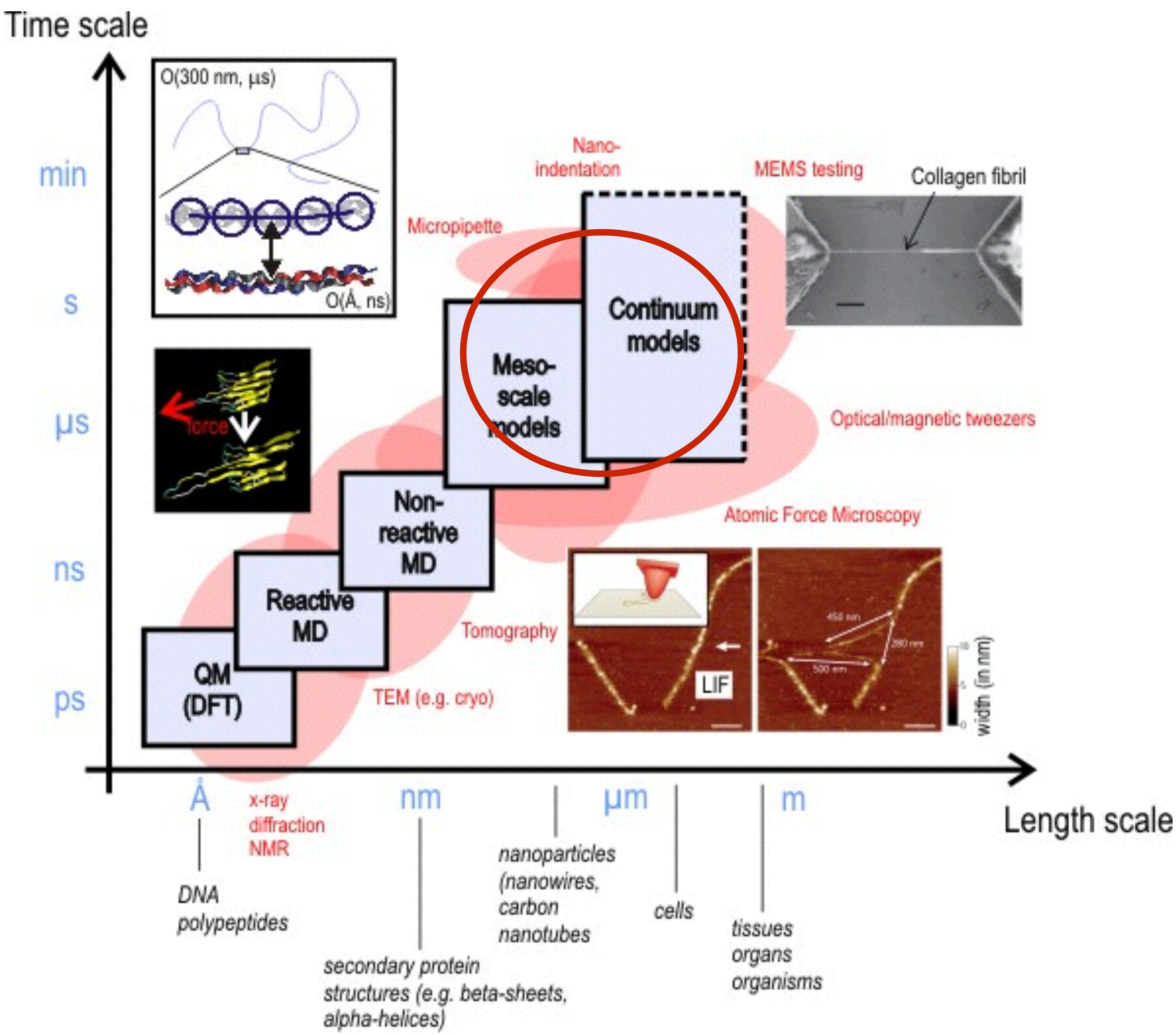
Brownian motion (cont.)

