function prototypes
Basic MPI functions

- **Initializing MPI:**
  - MPI_Init(ierr)
  - int MPI_Init(int *argc, char **argv)

- **Terminating MPI**
  - MPI_Finalize(ierr)
  - int MPI_Finalize()

- **Determine no. of processes**
  - MPI_Comm_Size(comm, size, ierr)
  - int MPI_Comm_Size(MPI_comm comm, int* size)

- **Determine rank of the process**
  - MPI_Comm_Rank(comm, rank, ierr)
  - int MPI_Comm_Rank(MPI_comm comm, int* rank)
Basic point-to-point communication

• **Sending data**
  - MPI_Send(buf, count, datatype, dest, tag, comm, ierr)
  - int MPI_Send(void *buf, int count, MPI_Datatype, int dest, int tag, MPI_comm comm)
    call MPI_Send(my_rank,1,MPI_INTEGER,0,0,MPI_COMM_WORLD,ierr)

• **Receiving data**
  - MPI_Recv(buf, count, datatype, source, tag, comm, status, ierr)
  - int MPI_Recv(void *buf, int count, MPI_Datatype, int source, int tag,
    MPI_comm comm, MPI_Status status)
    call MPI_Recv(n,1,MPI_INTEGER,i,0,MPI_COMM_WORLD,status,ierr)
Message send/recv

- Data (buffer, count)
- Sender / Recipient
- Message envelope
  - data type – see next two slides
  - tag – integer to differentiate messages
  - communicator – group of processes that take place in the communication
    default group communicator – MPI_COMM_WORLD
### Predefined data structures

<table>
<thead>
<tr>
<th>MPI Datatype</th>
<th>Fortran Datatype</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPI_BYTE</td>
<td></td>
</tr>
<tr>
<td>MPI_CHARACTER</td>
<td>CHARACTER</td>
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<tr>
<td>MPI_COMPLEX</td>
<td>COMPLEX</td>
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<tr>
<td>MPI_DOUBLE_PRECISION</td>
<td>DOUBLE PRECISION</td>
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<tr>
<td>MPI_REAL</td>
<td>REAL</td>
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<tr>
<td>MPI_INTEGER</td>
<td>INTEGER</td>
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<tr>
<td>MPI_LOGICAL</td>
<td>LOGICAL</td>
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<tr>
<td>MPI_PACKED</td>
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<tr>
<td>MPI Datatype</td>
<td>C Datatype</td>
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<td>--------------</td>
<td>------------</td>
</tr>
<tr>
<td>MPI_BYTE</td>
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<tr>
<td>MPI_CHAR</td>
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<tr>
<td>MPI_FLOAT</td>
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<tr>
<td>MPI_INT</td>
<td>int</td>
</tr>
<tr>
<td>MPI_LONG</td>
<td>long</td>
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<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>MPI_PACKED</td>
<td></td>
</tr>
</tbody>
</table>
Communication modes

• Four different
  ▪ standard: completion is system-dependent
  ▪ synchronous: send is not completed until the corresponding receive has started
  ▪ ready: send can be initiated only if the corresponding receive has been posted
  ▪ buffered: local, copies message into buffer and then sends it out

• NOTE: standard operations may not be buffered

• Contents of the send buffer can be safely modified after return from the send call
Nonblocking communication

- Initiates point-to-point operation and returns
  - overlap communication with computation
  - receive requires 2 function calls – initiate the communication, and finish it
  - all four communication modes available
  - usually completed at the point when the communicated data are to be used
  - consume system resources, which must be released (MPI_Wait, MPI_Test)
Example 2 – numerical integration

\[
\int_{a}^{b} f(x) \approx \sum_{i=1}^{n} \frac{1}{2} h [f(x_{i-1}) + f(x_{i})] = \frac{1}{2} h[f(x_{0}) + f(x_{n})] + \sum_{i=1}^{n-1} h[f(x_{i})]
\]
1. Initialize MPI
2. Get interval and no. of trapezoids
3. Broadcast input to all processes
4. Each process calculates its interval
5. Collect the results from all the processes

- Two new concepts:
  - collective communication – involves more processes
  - derived data types – more efficient data transfer
#include <stdio.h>
#include "mpi.h"

int main (int argc, char* argv[]){
    int p, my_rank, n , i , local_n;
    float a, b, h, x, integ, local_a, local_b, total;
    MPI_Datatype mesg_ptr;
    float f(float x);
    void Build_der_data_t(float *a,float *b,int *n,MPI_Datatype *mesg_ptr);

