PHY566 - Computational Physics
Group Project 1B

Team 2
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03/25/2016

2D Random Walker

- We begin with a program that simulates taking steps of $\pm x$ or $\pm y$ on a two dimensional square lattice.
- The simulation was run for up to 100 steps and various characteristics were examined by averaging the results for 10^4 walkers.
- The quantities of interest examined were:

1. The average of the x coordinate $\langle x_n \rangle$
2. The average of the square of the x coordinate $\langle (x_n)^2 \rangle$
3. The average of the square of the distance $\langle (r_n)^2 \rangle$

2D Random Walker

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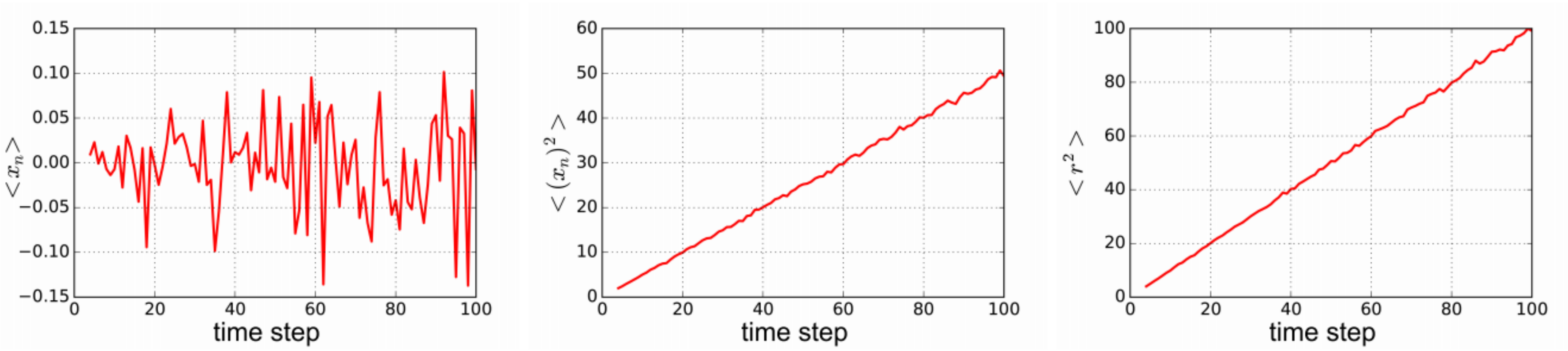
2. The average of the square of the x coordinate $<(x_n)^2>$
3. The average of the square of the distance $<(r_n)^2>$



(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.

1D Diffusion Equation

- The second problem involved simulation/solution of the 1D diffusion equation, given as the following:

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

- Or equivalently, in iterative form:

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

1D Diffusion Equation

- Starting from an initial “box” density profile, the equation was solved numerically.
- The density was then plotted at different times (t) and shown to be Gaussian.

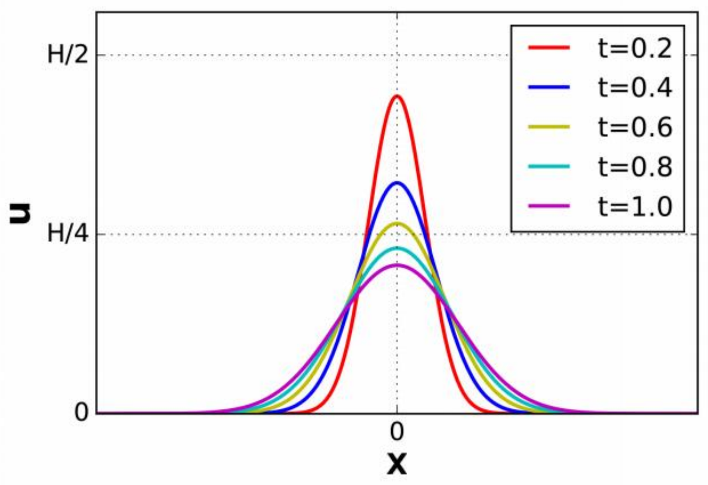


Figure 2: Solution of 1D diffusion equation at time 0, 0.2, 0.4, 0.6, 0.8, 1.0.

1D Diffusion Equation

The maximum value of u is related to the standard deviation in the following way:

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

And thus, the standard deviation can be extracted from the maximum u.

