Message Passing Interface (MPI) Programming

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MPI: Standard parallel programming language





Preparation

Minimal knowledge required for the hands-on projects in this course:

• Able to log in & use the Discovery computing cluster at USC Center for Advanced Research Computing (CARC) at the level of its "getting started" tutorial:

https://carc.usc.edu/user-information/user-guides/hpc-basics/getting-started-discovery

• Use shell commands to interact with the operating system at the level of "Chapter 1—Introduction to the Command Line" of Effective Computation in Physics by Scopatz and Huff; USC students have free access to the book through Safari Online: https://libraries.usc.edu/databases/safari-books

Contents

Overview

Logging in to the login node

Organizing files

Transferring files

Creating and editing files

Installing and running software

Jobs

Getting help

Chapter 1. Introduction to the Command Line

The command line, or *shell*, provides a powerful, transparent interface between the user and the internals of a computer. At least on a Linux or Unix computer, the command line provides total access to the files and processes defining the state of the computer—including the files and processes of the operating system.

How to Use USC CARC Cluster

Use text editor like vim, nano, emacs

System: Intel/AMD-based computing cluster

https://carc.usc.edu

Log in

> ssh anakano@discovery.usc.edu

Alternatively, you can use discovery2.usc.edu

To use MPI library:

If using Bash shell, add these in .bashrc

module purge
module load usc

To set up standard software environment

shells ls cut kemel grep date sort

Shell is a language you speak with the operating system

Type echo \$0 to find which shell you are using

Compile an MPI program

> mpicc -o mpi_simple mpi_simple.c

Execute an MPI program

> mpirun -n 2 mpi_simple

To find absolute path to mpicc command

[anakano@discovery ~]\$ which mpicc

 $/spack/apps/linux-centos 7-x86_64/gcc-8.3.0/openmpi-4.0.2-ipm3dnvlbtxawpi4ifz7jma6jgr7mexq/bin/mpicc-2.0.2-ipm3dnvlbtyawpi4ifz7jma6jgr7mexq/bin/mpicc-2.0.2-ipm3dnvlbtyawpi4ify7mexq/bin/mpicc-2.0.2-ipm3dnvlbtyawpi4ify7mexq/bin/mpicc-2.0.2-ipm3dnvlbtyawpi4ify7mexq/bin/mpic-2.0-ipm3dnvlbtyawpi4ify7mexq/bin/mpic-2.0-ipm3dnvlbtyawpi4ify7mexq/bin/mpic-2.0-ipm3dnvlbtyawpi4ify7mexq/b$

[anakano@discovery ~]\$ more /proc/cpuinfo

To find processor information

Email <u>carc-support@usc.edu</u> for assistance

Submit a Slurm Batch Job

Prepare a script file, mpi_simple.sl

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=2
#SBATCH --time=00:00:10
#SBATCH --output=mpi_simple.out
#SBATCH -A anakano_429
mpirun -n $SLURM_NTASKS ./mpi_simple
```

Slurm (Simple Linux Utility for Resource Management): Open-source job scheduler that allocates compute resources on clusters for queued jobs

Submit a Slurm job

Class project account; type myaccount to check all accounts

discovery: sbatch mpi simple.sl

Submitted batch job 63695

Check the status of a Slurm job

discovery: squeue -u anakano

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
63695 main mpi simple anakano PD 0:00 1 (Resources)

Cancel a Slurm job

discovery: scancel 63695

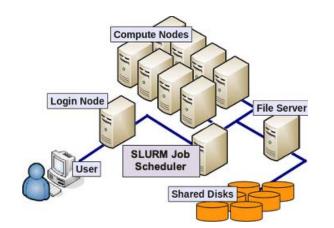
Check the output

discovery: more mpi_simple.out

n = 777

For detailed explanation, see the lecture note

https://aiichironakano.github.io/cs596/02MPI.pdf



Interactive Job at CARC

When debugging your MPI program, you may want to access computing nodes interactively, so that you can edit, compile & run MPI program in real time unlike the batch job

Reserve 2 processors for 20 minutes

Back to the login node

Type less /proc/cpuinfo to find what kind of node you got

Symbolic Link to Work Directory

- Your home directory has very small quota (type myquota to confirm), so please use the scratch file system (/scratch/anakano for user anakano) instead
- It is convenient to make a symbolic link to a directory you use often, rather than typing its long absolute path every time

