Computational Physics Group Assignment 1

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March 21, 2016

1 Introduction

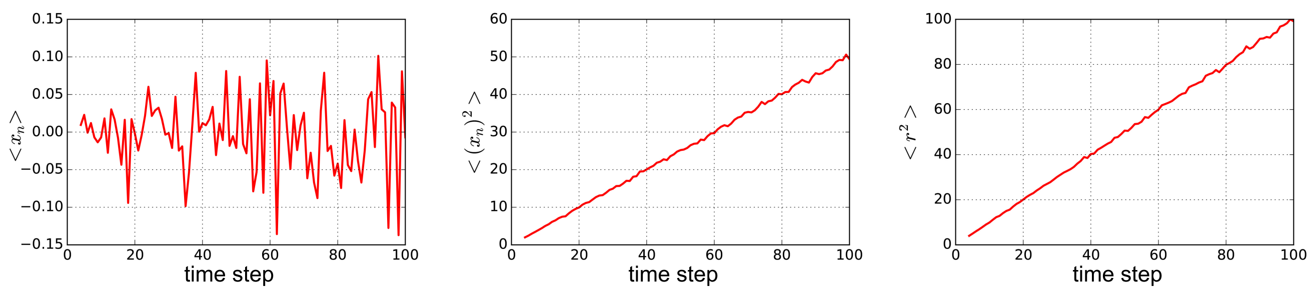
In this work, the 2D random walk, diffusion equation, and mixing of two gases are studied by Python programs.

2 2D Random Walk

A 2-dimensional random walker is a point continuously taking steps of unit length in $\pm x$ or $\pm y$ direction on a discrete square lattice. Random walkers taking up to 100 steps are simulated, then the properties of 2D random walk are investigated by averaging over 10^4 walks.

The average of x-coordinate $< x_n >$, of the square of x-coordinate $< (X_n)^2 >$, and of the square distance $< (r_n)^2 >$ of random walks with different steps are plotted in figure 1 (a), (b), and (c), respectively. $< x_n >$ oscillates around zero, consistent with the theoretical expectation. $< (x_n)^2 >$, by contrast, increases with steps with a slope of $\frac{1}{2}$.

Figure 1 (c) shows that $< (r_n)^2 >$ increases with steps as well, with a slope of 1. This can be explained by the symmetry between $< (y_n)^2 >$ and $< (x_n)^2 >$, leading the slope of $< (r_n)^2 >$ be $\frac{1}{2} + \frac{1}{2} = 1$.



(a) $< x_n >$ versus steps n

(b) $< (x_n)^2 >$ versus steps n

(c) $< (r_n)^2 >$ versus steps n

Figure 1: $< x_n >$, $< (x_n)^2 >$, and $< (r_n)^2 >$ of 2D random walk.

3 Diffusion Equation

a) Consider the 1D Normal Distribution

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

The spatial expectation value $< x^2(t) >$ can be computed by

$$
\begin{aligned}
< x^2(t) > &= \int_{-\infty}^{\infty} x^2 \rho(x,t) dt \\
&= \frac{1}{\sqrt{2\pi\sigma^2(t)}} \int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{2\sigma^2(t)}} dx \\
&= \frac{1}{\sqrt{2\pi\sigma^2(t)}} \frac{1}{2} (\sqrt{2}\sigma(t))^3 \sqrt{\pi} \\
&= \sigma^2(t)
\end{aligned}
$$

Here $\int_{-\infty}^{\infty} x^{2k} e^{-\frac{x^2}{a^2}} dx = \frac{(2k+1)!!}{(2k+1)2^k} a^{2k+1} \sqrt{\pi}$ $(k = 0, 1, 2, ...)$ is used.

b) The diffusion equation with a constant diffusion coefficient has the following form:

$$
\frac{\partial u(r,t)}{\partial t} = D \nabla^2 u(r,t) \tag{2}
$$

In one-dimensional case, equation (2) becomes

$$
\frac{\partial u(r,t)}{\partial t} = D \frac{\partial^2 u(x,t)}{\partial x^2} \tag{3}
$$

