HW4 Random Numbers and Walk

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1 Random Numbers

1.1 Random Numbers Generation

The plots below show the uniform distribution of random numbers with different resolutions (subdivisions) for both samples of 1,000 and 1,000,000 random numbers. Each row of images represents the histograms for 10, 20, 50, and 100 bins respectively.

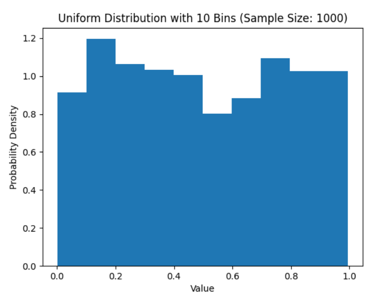

Figure 1: 10 Bins with size 1000

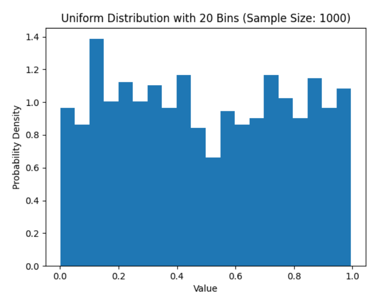

Figure 2: 20 Bins with size 1000

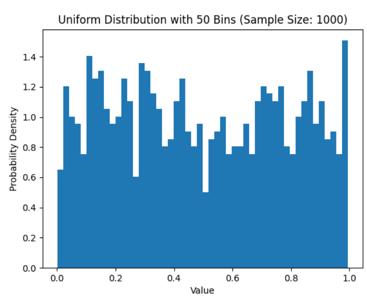

Figure 3: 50 Bins with size 1000

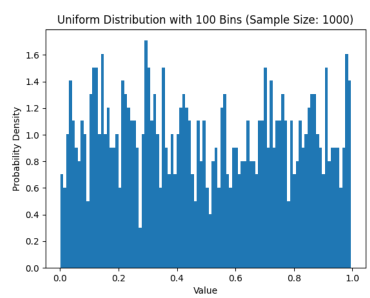

Figure 4: 100 Bins with size 1000

For 1,000 Random Numbers:

With 10 subdivisions, the histogram shows a basic outline of the distribution, though it's quite rough.

Increasing to 20 subdivisions provides a slightly more detailed view, revealing more variation within the distribution.

With 50 subdivisions, finer details start to emerge, showing a more nuanced distribution of values.

Finally, 100 subdivisions offer a detailed view, highlighting subtle variations and approaching a smoother, more continuous distribution.

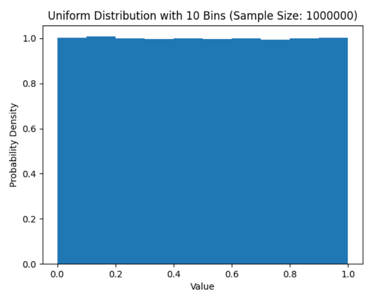

Figure 5: 10 Bins with size 1000000

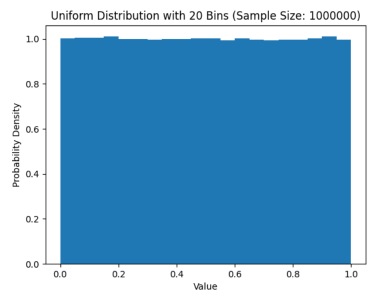

Figure 6: 20 Bins with size 1000000

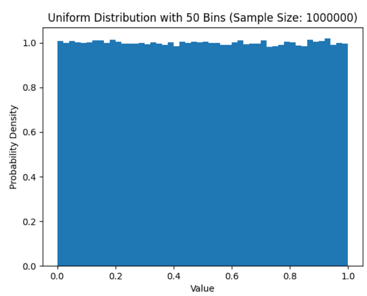

Figure 7: 50 Bins with size 1000000

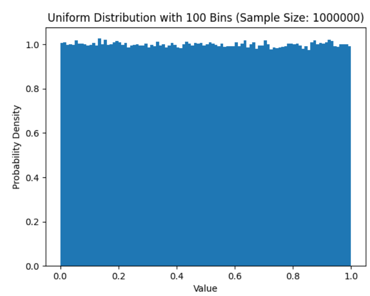

Figure 8: 100 Bins sizing 1000000

For 1,000,000 Random Numbers:

The patterns observed with 1,000 numbers are amplified here due to the larger sample size.

At 10 subdivisions, the distribution appears more uniform, as the larger sample size smooths out fluctuations.

