PHY566 - Diffusion Equation

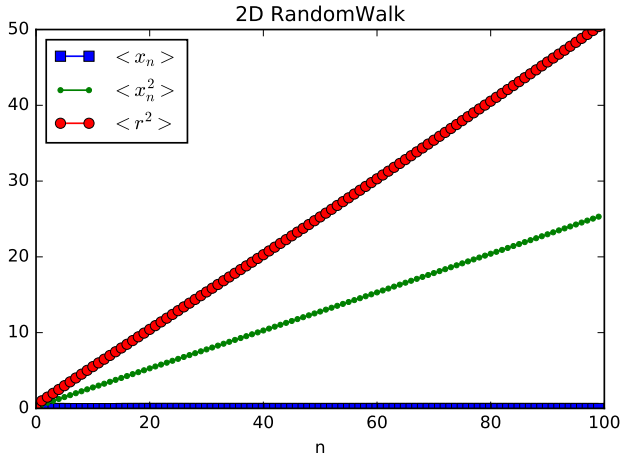
Tianyu Dai, Xiaoqing Li, Xuejian Ma, Yuheng Liao

1 Problem 1

To solve this problem, we first obtain x_n for one random walker. Put a random walker at the origin. Create a random number *movestep* in range (0,1,2,3), and these four numbers means moving one step right/left/up/down respectively.

We create a zero list to record the number of moving steps in every direction. After we know the moving direction of a step, we add the number of total steps in that certain direction by 1. If the total number of moving steps is n, we repeat the previous procedure n times. The number of total rightward steps minus the number of total leftward steps generates the x-component of the random walker's displacement, x_n. Likewise, the number of total upward steps minus the number of total downward steps generates the y-component of the random walker's displacement, y_n.

After that, x_n^2 and r_n^2 are easy to calculate. We use a function named random_walk to return the values of x_n, x_n^2, and r_n^2. Since our goal is averaging over 10^4 different walkers, we need a loop with 10^4 iterations to get the values of x_n, x_n^2, and r_n^2 of each walker, and then realize the average values, $\langle x_n \rangle$, $\langle x_n^2 \rangle$, and $\langle r_n^2 \rangle$.



2 Problem 2

2.1 Part A

To calculate $\langle x(t)^2 \rangle$, we can integrate it by part:

$$\begin{aligned}
\rho(x,t) &= \frac{1}{\sqrt{2\pi\sigma(t)^2}} exp\left(-\frac{x^2}{2\sigma(t)^2}\right) \\
\langle x(t)^2 \rangle &= \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{2\pi\sigma(t)^2}} exp\left(-\frac{x^2}{2\sigma(t)^2}\right) dx \\
\langle x(t)^2 \rangle &= \int_{-\infty}^{\infty} \sigma(t)^2 x \frac{1}{\sqrt{2\pi\sigma(t)^2}} d\left(\exp\frac{-x^2}{2\sigma(t)^2}\right) \\
\langle x(t)^2 \rangle &= \sigma(t)^2 \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma(t)^2}} exp\left(-\frac{x^2}{2\sigma(t)^2}\right) dx \\
\langle x(t)^2 \rangle &= \sigma(t)^2
\end{aligned}$$

Therefore,the spatial expectation value $\langle x(t)^2 \rangle$ of the 1D Normal Distribution equals $\sigma(t)^2$

2.2 Part B

The diffusion equation is:

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

where $D = 2$ is a diffusion constant.

For a linear diffusion equation:

$$\frac{\partial\phi(\vec{r},t)}{\partial t} = D\frac{d^2\phi(\vec{r},t)}{dx^2}$$

