mpicc -O -o hmd hmd.c -lm -fopenmp

$ salloc --nodes=2 --ntasks-per-node=1 --cpus-per-task=4 -t 29

Srun -n 2 ./hmd

Should be same: p16 in ppt

In hmd.h:

vproc = {1,1,1}, nproc = 1;

vthrd = {1,1,1}, nthrd = 1;

2 1 1 2

2 2 1 4

2 2 2 8

$ salloc --nodes=1 --ntasks-per-node=1 --cpus-per-task=8 -t 29

Changes in pmd.in

24 24 24 InitUcell[3]

0.8 Density

1.0 InitTemp

0.005 DeltaT

100 StepLimit

101 StepAvg

Srun -n 1 ./hmd1

23s

Srun -n 1 ./hmd8

10s