

EE582 sect. 3  
Homework # 1

The initial step in running an MD calculations requires the coordinates and velocities of the atoms. Assuming a Maxwell-Boltzmann distribution for the energies of the atoms at room temperature, use the rejection approach discussed in class to obtain the initial velocities of a system of 10,000 atoms. You will need a random number generator.

Useful links:

1. Molecular Dynamic Primer: <http://www.fisica.uniud.it/~ercolessi/md/>
2. Ames MD codes: [http://cmp.ameslab.gov/cmp/CMP\\_Theory/cmd/alcmd\\_source.html](http://cmp.ameslab.gov/cmp/CMP_Theory/cmd/alcmd_source.html)
3. Simple MD codes (LJ potential tutorial):  
<http://www.photon.t.u-tokyo.ac.jp/~maruyama/mdlecture/mdlecture.html>
4. [http://www.csupomona.edu/~hxue/publication/nmhff\\_xue99.pdf#search='micro%20heat%20conduction'](http://www.csupomona.edu/~hxue/publication/nmhff_xue99.pdf#search='micro%20heat%20conduction')  
a paper on heat conduction in thin films.
5. [http://www.ch.embnet.org/MD\\_tutorial/](http://www.ch.embnet.org/MD_tutorial/)