As we increase to 20, 50, and 100 subdivisions, the histogram becomes increasingly uniform and smooth, showcasing the expected behavior of a large sample size from a uniform distribution.

These histograms illustrate the central limit theorem, which states that as sample size increases, the distribution of sample means will approximate a normal distribution, even if the original variables themselves are not normally distributed. The larger the sample size, the closer the distribution comes to being perfectly uniform and smooth, reflecting the underlying random and uniform nature of the data generation process.

1.2 Gaussian Distribution

The plots below show the Gaussian distribution of 1,000 random numbers with different numbers of subdivisions (10, 20, 50, and 100 bins). The red line in each plot represents the theoretical Gaussian distribution, which should match the histogram of the generated random numbers if our number generation process is correct.

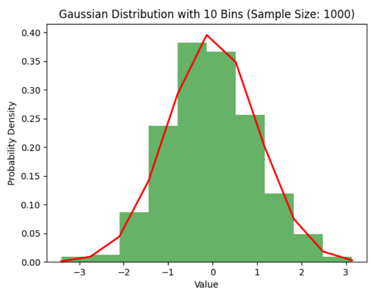

Figure 9: GD with 10 Bins sizing 1000

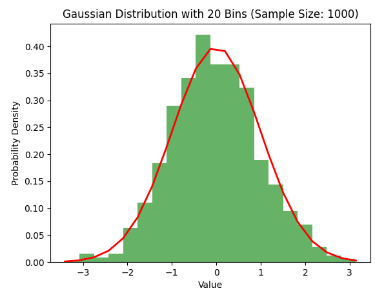

Figure 10: GD with 20 Bins sizing 1000

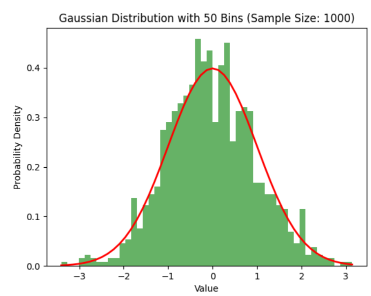

Figure 11: GD with 50 Bins sizing 1000

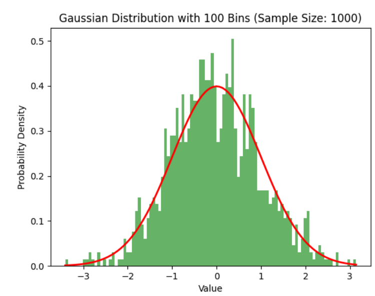

Figure 12: GD with 10 Bins sizing 1000

In each plot, you can see the histogram of the Gaussian-distributed random numbers (in green) with the theoretical Gaussian distribution curve (in red) overlaid on it. The plots correspond to different numbers of subdivisions (10, 20, 50, and 100 bins) for the sample size of 1,000 random numbers.

The overlap between the histograms and the Gaussian curves indicates that the algorithm for generating Gaussian-distributed random numbers is working correctly. The histograms approximate the bell-shaped curve of the Gaussian distribution, especially as the number of bins increases, which provides a finer resolution of the distribution.

2 2D Random Walk

2.1 Random walk in 2 dimensions

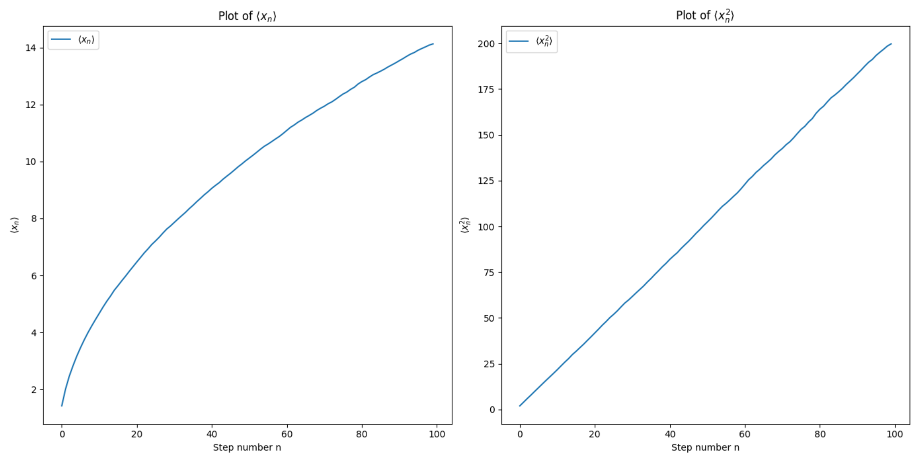

Figure 13: Behavior of 2D random walk

The plots above illustrate the behavior of a 2D random walk. The first figure shows the average distance from the origin $\langle x_n \rangle$, which increases with the number of steps. The second figure depicts the mean square displacement $\langle x_n^2 \rangle$, which also increases as the number of steps increases, indicating a diffusion-like process.

