Outline of Assignment 4, Part I

Deadlock-free communication

pmd.c

```
if even
  MPI_Send()
  MPI_Recv()
else if odd
  MPI_Recv()
  MPI_Send()
else (self)
  memory copy
```

No ifs & buts!
cleaner

pmd_irecv.c

```
MPI_Irecv()
MPI_Send()  // OK to send to self
MPI_Wait()
```

Where?

2 in atom_copy()
2 in atom_move()

4 code segments in total

Computation (ns)/communication (μs-ms) overlap

```
MPI_Irecv()
?
MPI_Send()
MPI_Wait()
```

[discovery ~]$ ping hpc-transfer.usc.edu
time=0.074 ms
...

Bash Programming

pmd_irecv.sl

```
counter=0

while [ $counter -lt 3 ]; do

  echo "***** Asynchronous *****"

  mpirun -n $SLURM_NTASKS ./pmd_irecv

  echo "***** Synchronous *****"

  mpirun -n $SLURM_NTASKS ./pmd

  let counter+=1

done
```

mpicc -O -o pmd_irecv pmd_irecv.c -lm

Value of a variable

Print to terminal

Input-parameter file `pmd.in` should be in the same directory

mpicc -O -o pmd pmd.c -lm

Evaluate a mathematical expression & stores its result into a variable

See “Bash scripting tutorial for beginners”
https://linuxconfig.org/bash-scripting-tutorial-for-beginners

Start programming scripts for your research!

Runtime Fluctuation

- Due to (1) network interference & (2) shared access to computing nodes, measured runtimes will fluctuate
- The latter could be avoided by exclusive access (#SBATCH --exclusive), but please do not use this since it will cause very low utilization of computing resources & slow down other users' work

```
***** Asynchronous *****
CPU & COMT = 4.626476e-01 1.115105e-01
***** Synchronous *****
CPU & COMT = 5.080977e-01 1.547345e-01

***** Asynchronous *****
CPU & COMT = 4.822192e-01 1.280804e-01
***** Synchronous *****
CPU & COMT = 4.952592e-01 1.424449e-01

***** Asynchronous *****
CPU & COMT = 4.679100e-01 1.141893e-01
***** Synchronous *****
CPU & COMT = 4.906234e-01 1.389465e-01
```

pmd_irecv.c

pmd.c

Run time:

pmd_irecv

0.471 ± 0.010 s

pmd

0.498 ± 0.010 s

CPU & COMT reports total run time & communication time, respectively

Removing Barrier

Q. Are MPI_Barrier() calls necessary in atom_copy() & atom_move()?

A. Not necessarily. To remove it, however, message tag needs be made unique across neighbors so that messages won't interfere.