18.S995 - L03



http://web.mit.edu/mbuehler/www/research/f103.jpg

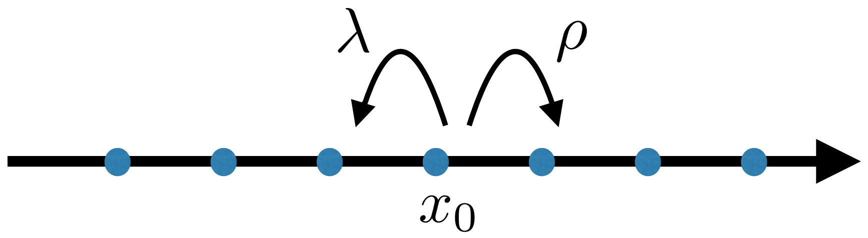
Basic idea

Split dynamics into

- deterministic part (drift)
- random part (diffusion)

$$\dot{x} = f(t, x(t)) + \text{noise} \qquad \text{SDE}$$

$$\partial_t p = -u\,\partial_x p + D\,\partial_{xx} p \qquad \text{PDE}$$



1.1.2 Biased random walk (BRW)

$$P(t+\tau, x) = (1-\lambda-\rho)\, P(t,x) + \rho\, P(t, x-\ell) + \lambda\, P(t, x+\ell). \tag{1.15}$$

Technically, ρ, λ and $(1-\lambda-\rho)$ are the non-zero-elements of the corresponding transition matrix $W = (W_{ij})$ with $W_{ij} > 0$ that governs the evolution of the column probability vector $P(t) = (P_j(t)) = (P(t,y))$ by

$$P_i(t+\tau) = W_{ij} P_j(t) \tag{1.16a}$$

or, more generally, for n steps

$$P(t+n\tau) = W^n P(t). \tag{1.16b}$$

The stationary solutions are the eigenvectors of W with eigenvalue 1. To preserve normalization, one requires $\sum_i W_{ij} = 1$.

Continuum limit Define the density $p(t,x) = P(t,x)/\ell$. Assume τ, ℓ are small, so that we can Taylor-expand

$$\begin{aligned} p(t+\tau,x) &\simeq p(t,x) + \tau\partial_t p(t,x) && (1.17a) \\ p(t,x\pm\ell) &\simeq p(t,x) \pm \ell\partial_x p(t,x) + \frac{\ell^2}{2}\partial_{xx}p(t,x) && (1.17b) \end{aligned}$$

Neglecting the higher-order terms, it follows from Eq. (1.15) that

$$\begin{aligned} p(t,x) + \tau\partial_t p(t,x) \simeq\; & (1-\lambda-\rho)\, p(t,x) + \\ & \rho\,[p(t,x) - \ell\partial_x p(t,x) + \frac{\ell^2}{2}\partial_{xx}p(t,x)] + \\ & \lambda\,[p(t,x) + \ell\partial_x p(t,x) + \frac{\ell^2}{2}\partial_{xx}p(t,x)]. \end{aligned} \tag{1.18}$$

Dividing by τ, one obtains the advection-diffusion equation

$$\partial_t p = -u\,\partial_x p + D\,\partial_{xx} p \tag{1.19a}$$

with drift velocity u and diffusion constant D given by[2]

$$u := (\rho-\lambda)\frac{\ell}{\tau}\,, \qquad D := (\rho+\lambda)\frac{\ell^2}{2\tau}. \tag{1.19b}$$

Time-dependent solution

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with drift velocity u and diffusion constant D given by[2]

$$u := (\rho - \lambda)\frac{\ell}{\tau}\ , \qquad D := (\rho + \lambda)\frac{\ell^2}{2\tau}. \tag{1.19b}$$

We recover the classical diffusion equation (1.12) from Eq. (1.19a) for $\rho = \lambda = 0.5$. The time-dependent fundamental solution of Eq. (1.19a) reads

$$p(t, x) = \sqrt{\frac{1}{4\pi D t}}\exp\left(-\frac{(x - ut)^2}{4Dt}\right) \tag{1.20}$$

Remarks Note that Eqs. (1.12) and Eq. (1.19a) can both be written in the current-form

$$\partial_t p + \partial_x j_x = 0 \tag{1.21}$$

with

$$j_x = up - D\partial_x p, \tag{1.22}$$

reflecting conservation of probability. Another commonly-used representation is

$$\partial_t p = \mathcal{L} p, \tag{1.23}$$

where $\mathcal{L}$ is a linear differential operator; in the above example (1.19b)

$$\mathcal{L} := -u\,\partial_x + D\,\partial_{xx}. \tag{1.24}$$

Stationary solutions, if they exist, are eigenfunctions of $\mathcal{L}$ with eigenvalue 0.

