Introduction

MPI

Presentation

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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 cluster (Arches)
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

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
Program output

```
da001:~> %
  /uufs/delicatearch.arches/sys/bin/mpif77 ex1.f -o ex1

da001:~> %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
```
MPI header files

- 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>
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<tr>
<td>MPI_CHARACTER</td>
<td>CHARACTER</td>
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<tr>
<td>MPI_COMPLEX</td>
<td>COMPLEX</td>
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<td>MPI_DOUBLE_PRECISION</td>
<td>DOUBLE PRECISION</td>
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<td>MPI_REAL</td>
<td>REAL</td>
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<tr>
<td>MPI_INTEGER</td>
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<tr>
<td>MPI_LOGICAL</td>
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<td>MPI_PACKED</td>
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<tr>
<td>MPI Datatype</td>
<td>C Datatype</td>
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<tr>
<td>MPI_BYTE</td>
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<td>MPI_CHAR</td>
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<td>MPI_LONG</td>
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<td>...</td>
<td>...</td>
</tr>
<tr>
<td>MPI_PACKED</td>
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</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

\[
\int_a^b f(x) \approx \sum_{i=1}^{n} \frac{1}{2} h \left[ f(x_{i-1}) + f(x_i) \right] = \\
\frac{1}{2} h [f(x_0) + f(x_n)] + \sum_{i=1}^{n-1} h [f(x_i)]
\]
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
Program core - code

```
#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);
   }
3. Build_der_data_t(&a,&b,&n, &mesg_ptr);
   MPI_Bcast(&a,1,mesg_ptr,0,MPI_COMM_WORLD);
```
4. h = (b-a)/n; local_n = n/p;
local_a = a + my_rank*h*local_n;
local_b = local_a + h*local_n;

integ = (f(local_a)+f(local_b))/2.;
x = local_a;
for (i=1;i<local_n;i++){
    x = x+h;
    integ = integ+ f(x);
}
integ = integ*h;
printf("Trapezoids n = %d, local integral from ",local_n);
printf("%f to %f is %f\n",local_a,local_b,integ);
total = 0.;

5. MPI_Reduce(&integ,&total,1,MPI_FLOAT,MPI_SUM,0,MPI_COMM_WORLD);
if (my_rank == 0)
    printf("Total integral = %f\n",total);
MPI_Finalize();
return 0;

da001:~>%/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.**
• 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)

\[
\begin{align*}
&\text{a} \quad \text{some data} \quad \text{b} \quad \text{some data} \quad \text{n} \\
\text{MPI\_DOUBLE} & \quad \text{MPI\_DOUBLE} & \quad \text{MPI\_INT}
\end{align*}
\]
void Build_der_data_t(float *a, float *b,
                      int *n, MPI_Datatype *mesg_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, mesg_ptr);
    MPI_Type_commit(mesg_ptr);
}
Derived data types

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

- **Derived date 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 date 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
  - MPI_Pack(pack_data, in_cnt, datatype, buf, buf_size, position, comm, ierr)
  - int MPI_Pack(void *pack_data, int in_cnt, MPI_Datatype datatype, void *buf, int buf_size,
     int *position, MPI_comm comm)
  - MPI_Pack(a,1,MPI_FLOAT,buffer,100,&position,MPI_COMM_WORLD);
- Unpack – after receive
  - MPI_Unpack(buf, size, position, unpack_data, cnt, datatype, comm, ierr)
  - int MPI_Unpack(void *buf, int size, int *position,
     void *unpack_data, int cnt, MPI_Datatype datatype, MPI_comm comm)
  - MPI_Unpack(buffer,100,&position,a,1,MPI_FLOAT,MPI_COMM_WORLD);
- position gets updated after every call to MPI_Pack/Unpack
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
- You may not share your account under any circumstances
- 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
• Report suspicions to CHPC (security@chpc.utah.edu)
• 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)?