The first derivative in time and second derivative in space can be approximated by the finite difference:

$$
\begin{aligned}
\frac{\partial u(r,t)}{\partial t} &= \frac{u(x, t + \Delta t) - u(x,t)}{\Delta t} \\
\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{u(x + \Delta x, t) + u(x - \Delta x, t) - 2u(x,t)}{(\Delta x)^2}
\end{aligned}
$$

Then equation (3) can be rewritten as

$$
\frac{u(x, t + \Delta t) - u(x,t)}{\Delta t} = D \cdot \frac{u(x + \Delta x, t) + u(x - \Delta x, t) - 2u(x,t)}{(\Delta x)^2}
$$

or equivalently,

$$
u(x, t + \Delta t) = u(x,t) + D \cdot \Delta t \cdot \frac{u(x + \Delta x, t) + u(x - \Delta x, t) - 2u(x,t)}{(\Delta x)^2} \tag{4}
$$

Starting from an initial box density profile, the 1D diffusion equation (3) is numerically solved based on equation (4). The density profile at later times is plotted in figure 2. The density are normally distributed, with different standard deviation σ. The value of σ at time t can be extracted from the maximum value of density u_{max} at $x = 0$.

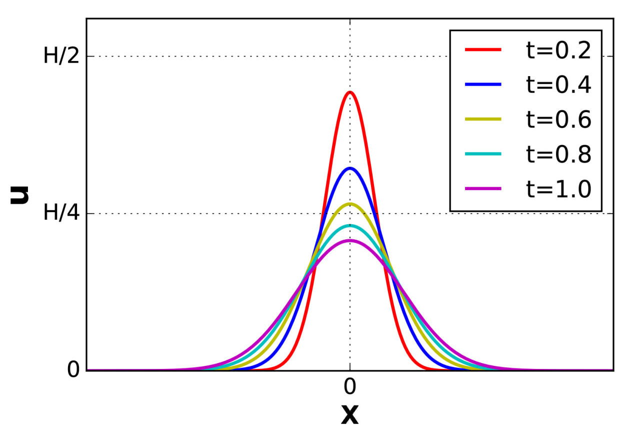


Figure 2: Solution of 1D diffusion equation at time 0, 0.2, 0.4, 0.6, 0.8, 1.0.

$$u_{max}(t) = \rho(0,t) = \frac{1}{\sqrt{2\pi\sigma^2(t)}}$$

$$\Rightarrow \sigma(t) = \frac{1}{\sqrt{2\pi u_{max}^2(t)}}$$

The maximum values u_{max} and derived *sigma* at time 0.2, 0.4, 0.6, 0.8, 1.0 are listed in table **??**. The $\sigma(t)$ versus time t is plotted (log scale) in figure 3 with a linear fit line, which has a scope of 0.478. This indicates that $\sigma(t) \propto \sqrt{t}$.

Table 1: u_{max} at time 0.2, 0.4, 0.6, 0.8, 1.0.

t	0.2	0.4	0.6	0.8	1.0
u_{max}	22.1449	16.0971	13.2666	11.5433	10.3539
σ $[\times 10^{-2}]$	1.8015	2.4783	3.0071	3.4560	3.8531

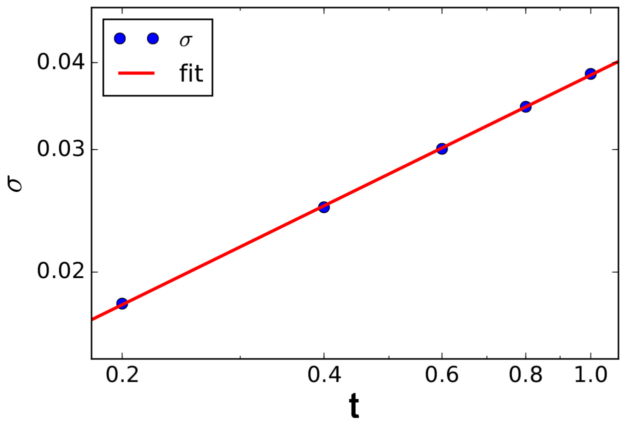


Figure 3: σ versus t (log plot).