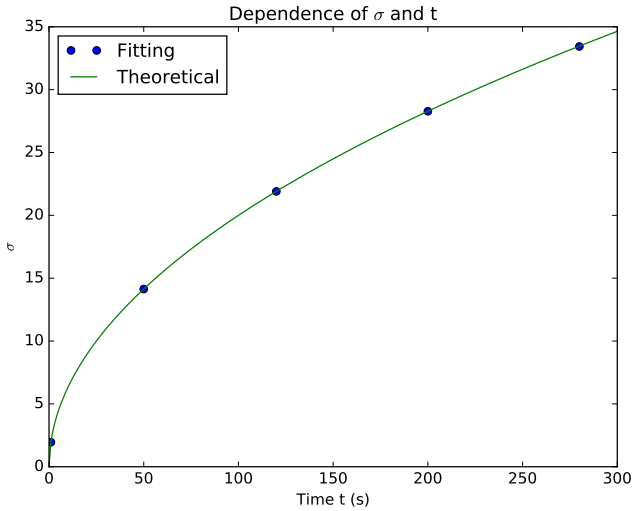
The numerical solution is:

$$\begin{aligned}
\frac{y_{j+1,i} - y_{j,i}}{\Delta t} &= D\frac{y_{j,i+1} + y_{j,i-1} - 2y_{j,i}}{\Delta x^2} \\
y_{j+1,i} &= y_{i,j} + \frac{D\Delta t}{\Delta x^2}(y_{j,i+1} + y_{j,i-1} - 2y_{j,i})
\end{aligned}$$

After getting y in each x for each time snapshot, we obtained $\sigma(t)$ by fitting it into equation:

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

We choose 5 time snapshots [1,50,120,200,280]($\Delta t = 0.01$) to get $\sigma(t)$ and plot them in following figure.



The fitting points match the analytical function perfectly.

3 Problem 3

3.1 Part A

First, we set up the initial condition by generating a matrix with 80 rows and 120 columns and assigning -1 and 1 to the first 40 columns and the last 40 columns respectively. Here, -1 means this site is occupied by a A-molecule, and 1 means it is occupied by a B-molecule. We also generate a matrix with $2 \times N$ rows and 2 columns, where N represents the number of molecules of each species.

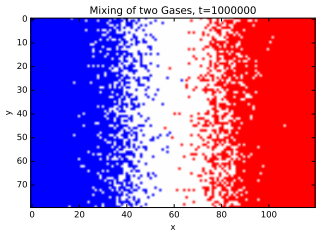
The first and second half 80×40 rows respectively record the coordinates of A molecules and B molecules. For every step, we generate a random number to decide which molecule to move in which direction. Since there are $2 \times N$ molecules and every molecule can move in up/down/left/right four different directions, we have to pick a random number, R, from the range $[0, 2 \times N \times 4 - 1]$. $m = R\%(2N)$ means the molecule decided by the random number R, and $move = R/(2N)$ means the moving direction decided by R. We can extract the coordinates of the molecule as $x = mol[m, 0]$, and $y = mol[m, 1]$. The next step is moving the picked molecule. $move = 0, 1, 2, 3$ means the moving direction is up/down/left/right, respectively.

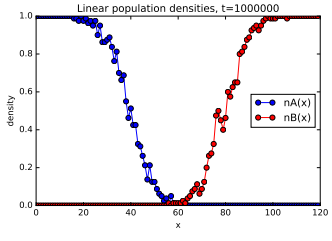
However, this grid has boundary. Specifically, a molecule on the upper side cannot move upward, a molecule on the lower side cannot move downward, a molecule on the left side cannot move leftward, and a molecule on the right side cannot move rightward. If $move = 0$, y cannot be 79, and we demand $y+1 < 80$. Then, if $sites[y + 1, x] = 0$, it means the site right above this molecule is not

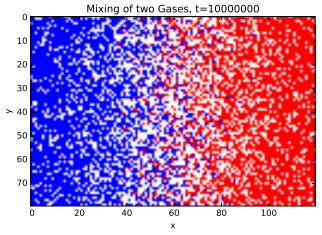
occupied and we can move the molecule to that site. After the movement, we have to update the molecule's coordinates by adding one the its y-coordinate, the update the distribution on the grid by assigning the value of $sites[y, x]$ to $sites[y + 1, x]$ and assigning 0 to $sites[y, x]$. If $move = 1$, y cannot be 0, and we demand $y - 1 > 0$, and if $sites[y - 1, x] = 0$, we move the molecule one step down and update its coordinates and the distribution. For $m = 1$ and $m = 2$, the procedure is the same.

