General form of Langevin equation

$$\dot{x} = + \overbrace{F(x(t))}^{\text{deterministic DRIFT term}} + \underbrace{\sqrt{\epsilon}\,\eta(t)}_{\text{stochastic term}}$$

$$\langle \eta(t)\,\eta(t')\rangle = \delta(t-t')$$ dimensions of $\eta = \frac{1}{\text{time}}$

ϵ is the variance of the noise

— e.g. the momentum equation in absence of force —

$$\dot{p} = \underbrace{-\gamma p}_{\text{drift}} + \underbrace{\xi(t)}_{\text{noise}}$$

noise $\longrightarrow \sqrt{\frac{2M\gamma}{\beta}}\,\eta(t)$

— the position equation in the overdamped limit —

$\gamma \gg \gamma_{pot}$ $\quad \gamma t \gg 1$

$$\cancel{M\ddot{x}} = -M\gamma\dot{x} - \frac{\partial \tilde{V}}{\partial x} + \xi$$

$$\xi \leftarrow \sqrt{\frac{2M\gamma}{\beta}}\,\eta(t)$$

$$\dot{x} = -\frac{1}{M\gamma}\frac{\partial \tilde{V}}{\partial x} + \sqrt{\frac{2}{\beta M\gamma}}\,\eta(t)$$

in absence of potential it can be integrated to give

$$x(t) - x(0) = \sqrt{\frac{2}{\beta M\gamma}}\int_0^t dt'\,\eta(t')$$

$$\langle |x(t)-x(0)|^2\rangle = \frac{2}{\beta M\gamma}\int_0^t dt'\int_0^t dt''\,\underbrace{\langle \eta(t)\,\eta(t')\rangle}_{\delta(t-t')} = \frac{2}{\beta M\gamma}\,t$$

the long-time limit of the MSD $\quad D = \frac{k_B T}{M\gamma}$

Discretization of Langevin eq.

(how to simulate it ...)

$$\dot{x}(t) = F(x) + \sqrt{\epsilon}\,\eta(t)$$

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

infinite variance

$$X(t_{k+1}) - X(t_k) = \int_{t_k}^{t_k+\Delta t} dt'\, F(x(t')) + \sqrt{\epsilon}\,\underbrace{\int_{t_k}^{t_k+\Delta t} dt'\,\eta(t')}_{\Delta W(t_k)}$$

$$\langle \Delta W(t_k)\,\Delta W(t_\ell) \rangle = \int_{t_k}^{t_k+\Delta t} dt_1 \int_{t_\ell}^{t_\ell+\Delta t} dt_2\, \langle \eta(t_1)\,\eta(t_2) \rangle =$$

$$= \delta_{k\ell}\,\Delta t$$

$$\langle \Delta W(t_k) \rangle = 0$$

$\Delta W(t_k)$ gaussian number of variance Δt

$$X(t_{k+1}) - X(t_k) = F(x(t_k))\,\Delta t + \sqrt{\epsilon}\,\sqrt{\Delta t}\, g_k \qquad \text{(ITÔ sense)}$$

gaussian of variance 1

this is Euler's method

In W. Rüemelin SIAM J. Numer. Anal. 19, 604 (1982) has been demonstrated that for a 1-d process the step error cannot be smaller than $O(\Delta t^3)$

for an n dimensional case the highest precision is that of a simple Euler's method

The Fokker-Planck equation

given Langevin eq

$$\dot{x} = F(x) + \sqrt{\varepsilon}\,\eta(t)$$

the distribution of x $P(x,t)$ satisfies

$$\frac{\partial P}{\partial t} = \underbrace{-\frac{\partial}{\partial x}(FP)}_{\text{DRIFT}} + \underbrace{\frac{\varepsilon}{2}\frac{\partial^2 P}{\partial x^2}}_{\text{DIFFUSION}}$$

for a particle in a potential

a) $P(p, t\to\infty) \propto e^{-\beta \frac{p^2}{2M}}$

b) $P(x, t\to\infty) \propto e^{-\beta \tilde{V}(x)}$

$\beta = \frac{1}{K_B T}$ Bath Temp.

To proof let's start with the fundamental probability formula

$$P(x) = \int dy\, P_c(x|y)\, P(y)$$

prob of x

CONDITIONAL probability of X GIVEN y

prob of y

let $x = X(t+\Delta t)$

$y = X(t)$

What is the conditional probability of $X(t+\Delta t)$ given $X(t)$?

We can write

$$P_c(\overbrace{X(t+\Delta t)}^{x}|\overbrace{X(t)}^{y}) = \langle \delta(\underbrace{X(t+\Delta t) - X(t) - F(X(t))\Delta t - \sqrt{\varepsilon}\Delta W(t)}_{\text{Constraint}}) \rangle$$

Euler's scheme

$$X(t+\Delta t) - X(t) = F(X(t))\Delta t + \sqrt{\varepsilon}\Delta W(t)$$

$\langle (\ldots) \rangle$ = average over the random variables ΔW which are gaussian zero mean and variance Δt

$$P_c(x|y) = \int_{-\infty}^{+\infty} \frac{d\Delta W}{\sqrt{2\pi\Delta t}} e^{-\frac{(\Delta W)^2}{2\Delta t}} \delta(x - y - F(y)\Delta t - \sqrt{\varepsilon}\Delta W)$$

$$= \frac{1}{\sqrt{2\pi\varepsilon\Delta t}} e^{-\frac{1}{2\varepsilon\Delta t}[x-y-F(y)\Delta t]^2}$$

$$z = \frac{x-y}{\sqrt{\varepsilon\Delta t}} \qquad y = x - \sqrt{\varepsilon\Delta t}\, z$$

$$P(x, t+\Delta t) = \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} e^{-\frac{1}{2}[z - \frac{F(x-\sqrt{\varepsilon\Delta t}z)}{\sqrt{\varepsilon}}\sqrt{\Delta t}]^2} P(x - \sqrt{\varepsilon\Delta t}\, z)$$

