Monte Carlo Solutions to Diffusion-Like Equations:
A Practical Application of the Itô Calculus

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1.   Introduction

In the process of developing a Monte Carlo kinetic code for the acceleration and heating of ions and electrons in the solar wind, I have encountered at least two pieces of physics that are *diffusive* in velocity space. (These processes are Coulomb collisions and quasi-linear wave-particle interactions.) When modeling the evolution of individual particles, one thus needs to apply some degree of randomness to their trajectories.

These notes describe how to take a given kind of partial differential equation (usually describing diffusion, with or without advection) and derive exact rules for how to update the positions of particles in a probabilistic manner. These derivations follow, in part, the mathematical theory known as the *Itô calculus* (see, e.g., Ikeda & Watanabe 1989; Rogers & Williams 1994), but I will not attempt to use the mathematical notation (or the large number of proofs and lemmas) commonly presented in developments of this theory. This kind of theory has been applied in astronomy (Spitzer & Hart 1971; Spitzer & Thuan 1972; Yi et al. 1991) space physics (Veltri et al. 1990, 1993; Barakat & Barghouthi 1994; Barghouthi et al. 1993, 1998), and theories of quantum gravity (e.g., Rumpf 1986). An Internet search for "Ito calculus" also brings up many sites devoted to using this theory for financial modeling and the prediction of derivative prices.

None of the results in these notes can be considered "new," so if a reader wishes to cite anything in this document, I would strongly suggest either contacting me for further information or investigating the references listed above. Furthermore, the excellent textbook on partial differential equations by Guenther & Lee (1988) contains many of the results derived below.

2.   One-dimensional Diffusion Equation

Let us begin with a simple example, then generalize it in various ways in the following sections. Consider the classical one-dimensional diffusion equation,

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2} \quad , \quad \text{where} \ -\infty < x < +\infty \ , \quad t > 0 \ , \tag{1}$$

and the initial condition is specified as $f(x, t = 0) = f_0(x)$. This equation, and many others like it, can be solved by Fourier transform. For completeness let us define the Fourier transform and its inverse transform as

$$g(k) = \int_{-\infty}^{+\infty} dx \, f(x) \, e^{ikx} \tag{2}$$

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \, g(k) \, e^{-ikx} \quad . \tag{3}$$

Multiply each term in the differential equation by e^{ikx}, group the terms on one side, and integrate over all x:

$$0 = \int_{-\infty}^{+\infty} dx \, e^{ikx} \left(\frac{\partial f}{\partial t} - D\frac{\partial^2 f}{\partial x^2} \right) \tag{4}$$

$$= \frac{\partial}{\partial t} \int_{-\infty}^{+\infty} dx \, e^{ikx} f - D \int_{-\infty}^{+\infty} dx \, e^{ikx} \frac{\partial^2 f}{\partial x^2} \tag{5}$$

If we assume that both $f(x)$ and $\partial f/\partial x$ go to zero as $x \to \pm\infty$, the last term above can be evaluated by integration by parts, and the differential equation becomes

$$0 = \frac{\partial g}{\partial t} + k^2 Dg \tag{6}$$

with its corresponding transformed initial condition $g_0(k)$. This is just a first-order ordinary differential equation, with solution

$$g(k, t) = g_0(k) \, e^{-k^2 Dt} \quad . \tag{7}$$

To obtain $f(x, t)$ we perform the inverse transform of eq. (7) and obtain

$$f(x, t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \, e^{-ikx} \, g_0(k) \, e^{-k^2 Dt} \tag{8}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \, e^{-ikx - k^2 Dt} \left[\int_{-\infty}^{+\infty} dx' \, f_0(x') \, e^{ikx'} \right] \tag{9}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx' \, f_0(x') \int_{-\infty}^{+\infty} dk \, e^{-k^2 Dt + ik(x' - x)} \quad . \tag{10}$$

If $D > 0$, the integral over k is a standard form found in tables of definite integrals (often with $e^{ik(x' - x)}$ replaced by its real part $\cos[k(x' - x)]$), and the solution is expressible as

$$f(x, t) = \int_{-\infty}^{+\infty} dx' \, f_0(x') \left\{ \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x - x')^2}{4Dt} \right] \right\} \quad . \tag{11}$$

The function in curly brackets plays the same role as a Green's function in diffusion problems with a finite spatial domain.

