Random Walks, the Diffusion Equation, and Cluster Growth

Tahoe Schrader, Ksenia , Xinmeng
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Abstract

In this assignment we blah blah blah

1 Theory

1.1 Diffusion Equations and the Finite Difference Form

The diffusion equation in $1D$ is written,

$$\frac{\partial \rho(x,t)}{\partial t} = D\nabla^2 \rho(x,t), \tag{1}$$

where D is the diffusion constant. Equation 1 is turned into an iterable form by noting: $\rho(x,t) = \rho(i\Delta x, n\Delta t) = \rho(i,n)$. This is the finite difference form[1].

After using the formal definition of derivatives and algebraically manipulating Equation 1 in the finite difference form, we get

$$\rho(i, n+1) = \rho(i,n) + \frac{D\Delta t}{\Delta x^2}\left(\rho(i+1,n) + \rho(i-1,n) - 2\rho(i,n)\right), \tag{2}$$

where Δt and Δx are the step sizes in an iteration. This solution requires knowledge of initial conditions. We must assume that the x displacement is known at times prior to and including $t_n = n\Delta t$. Two consecutive steps prior to the first unknown step is sufficient to solve such an equation.

We will use an initial density profile that is sharply peaked around $x = 0$, but extends over a few grid sites to resemble a box. This is sufficient for generating the solution to the diffusion equation. Interestingly, after a couple iterations, the box profile will diffuse into a Gaussian normal distribution. The $1D$ Gaussian normal distribution has the form,

$$\rho(x,t) = \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right), \tag{3}$$

where $\sigma(t) = \sqrt{2Dt}$.

The spatial expectation value, $\langle x(t)^2 \rangle$, of Equation 3 is equal to $\sigma(t)^2$.

2 Computations

2.1 Diffusion of a Box Density Distribution

Using the arguments in Section 1.1, we solve the $1D$ Diffusion Equation over a period of time. Five different snapshots in time were then fit against Equation **??** to show a box shaped density will eventually diffuse into a Gaussian normal distribution.

[1] The finite difference form must be used because the diffusion equation is time dependent. Therefore, a relaxation method cannot be used.