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

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This data, when plotted on a log scale, shows a linear relationship with slope ~0.5

This indicates a relationship of the standard deviation being proportional to the square root of t, as expected.

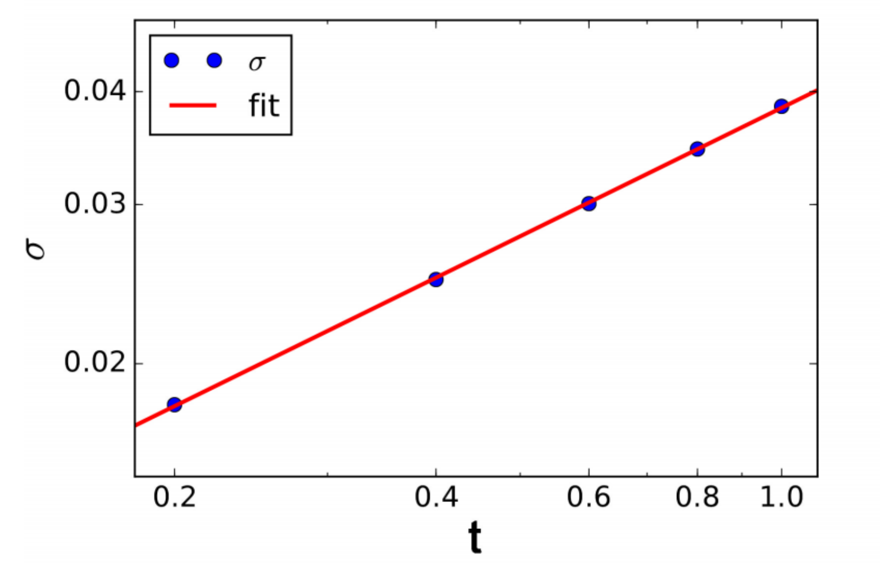

Figure 3: σ versus t (log plot).

1D Diffusion Equation

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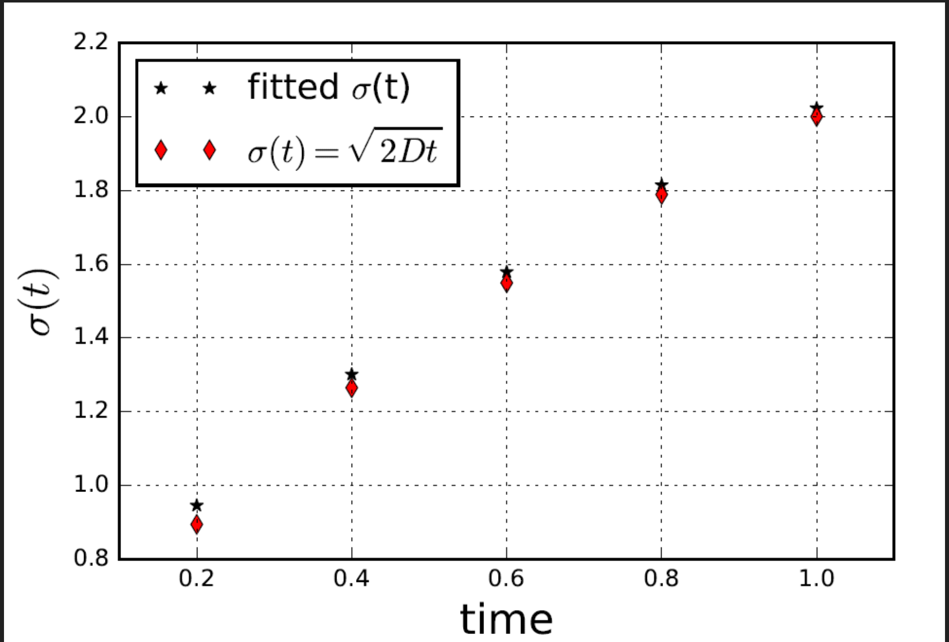
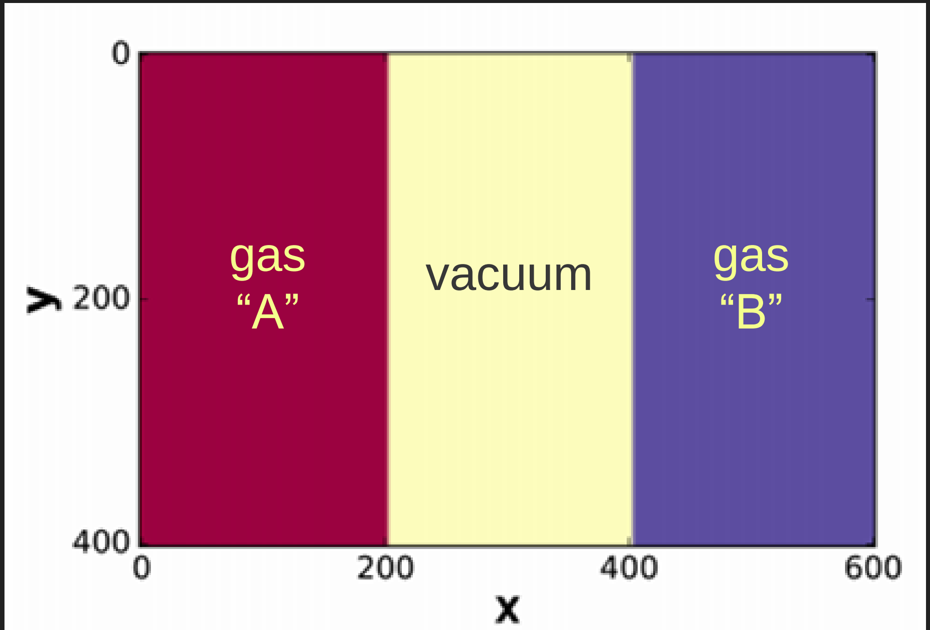
The standard deviation obtain from Gaussian fitting verifies this conclusion.