```
symbolic link
                                                          alias
                                         source
[anakano@discovery ~]$ ln -s /scratch/anakano/cs596 cs596
[anakano@discovery ~]$ ls -lt
                                               This directory has been created as
                                                  mkdir /scratch/anakano/cs596
total 2
lrwxrwx--- 1 anakano anakano 22 Aug 23 12:14 cs596 -> /scratch/anakano/cs596
drwxrwx--- 3 anakano anakano 1 Aug 20 10:07 FFTW
lrwxrwx--- 1 anakano anakano 16 Aug 14 15:48 scr -> /scratch/anakano
[anakano@discovery ~]$ cd cs596 ~
[anakano@discovery cs596]$ pwd -P
                                          Instead of typing
/scratch/anakano/cs596
                                           cd /scratch/anakano/cs596
```

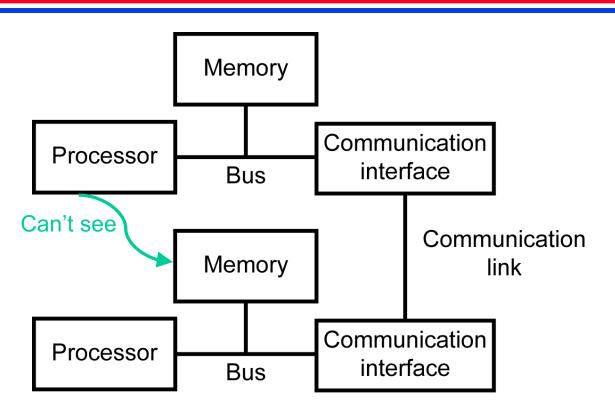
Print physical working directory

File Transfer

• Use secure file transfer protocol to transfer files between your laptop and Discovery

 To transfer files from remote computer to local computer, use get instead

Parallel Computing Hardware

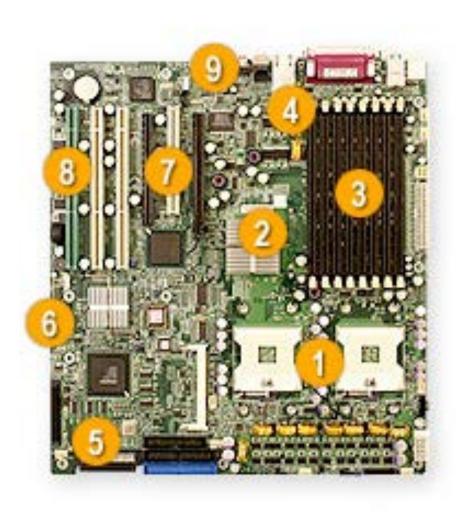






- **Processor**: Executes arithmetic & logic operations.
- Memory: Stores program & data.
- Communication interface: Performs signal conversion & synchronization between communication link and a computer.
- Communication link: A wire capable of carrying a sequence of bits as electrical (or optical) signals.

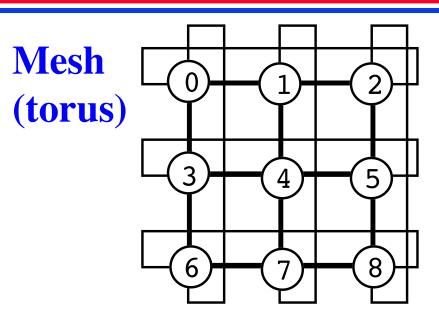
Motherboard



Key Features

- Dual Intel® Xeon™ EM64T Support up to 3.60 GHz
- Intel® E7525 (Tumwater) Chipset
- Up to 16GB DDRII-400 SDRAM
- Intel® 82546GB Dual-port Gigabit Ethernet Controller
- Adaptec AIC-7902 Dual Channel Ultra320 SCSI
- 2x SATA Ports via ICH5R SATA Controller
- 7. 1 (x16) & 1 (x4) PCI-Express, 1 x 64-bit 133MHz PCI-X, 2 x 64-bit 100MHz PCI-X, 1 x 32-bit 33MHz PCI Slots
- Zero Channel RAID Support
- AC'97 Audio, 6-Channel Sound

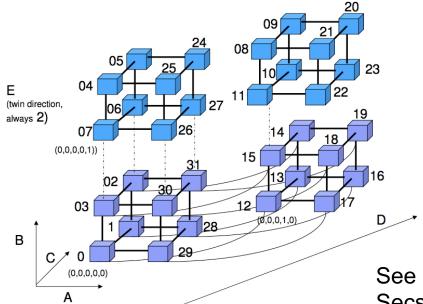
Communication Network





NEC Earth Simulator (640x640 crossbar)

IBM Blue Gene/Q (5D torus)



Crossbar_[
switch

See Grama, Secs. 2.4.2-2.4.4

Message Passing Interface

MPI (Message Passing Interface)

A standard message passing system that enables us to write & run applications on parallel computers

Download for Unix & Windows:

```
http://www.mcs.anl.gov/mpi/mpich
```

Compile

```
> mpicc -o mpi_simple mpi_simple.c
```

Run

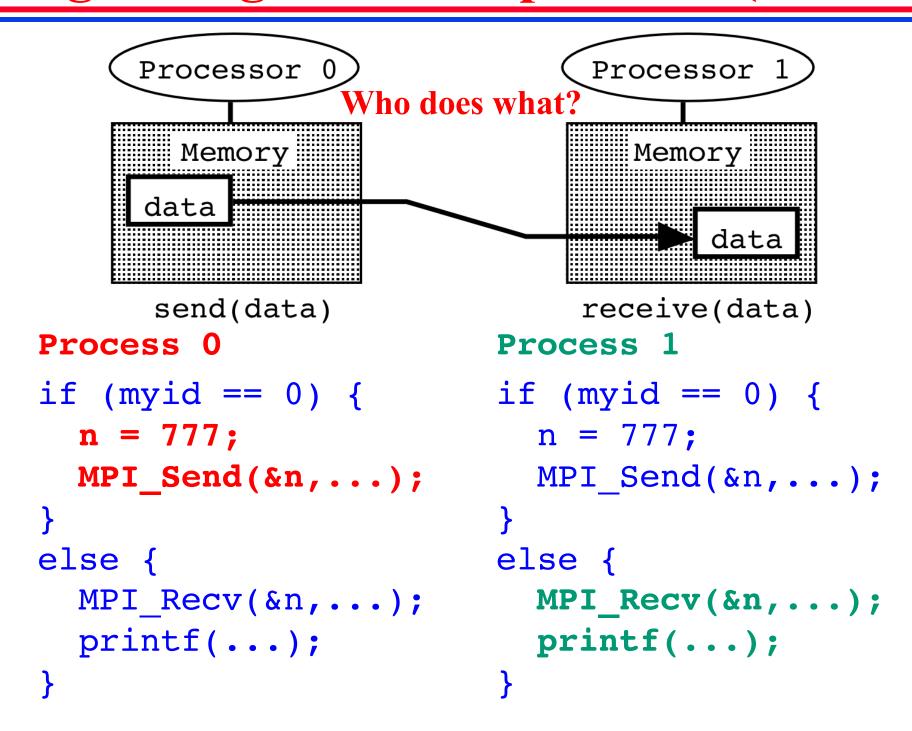
```
> mpirun -np 2 mpi_simple
```

MPI Programming

mpi_simple.c: Point-to-point message send & receive