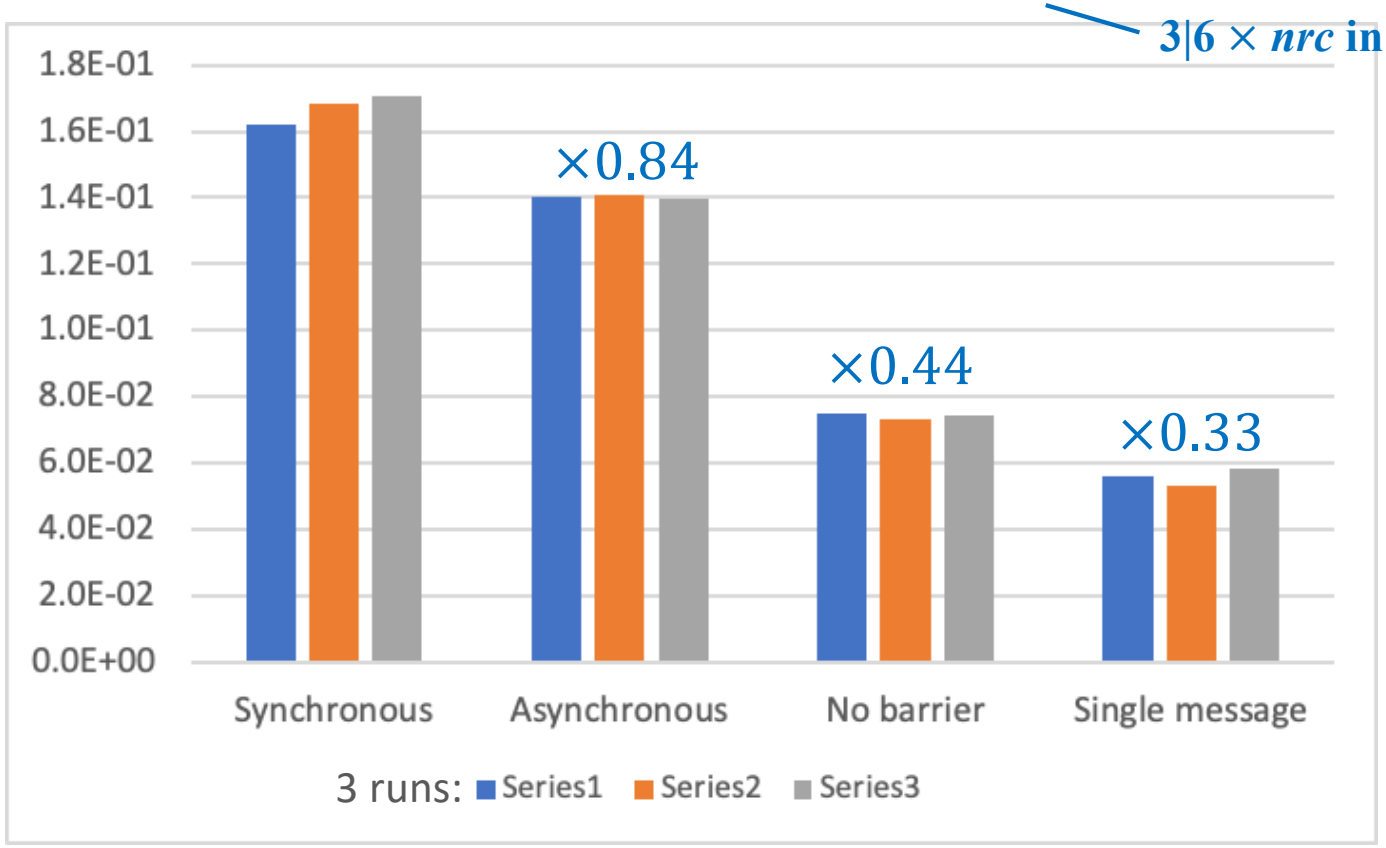
- **Message passing of *nsd* & *nrc* can be eliminated by enquiring the received message size.**

Receive up to the array size — Neighbor-specific tag

```
MPI_Irecv(dbufr,NDBUF,MPI_DOUBLE,MPI_ANY_SOURCE,120+ku,MPI_COMM_WORLD,&request);
MPI_Get_count(&status,MPI_DOUBLE,&doublesReceived);
```

Enquire the count of received doubles

3|6 × *nrc* in atom_copy|move()



Average 67% reduction of communication time thanks to Raghav

Resource Usage (1)

- **Start interactive job on discovery & start a MPI program on one of the allocated computing nodes**

```
[anakano@discovery cs596]$ salloc --nodes=4 --ntasks-per-node=4 -t 30
salloc: Nodes d05-[33-36] are ready for job
[anakano@d05-33 cs596]$ mpirun -n 16 ./pmd_irecv
...
```

- **In another terminal, log in to another allocated node & type 'top' to see running processes**

```
[anakano@discovery cs596]$ ssh d05-34
[anakano@d05-34 ~]$ top
top - 07:42:03 up 47 days, 18:34,  2 users,  load average: 4.37, 3.33, 3.15
Tasks: 315 total,   8 running, 307 sleeping,   0 stopped,   0 zombie

PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
 3262 rvandamm  20   0 1168000   1.0g  25228 R 100.0  0.5   1090:38 rna_denovo.stat
 3263 rvandamm  20   0 1344840   1.2g  25228 R  99.7  0.6   1090:38 rna_denovo.stat
23608 anakano   20   0  432324 110840   8660 R  99.7  0.1   0:26.48 pmd_irecv
23609 anakano   20   0  432332 108808   8672 R  99.7  0.1   0:26.41 pmd_irecv
23610 anakano   20   0  432324 110856   8676 R  99.7  0.1   0:26.51 pmd_irecv
23607 anakano   20   0  432328 108732   8604 R  99.3  0.1   0:26.43 pmd_irecv
15225 sgopalan  20   0   11.4g  11.2g   7576 R  99.0  5.9   2072:59 R
19675 telegraf  20   0 1507240  49764  18380 S   0.3  0.0  14:08.81 telegraf
23588 anakano   20   0  164372   2508   1612 R   0.3  0.0   0:00.12 top
    1 root      20   0   43572   3956   2528 S   0.0  0.0   2:02.10 systemd
```