Mixing of Two Gases

Using insights from the previous two activities, the diffusion and mixing of two gases was simulated with a grid of random walkers.



Mixing of Two Gases

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Several similar algorithms were implemented to this end:

1. Grid points selected at random, move is accepted if adjacent spot is available
2. Modified to include a list of available sites to reduce computational cost
3. Initial list of sites modified to only include near boundary sites early on
4. Step size increased - but accuracy lost

Mixing of Two Gases

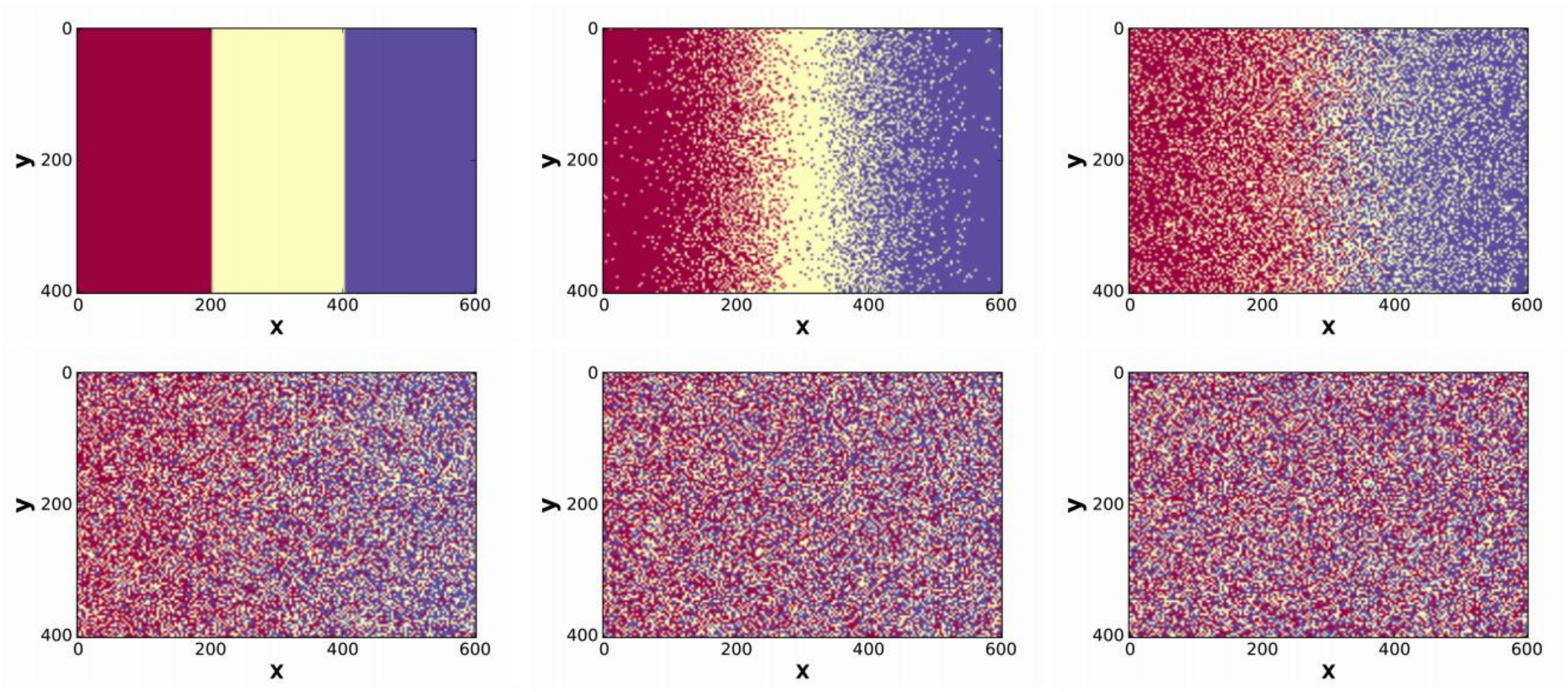


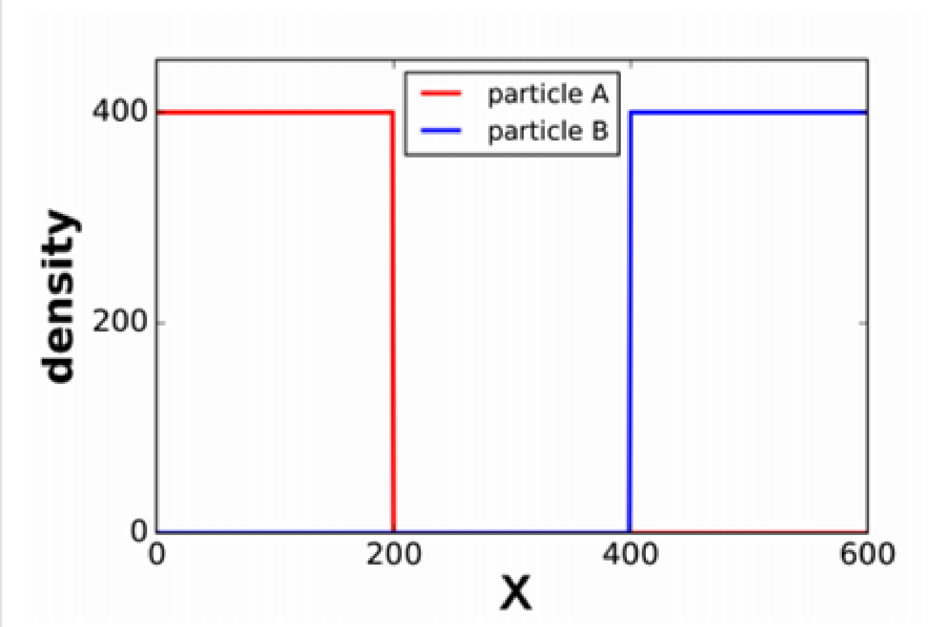
Figure 4: Gases mixing configurations after different number of steps.

Mixing of Two Gases

Gas mixing process was monitored quantatively by linear population density.

$n_A(x)$ = number of particle "A" at the x^{th} column (red)

$n_B(x)$ = number of particle "B" at the x^{th} column (blue)