1.  MPI_Init(&argc,&argv);
2.  MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
3.  MPI_Comm_size(MPI_COMM_WORLD,&p);
    if (my_rank == 0) {
        printf("Input integ. interval, no. of trap:\n");
        scanf("%f %f %d",&a,&b,&n);
    }
    Build_der_data_t(&a,&b,&n, &mesg_ptr);
    MPI_Bcast(&a,1,mesg_ptr,0,MPI_COMM_WORLD);
4. \[ h = \frac{(b-a)}{n}; \quad \text{local}_n = \frac{n}{p}; \]
\[ \text{local}_a = a + \text{my}_\text{rank} \times h \times \text{local}_n; \]
\[ \text{local}_b = \text{local}_a + h \times \text{local}_n; \]
\[ \text{integ} = \frac{(f(\text{local}_a)+f(\text{local}_b))}{2.}; \]
\[ x = \text{local}_a; \]
\[ \text{for} \ (i=1;i<\text{local}_n;i++) \{ \]
\[ \quad x = x+h; \]
\[ \quad \text{integ} = \text{integ} + f(x); \}
\[ \text{integ} = \text{integ} \times h; \]
\[ \text{printf}(\text{"Trapezoids n = %d, local integral from ",local}_n); \]
\[ \text{printf}(\text{"%f to %f is %f\n"},\text{local}_a,\text{local}_b,\text{integ}); \]
\[ \text{total} = 0.; \]
\[ \text{MPI\_Reduce}(&\text{integ},&\text{total},1,\text{MPI\_FLOAT},\text{MPI\_SUM},0,\text{MPI\_COMM\_WORLD}); \]
\[ \text{if} \ (\text{my}_\text{rank} == 0) \]
\[ \quad \text{printf}(\text{"Total integral = %f\n"},\text{total}); \]
\[ \text{MPI\_Finalize}(); \]
\[ \text{return} \ 0; \} \]
Program output

da1:~>%/uufs/delicatearch.arches/sys//bin/mpicc trapp.c
    -o trapp
da001:~>%/uufs/delicatearch.arches/sys/bin/mpirun.ch_gm
    -np 4 -machinefile $PBS_NODEFILE trapp
Input integ. interval, no. of trap:
0 10 100
Trapezoids n = 25, local integral from 0.000000 to
    2.500000 is 5.212501
Total integral = 333.350098
Trapezoids n = 25, local integral from 2.500000 to
    5.000000 is 36.462475
Trapezoids n = 25, local integral from 5.000000 to
    7.500000 is 98.962471
Trapezoids n = 25, local integral from 7.500000 to
    10.000000 is 192.712646
Collective communication

- **Broadcast** – from one node to the rest
  - MPI_Bcast(buf, count, datatype, root, comm, ierr)
  - int MPI_Bcast(void *buf, int count, MPI_Datatype datatype, int root, MPI_comm comm)

  On root, buf is data to be broadcast, on other nodes it's data to be received

- **Reduction** – collect data from all nodes
  - MPI_Reduce(sndbuf, rcvbuf, count, datatype, op, root, comm, ierr)
  - int MPI_Reduce(void *sndbuf, void *recvbuf, int count, MPI_Datatype datatype, MPI_Op op, int root, MPI_comm comm)

  `MPI_Reduce(&integ,&total,1,MPI_FLOAT,MPI_SUM,0,MPI_COMM_WORLD);`

  Supported operations, e.g. MPI_MAX, MPI_MIN, MPI_SUM,...
  Result stored in rcvbuf only on processor with rank root.
More collective communication

• Communication operations that involve more than one process
  ▪ broadcast from one process to all the others in the group
  ▪ reduction collect data from all the processes in certain manner (sum, max,...)
  ▪ barrier synchronization for all processes of the group
  ▪ gather from all group processes to one process
  ▪ scatter distribute data from one process to all the others
  ▪ all-to-all gather/scatter/reduce across the group

• NOTE: There is no implicit barrier before collective communication operations
Derived data types

- Used to group data for communication
- Built from basic MPI data types
- Must specify:
  - number of data variables in the derived type and their length (1,1,1)
  - type list of these variables (MPI_DOUBLE, MPI_DOUBLE, MPI_INT)
  - displacement of each data variable in bytes from the beginning of the message (0,24,56)
void Build_der_data_t(float *a, float *b, 
                    int *n, MPI_Datatype *msg_ptr) {

  int blk_len[3] = {1, 1, 1};
  MPI_Aint displ[3], start_addr, addr;
  MPI_Datatype typel[3] = {MPI_FLOAT, MPI_FLOAT, MPI_INT};

  displ[0] = 0;
  MPI_Address(a, &start_addr);
  MPI_Address(b, &addr);
  displ[1] = addr - start_addr;
  MPI_Address(n, &addr);
  displ[2] = addr - start_addr;

  MPI_Type_struct(3, blk_len, displ, typel, msg_ptr);
  MPI_Type_commit(msg_ptr);
}
Derived data types

• **Address displacement**
  - `MPI_Address(location, address)`
  - `int MPI_Address(void *location, MPI_Aint *address)`