```
#include "mpi.h"
#include <stdio.h>
int main(int argc, char *argv[]) {
  MPI Status status;
  int myid;
                                          MPI rank
  int n;
  MPI Init(&argc, &argv);
  MPI Comm rank(MPI COMM WORLD, &myid);
  if (myid == 0) {
                                         Matching message labels
    n = 777;
    MPI_Send(&n, 1, MPI_INT, 1, 10, MPI_COMM WORLD);
  }
                                  To/from whom
                Data triplet
  else {
    MPI Recv(&n, 1, MPI INT, 0, 10, MPI COMM WORLD, &status);
    printf("n = %d\n", n);
                                          MPI daemon
  MPI Finalize();
                                                           recv
                                  send
                                            requests)
 return 0;
                                                          from 0
                                   to 1
}
```

Single Program Multiple Data (SPMD)



Single Program Multiple Data (SPMD)

What really happens?

node 1 node 2

start executing line-by-line independently

node 3

mpi_simple

rank0

node 4

mpi_simple

rank1

sbatch allocates backend nodes

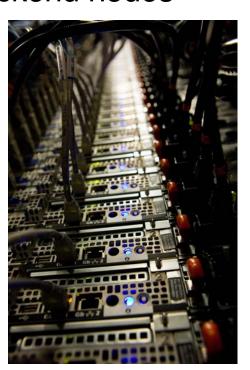
discovery

%mpirun -n 2 mpi_simple



%ssh discovery.usc.edu
My laptop





MPI Minimal Essentials

```
We only need MPI_Send() & MPI_Recv() within MPI_COMM_WORLD
```

```
MPI_Send(&n, 1, MPI_INT, 1, 10, MPI_COMM_WORLD);
MPI_Recv(&n, 1, MPI_INT, 0, 10, MPI_COMM_WORLD, &status);

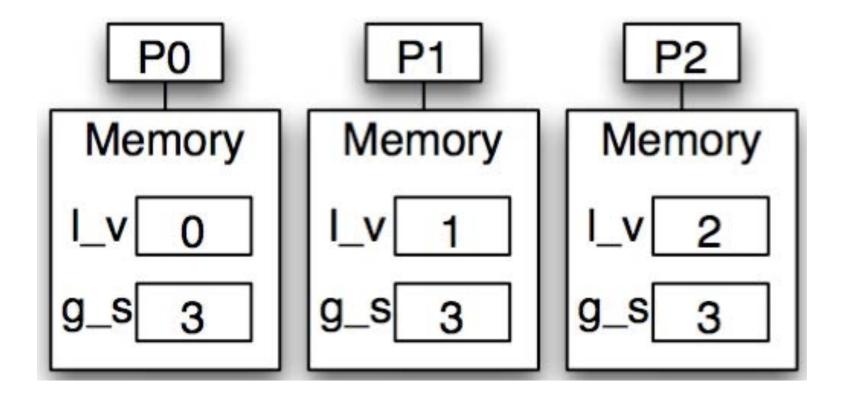
Data triplet To/from whom Information
```

Global Operation

All-to-all reduction: Each process contributes a partial value to obtain the global summation. In the end, all the processes will receive the calculated global sum.

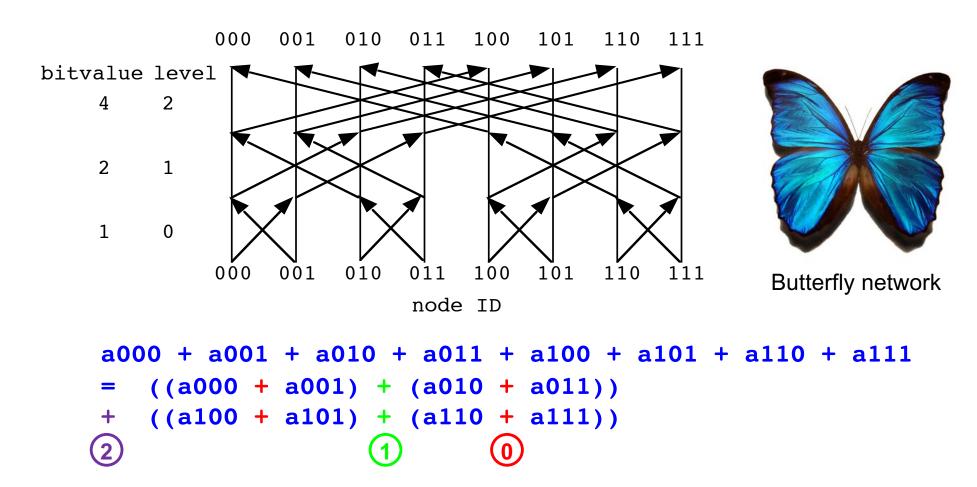
```
MPI_Allreduce(&local_value, &global_sum, 1, MPI_INT, MPI_SUM, MPI_COMM_WORLD)
```