Let us consider the evolution of a particle, in time t and space x, which obeys the diffusion equation (eq. [1]). At time $t = 0$ let us assume we know the position x_0 of the particle. Thus, $f_0(x) = \delta(x - x_0)$, the Dirac delta function. At a small increment of time in the future $t = \Delta t$, the solution $f(x, t)$ can be thought of as the *probability density* of finding the particle at any position x. Using the Dirac delta function for f_0, we obtain

$$f(\Delta x, \Delta t) = \frac{1}{\sqrt{4\pi D \, \Delta t}} \exp\left[-\frac{(\Delta x)^2}{4D \, \Delta t} \right] \quad , \tag{12}$$

where $\Delta x = x - x_0$, the incremental displacement over time-step Δt. It is trivial to confirm that f above is normalized to unity, so it is an actual probability density.

Thus, the "recipe" for updating the position of a particle (initially at x_0 and $t = 0$) is to increment x_0 by an amount

$$\Delta x = \mathcal{N}(\xi)\sqrt{2D\,\Delta t}$$

where $\mathcal{N}(\xi)$ is a random sample from a normal distribution

$$\mathcal{N}(\xi) = \frac{1}{\sqrt{2\pi}}\,e^{-\xi^2/2} \quad . \tag{13}$$

with zero mean and unit variance. It is a simple matter to transform a uniformly distributed random number (e.g., between 0 and 1 as in most computer RAN functions) into a normally distributed random number (see Press et al. 1992, and many others, for descriptions of the Box-Muller transformation).

3. One-dimensional "N-Diffusion" Equations

Let us generalize the above analysis to a class of differential equations with an arbitrary number of differentiations:

$$\frac{\partial f}{\partial t} = D\frac{\partial^n f}{\partial x^n} \quad , \tag{14}$$

with the same boundary and initial conditions as eq. (1) above. The Fourier transform and integration by parts can be done similarly to obtain the transformed differential equation

$$0 = \frac{\partial g}{\partial t} - D(-ik)^n g \tag{15}$$

with solutions

$$g(k,t) = g_0(k)\,e^{+Dt(-ik)^n} \quad . \tag{16}$$

Let us examine several specific values for n:

The advection equation ($n = 1$):

Upon performing the inverse Fourier transform of the above solution for $n = 1$, we obtain

$$f(x,t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dx'\,f_0(x')\left[\int_{-\infty}^{+\infty} dk\,e^{-ik(x-x'+Dt)}\right] \quad . \tag{17}$$

However, the quantity in square brackets above can be expressed as a form of the Dirac delta function:

$$\delta(x) = \int_{-\infty}^{+\infty} dk\,e^{-2\pi ikx} \quad . \tag{18}$$

Thus,

$$f(x,t) = \int_{-\infty}^{+\infty} dx'\,f_0(x')\,\delta(x - x' + Dt) = f_0(x + Dt) \quad , \tag{19}$$

i.e., it is an advected "copy" of the the initial condition. For our particle recipe, the initial condition is itself a delta function, so the particle displacement at a later time Δt is given deterministically by

$$\Delta x = -D\,\Delta t \quad .$$

A Kortweg-DeVries equation ($n = 3$):

