Homework 1 — Solution

3.016 Mathematical Methods for Materials Scientists and Engineers
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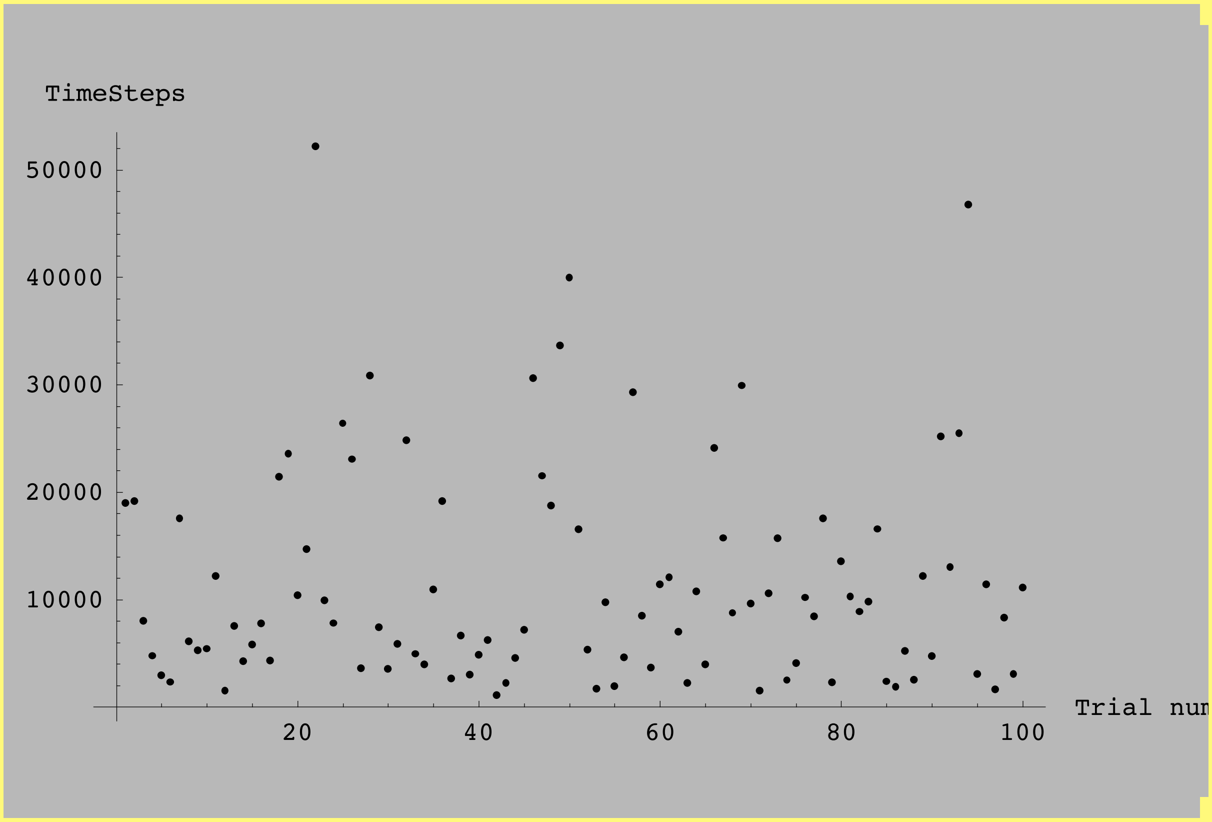
Individual Exercise I-1:

First, recognize that you will need to use ListPlot to make the final plot of your data. ListPlot produces a plot from (x,y) pairs that are stored in a Table. The program you need to write has to produce output that will be written to a Table with the proper format.

The function Random[Integer] is used here; it returns either 0 or 1 with probability 1/2.

Quoting Charles Cantrell: "All of the problem is contained in one line of input. First I create a table of data members that contains the trial number and the number of required steps to reach the end-point. Then I plot the data using the ListPlot command. The While loop runs until the position is either 100 or -100, and the Table command is run 100 times--giving us 100 data points."

```
data = Table[{i, location = 0; timestep = 0;
        While[Abs[location] < 100, If[Random[Integer] == 0,
            location = location + 1, location = location – 1];
          timestep = timestep + 1]; timestep}, {i, 100}];
ListPlot[data, AxesLabel → {"Trial number", "TimeSteps"}]
```




```
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```

Individual Exercise I-2:

Note: Some features of Omar Fabian's work were incorporated in the solution to this exercise.

1.

Input the LJ potential, differentiate and set derivative == 0 to find minima.

```
LJ = a/r^12 - b/r^6
```

$$\frac{a}{r^{12}} - \frac{b}{r^6}$$

```
MinimaOfLJ = Solve[D[LJ, r] == 0, r]
```

$$\left\{\left\{r \to -\frac{2^{1/6}\, a^{1/6}}{b^{1/6}}\right\}, \left\{r \to \frac{2^{1/6}\, a^{1/6}}{b^{1/6}}\right\}, \left\{r \to -\frac{(-1)^{1/3}\, 2^{1/6}\, a^{1/6}}{b^{1/6}}\right\}, \left\{r \to \frac{(-1)^{1/3}\, 2^{1/6}\, a^{1/6}}{b^{1/6}}\right\}, \left\{r \to -\frac{(-1)^{2/3}\, 2^{1/6}\, a^{1/6}}{b^{1/6}}\right\}, \left\{r \to \frac{(-1)^{2/3}\, 2^{1/6}\, a^{1/6}}{b^{1/6}}\right\}\right\}$$

Note that there are six roots but only one of them is "physical" — i.e., real and positive (the second root). Use this to set rmin. Note how Replace is used to extract the value of the second root.

