Semi-stochastic simulation of Brownian motion

The aggregate behavior of many rapid collisions causes particles to move about randomly in a manner known as Brownian motion. This random movement is the underlying cause of the macroscopic phenomenon we call diffusion. After a statistically large number of fluctuations have occurred, a particle will move from the origin to a position r, θ in time interval t with probability

$$\rho(r, \theta, t) = \frac{1}{4\pi Dt} e^{-r^2/4Dt} \tag{1}$$

where D is the diffusion coefficient. This probability density is simply the solution to the diffusion equation from a point source in the r, θ plane, normalized to unity such that:

$$\int_0^{2\pi} \int_0^{\infty} \rho(r, \theta, t) r dr d\theta = 1 \tag{2}$$

Normalizing the distribution to unity shifts our point of view from *how many* particles diffuse to a radius r at time t to *how likely* it is that any one particle will move a distance r in time t.

We can simulate diffusion by using this probability distribution to move particles stochastically. Since all directions are equally likely, θ for each move can be related to a uniformly distributed random number $\mathcal{R}$:

$$\theta = 2\pi\mathcal{R} \quad 0 \leq \mathcal{R} \leq 1 \tag{3}$$

To determine the distance r moved by a particle at each step, we note that each interval $dP = \rho d\rho$ should occur with equal probability. Integrating gives a function that we can equate to a uniformly distributed random number $\mathcal{Q}$:

$$P = \frac{1}{2}\rho^2 = \frac{1}{2}\rho_{\max}^2 \mathcal{Q} \quad 0 \leq \mathcal{Q} \leq 1 \tag{4}$$

Substituting the probability density gives

$$\mathcal{Q} = \frac{\rho^2}{\rho_{\max}^2} = \left(e^{-r^2/4Dt}\right)^2 = e^{-r^2/2Dt} \tag{5}$$

which, rearranged, gives the distance of the move

$$r = \sqrt{-ln(\mathcal{Q})2Dt} \tag{6}$$

It is convenient to convert distance to velocity:

$$u_r = r/t = \sqrt{-ln(\mathcal{Q})2D/t} \tag{7}$$

This velocity can be mapped from the local polar coordinates centered on the particle to the Cartesian coordinates of the computational domain:

$$U = u_r cos(\theta), \quad V = u_r sin(\theta) \tag{8}$$

and added to the convective flow velocity during particle path integration to simulate diffusion.

In a fully stochastic method, particle velocities are updated on the time scale of thermal fluctuations to satisfy a Boltzmann probability distribution. In the semi-stochastic method described here, particle velocities are updated every t time units using the diffusion equation as a probability distribution, which is valid only if t is much longer than the fluctuation time scale. Stochastic behavior at smaller time scales is replaced by deterministic statistical behavior. To succeed there must be sufficiently many changes of directions and velocities to obtain statistically representative behavior. This can be achieved if t is much shorter than the diffusion time, essentially the same criterion that applies to the time step size when integrating the diffusion equation numerically.

Andrew Yeckel
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