4 instances (ranks) of pmd_irecv are running per node

Resource Usage (2)

- **Type ‘1’ (toggle to show detailed core usage): two users (including myself) are not making full use of cores; let others utilize the unused resources by avoiding exclusive access**

```
%Cpu0  :  0.0 us,  0.0 sy,  0.0 ni, 99.7 id,  0.0 wa,  0.0 hi,  0.3 si,  0.0 st
%Cpu1  :100.0 us,  0.0 sy,  0.0 ni,  0.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu2  :100.0 us,  0.0 sy,  0.0 ni,  0.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu3  :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu4  : 76.3 us, 23.0 sy,  0.0 ni,  0.7 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu5  :100.0 us,  0.0 sy,  0.0 ni,  0.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu6  :100.0 us,  0.0 sy,  0.0 ni,  0.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu7  : 99.7 us,  0.3 sy,  0.0 ni,  0.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu8  : 99.7 us,  0.3 sy,  0.0 ni,  0.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu9  :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu10 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu11 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu12 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu13 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu14 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu15 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu16 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu17 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu18 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu19 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu20 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu21 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu22 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
%Cpu23 :  0.0 us,  0.0 sy,  0.0 ni,100.0 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
```

17 out of 24 cores unused

Note on Assignment 4, Part II

- **Hands-on experience in a common situation of adding new analysis functionality to an existing MPI simulation code, *via* minimally invasive surgery of the code**
- **Note the header, pmd.h, in the homework package, csci596-as04, was set for Part I:**

```
int vproc[3] = {2,2,4}, nproc = 16;
```

The number of MPI ranks should match nproc in pmd.h:

```
mpirun -n 16 ./pmd (also ./pmd_irecv)
```

- **Due to 'shadow' analysis ranks, the total number of ranks to be spawned by mpirun in Part II should instead be twice the number of spatial subsystems, nproc, in pmd_split.c:**

In pmd_split.h:

```
int vproc[3] = {2,2,2}, nproc = 8;
```

Run:

```
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=8
mpirun -n $SLURM_NTASKS ./pmd_split // $SLURM_NTASKS = 16
```

Note on Assignment 4, Part II

- **Input-parameter file, `pmd.in`, needs be edited for part II**

`pmd.in` for part I

```
3  3  3   InitUcell[0[1[2]
0.8
1.0
0.005
1000     StepLimit
1001     StepAvg
```

To measure run time only for simulation itself, but not for calculating other quantities

`pmd.in` for part II

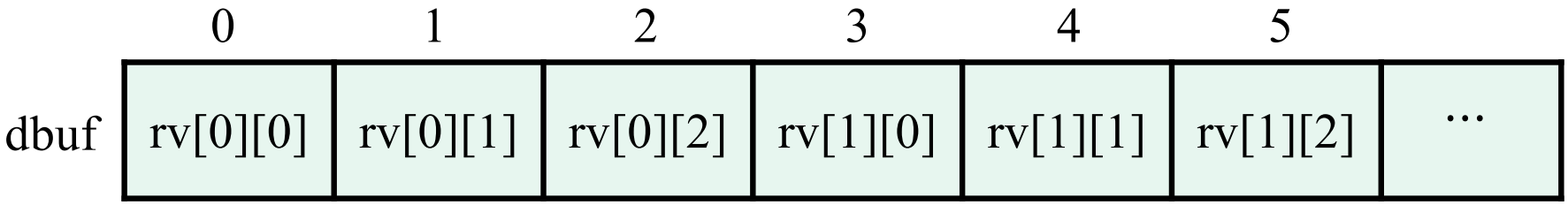
```
5  5  5   InitUcell[0[1[2]
0.8
1.0
0.005
30       StepLimit
10       StepAvg
```

To compute rapidly equilibrating velocity probability density at every 10th time steps

Message Composition

- **Multidimensional arrays are sent as one-dimensional arrays**

```
double rv[NMAX][3];
double dbuf[NDBUF], dbufr[NDBUF];
```



MD world (*md* = 1)

dbuf[3**i*+*a*] ← *rv*[*i*][*a*] ($i = 0, \dots, n-1; a = 0,1,2$)

Send *dbuf*[]

Analysis world (*md* = 0)

Receive *dbufr*[]

rv[*i*][*a*] ← *dbufr*[3**i*+*a*] ($i = 0, \dots, n-1; a = 0,1,2$)