

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

**Mathematical Methods
for Materials Scientists and Engineers**

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Problem Set 1: Due Friday Sept. 16, Before 5PM: email to **the TA**.

There will be no group assignments for this first problem set. You should submit your homework by attaching a Mathematica notebook as an attachment of an email to **the TA**. To ensure that you receive credit, you should name your notebook **HW01 Lastname.nb** before you attach it.

Individual Exercise I1-1

Design a random walk on a finite one-dimensional lattice simulator. Suppose a particle begins at position 0 at iteration 0. At each iteration, the particle will either jump to the right (occupying position 1 at iteration 1) with probability $\frac{1}{2}$ or to the left (occupying position -1 at iteration 1) with probability $\frac{1}{2}$.

Suppose the lattice occupies positions -100 to $+100$ and simulate how many iterations are required for the particle to exit the lattice by reaching the ends of the lattice.

Each simulation is called “a trial.” Plot the number of steps for each trial versus the trials for 100 trials.

Individual Exercise I1-2

In many simple models, the potential between two atoms is taken to be the Lennard-Jones potential

$$LJ(r) = \frac{a}{r^{12}} - \frac{b}{r^6}$$

1. Calculate the distance r_{\min} at which the Lennard-Jones potential is a minimum in terms of a and b
2. Calculate the minimum energy $E_{\min} = LJ(r_{\min})$ in terms of a and b
3. The parameters a and b are not very “physical.” Re-express the Lennard-Jones potential in terms of the minimum energy (E_{\min}) and the equilibrium two-atom separation (r_{\min})—in other words what is $LJ(r)$ written with parameters E_{\min} and r_{\min} instead of a and b .

4. Calculate the force, F , between two atoms as a function of their separation r .
5. It is good practice to create “normalized” or “dimensionless” representations of physical variables. Explain why $\bar{F} \equiv Fr_{\min}/E_{\min}$ and $\bar{r} \equiv r/r_{\min}$ are normalized variables.
6. Plot $LJ(\bar{r})/E_{\min}$ and $\bar{F}(\bar{r})$ together.
7. A mass m in a simple linear spring system has potential energy given by

$$U(x) = A + Bx + \frac{k}{2}x^2$$

and kinetic energy given by

$$K(\dot{x}) = \frac{m}{2}\dot{x}^2$$

and will have a vibrational frequency near its equilibrium position given by

$$\nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$$

Rewrite the potential energy of a spring system with a more physical parameterization.

8. The kinetic energy of a single atom has the same form as that of a simple mass

$$K(\dot{x}) = \frac{m}{2}\dot{x}^2$$

Expand the Lennard-Jones potential about the equilibrium separation, r_{\min} , to second-order to find the effective spring constant for small forces.

9. Calculate the vibrational frequency for a atom near its equilibrium position.