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Center for High-Performance Computing

Introduction to MPI

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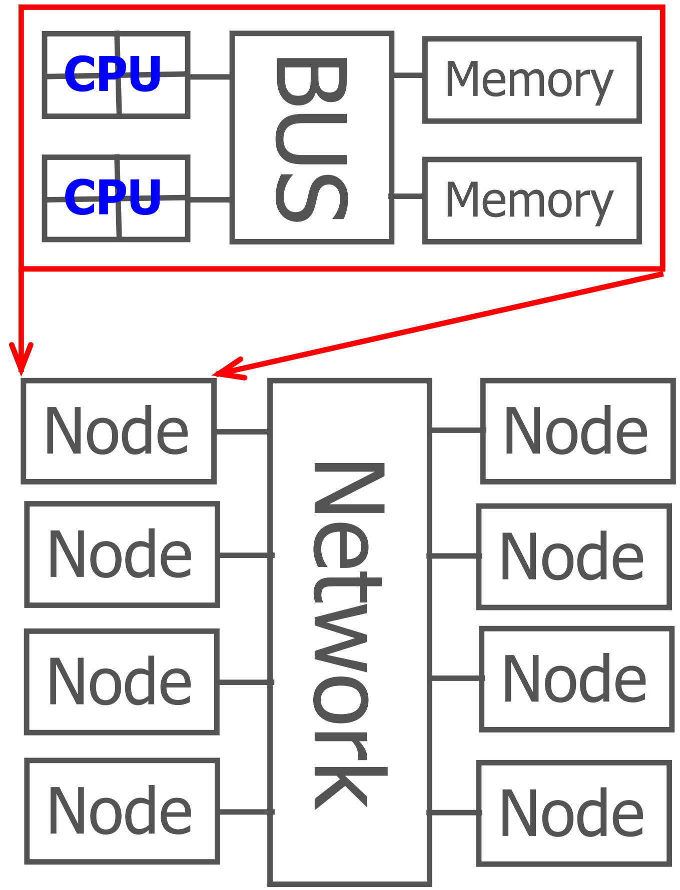
Overview

- 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.
- Survey

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



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
  - one sided communication (RMA)
  - parallel I/O

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

```
notchpeak1:~>%module load mpich
notchpeak1:~>%mpif77 ex1.f -o ex1
notchpeak1:~>%salloc -n 4 -N 1 -A notchpeak-shared-
  short -p notchpeak-shared-short -t 1:00:00
notch081:~%>mpirun -np $SLURM_NTASKS 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

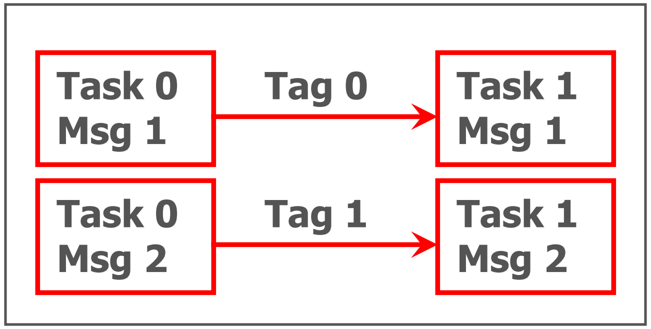
- Sending data
  - `MPI_Send(buf, count, datatype, dest, tag, comm, ierr)`
  - `int MPI_Send(void *buf, int count, MPI_Datatype, int dest, int tag, MPI_comm comm)`

```
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

MPI Datatype	Fortran Datatype
MPI_BYTE	
MPI_CHARACTER	CHARACTER
MPI_COMPLEX	COMPLEX
MPI_DOUBLE_PRECISION	DOUBLE PRECISION
MPI_REAL	REAL
MPI_INTEGER	INTEGER
MPI_LOGICAL	LOGICAL
MPI_PACKED	

Predefined data structures

MPI Datatype	C Datatype
MPI_BYTE	
MPI_CHAR	char
MPI_DOUBLE	double
MPI_FLOAT	float
MPI_INT	int
MPI_LONG	long
…	…
MPI_PACKED	

Non-blocking communication

- Initiates operation and returns
  - overlap communication with computation
  - receive requires 2 function calls – initiate the communication, and finish it
  - prepend function name with I and use request handle at the end of message

```
call MPI_Irecv(n,1,MPI_INTEGER,i,0,MPI_COMM_WORLD,status,req,ierr)
```

