Home work 8: Monte Carlo

Create your own Monte Carlo program to perform a Monte Carlo Simulation of a harmonic oscillator:

$$U(x) = \frac{1}{2}k(x - x_0)^2 \tag{1}$$

with Boltzman constant $k_\mathrm{B} = 0.0083\,\mathrm{kJmol^{-1}1K^{-1}}$. We use $k = 1.0\times10^7$ $\mathrm{kJmol^{-1}nm^{-2}}$, $k_\mathrm{B} = 0.0083$ $\mathrm{kJmol^{-}1K^{-1}}$ and $x_0 = 0.136$ nm, models a C=O bond.

Perhaps it is easiest to use Mathematica, unless you're confortamble programming. The relevant functions for this exercise in Mathematica are:

```
RandomReal[]
```

```
For[]
```

```
If[]
```

```
Print[]
```

Use the help function if you are not sure how to use these. Think about how you want to make the trial move. Perhaps some randomness withing certain boundaries, *i.e.* $x(n) = x(o) + R \times \delta$, with R a random number between -1 and 1, and δ the maximum displacement in x? Try to determine the optimal δ.

Use your program to evaluate the following properties and compare to the analytic result (Homework week 4, exercise 3).

- Average potential energy at $T = 300$ K
- heat capacity (Hint plot the average energy as a function of temperature and use finite differencing to obtain the gradient), assuming equipartition for the kinetic energy: $\frac{1}{2}k_\mathrm{B}T$.
- the average displacement of x: $\langle x - x_0 \rangle$

- the root-mean-square displacement of x: $\sqrt{\langle (x - x_0)^2 \rangle - \langle x - x_0 \rangle^2}$. How does it depend on temperature?