The third-order version of eq. (14) is related to the Kortweg-DeVries (KdV) equation for soliton propagation in various nonlinear media (see, e.g., Webb & Zank 1992). The inverse transform of the general solution for $g(k,t)$ is

$$f(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx' \, f_0(x') \int_{-\infty}^{+\infty} dk \, \exp\left[ik(x'-x) + ik^3 Dt\right] \tag{20}$$

and the variables in the latter integration can easily be transformed into the form required for the definition of the Airy function:

$$\text{Ai}(z) \equiv \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\tau \, \exp\left[i(z\tau + \tau^3/3)\right] \ , \tag{21}$$

and

$$f(x,t) = \int_{-\infty}^{+\infty} dx' \, f_0(x') \left\{ \frac{1}{(3Dt)^{1/3}} \, \text{Ai}\left[-\frac{x - x'}{(3Dt)^{1/3}}\right] \right\} \ . \tag{22}$$

Ideally, sampling from the normalized distribution in curly brackets gives the particle update Δx. However, the Airy function exhibits negative values for some values of its argument, so it is unclear how to interpret the above quantity as a probability. (The actual KdV equation contains lower-order derivatives that may change this result and make the particle updates more straightforwardly computable.)

A hyper-diffusion equation ($n = 4$):

I will just state the result without derivation, and note that I have not checked to see if the integral over κ below corresponds to any known "special function." Note, though, that we must require $D < 0$ for this solution to converge. Defining $C \equiv -D > 0$,

$$f(x,t) = \int_{-\infty}^{+\infty} dx' \, f_0(x') \left\{ \frac{1}{2\pi(Ct)^{1/4}} \int_{-\infty}^{+\infty} d\kappa \, e^{-\kappa^4} \cos\left[\frac{\kappa(x'-x)}{(Ct)^{1/4}}\right] \right\} \ . \tag{23}$$

Like the solution to the classical ($n = 2$) diffusion equation, the above function in curly brackets is symmetric about $x = x'$ and is sharply peaked. However, it exhibits negative values—qualitatively similar to the Bessel function $J_0(x)$—thus its interpretation as a probability is questionable.

4. Useful Variable Transformations in 1D

Let us define the variables $u \equiv x - at$ and $\tau \equiv t$ and examine the behavior of $f(u,\tau)$. The original variables are expressed as

$$x = u + a\tau \ , \qquad t = \tau \ , \tag{24}$$

and the partial derivatives of f with respect to the new variables are given by

$$\frac{\partial f}{\partial u} = \frac{\partial f}{\partial x} \ , \qquad \frac{\partial f}{\partial \tau} = a\frac{\partial f}{\partial x} + \frac{\partial f}{\partial t} \ . \tag{25}$$

Thus, the standard advection equation is equivalent to

$$\frac{\partial f}{\partial \tau} = 0 \ , \tag{26}$$

which means that $f(u, \tau)$ is independent of τ, and thus is a function of u only; i.e., $f = f(x - at)$, which we essentially derived above in eq. (19) with $a = -D$.

A more interesting use of the above variables is to write the standard diffusion equation as

$$\frac{\partial f}{\partial \tau} = D\frac{\partial^2 f}{\partial u^2} \ , \tag{27}$$

for which we know the solution $f(u, \tau)$. However, this equation is equivalent to the **advection-diffusion equation** in the original variables:

$$\frac{\partial f}{\partial t} = -a\frac{\partial f}{\partial x} + D\frac{\partial^2 f}{\partial x^2} \ . \tag{28}$$

Thus, the update recipe for the advection-diffusion equation is obtainable from the simpler update recipe for $\Delta u = \Delta x - a\Delta t$, and

$$\boxed{\Delta x = a\,\Delta t + \mathcal{N}(\xi)\,\sqrt{2D\,\Delta t} \ .}$$

This expression is the most typical practical result from the Itô calculus. Further, the Itô calculus shows that, for small time steps Δt, the above update scheme is valid even for a and D being functions of x and t:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x}\left[a(x, t)f(x, t)\right] + \frac{\partial}{\partial x}\left[D(x, t)\frac{\partial f}{\partial x}\right] \ , \tag{29}$$