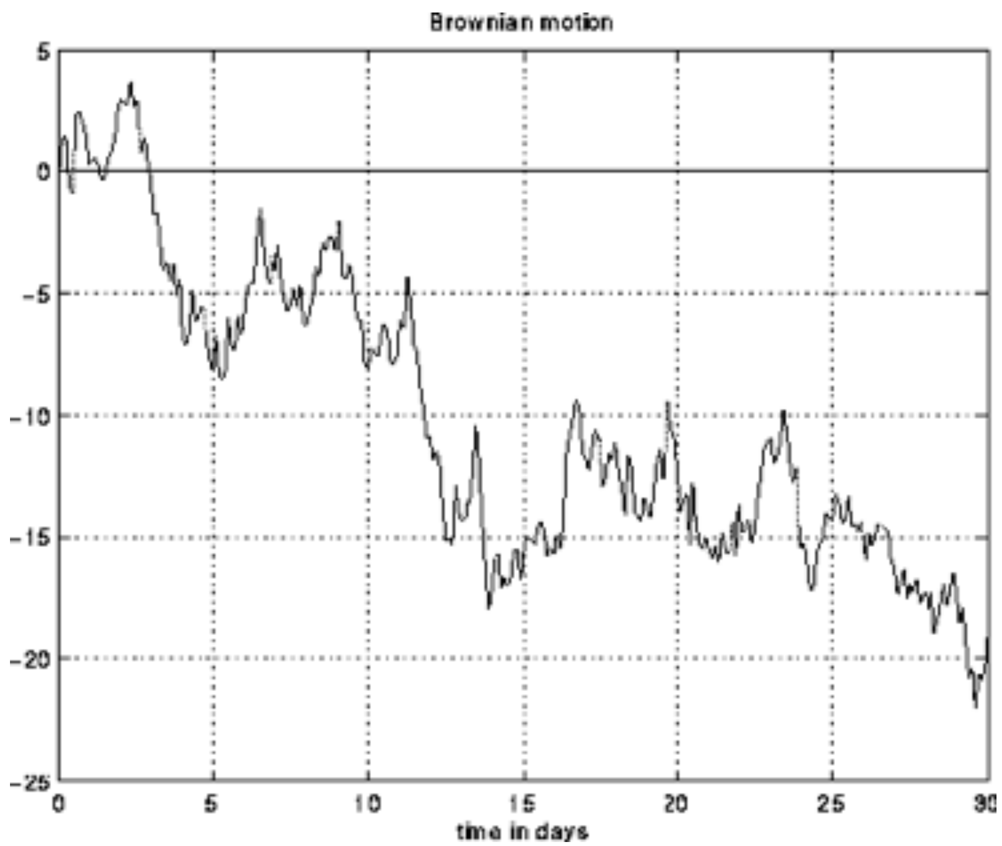
(useful later when discussing Brownian motors)

1.2 Brownian motion

Diffusion equation with constant drift

$$\partial_t p = -u\,\partial_x p + D\,\partial_{xx} p \tag{1.19a}$$

Path-wise representation of typical trajectories ?



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1.2.1 SDEs and discretization rules

The continuous stochastic process $X(t)$ described by Eq. (1.19a) or, equivalently, Eq. (1.20) can also be represented by the stochastic differential equation

$$dX(t) = u\,dt + \sqrt{2D}\,dB(t). \tag{1.25}$$

1.2 Brownian motion

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$$dX(t) = u\,dt + \sqrt{2D}\,dB(t). \tag{1.25}$$

Here, $dX(t) = X(t+dt) - X(t)$ is increment of the stochastic particle trajectory $X(t)$, whilst $dB(t) = B(t+dt) - B(t)$ denotes an increment of the standard Brownian motion (or Wiener) process $B(t)$, uniquely defined by the following properties[3]:

(i) $B(0) = 0$ with probability 1.