```
Minr = r /. MinimaOfLJ[[2]]
```

$$\frac{2^{1/6}\,a^{1/6}}{b^{1/6}}$$

■ 2.

Replace r with rmin in LJ to get EMin = LJ(rmin).

```
MinE =  LJ /. r -> Minr
```

$$-\frac{b^2}{4\,a}$$

■ 3.

The Solve function can be used to eliminate specific variables from a set of equations. Here we have the equation for rMin in terms of (a,b) and the equation for EMin in terms of (a,b). Solve is used to find expressions for a and b in terms of rMin and EMin.

```
Clear[rMin, EMin]
```

```
NewVars = Solve[{rMin == Minr, EMin == MinE}, {a, b}]
```

$$\{\{a \to -\text{EMin}\,\text{rMin}^{12},\ b \to -2\,\text{EMin}\,\text{rMin}^{6}\}\}$$

All that remains is to Replace a and b with these new variables.

```
LJModified = LJ /. NewVars[[1]]
```

$$\frac{2\,\text{EMin}\,\text{rMin}^6}{r^6} - \frac{\text{EMin}\,\text{rMin}^{12}}{r^{12}}$$

4.

The force is obtained by differentiation

```
Force := -∂r LJModified
Force
```

$$\frac{12\,\text{EMin}\,\text{rMin}^6}{r^7} - \frac{12\,\text{EMin}\,\text{rMin}^{12}}{r^{13}}$$

5.

Define new "normalized" variables rNorm = r / rMin and LJNorm = LJ / EMin and use them to define a normalized LJ function LJNorm(rNorm). Recongnizing that I will eventually want to plot these functions, I define them with delayed assignment :=

```
LJNorm :=
  Simplify[-(LJModified / EMin) /. rMin → r / rNorm,
    Assumptions → {a > 0 && b > 0}]
LJNorm
```

$$\frac{1}{rNorm^{12}} - \frac{2}{rNorm^{6}}$$

```
ForceNorm :=
  Simplify[-(Force rMin / EMin) /. rMin → r / rNorm,
    Assumptions → {a > 0 && b > 0}]
ForceNorm
```

$$-\frac{12\,(-1 + rNorm^{6})}{rNorm^{13}}$$

To demonstrate that LJNorm and ForceNorm are dimensionless:

```
EMinUnits = Mass Length^2 / Time^2;
ForceUnits = Mass Length^2 / (Time^2 Length);
rUnits = Length;
rMinUnits = Length;
```

```
rBarUnits = rUnits / rMinUnits;
rBarUnits == 1
```

True

```
FBarUnits = ForceUnits rMinUnits / EMinUnits;
FBarUnits == 1
```

```
True
```

So, the variables $\bar{r}$ and $\overline{F}$ are dimensionless.

6.

Now for the plot. Note in the use of the DisplayFunction option to control whether or not the graphics are rendered to the screen.

```
NewPlot = Plot[{LJNorm, ForceNorm},
    {rNorm, 0, 2}, PlotRange → {−4, 4},
    PlotStyle → {{Thickness[.01], Hue[0.3]},
        {Thickness[.01], Hue[1]}},
    AxesLabel −> {"r/rMin", "Normalized LJ and F"},
    DisplayFunction → Identity]
```

