Exercise 1

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Diffusion equation

During the first lecture, we derived the Diffusion equation for the one-dimensional Brownian motion

$$\frac{\partial f(x,t)}{\partial t} = D\frac{\partial^2 f(x,t)}{\partial x^2}\,, \tag{1}$$

where $f(x,t)$ is a density function that describes the time-evolution of a Brownian particle (e.g. a pollen grain suspended in a liquid) and D is the diffusion constant. The solution of the diffusion equation is the Gaussian function

$$f(x,y) = \frac{1}{\sqrt{4\pi D}}\exp\left(-\frac{x^2}{4Dt}\right)\,. \tag{2}$$

Theoretical exercise

- Solve eq. 1 and derive eq. 2. Hint: use the Fourier transform method.
- Calculate the average position $\langle x\rangle$ of a particle from $f(x,t)$.
- Calculate the average displacement $\sqrt{\langle x^2\rangle}$ from $f(x,t)$.

Numerical exercise

Using your favorite programming language:

- Write a program to plot eq. 2.
- Write a program that simulates the one-dimensional Brownian motion.
  Hint: Trajectories that simulate the Brownian motion can be generated using the Euler-Maruyama scheme:

  $$x_{k+1} = x_k + \sqrt{2D\,\tau}\,\eta\,, \tag{3}$$

  where x_k denotes the position of the particle at time $t = k\cdot\tau$, x_{k+1} denotes the position of the particle at time $t = k\tau+\tau$, τ is a small timestep and η is a random number drawn from a standard normal distribution $\mathcal{N}(0,1)$.
- Generate a large number of trajectories, and build the time-evolution distribution using the histogram function.
- Compare the results from your numerical experiment with the analytical solution.
- Stress your program by changing the input parameters, and test the conditions under which the analytical solution accurately reproduces the numerical results.