(ii) $B(t)$ is stationary, i.e., for $t > s \geq 0$ the increment $B(t) - B(s)$ has the same distribution as $B(t-s)$.

(iii) $B(t)$ has independent increments. That is, for all $t_n > t_{n-1} > \ldots > t_2 > t_1$, the random variables $B(t_n) - B(t_{n-1}), \ldots, B(t_2) - B(t_1)$, $B(t_1)$ are independently distributed (i.e., their joint distribution factorizes).

(iv) $B(t)$ has Gaussian distribution with variance t for all $t \in (0, \infty)$.

(v) $B(t)$ is continuous with probability 1.

The probability distribution $\mathbb{P}$ governing the driving process $B(t)$ is commonly known as the Wiener measure.

SDEs in physicist's notation

$$dX(t) = u\,dt + \sqrt{2D}\,dB(t). \tag{1.25}$$

Although the derivative $\xi(t) = dB/dt$ is not well-defined mathematically, Eq. (1.25) is in the physics literature often written in the form

$$\dot{X}(t) = u + \sqrt{2D}\,\xi(t). \tag{1.26}$$

The random driving function $\xi(t)$ is then referred to as Gaussian white noise, characterized by

$$\langle \xi(t) \rangle = 0\ , \qquad \langle \xi(t)\xi(s) \rangle = \delta(t-s), \tag{1.27}$$

with $\langle \cdot \rangle$ denoting an average with respect to the Wiener measure.

Stochastic differential calculus

$$dX(t) = u\,dt + \sqrt{2D}\,dB(t). \tag{1.25}$$

Ito's formula Note that property (iv) implies that $\mathbb{E}[dB^2] = dt$. This justifies the following heuristic derivation of Ito's formula for the differential change of some real-valued function $F(x)$

$$\begin{aligned}
dF(X(t)) &:= F(X(t+dt)) - F(X(t)) \\
&= F'(X(t))\,dX + \frac{1}{2}F''(X(t))\,dX^2 + \dots \\
&= F'(X(t))\,dX + \frac{1}{2}F''(X(t))\left[u\,dt + \sqrt{2D}\,dB\right]^2 + \dots \\
&= F'(X(t))\,dX + DF''(X(t))\,dB^2 + \mathcal{O}(dt^{3/2}); \qquad (1.28)
\end{aligned}$$

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hence, in a probabilistic sense, one has to leading order in dt

$$\begin{aligned} dF(X(t)) &= F'(X(t))\,dX + D\,F''(X(t))\,dt \\ &= [u\,F'(X(t)) + D\,F''(X(t))]\,dt + F'(X(t))\,\sqrt{2D}\,dB(t). \end{aligned} \tag{1.29}$$

It is crucial to note that, due to the choice of the expansion point, the coefficient $F'(X)$ in front of $dB(t)$ is to be evaluated at $X(t)$. This convention is the so-called Ito integration rule. In particular, it is important to keep in mind that nonlinear transformations of Ito SDEs must feature second-order derivatives.

Numerical integration

Discretization dilemma To clarify the importance of discretization rules when dealing with SDEs, let us consider a simple generalization of Eq. (1.25), where drift u and diffusion coefficient D are position dependent. Adopting the Ito convention, the corresponding SDE reads

$$dX(t) = u(X)\,dt + \sqrt{2D(X)} * dB(t), \tag{1.30a}$$

where from now on the $*$-symbol signals that $D(X)$ is to be evaluated at $X(t)$. The simplest numerical integration procedure for Eq. (1.30a) is the stochastic Euler scheme

$$X(t+dt) = X(t) + u(X(t))\,dt + \sqrt{2D(X(t))}\,\sqrt{dt}\,Z(t), \tag{1.30b}$$

$$Z(t) \sim \mathcal{N}(0,1)$$

When you see an equation like (1.30a), then always ask which discretization rule has been adopted!