```
int l_v, g_s; // local variable & global sum
l_v = myid; // myid is my MPI rank
MPI_Allreduce(&l_v, &g_s, 1, MPI_INT, MPI_SUM, MPI_COMM_WORLD);
```



Hypercube Algorithm

Hypercube algorithm: Communication of a reduction operation is structured as a series of pairwise exchanges, one with each neighbor in a hypercube (**butterfly**) structure. Allows a computation requiring all-to-all communication among p processes to be performed in log_2p steps.



Barrier

```
<A>;
                    barrier();
                     <B>;
       Process 0
                    Process 1
                             Process 2
                                            Process 3
                   barrier();
time
                               barrier();
       barrier();
                                            barrier();
```

MPI_Barrier(MPI_Comm communicator)

Useful for debugging (but would slow down the program)

MPI Communication

MPI communication functions:

1. Point-to-point

```
MPI_Send()
MPI_Recv()
```

2. Global

```
MPI_Allreduce()
MPI_Barrier()
MPI_Bcast()
```

Hypercube Template

```
procedure hypercube(myid, input, log<sub>2</sub>P, output)
begin
                                               001 010 011 100 101 110
  mydone := input;
                                 bitvalue level
                                        2
  for l := 0 to log_2P-1 do
  begin
                                    2
                                        1
     partner := myid XOR 2^{1};
     send mydone to partner;
                                           000
                                               001
                                                   010
                                                       011
                                                          100
                                                               101
     receive hisdone from partner;
                                                       node ID
     mydone = mydone OP hisdone
                                       level 21 bitvalue
  end
  output := mydone
                                               001
end
                                              010
                                            2 100
                     Associative operator
   Exclusive OR
                     (e.g., sum, max)
                                        (a 	ext{ OP } b) 	ext{ OP } c = a 	ext{ OP } (b 	ext{ OP } c)
   b a XOR b
                     abcdefg XOR 0000100 = abcdefg
         b
                    In C, ^ (caret operator) is bitwise XOR applied to int
```

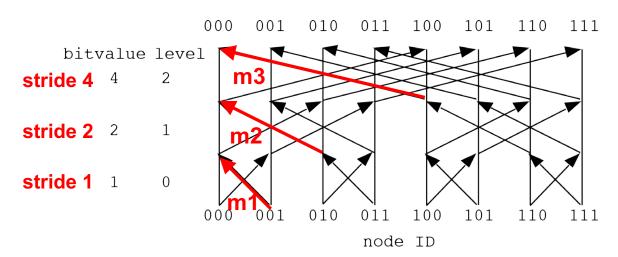
Driver for Hypercube Test

```
#include "mpi.h"
#include <stdio.h>
int nprocs; /* Number of processes */
int myid; /* My rank */
double global sum(double partial) {
  /* Implement your own global summation here */
}
int main(int argc, char *argv[]) {
  double partial, sum, avg;
  MPI Init(&argc, &argv);
 MPI Comm rank (MPI COMM WORLD, &myid); Who am I?
 MPI Comm size(MPI COMM WORLD, &nprocs); How big is the world? (see
  partial = (double) myid;
                                     p. 5 in lecture note)
  printf("Rank %d has %le\n", myid, partial);
  sum = global sum(partial);
  if (myid == 0) {
    avg = sum/nprocs;
    printf("Global average = %d\n", avg);
 MPI Finalize();
 return 0;
```

C Implementation of global_sum()

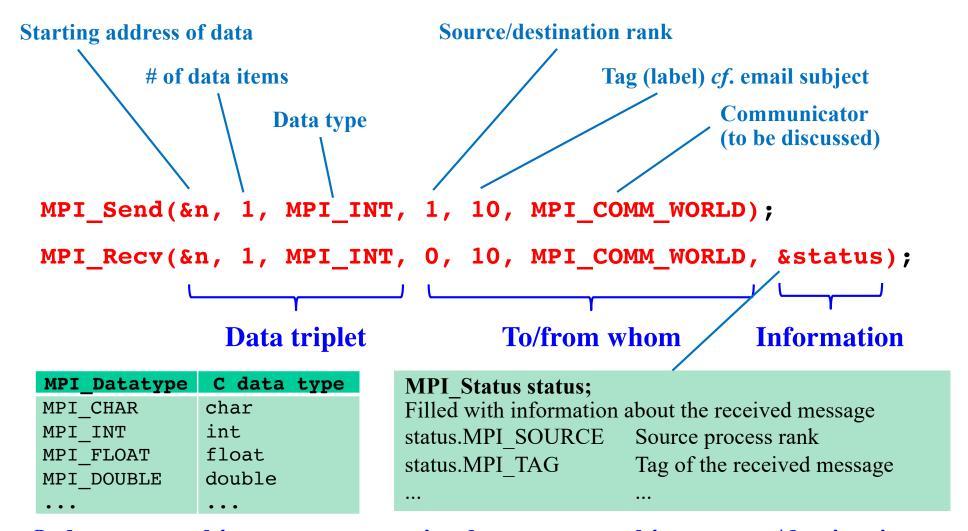
```
mydone = partial;
for (bitvalue=1; bitvalue<nprocs; bitvalue*=2)</pre>
{
   partner = myid ^ bitvalue;
                                                      <u>1</u> 2<sup>1</sup>
                                                 level
                                                                 bitvalue
   send mydone to partner;
   receive hisdone from partner;
                                                         001
   mydone = mydone + hisdone
                                                          010
}
                                                           100
return mydone;
                                  Implement with MPI Send() & MPI Recv()
```

Use bitvalue as counter & bitmask



It is recommended to use distinct labels (tags) for different messages, e.g. (bitmask = stride) as a tag

MPI Send & Receive Revisited



- Only tag-matching message passing between matching source/destination pair of ranks take place
- It is recommended to use distinct tags for different messages to avoid accidental receipt of unintended messages

Sample Slurm Script

Run two MPI runs in a single Slurm job

Total number of processors = ntasks-per-node (4) × nodes (2) = 8

• Type sbatch global_avg.sl in the directory where the executable global_avg resides, or cd (change directory) to where it is

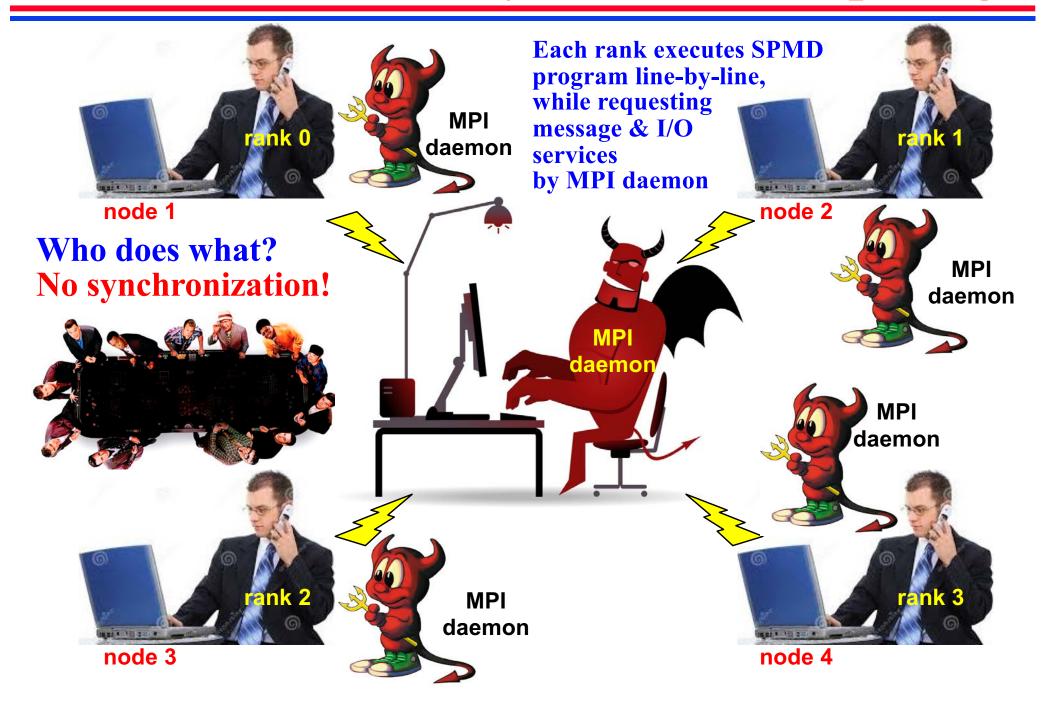
Output of global.c

