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E4 Brownian motion and the Fokker-Planck equation

Here you will implement an algorithm for Brownian dynamics simulation, using random numbers from a Gaussian distribution and solve for two cases which has been measured experimentally.

Langevin's equation

Consider the motion of a heavy particle, a Brownian particle, immersed in a fluid, the solvent. Assume that the particle is hold in place by a trap, *e.g.* an optical trap created by laser beams. For simplicity consider motion in one dimension and assume that the trap can be described by an harmonic potential well

$$V(x) = \frac{k}{2}x^2 = \frac{m\omega_0^2}{2}x^2$$

The force on the particle can be split into the restoring force

$$F^{ext}(t) = -kx(t)$$

a smooth friction term $-m\eta v(t)$, which is assumed to be proportional to the velocity of the particle, and a rapidly fluctuating force $F^{st}(t) = m\xi(t)$, a stochastic force. The two latter forces both arise from the collisions of the individual solvent molecules. The equation of motion, the Langevin's equation, is then given by

$$\frac{d}{dt}x(t) = v(t) \tag{1}$$

$$\frac{d}{dt}v(t) = -\omega_0^2 x(t) - \eta v(t) + \xi(t) \tag{2}$$

where $\xi(t)$ is a Gaussian random process with

$$\langle \xi(t) \rangle = 0$$

and

$$\left\langle \xi(t)\xi(t') \right\rangle = 2\eta \frac{k_B T}{m} \delta(t - t')$$

Fokker-Planck equation

The corresponding equation for the probability distribution function $f(x, v, t)$ is the Fokker-Planck equation

$$\left[\frac{\partial}{\partial t} + v\frac{\partial}{\partial x} - \omega_0^2 x \frac{\partial}{\partial v} \right] f(x, v, t) = \eta \frac{\partial}{\partial v} \left[v + \frac{k_B T}{m} \frac{\partial}{\partial v} \right] f(x, v, t) \tag{3}$$

This is a partial differential equation. By solving the Langevin's equation we get information on the trajectory of the particle. This can be used to solve the Fokker-Planck equation by generating a lot of trajectories and then taking an average.

Measurements

The instantaneous velocity of a Brownian particle has been measured with a resolution such that both the ballistic and diffusive regime of the Brownian motion could be detected (Li *et al.*, Science **328**, 1673 (2010)). They studied the motion of a silica particle with the size of about one μm in diameter. If it is dissolved in a liquid the motion becomes too overdamped and therefore they considered air as the solvent, which has a much lower viscosity. The managed to trap and monitor the motion of the silica particles using optical tweezers. Long-duration, ultra-high resolution measurements where performed over a wide range of air pressures and at room temperature.

Task

1. Consider the motion of the silica (SiO_2) particles studied by Li *et al.* (Science **328**, 1673 (2010)). The particles have a diameter of 2.79 μm in average and their density is ρ=2.65 g/cm^3. The measurements where performed at room temperature (297 K) and at two different pressures, 99.8 kPa and 2.75 kPa. They obtained the relaxation times τ=48.5 μs and τ=147.3 μs, respectively. The relaxation time is related to the friction coefficient η, introduced in the Langevin's equation, via $\tau = 1/\eta$. The viscosity of air is $\nu = 18.6$ μNsm^{-2} at 25 °C and at normal pressure 101 kPa. Is this consistent with the Stokes law from macroscopic hydrodynamics? (0p)

2. You are now asked to simulate the motion of the Brownian particle. You should use the **Algorithm BD3** in the Lecture notes "Brownian motion". You should consider two cases defined by the two different relaxation times,

$$\begin{aligned} \text{A: } \tau &= 48.5\ \mu\text{s} \\ \text{B: } \tau &= 147.3\ \mu\text{s} \end{aligned}$$

For each case you should generate trajectories with the initial conditions

$$\begin{aligned} x(0) = x_0 &= 0.1\ \mu\text{m} \\ v(0) = v_0 &= 2.0\ \mu\text{m/ms} \end{aligned}$$

The trap generates a harmonic potential well with a vibrational frequency of about $f_0 = 3$ kHz for the Brownian particle. Use this value

for both case A and case B. Notice that the frequency is the ordinary frequency, not the angular frequency.

Generate first 5 trajectories for each case A and B. Plot the result for $x(t)$ and $v(t)$ as function of time. Generate then many trajectories and determine the averages

$$\begin{aligned}
\mu_x(t) &= \langle x(t) \rangle \\
\sigma_x^2(t) &= \left\langle [x(t) - \langle x(t) \rangle]^2 \right\rangle \\
\mu_v(t) &= \langle v(t) \rangle \\
\sigma_v^2(t) &= \left\langle [v(t) - \langle v(t) \rangle]^2 \right\rangle
\end{aligned}$$

and plot the result for the mean values $\mu_{x,v}(t)$ and plus-minus one standard deviation $\sigma_{x,v}(t)$ for the two different cases together with the 5 different trajectories. Do you obtain what you expect? (3p)

3. Determine now the probability distribution function $f(x, v, t)$, based on the generated trajectories. Plot the result for

$$\begin{aligned}
\rho_x(x, t_i) &= \int f(x, v, t_i) dv \\
\rho_v(v, t_i) &= \int f(x, v, t_i) dx
\end{aligned}$$

for a few different well chosen times t_i. Do you obtain what you expect? In particular, what do you obtain for the largest time? (1p)