Ito *vs.* backward-Ito

Compare

$$dX(t) = u(X)\,dt + \sqrt{2D(X)} * dB(t), \tag{1.30a}$$

$$X(t+dt) = X(t) + u(X(t))\,dt + \sqrt{2D(X(t))}\,\sqrt{dt}\,Z(t), \tag{1.30b}$$

with

the so-called backward Ito SDE with coefficients u_B and D_B, denoted by

$$dX(t) = u_B(X)\,dt + \sqrt{2D_B(X)} \bullet dB(t), \tag{1.31a}$$

is defined as the upper Riemann sum[6]

$$X(t+dt) = X(t) + u_B(X(t+dt))\,dt + \sqrt{2D_B(X(t+dt))}\,\sqrt{dt}\,Z(t). \tag{1.31b}$$

do NOT give same results when *dt* → *0*

Ito *vs.* backward-Ito

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For instance, the so-called backward Ito SDE with coefficients u_B and D_B, denoted by

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In particular

$$\begin{aligned} dF(X) &= F'(X) \bullet dX - D_B\,F''(X)\,dt \\ &= [u_B\,F'(X) - D_B\,F''(X)]\,dt + F'(X)\,\sqrt{2D_B} \bullet dB(t). \end{aligned} \tag{1.32}$$

Stratonovich SDE

Another discretization convention, that is popular in the physics literature is the Stratonovich-Fisk discretization, denoted by

$$dX(t) = u_S(X)\,dt + \sqrt{2D_S(X)} \circ dB(t), \tag{1.34a}$$

and defined as the mean value of lower and upper Riemann sum[8]

$$\begin{aligned} X(t+dt) \quad = \quad & X(t) + \frac{u_S(X(t)) + u_S(X(t+dt))}{2}\,dt + \\ & \frac{\sqrt{2D_S(X(t))} + \sqrt{2D_S(X(t+dt))}}{2}\,\sqrt{dt}\,Z(t). \end{aligned} \tag{1.34b}$$

From a numerical perspective, the non-anticipatory Ito scheme (1.30b) is advantageous for it allows to compute the new position directly from the previous one. For analytical calculations, the Stratonovich-Fisk scheme is somewhat preferable as it preserves the rules of ordinary differential calculus,[9]

$$dF(X) = F'(X) \circ dX(t) \tag{1.36}$$

each SDE formulation has advantages & disadvantages

Summary

Ito

$$dX(t) = u(X)\,dt + \sqrt{2D(X)} * dB(t), \qquad (1.30a)$$

$$X(t+dt) = X(t) + u(X(t))\,dt + \sqrt{2D(X(t))}\,\sqrt{dt}\,Z(t), \qquad (1.30b)$$

backward-Ito

$$dX(t) = u_B(X)\,dt + \sqrt{2D_B(X)} \bullet dB(t)$$

$$X(t+dt) = X(t) + u_B(X(t+dt))\,dt + \sqrt{2D_B(X(t+dt))}\,\sqrt{dt}\,Z(t).$$

Stratonovich

$$dX(t) = u_S(X)\,dt + \sqrt{2D_S(X)} \circ dB(t)$$

$$\begin{aligned} X(t+dt) \;&=\; X(t) + \frac{u_S(X(t)) + u_S(X(t+dt))}{2}\,dt + \\ &\quad \frac{\sqrt{2D_S(X(t))} + \sqrt{2D_S(X(t+dt))}}{2}\,\sqrt{dt}\,Z(t) \end{aligned}$$

1.2.2 Fokker-Planck equations

Since other types of SDEs can be transformed into an equivalent Ito SDE, we shall focus in this part on discussing how one can derive a Fokker-Planck equation (FPE) for the probability density function (PDF) $p(t,x)$ for a process $X(t)$ described by the Ito SDE

$$dX(t) = u(X)\,dt + \sqrt{2D(X)} * dB(t). \tag{1.37}$$

The PDF can be formally defined by

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To evaluate the rhs., we apply Ito's formula to the differential $d[\delta(X(t)-x)]$ and find

$$\begin{aligned}
\mathbb{E}[d[\delta(X-x)]] &= \mathbb{E}\big[(\partial_X\delta(X-x))\,dX + D(X)\,\partial_X^2\delta(X(t)-x)\,dt\big] \\
&= \mathbb{E}\big[(\partial_X\delta(X-x))\,u(X) + D(X)\,\partial_X^2\delta(X(t)-x)\big]\,dt.
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Here, we have used that $\mathbb{E}[g(X(t)) * dB] = 0$,