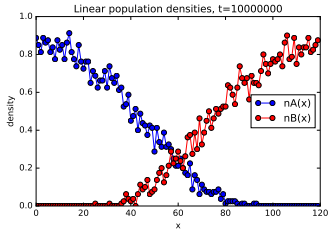
3.2 Part b

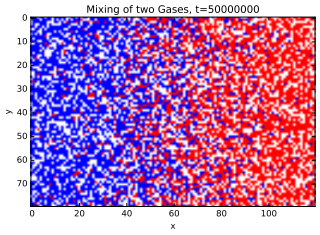
To plot the linear population densities $n_A(x)$ and $n_B(x)$, we need to know there are how many A-molecules and B-molecules on each column respectively. We use a nested loop to complete this job, the inner one is to count there are how many 1 and -1 on each column respectively. The number of 1 means the number of B-molecules, and the number of -1 means the number of A-molecules. Then record the values in two lists maned sumA and sumB. For example, if loop is running for the i^{th} column, sumA[i] is the number of A-molecules on the i^{th} column, and sumB[i] is the number of B-molecules on this column. The outer loop makes the inner one runs for each column. Finally, divide sumA[i] and sumB[i] by the length of the left or right side, 80.0, we obtain the linear population densities $n_A(x)$ and $n_B(x)$. The distribution figures and the density figures of the two gases on the grid are shown below. Here, we plot the matrix, $sites$, with imshow to generate the distribution figures.

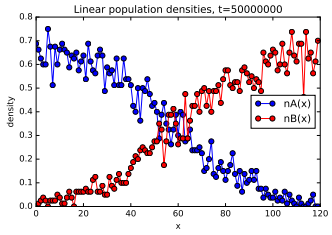


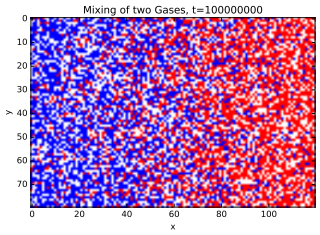


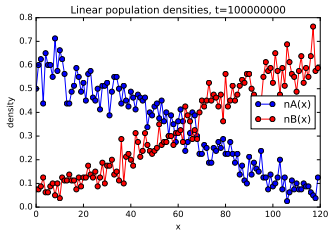


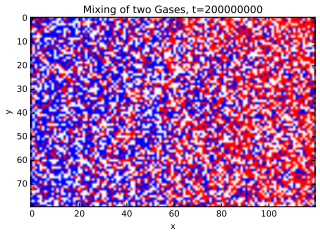


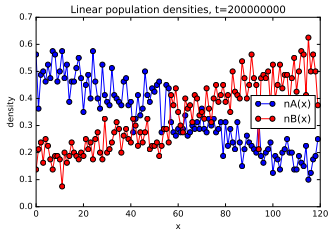

Mixing of two Gases, t=50000000
y
x

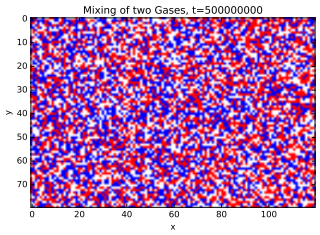

Linear population densities, t=50000000
density
x
nA(x)
nB(x)

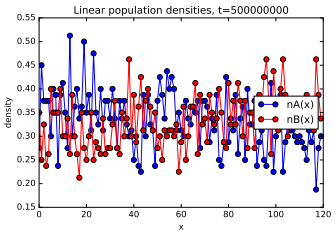

Mixing of two Gases, t=100000000
y
x


Linear population densities, t=100000000
density
x
nA(x)
nB(x)


Mixing of two Gases, t=200000000
y
x


Linear population densities, t=200000000
density
x
nA(x)
nB(x)


Mixing of two Gases, t=500000000
y
x


Linear population densities, t=500000000
density
x
nA(x)
nB(x)

3.3 Part C

To average the densities over 100 trials for added accuracy, we only need a bigger loop outside the program of part (b) to run the code 100 times average them. We make a comparison of linear population densities between one trial and the average of 100 trials as following.