

HPC

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The Gateway used in the cluster for the homework was vmeps09.vampire with an Intel® Xeon® CPU 2.40GHz

1)

gcc no opt	gcc -O2	Compiling/time (min + secs)
1 + 32.402	0 + 52.4465	
Intel -O3	Intel -xHost	
0 + 6.732	0 + 6.007	
gcc -O3	Intel -O0	Intel -O2
0 + 20.9765	1 + 32.265	0 + 6.266

2)

- Type make.

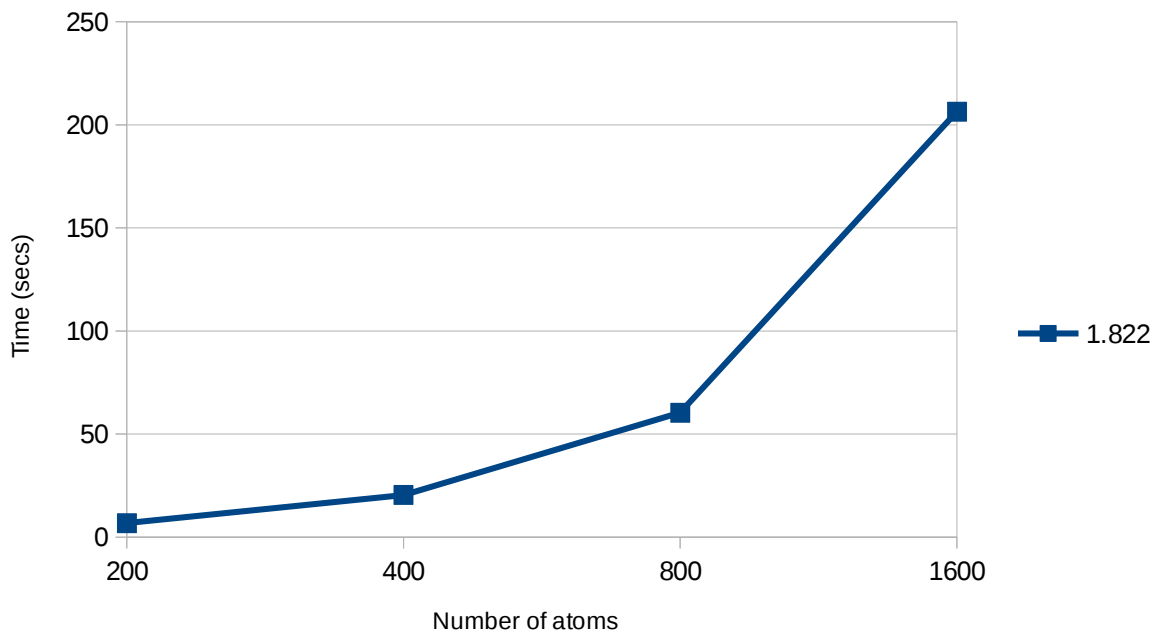
If there are modifications within the source code type, make.

If there are modifications within the make file, type make cleanall, and then make.

-Accepted CL are Number of atoms (default 125 in .sh, 100 in src), number of time steps (default 10000), output freq. (default 100), thermo output freq. (default 100).

-They are defined in Atoms.h and Params.h, they are initialized in Initialization.c.

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This problem scales exponentially as the number of atoms increases.

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100	200	Atoms/secs/FLOP/FLOPS
1.822	6.775	
1314971355	3988980471	
721718636.11416	588779405.313653	
400	800	1600
20.426	60.296	206.375
11161150536	-	-
546418806.227357	-	-