```
• 4-processor job
 Rank 0 has 0.000000e+00
 Rank 1 has 1.000000e+00
 Rank 2 has 2.000000e+00
 Rank 3 has 3.000000e+00
 Global average = 1.500000e+00
• 8-processor job
 Rank 0 has 0.000000e+00
 Rank 1 has 1.000000e+00
 Rank 2 has 2.000000e+00
                              Actual output
 Rank 3 has 3.000000e+00
                              is random
                              order in ranks
 Rank 5 has 5.000000e+00
                              — Why?
 Rank 6 has 6.000000e+00
 Rank 4 has 4.000000e+00
 Rank 7 has 7.000000e+00
 Global average = 3.500000e+00
```

References on Hypercube Algorithms

- 1. https://en.wikipedia.org/wiki/Hypercube (communication pattern)
- 2. I. Foster, *Designing and Building Parallel Programs* (Addison-Wesley, 1995) Chap. 11 Hypercube algorithms: https://www.mcs.anl.gov/~itf/dbpp/text/node123.html

Distributed-Memory Parallel Computing



Communicator

mpi_comm.c: Communicator = process group + context

For detail, see p. 4 in https://aiichironakano.github.io/cs596/02MPI.pdf

```
#include "mpi.h"
                                            Usage
#include <stdio.h>