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To evaluate the rhs., we apply Ito's formula to the differential $d[\delta(X(t) - x)]$ and find

$$\begin{aligned} \mathbb{E}[d[\delta(X - x)]] &= \mathbb{E}\big[(\partial_X \delta(X - x))\,dX + D(X)\,\partial_X^2 \delta(X(t) - x)\,dt\big] \\ &= \mathbb{E}\big[(\partial_X \delta(X - x))\,u(X) + D(X)\,\partial_X^2 \delta(X(t) - x)\big]\,dt. \end{aligned}$$

Here, we have used that $\mathbb{E}[g(X(t)) * dB] = 0$.

$$\boxed{\partial_t p \;=\; \mathbb{E}\big[(\partial_X \delta(X - x))\,u(X) + D(X)\,\partial_X^2 \delta(X(t) - x)\big]}$$

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Furthermore, by recalling that

$$\partial_X \delta(X - x) = -\partial_x \delta(X - x), \tag{1.40}$$

we may write

$$\begin{aligned} \mathbb{E}[d[\delta(X - x)]] &= \mathbb{E}\big[(-\partial_x \delta(X - x))\, u(X) + D(X)\, \partial_x^2 \delta(X(t) - x)\big]\, dt \\ &= -\partial_x\, \mathbb{E}[\delta(X - x)\, u(X)]\, dt + \partial_x^2\, \mathbb{E}[D(X)\, \delta(X(t) - x)]\, dt. \end{aligned}$$

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&= -\partial_x\, \mathbb{E}[\delta(X-x)\, u(X)]\, dt + \partial_x^2\, \mathbb{E}[D(X)\, \delta(X(t)-x)]\, dt.
\end{aligned}$$

Using another property of the δ-function

$$f(y)\delta(y-x) = f(x)\delta(y-x) \tag{1.41}$$

we obtain

$$\begin{aligned}
\mathbb{E}[d[\delta(X-x)]] &= -\partial_x\, \mathbb{E}[\delta(X-x)\, u(x)]\, dt + \partial_x^2\, \mathbb{E}[D(x)\, \delta(X(t)-x)]\, dt \\
&= -\partial_x \{u(x)\, \mathbb{E}[\delta(X-x)]\}\, dt + \partial_x^2 \{D(x)\, \mathbb{E}[\delta(X(t)-x)]\}\, dt \\
&= -\partial_x \{u(x)\, p - \partial_x [D(x) p]\}\, dt.
\end{aligned}$$

$$\partial_t p \;=\; \mathbb{E}\Big[(\partial_X \delta(X-x))\,u(X) + D(X)\,\partial_X^2 \delta(X(t)-x)\Big]$$

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&= -\partial_x\,\{u(x)\,p - \partial_x[D(x)p]\}\,dt.
\end{aligned}$$

Combining this with Eq. (1.39) yields the Fokker-Planck (or Smoluchowski) equation

$$\boxed{\partial_t p = -\partial_x\,\{u(x)\,p - \partial_x[D(x)p]\}\,.} \tag{1.42}$$

Ito-FPE

$$\partial_t p = -\partial_x \left\{ u(x)\, p - \partial_x [D(x) p] \right\}$$

Backward-Ito FPE

For comparison, an analogous calculation for the backward-Ito SDE

$$dX(t) = u_B(X)\, dt + \sqrt{2D_B(X)} \bullet dB(t), \tag{1.43}$$

gives

$$\partial_t p = -\partial_x \left[u_B(x)\, p - D_B(x)\, \partial_x p \right]. \tag{1.44}$$

Compared with the Ito FPE (1.42), the diffusion coefficient D_B now enters in front of the gradient $\partial_x p$. Note, however, that the two different FPEs coincide if one identifies the coefficients as in Eq. (1.33):

$$u = u_B + \partial_x D_B, \qquad D = D_B$$