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

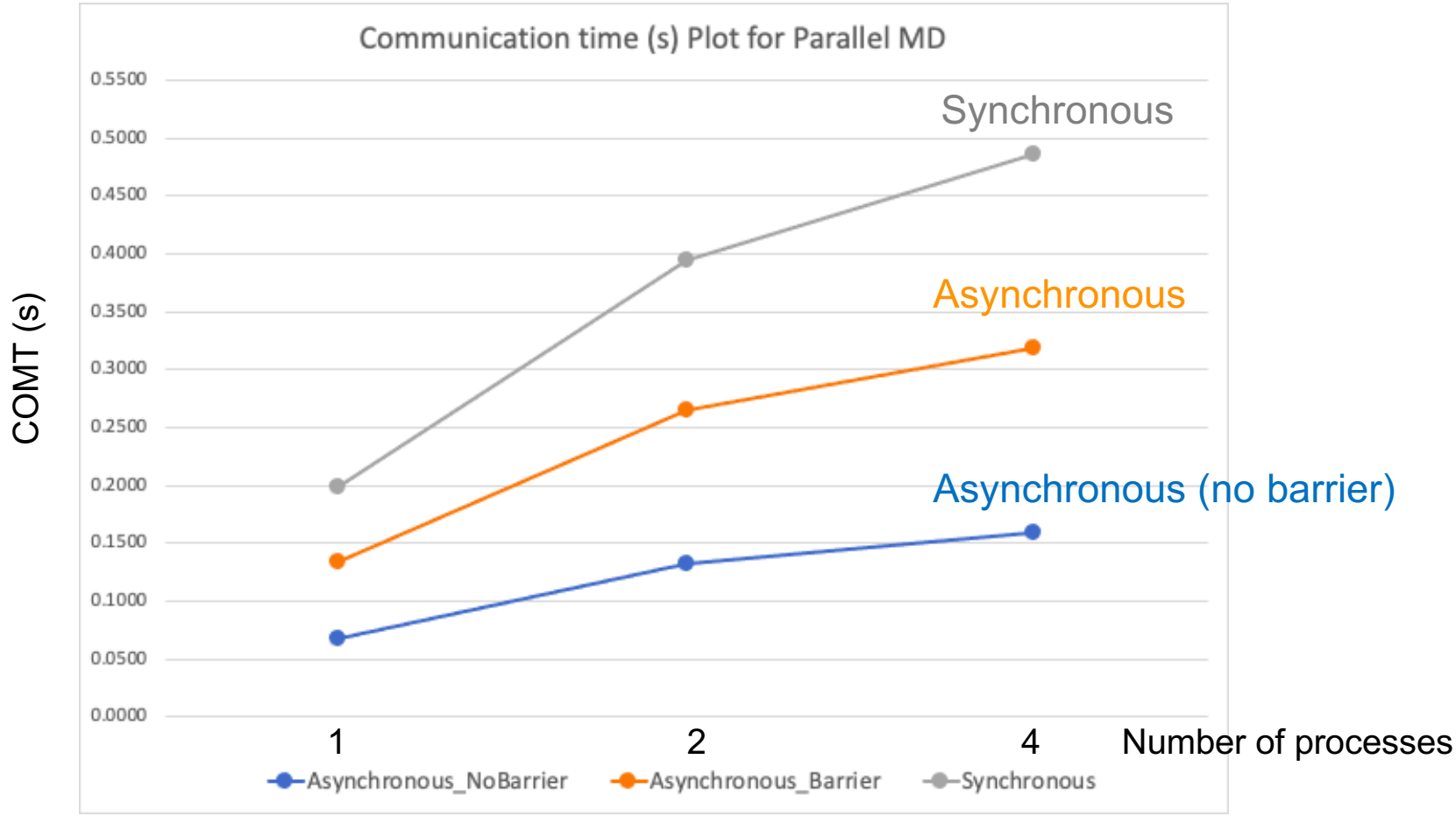
0.498 ± 0.010 s

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 MD time steps so that messages across MD steps won't interfere.



COMT is halved by removing the barrier (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
```

Message Composition

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

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