    Avoid accidental match of

#define N 64
                                              unintended Send-Receive pairs
int main(int argc, char *argv[]) {
  MPI Comm world, workers;
                                              Global operations in a subgroup
  MPI Group world group, worker group;
                                              of processes
  int myid, nprocs;
  int server, n = -1, ranks[1];
  MPI Init(&argc, &argv);
  world = MPI COMM WORLD;
  MPI Comm rank(world, &myid);
  MPI Comm size(world, &nprocs);
  server = nprocs-1;
  MPI Comm group(world, &world group);
  ranks[0] = server;
  MPI Group excl(world group, 1, ranks, &worker group);
  MPI Comm create(world, worker group, &workers);
  MPI Group free(&worker group);
  if (myid != server)
    MPI Allreduce(&myid, &n, 1, MPI INT, MPI SUM, workers);
  printf("process %2d: n = %6d n", myid, n);
  MPI Comm free(&workers);
  MPI Finalize();
                    Code at <a href="https://aiichironakano.github.io/cs596/src/mpi/">https://aiichironakano.github.io/cs596/src/mpi/</a>
  return 0;
```

Example: Ranks in Different Groups

1 1		/Region	Rank	Total Score	Score on Alumni _
(12)	Harvard University		1	100	100
2 5	Stanford University		2	72.1	41.8
3 1	Massachusetts Institute of Technology (MIT)		3	70.5	68.4
4	University of California-Berkeley		4	70.1	66.8
5 (University of Cambridge	>K	1	69.2	79.1
51	University of Southern California		33	31	31.7

Rank is relative in each communicator!

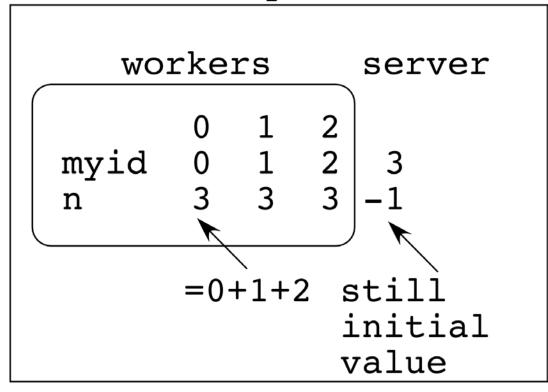
Output from mpi_comm.c

#SBATCH --nodes=2

world: nprocs = 4

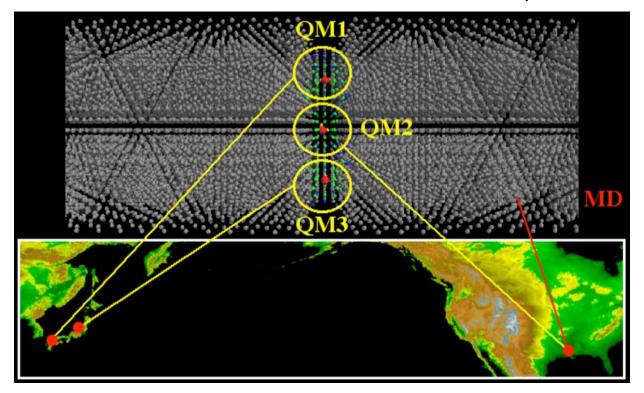
What Has Happened?

process 2: n =



Grid Computing & Communicators

H. Kikuchi *et al.*, "Collaborative simulation Grid: multiscale quantum-mechanical/classical atomistic simulations on distributed PC clusters in the US & Japan, *IEEE/ACM SC02*

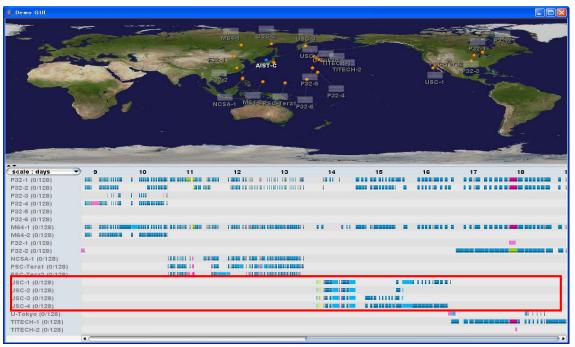


Communicator = a nice migration path to distributed computing

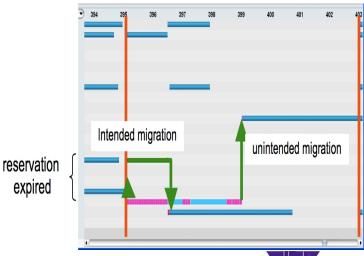
- Single MPI program run with the Grid-enabled MPI implementation, MPICH-G2
- Processes are grouped into MD & QM groups by defining multiple MPI communicators as subsets of MPI_COMM_WORLD; a machine file assigns globally distributed processors to the MPI processes

Global Grid QM/MD

• One of the largest (153,600 cpu-hrs) sustained Grid supercomputing at 6 sites in the US (USC, Pittsburgh, Illinois) & Japan (AIST, U Tokyo, Tokyo IT)



Automated resource migration & fault recovery



USC

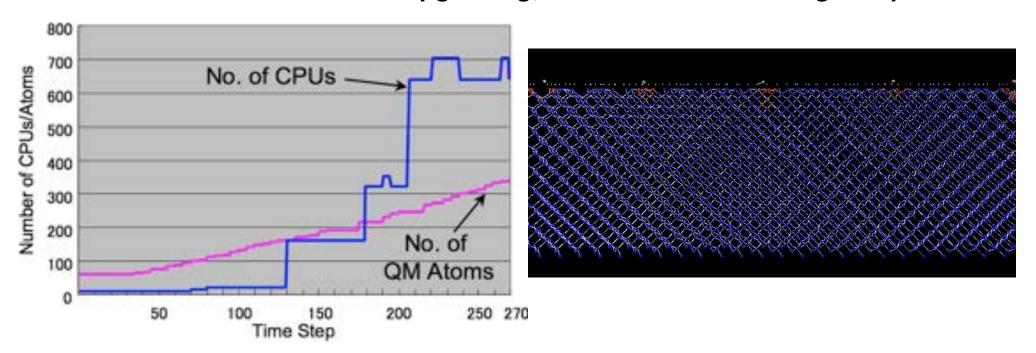


Takemiya et al., "Sustainable adaptive Grid supercomputing: multiscale simulation of semiconductor processing across the Pacific," IEEE/ACM SC06

Sustainable Grid Supercomputing

- Sustained (> months) supercomputing (> 10³ CPUs) on a Grid of geographically distributed supercomputers
- Hybrid Grid remote procedure call (GridRPC) + message passing (MPI) programming
- Dynamic allocation of computing resources on demand & automated migration due to reservation schedule & faults

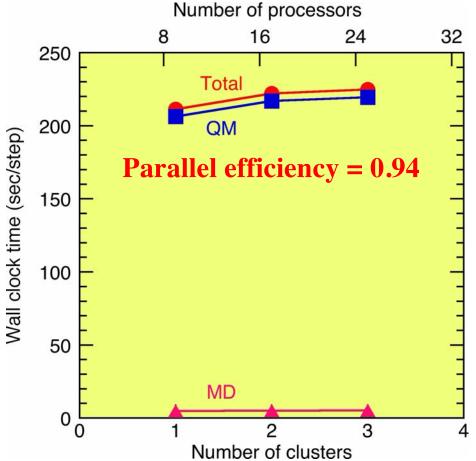
Ninf-G GridRPC: ninf.apgrid.org; MPICH: www.mcs.anl.gov/mpi



Multiscale QM/MD simulation of high-energy beam oxidation of Si

Computation-Communication Overlap

H. Kikuchi *et al.*, "Collaborative simulation Grid: multiscale quantum-mechanical/classical atomistic simulations on distributed PC clusters in the US & Japan, *IEEE/ACM SC02*





 $\frac{\text{Earth's circumference}}{\text{Light speed}}$ $= \frac{40,000 \text{ [km]} = 4 \times 10^7 \text{ [m]}}{3 \times 10^8 \text{ [m]}} = 0.1 \text{ s} = 100 \text{ ms}$

Try on Discovery: traceroute www.u-tokyo.ac.jp

vs. ping hpc-transfer.usc.edu

- How to overcome 200 ms latency & 1 Mbps bandwidth?
- Computation-communication overlap: To hide the latency, the communications between the MD & QM processors have been overlapped with the computations using asynchronous messages

Synchronous Message Passing

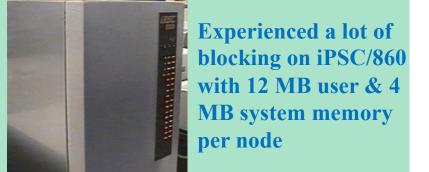
MPI_Send(): (blocking), synchronous

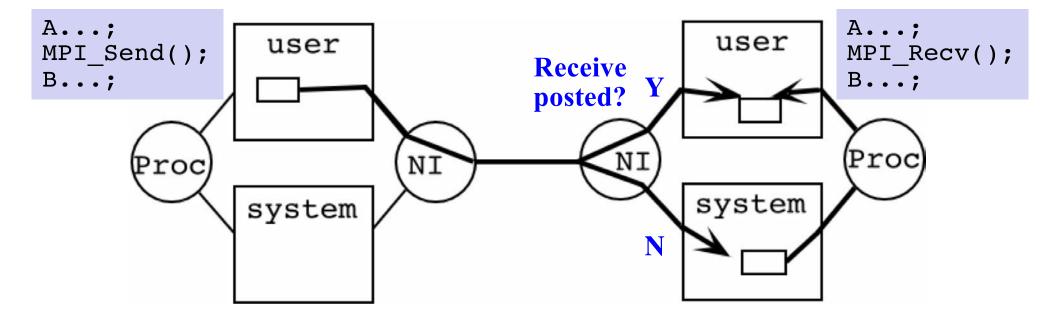
- Safe to modify original data immediately on return
- Depending on implementation, it may return whether or not a matching receive has been posted, or it may block (especially if

no buffer space available)

MPI_Recv(): blocking, synchronous

- Blocks for message to arrive
- Safe to use data on return





Asynchronous Message Passing

Allows computation-communication overlap

MPI_Isend(): non-blocking, asynchronous

- Returns immediately whether or not a matching receive has been posted
- Not safe to modify original data immediately (use MPI_Wait() system call)

MPI_Irecv(): non-blocking, asynchronous

- Does not block for message to arrive
- Cannot use data before checking for completion with

MPI_Wait()