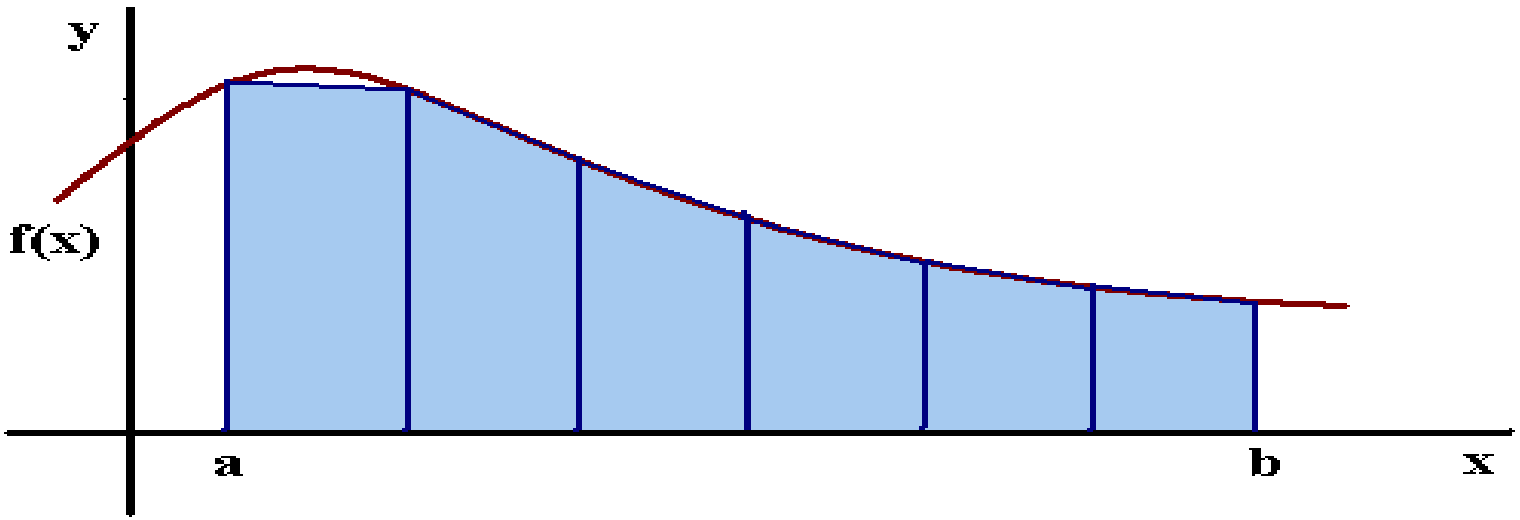
  - usually completed at the point when the communicated data are to be used
  - consume system resources, which must be released (MPI_Wait, MPI_Test)

```
call MPI_Wait(req,status, ierr)
```

Example 2 numerical integration

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

$$\frac{1}{2} h\left[f(x_0) + f(x_n)\right] + \sum_{i=1}^{n-1} h\left[f(x_i)\right]$$



Program core

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

- New concepts:
  - collective communication – involves more processes
  - explicit work distribution
  - 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);
    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);
```

Program core - code

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;}
```

Program output

```
notch081:~>% mpicc trapp.c -o trapp
notch081:~>% mpirun -np 4 ./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,…

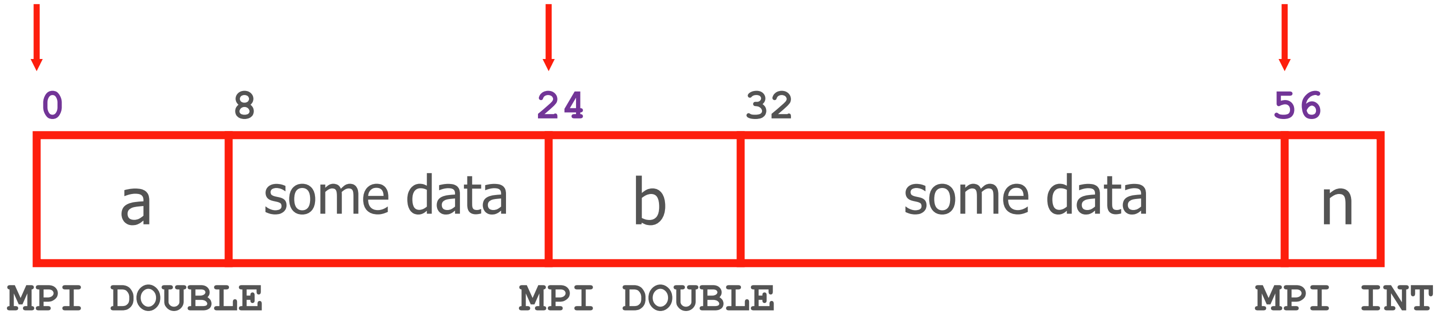
Result stored in `rcvbuf` only on processor with rank `root`.

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, but there is a barrier after

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)



Derived data types

