

Here, we show how to solve the stochastic differential equation corresponding to a free Brownian particle without having to resort to stochastic Itô calculus. Note that the treatment will not be entirely mathematically rigorous, but it should suffice for the purposes of deriving the BAOAB integrator. So, consider the stochastic differential equation

$$\dot{p} = -\gamma p + \sigma \eta(t) \quad (1)$$

where p is the momentum of the particle, γ is the friction, $\sigma = \sqrt{2\gamma k_B T}$, and $\eta(t)$ is a Gaussian random process applied at time t . Recall that, by definition, the following conditions are satisfied

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

$$\langle p(0)\eta(t) \rangle = 0$$

$$\langle \eta(t)\eta(t') \rangle = \delta(t - t') \quad (2)$$

Since the random force is meant to be applied as random “kicks” in infinitesimal time intervals Δt , a more rigorous way to write the stochastic differential equation is in differential form:

$$dp = -\gamma p dt + \sigma d\eta(t) \quad (3)$$

where $d\eta(t)$ indicates a random kick applied in an infinitesimal interval dt centered on t . However, suppose, for the moment, that we were to treat $\eta(t)$ as a continuous, deterministic process. In this case, the solution of the first-order equation is straightforward to derive for a given initial momentum $p(0)$:

$$p(t) = p(0)e^{-\gamma t} + \sigma \int_0^t d\tau \eta(\tau) e^{-\gamma(t-\tau)} \quad (4)$$

This is not the correct solution for a stochastic equation with a Gaussian random process, but we can be guided by its form to help us create an *ansatz* for the stochastic equation. First, if we evaluate this for $t = \Delta t$, where Δt is the time step of a numerical simulation, the solution would be

$$p(\Delta t) = p(0)e^{-\gamma \Delta t} + \sigma \int_0^{\Delta t} d\tau \eta(\tau) e^{-\gamma(\Delta t-\tau)} \quad (5)$$

and the (not so rigorous) assumption we will make is for small enough Δt , $\eta(\tau)$ does not undergo any discontinuous change so that the integral involving $\eta(\tau)$ can be performed. With this in mind, let us take a solution of the form

$$p(\Delta t) = p(0)e^{-\gamma \Delta t} + r\Sigma(\Delta t) \quad (6)$$

where r is a Gaussian random number of zero mean and unit width, and $\Sigma(t)$ is an unknown function of time we need to determine at $t = \Delta t$. We interpret $\Sigma(\Delta t)$ as a width in the sense that

$$\langle p^2(\Delta t) \rangle - \langle p(\Delta t) \rangle^2 = \Sigma^2(\Delta t) \quad (7)$$

Since $\langle r^2 \rangle = 1$, this relation can be shown by direct substitution of Eq. (6) into Eq. (7). To determine $\Sigma(\Delta t)$, let us consider an ensemble of trajectories carried out for a single step Δt described by Eq. (6) but each one starting from the exact same initial condition

$p(0)$. Because the random force will be different for each trajectory, we use Eq. (5) to compute the average of $p(\Delta t)$ and $p^2(\Delta t)$ over this ensemble of trajectories:

$$\begin{aligned}\langle p(\Delta t) \rangle &= p(0)e^{-\gamma\Delta t} + \sigma \int_0^{\Delta t} e^{-\gamma(\Delta t-\tau)} \langle \eta(\tau) \rangle d\tau \\ \langle p^2(\Delta t) \rangle &= p^2(0)e^{-2\gamma\Delta t} + \frac{2\sigma}{m} \int_0^{\Delta t} p(0) \langle \eta(\tau) \rangle e^{-\gamma(\Delta t-\tau)} d\tau \\ &\quad + \sigma^2 \int_0^{\Delta t} d\tau \int_0^{\Delta t} d\tau' \langle \eta(\tau) \eta(\tau') \rangle e^{-2\gamma\Delta t} e^{\gamma(\tau+\tau')}\end{aligned}\tag{8}$$

Using Eq. (2), for $\langle p(\Delta t) \rangle$, we obtain

$$\langle p(\Delta t) \rangle = p(0)e^{-\gamma\Delta t}\tag{9}$$

and for $\langle p^2(\Delta t) \rangle$, we find

$$\begin{aligned}\langle p^2(\Delta t) \rangle &= p^2(0)e^{-2\gamma\Delta t} + \sigma^2 e^{-2\gamma\Delta t} \int_0^{\Delta t} d\tau \int_0^{\Delta t} d\tau' \delta(\tau - \tau') e^{\gamma(\tau+\tau')} \\ &= p^2(0)e^{-2\gamma\Delta t} + \sigma^2 e^{-2\gamma\Delta t} \int_0^{\Delta t} d\tau e^{2\gamma\tau} \\ &= p^2(0)e^{-2\gamma\Delta t} + \sigma^2 \frac{1}{2\gamma} e^{-2\gamma\Delta t} (e^{2\gamma\Delta t} - 1) \\ &= p^2(0)e^{-2\gamma\Delta t} + \sigma^2 \frac{1}{2\gamma} (1 - e^{-2\gamma\Delta t})\end{aligned}\tag{10}$$

From these results, if we compute $\langle p^2(\Delta t) \rangle - \langle p(\Delta t) \rangle^2$, we find

$$\langle p^2(\Delta t) \rangle - \langle p(\Delta t) \rangle^2 = \sigma^2 \frac{1}{2\gamma} (1 - e^{-2\gamma\Delta t})\tag{11}$$

which means that

$$\Sigma^2(\Delta t) = \frac{\sigma^2}{2^2\gamma} (1 - e^{-2\gamma\Delta t})\tag{12}$$

or

$$\Sigma(\Delta t) = \sigma \sqrt{\frac{1 - e^{-2\gamma\Delta t}}{2\gamma}}\tag{13}$$

so that

$$p(\Delta t) = p(0)e^{-\gamma\Delta t} + \sigma \sqrt{\frac{1 - e^{-2\gamma\Delta t}}{2\gamma}} r\tag{14}$$

Note that, as $\Delta t \rightarrow 0$, the factor multiplying the random number, r , tends to 0, which tells us that the magnitude of the “kick” depends on the size of the interval. Conversely, as we make Δt larger, the prefactor tends to $\sigma/\sqrt{2\gamma}$, independent of Δt .