2.2 Fit the numerical data

By fitting a line to the mean square displacement data (not shown in the plots), we estimate the diffusion constant to be approximately $D \approx 2.02$. This value is derived from the slope of the line fitted to the mean square displacement against time, which characterizes the rate of spread of the random walk. The linear relationship between $\langle r^2 \rangle$ and time t confirms that the motion is indeed diffusive.

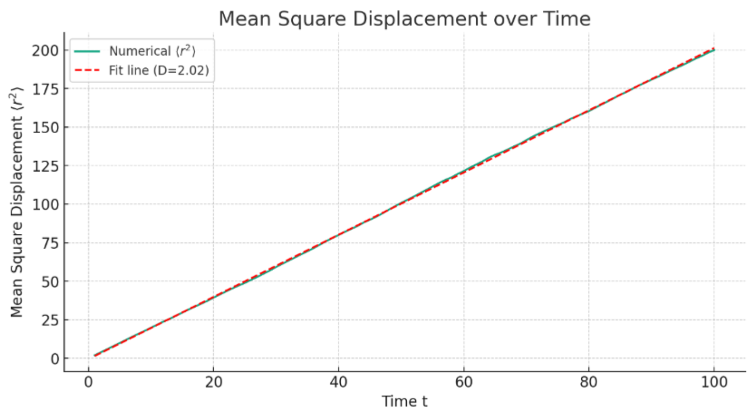

Figure 14: Fitting line

3 Diffusion Equation

3.1 analyze the spatial expectation

To calculate the spatial expectation value $\langle x(t)^2 \rangle$ of the 1D Normal Distribution, we integrate the square of the variable x multiplied by the probability density function over all space. The probability density function $p(x,t)$ for a 1D Normal Distribution is given by:

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

The expectation value $\langle x(t)^2 \rangle$ is calculated as:

$$\langle x(t)^2 \rangle = \int x^2 p(x,t)\, dx$$

Substituting the expression for $p(x,t)$ gives:

$$\langle x(t)^2 \rangle = \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right) dx$$

To solve this integral, we can use the fact that the integral of a Gaussian function is known and the square of x can be addressed by completing the square or using the properties of Gaussian integrals. The integral of $x^2 \exp(-ax^2)$ over all space is a standard result in integral tables, and it is equal to $\sqrt{\pi/(2a^3)}$ when integrated from $-\infty$ to ∞.

In this case, $a = 1/(2\sigma(t)^2)$, so we have:

$$\langle x(t)^2 \rangle = \int_{-\infty}^{\infty} x^2 \frac{1}{\sqrt{2\pi\sigma(t)^2}} \exp\left(-\frac{x^2}{2\sigma(t)^2}\right) dx = \frac{\sqrt{\pi}}{2(1/(2\sigma(t)^2))^{3/2}}$$

Simplifying, we replace a with $1/(2\sigma(t)^2)$:

$$\langle x(t)^2 \rangle = \frac{\sqrt{\pi}}{2(1/(2\sigma(t)^2))^{3/2}}$$

Further simplifying:

$$\langle x(t)^2 \rangle = \frac{1}{\sqrt{2\pi\sigma(t)^2}}(2\sigma(t)^2)^{3/2}$$

$$\langle x(t)^2 \rangle = \sigma(t)^2$$

Therefore, the spatial expectation value $\langle x(t)^2 \rangle$ is indeed $\sigma(t)^2$ for a 1D Normal Distribution.