```
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```
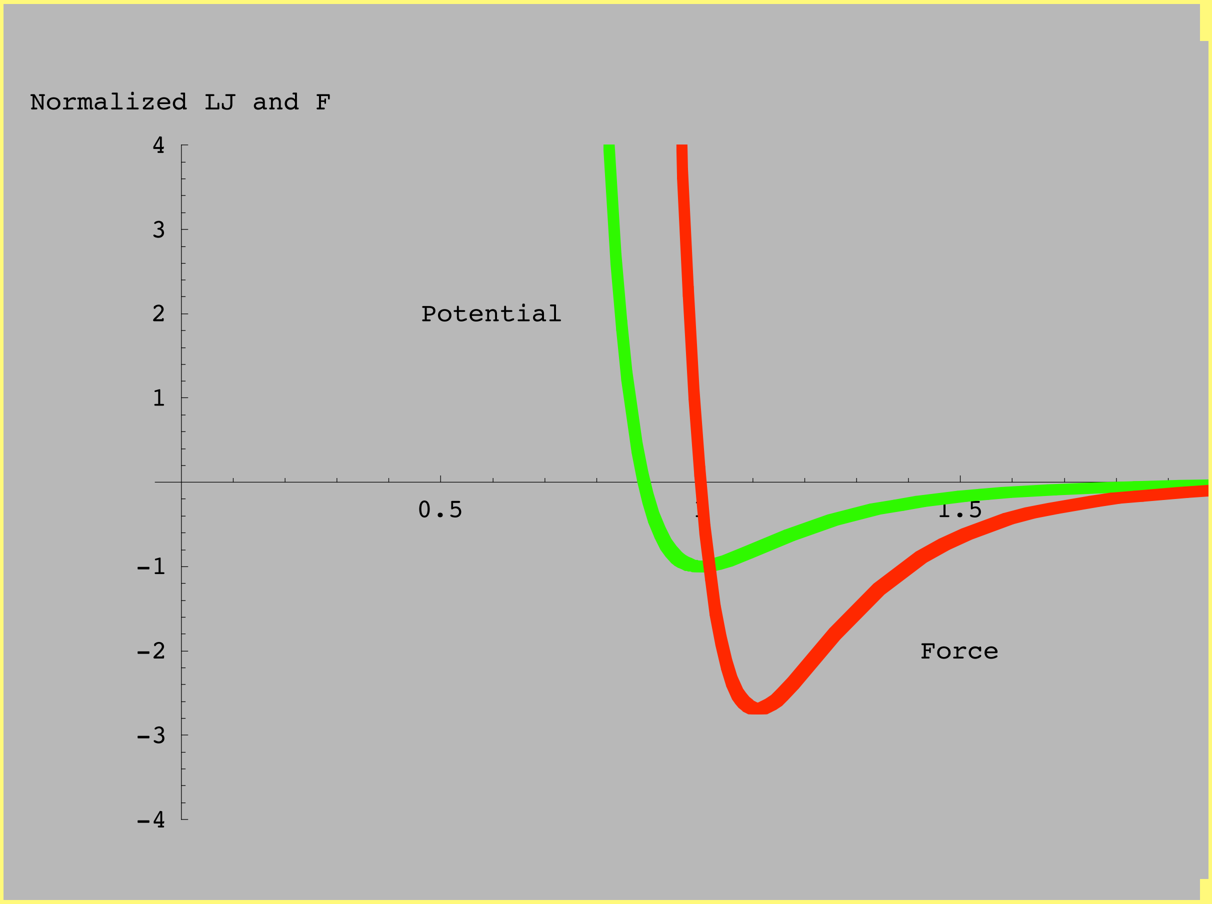

```
Show[NewPlot, Graphics[Text["Force", {1.5 , -2}]],
  Graphics[Text["Potential", {.6, 2}]],
  DisplayFunction → $DisplayFunction]
```



- Graphics -

■ 7.

I will use the same approach as above, using as my constants the equilibrium position, xMin, and minimum potential energy,

```
PotEnergy = A + B x + k x^2/2
```

$$A + B\,x - \frac{36\,\text{EMin}\,x^2}{\text{rMin}^2}$$

```
SpringForceEq = (D[PotEnergy, x] /. x -> xMin ) == 0
```

$$B - \frac{72\,\text{EMin}\,\text{xMin}}{\text{rMin}^2} == 0$$

```
MinEnergyEq = ( PotEnergy /. x → xMin) == -PotMin
```

$$A + B\,\text{xMin} - \frac{36\,\text{EMin}\,\text{xMin}^2}{\text{rMin}^2} == -\text{PotMin}$$

```
SolutionPot =
  Solve[{SpringForceEq, MinEnergyEq}, {A, B}]
```

$$\left\{\left\{A \to -\text{PotMin} - \frac{36\,\text{EMin}\,\text{xMin}^2}{\text{rMin}^2},\ B \to \frac{72\,\text{EMin}\,\text{xMin}}{\text{rMin}^2}\right\}\right\}$$

```
ModifiedPotEnergy = PotEnergy /. SolutionPot[[1]]
```

$$-\text{PotMin} - \frac{36\ \text{EMin}\ x^2}{\text{rMin}^2} + \frac{72\ \text{EMin}\ x\ \text{xMin}}{\text{rMin}^2} - \frac{36\ \text{EMin}\ \text{xMin}^2}{\text{rMin}^2}$$

8.

Use function Series to get the Taylor series representation, include Normal to eliminate the O[r - rMin]^3 term.

```
HarmonicApprox = Normal[Series[LJModified, {r, rMin, 2}]]
```

$$\text{EMin} - \frac{36\ \text{EMin}\ (r - \text{rMin})^2}{\text{rMin}^2}$$

Note that this expression is a parabolic fit to the bottom of the potential well for the LJ function.

■ **9.**

The coefficient of the second-order term of HarmonicApprox is equal to k/2, where k is the spring constant. We can use the relation between vibrational frequency and spring constant to get the desired expression.

```
k = 2 SeriesCoefficient[Series[LJModified, {r, rMin, 2}], 2]
```

$$-\frac{72\,\text{EMin}}{\text{rMin}^2}$$

$$\text{VibFrequency} = \frac{1}{2\pi}\sqrt{\frac{k}{\text{Mass}}}$$

$$\frac{3\sqrt{2}\sqrt{-\frac{\text{EMin}}{\text{Mass}\,\text{rMin}^2}}}{\pi}$$