```
A...;
MPI_Isend();
B...;
MPI_Wait();
C...; // Reuse the send buffer
```

MPI_Irecv() is just a "request" for data delivery, when a matching message arrives

```
A...;
MPI_Irecv();
B...;
MPI_Wait();
C...; // Use the received message
```

Program irecv_mpi.c

```
#include "mpi.h"
#include <stdio.h>
#define N 1000
int main(int argc, char *argv[]) {
  MPI Status status;
 MPI Request request;
                                                  Wrap-around/torus
  int send buf[N], recv buf[N];
                                                via modulo (%) operator
  int send sum = 0, recv sum = 0;
                                            (cf. periodic boundary condition)
  long myid, left, Nnode, msg id, i;
 MPI Init(&argc, &argv);
                                              myid
                                                      myid
                                                              myid
                                                                       myid
 MPI Comm rank(MPI COMM WORLD, &myid);
                                              =0
                                                       =1
                                                               =2
                                                                        =3
  MPI Comm size(MPI COMM WORLD, &Nnode);
  left = (myid + Nnode - 1) % Nnode;
  for (i=0; i<N; i++) send buf[i] = myid*N + i;
  MPI Irecv(recv buf, N, MPI INT, MPI ANY SOURCE, 777, MPI COMM WORLD,
            &request); /* Post a receive */
  /* Perform tasks that don't use recv buf */
  MPI Send(send buf, N, MPI INT, left, 777, MPI COMM WORLD);
  for (i=0; i<N; i++) send sum += send buf[i];
 MPI Wait(&request, &status); /* Complete the receive */
  /* Now it's safe to use recv buf */
  for (i=0; i<N; i++) recv sum += recv buf[i];
  printf("Node %d: Send %d Recv %d\n", myid, send sum, recv sum);
 MPI Finalize();
  return 0;
                         Code at https://aiichironakano.github.io/cs596/src/mpi/
```

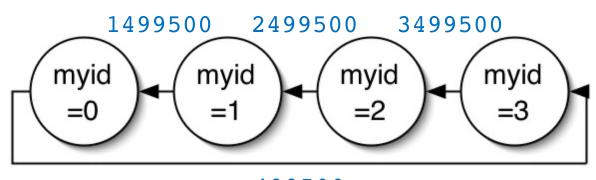
Output from irecv_mpi.c

Node 1: Send 1499500 Recv 2499500

Node 3: Send 3499500 Recv 499500

Node 0: Send 499500 Recv 1499500

Node 2: Send 2499500 Recv 3499500



499500

Multiple Asynchronous Messages