4 Mixing of two Gases

Figure 4: Gases mixing configurations after different number of steps.

5 Conclusions

References

[1] Notes of ***Computational Physics*** by Prof. S.A. Bass.

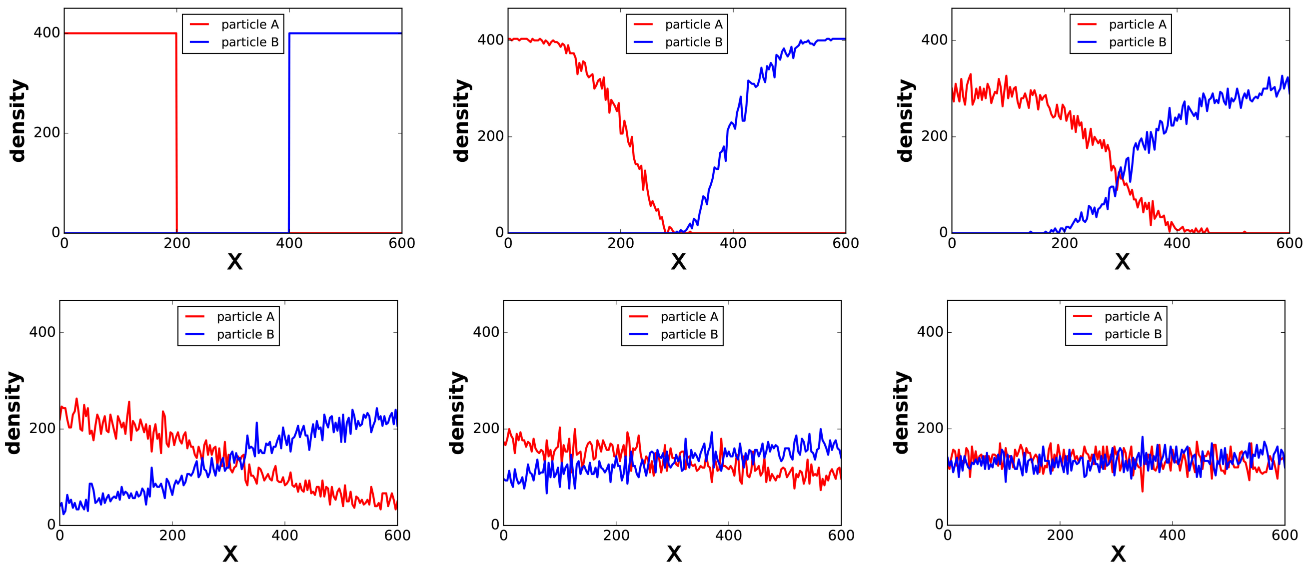


Figure 5: Linear population densities after different number of steps.

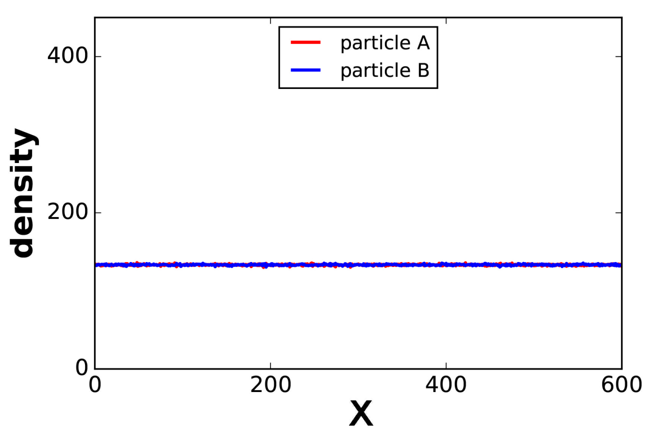


Figure 6: Linear population densities averaged over 100 trials.