• **Derived data type create**
  - `MPI_Type_Struct(count, bl_len, displ, typelist, new_mpi_t)`
  - `int MPI_Type_Struct(int count, int bl_len[], MPI_Aint displ[], MPI_Datatype typelist[], MPI_Datatype *new_mpi_t)`

  ```c
  MPI_Type_struct(3, blk_len, displ, typel, mesg_ptr);
  ```

• **Derived data type commit**
  - `MPI_Type_Commit(new_mpi_t)`
  - `int MPI_Type_Commit(MPI_Datatype *new_mpi_t)`
Derived data types

- Simpler d.d.t. constructors
  - MPI_Type_contiguous
    = contiguous entries in an array
  - MPI_Type_vector
    = equally spaced entries in an array
  - MPI_Type_indexed
    = arbitrary entries in an array
void Exch_data(float *a, float *b, int *n, int my_rank) {
    char buffer[100];
    int position = 0;

    if (my_rank == 0) {
        MPI_Pack(a, 1, MPI_FLOAT, buffer, 100, &position, MPI_COMM_WORLD);
        MPI_Pack(b, 1, MPI_FLOAT, buffer, 100, &position, MPI_COMM_WORLD);
        MPI_Pack(n, 1, MPI_INT, buffer, 100, &position, MPI_COMM_WORLD);
        MPI_Bcast(buffer, 100, MPI_PACKED, 0, MPI_COMM_WORLD);
    } else {
        MPI_Bcast(buffer, 100, MPI_PACKED, 0, MPI_COMM_WORLD);
        MPI_Unpack(buffer, 100, &position, a, 1, MPI_FLOAT, MPI_COMM_WORLD);
        MPI_Unpack(buffer, 100, &position, b, 1, MPI_FLOAT, MPI_COMM_WORLD);
        MPI_Unpack(buffer, 100, &position, n, 1, MPI_INT, MPI_COMM_WORLD);
    }
}
**MPI_Pack/Unpack**

- **Explicit storing of noncontiguous data for communication**
- **Pack – before send**
  - $\text{MPI\_Pack}(\text{pack\_data}, \text{in\_cnt}, \text{datatype}, \text{buf}, \text{buf\_size}, \text{position}, \text{comm}, \text{ierr})$
  - int $\text{MPI\_Pack}(\text{void *pack\_data}, \text{int in\_cnt}, \text{MPI\_Datatype datatype}, \text{void *buf}, \text{int buf\_size}$,$\text{int *position}, \text{MPI\_comm comm})$

  $\text{MPI\_Pack}(\text{a}, \text{1}, \text{MPI\_FLOAT}, \text{buffer}, \text{100}, &\text{position}, \text{MPI\_COMM\_WORLD});$

- **Unpack – after receive**
  - $\text{MPI\_Unpack}(\text{buf}, \text{size}, \text{position}, \text{unpack\_data}, \text{cnt}, \text{datatype}, \text{comm}, \text{ierr})$
  - int $\text{MPI\_Unpack}(\text{void *buf}, \text{int size}, \text{int *position}, \text{void *unpack\_data}, \text{int cnt}, \text{MPI\_Datatype datatype}, \text{MPI\_comm comm})$

- **position gets updated after every call to MPI_Pack/Unpack**

  $\text{MPI\_Unpack}(\text{buffer, 100, &position, a, 1, MPI\_FLOAT, MPI\_COMM\_WORLD});$

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Which communication method to use

• count and datatype
  ▪ sending contiguous array or a scalar

• MPI_Pack/Unpack
  ▪ sending heterogeneous data only once
  ▪ variable length messages (sparse matrices)

• Derived data types
  ▪ everything else, including:
    ▪ repeated send of large heterogeneous data
    ▪ sending of large strided arrays
Advanced topics

- Advanced point-to-point communication
- Specialized collective communication
- Process groups, communicators
- Virtual processor topologies
- Error handling
- MPI I/O (MPI-2)
- Dynamic processes (MPI-2)
Summary

• Basics
• Point-to-point communication
• Collective communication
• Grouping data for communication

http://www.chpc.utah.edu/short_courses/intro_mpi
References

• MPI
  http://www-unix.mcs.anl.gov/mpi/
  Pacheco - Parallel Programming with MPI
  Gropp, Lusk, Skjellum – Using MPI 1, 2

• CHPC
  http://www.chpc.utah.edu/index.php?currentNumber=3.2.200
Security Policies

- No clear text passwords use ssh and scp
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- Don’t leave your terminal unattended while logged into your account
- Do not introduce classified or sensitive work onto CHPC systems
- Use a good password and protect it
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- Do not distribute or copy privileged data or software
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- Please see http://www.chpc.utah.edu/docs/policies/security.html for more details
Future Presentations

• Debugging with Totalview
• Profiling with Vampir
• Mathematical Libraries at the CHPC
• MPI-IO
• Introduction to OpenMP
• Hybrid MPI/OpenMP programming
• Intermediate MPI (if interested)?