```
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_Get_address(a,&start_addr);
MPI_Get_address(b,&addr);
displ[1] = addr - start_addr;
MPI_Get_address(n,&addr);
displ[2] = addr - start_addr;

MPI_Type_create_struct(3,blk_len,displ,typel,mesg_ptr);
MPI_Type_commit(mesg_ptr);
}
```

Derived data types

- Address displacement
  - `MPI_Get_address(location, address)`
  - `int MPI_Get_address(void *location, MPI_Aint *address)`
- Derived date type create
  - `MPI_Type_create_struct(count, bl_len, displ, typelist, new_mpi_t)`
  - `int MPI_Type_create_struct(int count, int bl_len[], MPI_Aint displ[], MPI_Datatype typelist[], MPI_Datatype *new_mpi_t)`

```
MPI_Type_create_struct(3,blk_len,displ,typel,mesg_ptr);
```

- Derived date type commit/free
  - `MPI_Type_commit(new_mpi_t)`
  - `int MPI_Type_commit(MPI_Datatype *new_mpi_t)`
  - `MPI_Type_free(new_mpi_t)`
  - `int MPI_Type_free(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

User-controlled data packing

```
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)`
- `position` gets updated after every call to `MPI_Pack/Unpack`

```
MPI_Unpack(buffer,100,&position,a,1,MPI_FLOAT,MPI_COMM_WORLD);
```

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
- Dynamic processes
- One sided communication

Collective non-blocking communication example

Distributed matrix-vector multiply, vecout[M]=A[M][M]*vecin[M]

```
double _Complex out1[FNxy], out2[FNxy], *commbuf, *compbuf;

for (iis=0; iis <= FNlocs; iis++) {
  if (iis%2==1) commbuf=out2; else commbuf=out1;
  xind = iis*FNxy;
  MPI_Iallgatherv(&(vecin[xind]), FNxy, MPI_DOUBLE_COMPLEX, commbuf, counts,
stride, MPI_DOUBLE_COMPLEX, MPI_COMM_WORLD,&allg_handle);

  if (iis%2==0) compbuf=out2; else compbuf=out1;
  if (iis>0) {
  for (iir=0;iir<FNloc;iir++) {
    iy = iir*FNxy;
    for (ip=0;ip<numprocs;ip++) {
      ia = iy + ipoffA[ip] * Fnxy*FNloc;
      for (ix=0;ix<FNxy;ix++)
        vecout[iy+ix] += A[(ia+ix)] * compbuf[ipoffV[ip]+ix];
    }
  MPI_Wait(&allg_handle,&allg_status);
  }}
```

2 communication buffers + comm and comp pointers

swap comm. buffer

Gather vecin into commbuf

swap comp. buffer

vector offset

matrix offset

use current compbuf (part of vector vecin) in M-V product

To learn more

- MPI spec and text book
  - https://www.mpi-forum.org/
  - Pacheco – Introduction to Parallel Programming
- XSEDE HPC Summer Boot Camp
  - OpenMP, OpenACC, MPI
  - https://www.youtube.com/XSEDETraining
- XSEDE online training
  - https://www.xsede.org/web/xup/online-training

Summary

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

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

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

Security Policies

- Do not try to break passwords, tamper with files etc.
- Do not distribute or copy privileged data or software
- Report suspicians to CHPC (security@chpc.utah.edu)
- Please see http://www.chpc.utah.edu/docs/policies/security.html for more details

Future Presentations

- MPI-IO
- Introduction to OpenMP
- Hybrid MPI/OpenMP programming
- Debugging
- Profiling
- Mathematical Libraries at the CHPC