Brownian simulation results

Iraj Eshghi

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I. SET-UP

We have an overdamped Langevin equation for the positions of our particles. $\{x_1, x_2\}$ at respective temperatures $\{T_1, T_2\}$:

$$\gamma x_1 = -k(x_1 - x_2) - \partial_x \phi(x_1) + \sqrt{2\gamma T_1}\xi$$

$$\gamma x_2 = -k(x_2 - x_1) - \partial_x \phi(x_2) + \sqrt{2\gamma T_2}\xi$$

Where ϕ is a periodic potential such that $\phi(x + 10) = \phi(x)$, of a sawtooth shape so that

$$\phi(x) = x/9 \text{ if } 0 < x \leq 9, \quad \phi(x) = -x \text{ if } 9 < x \leq 10$$

We also consider ξ to be delta-correlated with mean of 0 and variance 1

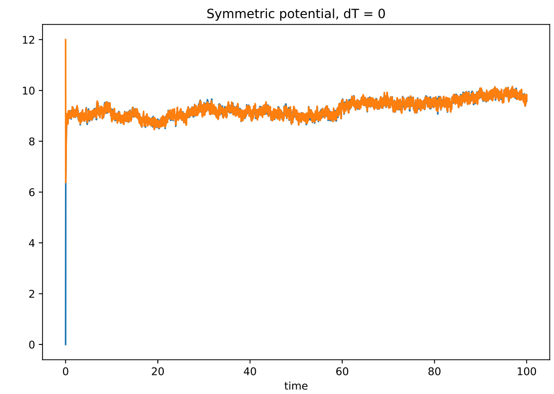
To time-evolve this, we use a simple RK4 scheme. We plug in some values for the parameters that we found were convenient when simulating: $T_1 = 1, \quad T_2 = 1 + \delta T, \quad \gamma = 0.01, \quad k = 1$. To guarantee that the particles never jumped from tooth to tooth in the potential, since the resolution of the potential (size of the smallest section of constant force) is of length 1, and we want the particle to feel it, we choose $\delta t = 0.001$.

II. TESTS

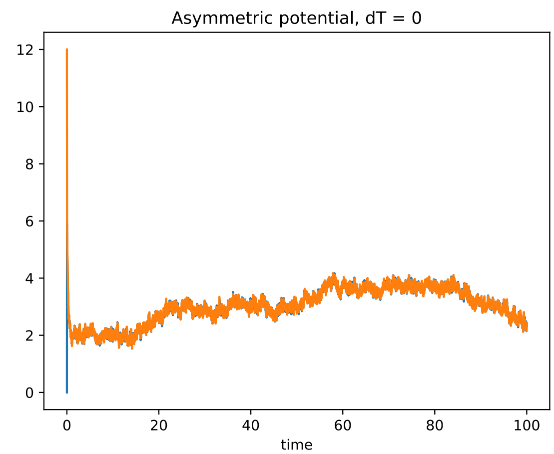
The first test was to establish there was no net drift if the particle was at equilibrium ($\delta T = 0$), and in a symmetric potential. To make the potential symmetric we define

$$\phi_s(x) = x/5 \text{ if } 0 < x \leq 5, \quad \phi_s(x) = -x/5 \text{ if } 5 < x \leq 10$$

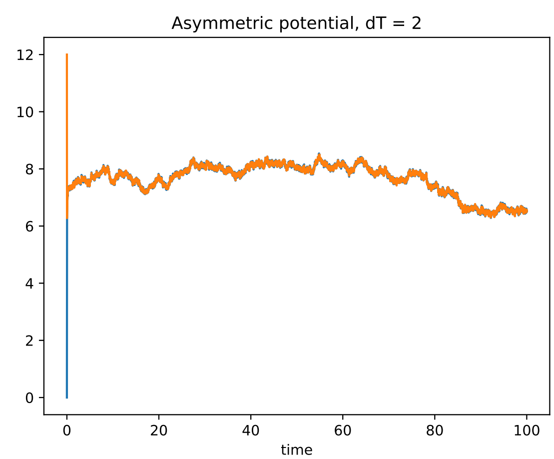
. We start particles at positions $x_1 = 1000, x_2 = 1012$ because for some reason the simulation behaves oddly around the origin (an issue worth exploring). We plot the position of the particles as a function of time with respect to $x = 1000$. The data in Figure 1 is averaged over $N = 100$ particles.



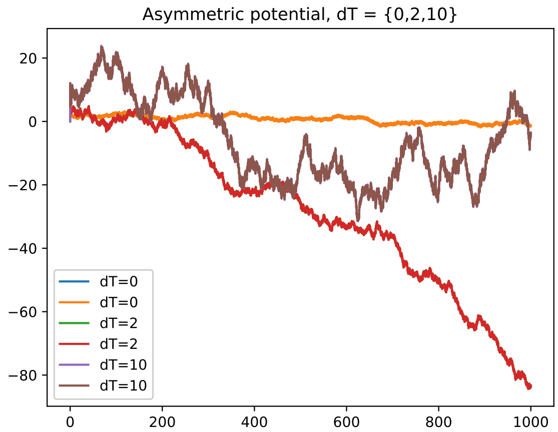
We then repeated the same experiment with the asymmetric potential, and observed the same no-drift average motion.



Finally, we also tested the symmetric potential with $\delta T = 2$, to check that non-equilibrium dynamics produce no drift if the potential is symmetric.



Again, it is visible that there is no drift here. Next, we moved back to an asymmetric potential and this time applied a temperature difference between the thermostats, $\delta T = 2, 5, 10$.



We observe here something interesting. There is a clear change of regime between $\delta T = 0$ and $\delta T = 2$, where the nonequilibrium situation produces obvious drift. However, the $\delta T = 10$ system seems to be moving around randomly with no clear direction. This could be because the temperature is high enough that the particles don't even feel the potential significantly anymore. Or it could be because the larger amount of noise requires that we give more statistics, or some combination of both.

III. ADDING A UNIFORM FIELD

If we now assume the system is given an extra linear potential, like a constant electric field or the influence of gravity, we can see if the heat engine can perform work with or against this force.

We add the a constant term to the force law described in the "set-up" section, as follows:

$$\gamma x_1 = -k(x_1 - x_2) - \partial_x \phi(x_1) + \sqrt{2\gamma T_1}\xi - g$$

And identically for particle 2.

We first reproduced the results from the previous part for a temperature difference $\delta T = 2$. We saw the same trend, using this time 20 walkers over the same time. Then, we applied a field and tuned temperature to 0. To get a similar amount of deviation in the same amount of time, it took a field of about $g = -0.02$. The negative sign is there to guarantee the field will go in the opposite direction to the walkers once their temperature difference is turned on again.

Then we turned on the temperature difference again. The interesting thing that happened here is that when the field is set at $g = -0.02$ with $\delta T = 2$, we actually first see a *stronger* deviation in the direction of the applied field. We suppose that this is because the higher temperature on one of the beads is getting the device unstuck from minima easier, thus allowing for easier drift for the system under a constant force. So we had to tune down the field to $g = -0.003$ before we recovered a no-drift situation.

We tried slightly different values of δT, but they didn't seem to produce stronger drift or be better at opposing the applied field. So we suppose that the strength of the heat engine might be determined by the potential rather than the temperature difference? This is still a question worth exploring.