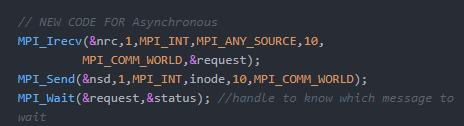
Minh Tran

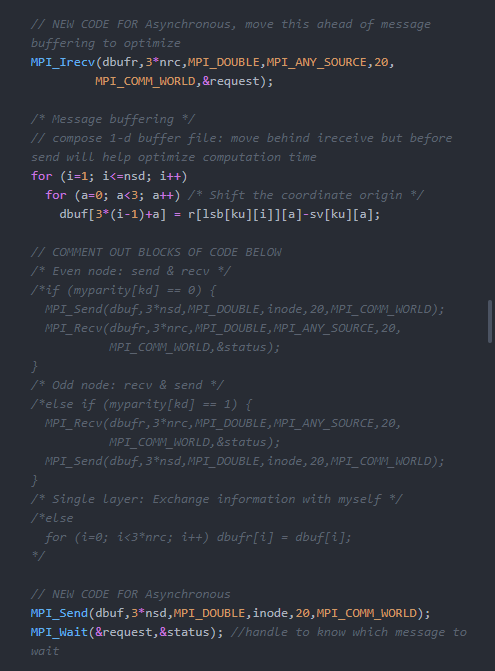
Assignment 4 CSCI 596: Parallel Molecular Dynamics

1. Asynchronous Messages

The new program pmd\_irecv.c is modifed from pmd.c by inserting proper asynchronous messaging lines of code. Note that nrc is number of atoms received while nsd is number of atoms sent. The MPI\_Irecv requires adjustment from MPI\_Recv by changing &status to &request and adding MPI\_Wait. The changes are marked by //NEW CODE



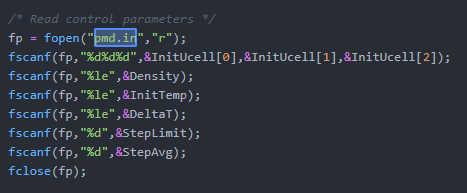
A similar adjustment is made for the buffer (note the commented out code as we do not need the deadlock-avoidance scheme anymore)



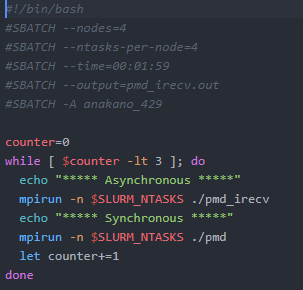
To complete this part, run the following on cluster:

* Compile the program by: (The input file pmd.in and header pmd.h are automatically read by the following scripts in both C programs: pmd.c and pmd\_irecv.c)

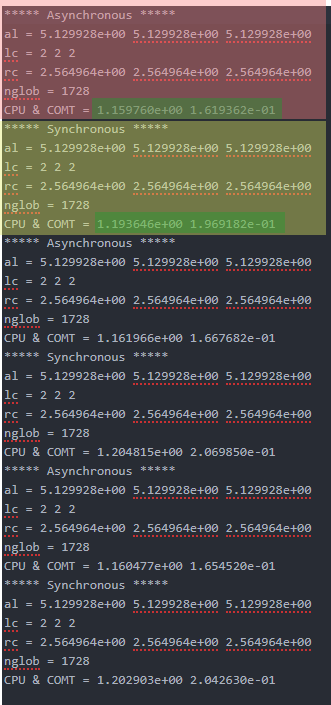




* + **Mpicc -o pmd pmd.c -lm**
  + **Mpicc -o pmd\_irecv pmd\_irecv.c -lm**
* Run sbatch:
  + **Sbatch pmd\_irecv.sl**
  + This sbatch will get 4 computing nodes, each with 4 processors. The job consists of 3 runs, each run has two tasks: pmd\_irecv and pmd. Then it will generate output pmd\_recv.out.



Below is the output pmd\_irecv.out. Note that each run consits of one asynchronous part (in red shadow) and one synchronous part (in yellow shadow). The processing computational and the communication time is highlighted in green.

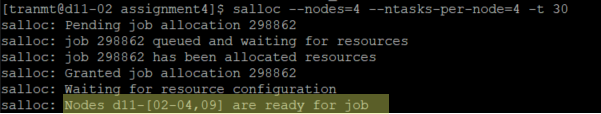


The results of computing time is shown below:

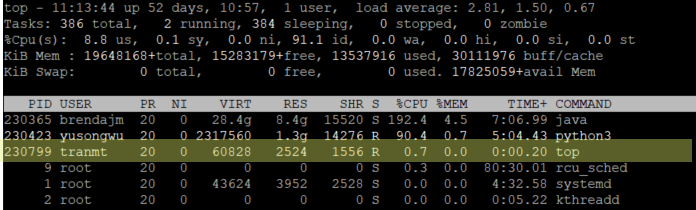


This part can be done interactively:

* **Run salloc –nodes=4 –ntasks-per-node=4 -t 30**



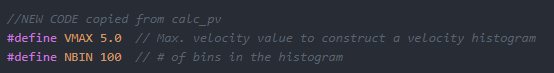
* In another terminal, run **ssh d11-02** and **top** to see the reserved nodes



1. Communicators
2. Modified source code

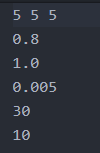
The modifications are clearly marked with //NEW CODE, which are in several places:

* In the header file pmd\_split.h, the variable definition is added from calc\_pv() as well as the change in the number of processors





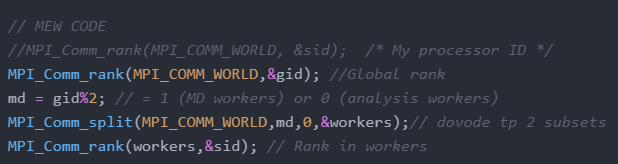
* In the input file pmd\_split.in, I change the parameters to the following:



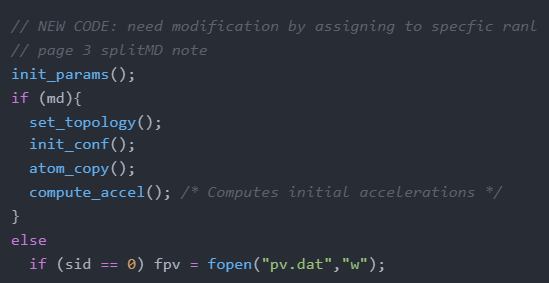
* In the program file pmd\_split.c (the original copy is from pmd\_irecv.c), the major changes are:
  + Change input file name



* + Add this following the initialization part

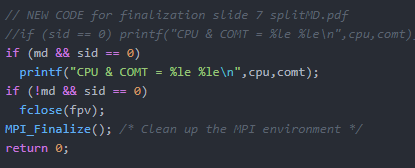


* + Modify to add rank-dependent task assignment





* + Add this to the finalization



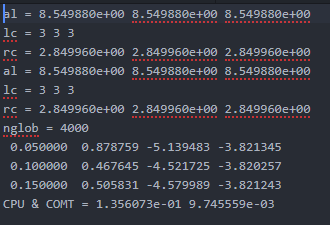
* + Change most MPI\_COMM\_WORLD to workers

1. Run the program

Compile it by **mpicc -o pmd\_split pmd\_split.c -lm**

Then run **sbatch pmd\_split.sl** on the computing node

The first output is pmd\_split.out, stating the computational time



The second output is the pv.dat, which can be post-processed in excel by separating data of the three timesteps to plot the pdf:

