
The following method is based on “Simulation of a Brownian particle in an optical trap” by Giorgio Volpe and Giovanni Volpe.
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Brownian Motion Simulation: Working Principle

To simulate confined Brownian motion, we numerically compute a solution to the Langevin equation (with confinement):

$$F = m\ddot{x}(t) = -\gamma\dot{x}(t) - k_{sp}x(t) + \sqrt{2k_B T \gamma}W(t) \quad (1)$$

where $W(t)$ is white noise: effectively a random number with a probability distribution given by a normal distribution with a standard deviation of $1/\Delta t$. k_B is the Boltzmann constant, T is the temperature in Kelvin, k_{sp} is the spring constant of your trap, and γ is friction coefficient which is related to the diffusion coefficient, D , by $D\gamma = k_B T$.

In order to numerically compute this solution, we plan to take steps of size Δt and compute the new position after each step. We do the following substitutions:

- $x(t) \rightarrow x_i$.
- $\dot{x}(t) \rightarrow \frac{x_i - x_{i-1}}{\Delta t}$.
- $\ddot{x}(t) \rightarrow \left[\frac{x_i - x_{i-1}}{\Delta t} - \frac{x_{i-1} - x_{i-2}}{\Delta t} \right] / \Delta t = \frac{x_i - 2x_{i-1} + x_{i-2}}{\Delta t^2}$
- $W(t) \rightarrow W_i$

Now, we can write out the discretized Langevin equation:

$$m \frac{x_i - 2x_{i-1} + x_{i-2}}{\Delta t^2} = -\gamma \frac{x_i - x_{i-1}}{\Delta t} + \sqrt{2k_B T \gamma} W_i \quad (2)$$

Solving for x_i , we find:

$$\begin{aligned} x_i &= -\frac{1}{1 + \frac{\gamma}{m}\Delta t + \frac{k}{m}\Delta t^2} x_{i-2} + \frac{2 + \frac{\gamma}{m}\Delta t}{1 + \frac{\gamma}{m}\Delta t + \frac{k}{m}\Delta t^2} x_{i-1} + \frac{\sqrt{2k_B T \gamma} \Delta t^2 W_{i-1}}{m \left(1 + \frac{\gamma}{m}\Delta t + \frac{k}{m}\Delta t^2 \right)} \\ &= -\frac{1}{1 + \tau \Delta t + \omega^2 \Delta t^2} x_{i-2} + \frac{2 + \tau \Delta t}{1 + \tau \Delta t + \omega^2 \Delta t^2} x_{i-1} + \frac{\sqrt{2k_B T \gamma} \Delta t^2 W_{i-1}}{m (1 + \tau \Delta t + \omega^2 \Delta t^2)} \end{aligned} \quad (3)$$

where τ is the momentum relaxation time (i.e. the time it takes for the velocity autocorrelation function to decay) and ω is the angular frequency of the mass spring system with the particle mass and trap spring constant.

Now that we have equation 3, we can create the following procedure:

- Set $x_0 = x_1 = 0$.
- Create an initial random kick W_1 .

↪ **Loop starts here!**

- Use equation 3 to create a new position x_i based on x_{i-1} , x_{i-2} , and W_{i-1} .
- Generate a new random push W_i .

↪ **Repeat loop for the desired number of iterations**