which is the most general form of the **Fokker-Planck equation.**

5. Multi-Dimensional Diffusion Equations

One can use multi-dimensional Fourier transforms to generalize the above 1D results to additional dimensions in the spatial coordinates (now described as a vector $\mathbf{x}$). The generalized diffusion equation for $f(\mathbf{x}, t)$ is

$$\frac{\partial f}{\partial t} = D\,\nabla^2 f \tag{30}$$

where the Laplacian operator ∇^2 is defined in m dimensions. The general solution is an m-dimensional integral over the initial condition $f_0(\mathbf{x})$, i.e.,

$$f(\mathbf{x}, t) = \int d\mathbf{x}'\, f_0(\mathbf{x}') \left\{\frac{1}{(4\pi Dt)^{m/2}}\exp\left[-\frac{|\mathbf{x} - \mathbf{x}'|^2}{4Dt}\right]\right\} \ . \tag{31}$$

If one expresses $\mathbf{x}$ in Cartesian coordinates and assumes that $f_0(\mathbf{x})$ is a separable product of functions of each coordinate, then the above solution is separable into the product of m functions each identical to eq. (11).

Thus, for a 3D diffusion equation of the form

$$\frac{\partial f}{\partial t} = D \left(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \right) \quad , \tag{32}$$

the particle updates are independent of one another and are given by

$$\boxed{\begin{aligned} \Delta x &= \mathcal{N}_1(\xi)\,\sqrt{2D\,\Delta t} \\ \Delta y &= \mathcal{N}_2(\xi)\,\sqrt{2D\,\Delta t} \\ \Delta z &= \mathcal{N}_3(\xi)\,\sqrt{2D\,\Delta t} \end{aligned}}$$

where the numerical subscripts of $\mathcal{N}(\xi)$ indicate that there should be three independent samplings of the normal distribution.

6.   Mixed Second Derivatives

Some diffusion equations contain mixed second derivatives of the form

$$\frac{\partial^2 f}{\partial x \partial y}$$

but we will restrict ourselves to a specific "parabolic" sub-class of these equations. Let us build up this type of equation by defining two new variables p and q:

$$p \equiv \frac{1}{2} \left(\frac{x}{a} - \frac{y}{b} \right) \quad , \quad q \equiv \frac{1}{2} \left(\frac{x}{a} + \frac{y}{b} \right) \tag{33}$$

with the inverse relation

$$x = a(q + p) \quad , \quad y = b(q - p) \quad . \tag{34}$$

The second derivative of f with respect to q is found to be

$$\frac{\partial^2 f}{\partial q^2} = a^2 \frac{\partial^2 f}{\partial x^2} + 2ab \frac{\partial^2 f}{\partial x \partial y} + b^2 \frac{\partial^2 f}{\partial y^2} \quad . \tag{35}$$

This allows us to solve a diffusion equation with mixed second partials of the above form, because the solution to

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial q^2} \tag{36}$$

is known. The particle updates for this equation are

$$\Delta q = \mathcal{N}(\xi)\,\sqrt{2D\,\Delta t} \tag{37}$$

$$\Delta p = 0 \tag{38}$$

which transforms to the original coordinates as

$$\boxed{\begin{aligned} \Delta x &= a\,\mathcal{N}(\xi)\,\sqrt{2D\,\Delta t} \\ \Delta y &= b\,\mathcal{N}(\xi)\,\sqrt{2D\,\Delta t} \end{aligned}}$$

Unlike the 2-dimensional diffusion equation with $\nabla^2 f$ on the right-hand side, the particle updates for Δx and Δy here are *correlated* with one another—i.e., only one sampling from the normal distribution is performed.

One can think of this particle update as diffusion in a direction which has been rotated by an angle θ from the x axis, and the angle θ is given simply $\tan^{-1}(b/a)$. This result is useful in the update of particle velocities for ions and electrons under the influence of quasi-linear wave-particle resonances.

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