# Massachusetts Institute of Technology

# Mathematical Methods for Materials Scientists and Engineers

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Problem Set 1: Due Thursday Sept. 14, Before 9PM: email to mingtang(the symbol at)mit.edu

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 mingtang(-at-)mit.edu. To ensure that you receive credit, you should name your notebook **HW01_Lastname.nb** before you attach it.

## Individual Exercise I1-1

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

$$LJ(r) = \frac{a}{r^{12}} - \frac{b}{r^{6}} \tag{1}$$

1. Calculate the distance $0 < r_{\mathrm{o}} < \infty$ at which the Lennard-Jones potential is an extremum in terms of $a$ and $b$

2. Calculate the energy $E_{\mathrm{o}} = LJ(r_{\mathrm{o}})$ at the extremal position in terms of $a$ and $b$

3. The parameters $a$ and $b$ are not very "physical." In other words, it is not easy to look at Equation 1 and determine its characteristic physics if it written in terms of $a$ and $b$. On the other hand, the variables $r_{\mathrm{o}}$ and $E_{\mathrm{o}}$ are physical.

   Re-express the Lennard-Jones potential in terms of the energy ($E_{\mathrm{o}}$) and the two-atom separation ($r_{\mathrm{o}}$)—in other words what is $LJ(r)$ written with parameters $E_{\mathrm{o}}$ and $r_{\mathrm{o}}$ instead of $a$ and $b$.

4. Calculate the force, $F$, between two atoms as a function of their separation $r$ in terms of $r_{\mathrm{o}}$ and $E_{\mathrm{o}}$.

5. Determine any conditions on $r_{\mathrm{o}}$ and $E_{\mathrm{o}}$ such that $LJ(r_{\mathrm{o}})$ is a minimum. This is also the condition that $r_{\mathrm{o}}$ is an *equilibrium* separation—explain why.

6. It is good practice to create "normalized" or "dimensionless" representations of physical variables. Explain why $\overline{F} \equiv F r_{\mathrm{o}}/E_{\mathrm{o}}$ and $\overline{r} \equiv r/r_{\mathrm{o}}$ are normalized variables.

7. Plot $LJ(\overline{r})/E_{\mathrm{o}}$ and $\overline{F}(\overline{r})$ together.

## Individual Exercise I1-2

This homework problem is a type of "simulated experiment."

Suppose that you wish to determine the density of a small sphere with very high confidence and with an estimate of the error of your determination.

One method to increase your confidence in your determined density is to repeat your measurement many many times.

Suppose that you determine density by the following process

**find mass** Weigh the small sphere and record its mass. Your scale can resolve 0.001 grams (i.e., there is a digital read-out that reports numbers like this: 1.234 grams)

**find diameter** Measure the small sphere and record its diameter. Your resolution is 0.1 millimeters.

**calculate** Using an appropriate formula, you calculate the density.

which is repeated over and over.

Suppose that by averaging and taking the standard deviation of your data, your mass determination is $m = 0.1256 \pm 0.0005$ grams and your determination of diameter is $D = 2.04 \pm 0.08$ millimeters.

How do you relate the average density and its variation to those of the mass and diameter?

Answer this question by assuming that your data are "normally" (in other words Gaussian) distributed and producing "simulated" data.

Find the appropriate discussion in MATHEMATICA® 's help browser for the function `Random` and extend `NormalDistribution` example found there in "Further Examples" to your case.

Your simulated experiment consists of

**generate mass** Generate a random mass from a normal distribution with the appropriate average and standard deviation.

**generate diameter** Generate a random diameter from a normal distribution with the appropriate average and standard deviation.

**calculate** Using an appropriate formula, calculate the density.

1. Repeat your simulated experiment 10000 times. Plot histograms of the simulated mass, diameter, and density.

2. Calculate the average and standard deviation of your density.

3. (extra credit) See if you can generalize the problem by letting the standard deviation of the mass and diameter be variables $\sigma_m$ and $\sigma_D$. Run your simulated experiment by fixing $\sigma_m$ and letting $\sigma_D$ take on different values, and by by fixing $\sigma_D$ and letting $\sigma_m$ take on different values Plot the resulting $\sigma_\rho$ and descibe the relationships $\partial\sigma_\rho/\partial\sigma_D$ and $\partial\sigma_\rho/\partial\sigma_D$.