```
MPI_Request requests[N_message];
MPI_Status statuses[N_message];
MPI_Status status;
int index;

/* Wait for all messages to complete */
MPI_Waitall(N_message, requests, statuses);

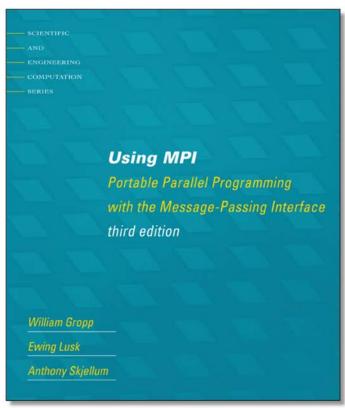
/* Wait for any specified messages to complete */
MPI_Waitany(N_message, requests, &index, &status);
```

returns the index (\in [0,N_message-1]) of the message that completed

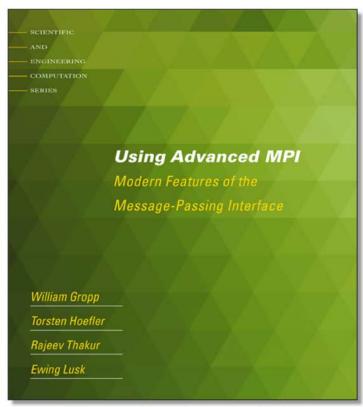
Polling MPI_Irecv

```
int flag;
/* Post an asynchronous receive */
MPI Irecv(recv buf, N, MPI INT, MPI ANY SOURCE, 777,
          MPI COMM WORLD, &request);
/* Perform tasks that don't use recv buf */
/* Polling */
MPI_Test(&request, &flag, &status); /* Check completion */
if (flag) { /* True if message received */
  /* Now it's safe to use recv buf */
}
```

Where to Go from Here







Advanced MPI, including MPI-3

- Complete MPI reference at http://www.netlib.org/utk/papers/mpi-book/mpi-book.html
- MPI is evolving (MPI-2 to MPI-3) to include advanced features like remote memory access (MPI_Put() & MPI_Get(); cf. sftp), parallel I/O and dynamic process management
- Various versions of MPI standard are specified at https://www.mpi-forum.org/docs/

MPI Basics: Recap

- Parallel computing = Who does what
- Single program multiple data (SPMD) programming: Do it with MPI rank (who am I) & selection constructs (if, etc.)
- Only need MPI_Send() & MPI_Recv() within communicators to implement any distributed-memory parallel computing
- Asynchronous message passing (MPI_Isend() & MPI_Irecv())
 to overlap computation & communication
- You can survive professionally only with a few global communication functions, e.g., MPI_Allreduce(), MPI_Barrier() & MPI_Bcast()

Start using MPI for your research & projects!

20 Years-Unleashing the Power of HPC

A discrete particle simulation of 1.5 billion atoms Adaptive mesh simulation of advecting sinusoidal density contours

2001 Chair Charles Slocomb Denver, CO





A WINE-2 system board

2001

Notable Systems first mentioned this year

in the proceedings:

- SGI Origin 3000
- Sun Fire 6000
- ASCI White
- Blue Horizon
- ASCI Blue Mountain



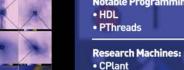
- MIPS R 12000
- Intel Pentium 4
- Intel Itanium



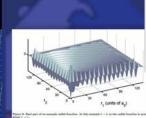
Noteworthy Architecture Topics:

- · Cache coherence through snooping
- Application speedups through custom on-the-fly FPGA function units
- Interactive program steering
- Grid-enabled parallel computing

Notable Programming Languages:



Adaptive mesh simulation of star formation



Best Research Poster

Solution of a three body quantum mechanics problem

S62001

SC01

Best Paper

Best Student Paper

ACM Gordon Bell Prize

Shimojo, and Subhash Saini Scalable atomistic simulation algorithms for materials research

Shava Smallen, Henri Cazsanova and Francine Berman Applying Scheduling and Tuning to On-line Parallel Tomography

See list of ACM Gordon Bell Prize winners

10⁶

20

(sec/MD-step)

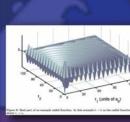
Wall-clock time

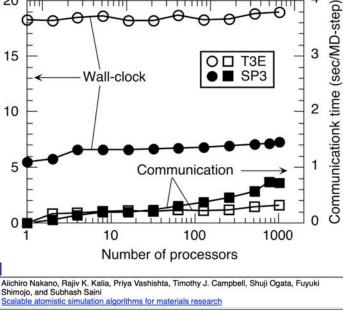
Sumir Chandra, Johan Steensland, and Manish Parashar ??? If you know, please contact chair@SIGHPC.org



The MDM system

Adaptive mesh simulation of a spherical shock





Number of atoms

10⁸

10⁷