Mixing of Two Gases

Linear population density   A -- red   B -- blue

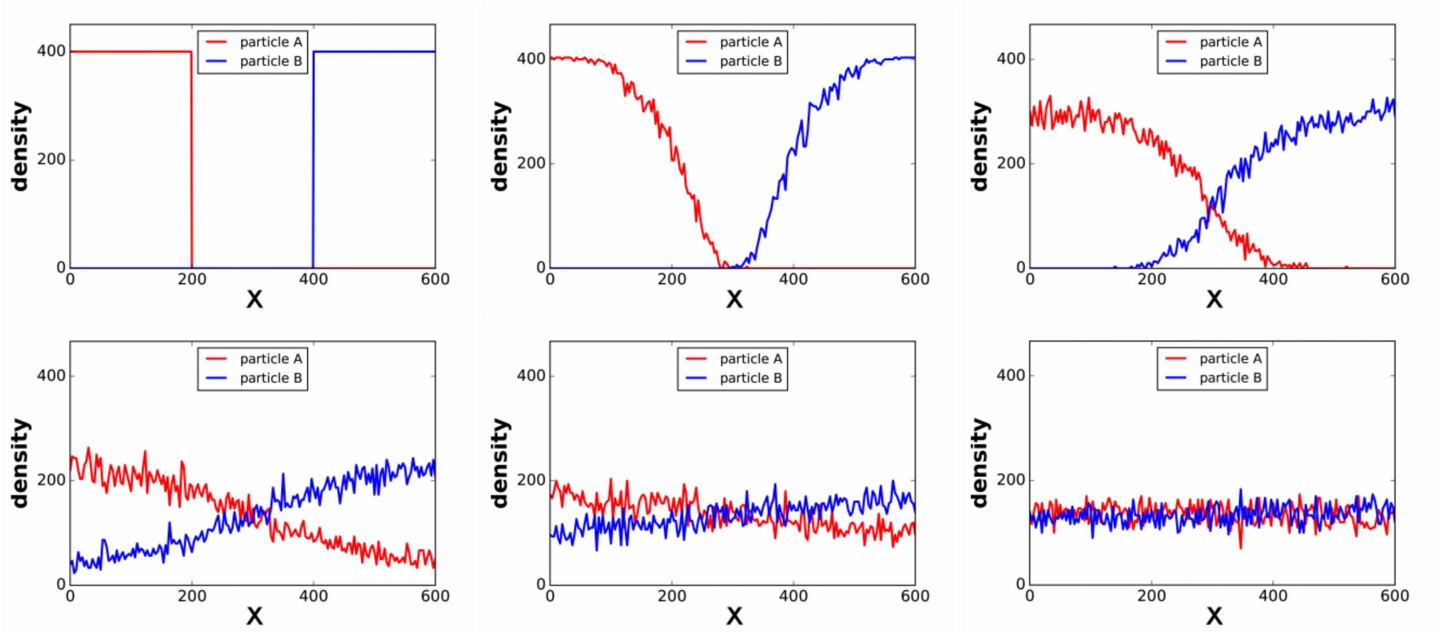


Figure 5: Linear population densities after different number of steps.

Mixing of Two Gases

Ideally, mixed gases should be uniformly distributed, but due to the random nature of the mixing process, the distribution was rough and oscilating until averaged over a large number of trials.

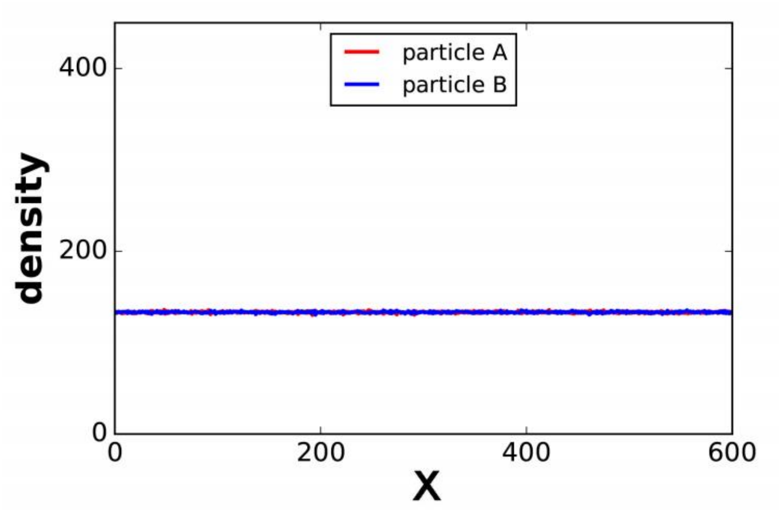


Figure 6: Linear population densities averaged over 100 trials.

Conclusions

- $\langle x_n \rangle$ of 2D random walk oscillates around zero, while $\langle (x_n)^2 \rangle$ and $\langle (r_n)^2 \rangle$ increases linearly with steps.
- The solutions of 1D diffusion equation with an initial box density profile are normal distributions. The standard variance of the normal distribution is proportional to the square root of time.
- In the gases mixing simulation, two gases are fully mixed after a large number of iterations. The final linear population density of each gas averaged over 100 simulations approaches a uniform distribution.

Thanks!

Source code:

github.com/vyu16/PHY566-DUKE

Questions?