Carefully develop the exponential and the P in Δt to get a differential equation for P

$$P(x,t+\Delta t)=\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}e^{-z^2/2}\left[P(x,t)+U(z)\sqrt{\Delta t}+W(z)\Delta t\right]$$

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$$\boxed{U(z)=-z\frac{\partial P}{\partial x}\sqrt{\varepsilon}+z\frac{F(x)}{\sqrt{\varepsilon}}P}$$

$$\boxed{W(z)=-z^2F\frac{\partial P}{\partial x}+\left(\frac{z^2}{2\varepsilon}F^2-\frac{F^2}{2\varepsilon}-z^2\frac{\partial F}{\partial x}\right)P+\frac{1}{2}\varepsilon\frac{\partial^2 P}{\partial x^2}z^2}$$

- the term in U is linear in z and vanishes once integrated
- the term in W contains only z^2 terms that gives 1 after average

$$P(x,t+\Delta t)=P(x,t)+\Delta t\int_{-\infty}^{+\infty}\frac{dz}{\sqrt{2\pi}}e^{-z^2/2}W(z)=$$

$$=P(x,t)+$$

$$+\Delta t\left[\underbrace{-F\frac{\partial P}{\partial x}+\left(\cancel{\frac{F^2}{2\varepsilon}}-\cancel{\frac{F^2}{2\varepsilon}}-\frac{\partial F}{\partial x}\right)P}_{-\frac{\partial}{\partial x}(FP)}+\frac{1}{2}\varepsilon\frac{\partial^2 P}{\partial x^2}\right]$$

$$\boxed{\frac{\partial P}{\partial t}=-\frac{\partial}{\partial x}(FP)+\frac{\varepsilon}{2}\frac{\partial^2}{\partial x^2}P}$$

Fokker-Planck equation for additive state independent noise → Gardiner

Equilibrium distribution of the ~~velocity~~ position from F-P equation

overdamped equation for the position
(Meets diffusion at long times)

$$\dot{x} = -\frac{1}{M\gamma}\frac{\partial \tilde{V}}{\partial x} + \sqrt{\frac{2}{\beta M\gamma}}\,\eta(t)$$

$$\langle \eta(t)\,\eta(t')\rangle = \delta(t-t') \qquad \varepsilon = \frac{2}{\beta M\gamma}$$

Stationary Solution of F-P Eq

$$\cancel{\frac{\partial P}{\partial t}} = -\frac{\partial}{\partial x}(FP) + \frac{\varepsilon}{2}\frac{\partial^2 P}{\partial x^2}$$

$$F = -\frac{\partial V}{\partial x}$$

$$-\frac{\partial}{\partial x}(FP) = \frac{\partial}{\partial x}\left(\frac{\partial V}{\partial x}P\right) = V''P + V'P'$$

$$V''P + V'P' + \frac{\varepsilon}{2}P'' = 0$$

$$P(x) = f(V(x))$$

$$P' = \cancel{f'}\frac{\partial f}{\partial V}V'$$

$$P'' = \frac{\partial^2 f}{\partial V^2}(\cancel{V'}V')^2 + \frac{\partial f}{\partial V}V''$$

$$\frac{\varepsilon}{2}\left(\frac{\partial^2 f}{\partial V^2}(V')^2 + \frac{\partial f}{\partial V}V''\right) + (V')^2\frac{\partial f}{\partial V} + V''f = 0$$

- $\frac{\varepsilon}{2}\frac{\partial^2 f}{\partial V^2} = -\frac{\partial f}{\partial V}$
- $\frac{\varepsilon}{2}\frac{\partial f}{\partial V} = -f$ not independent

$$\boxed{f(V) = e^{-\frac{2}{\varepsilon}V}\,\mathcal{N}}$$

Stationary solution of FP Equation

normalisation constant

$$V = \frac{\tilde{V}}{M\gamma} \qquad \varepsilon = \frac{2}{\beta M\gamma}$$

$$\frac{2}{\varepsilon}V = \beta \cancel{M\gamma}\frac{\tilde{V}}{\cancel{M\gamma}} \qquad P(x, t\to\infty) \propto e^{-\beta\tilde{V}(x)}$$

Stationary distribution of the velocities

$$\dot{p} = -\gamma p + \sqrt{\frac{2M}{\beta}}\gamma\,\eta(t)$$

$$\varepsilon = \frac{2M}{\beta}\gamma$$

$$F(p) = -\gamma p$$

$$V(p) = \frac{\gamma p^2}{2}$$

$$P(p) \propto e^{-\underbrace{\frac{2\beta}{2M\gamma}}_{\frac{2}{\varepsilon}}\underbrace{\frac{\gamma}{2}p^2}_{V}} = e^{-\beta\frac{p^2}{2M}}$$

Maxwell's distribution