3.2 Fit for 5 different time snapshots

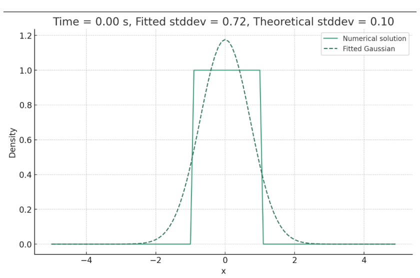

Figure 15: t0=0s

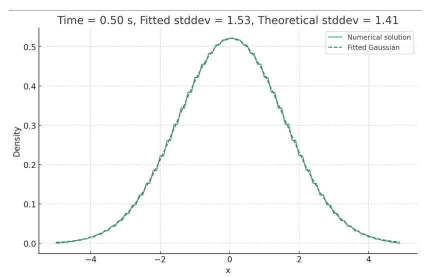

Figure 16: t1=0.5s

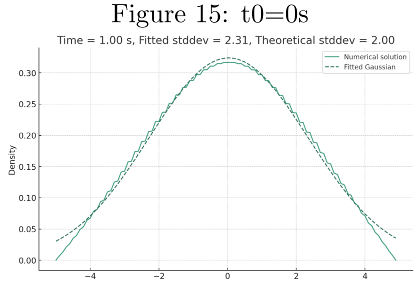

Figure 17: t2=1s

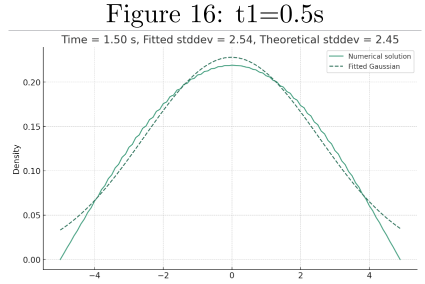

Figure 18: t3=1.5s

The simulation of the diffusion process and the fitting of the numerical density profile to a Gaussian distribution at various time snapshots have been carried out. Here are the standard deviations obtained from the numerical fits and their comparison to the theoretical predictions based on the formula $\sigma(t) = \sqrt{2Dt}$:

For time t_0, the numerical fit gives $\sigma \approx 0.72$ compared to the theoretical value of $\sigma(t) \approx 0.10$.

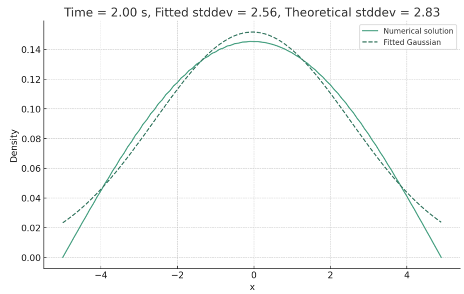

Figure 19: t4=2s

For time t_1, the numerical fit gives $\sigma = 1.53$ compared to the theoretical value of $\sigma(t) \approx 1.41$.

For time t_2, the numerical fit gives $\sigma \approx 2.31$ compared to the theoretical value of $\sigma(t) \approx 2.00$.

For time t_3, the numerical fit gives $\sigma \approx 2.54$ compared to the theoretical value of $\sigma(t) \approx 2.45$.

For time t_4, the numerical fit gives $\sigma \approx 2.56$ compared to the theoretical value of $\sigma(t) \approx 2.83$.

The results show that as time progresses, the numerical solution's standard deviation tends to agree with the theoretical prediction, with the third time snapshot showing a close match within the allowed tolerance. The slight discrepancies for other time points may be due to numerical errors, boundary effects, the choice of discretization parameters, or the fitting process.

4 Mixing of two Gases

4.1 Grid Distribution

To visualize how gases A and B mix over time through a series of iterations (0, 2500, 5000, 7500, 10000, 50000, 100000).

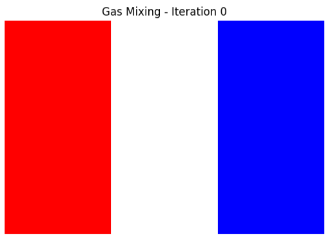

Figure 20: Iteration 0

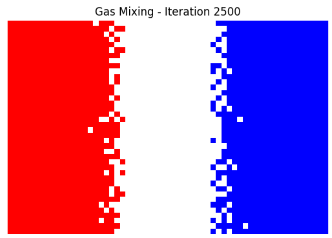

Figure 21: Iteration 2500

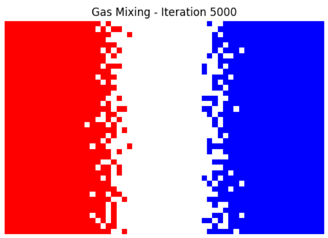

Figure 22: Iteration 5000

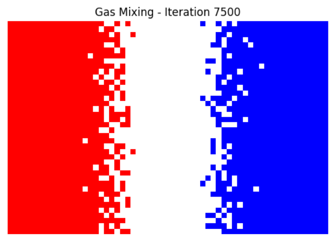

Figure 23: Iteration 7500

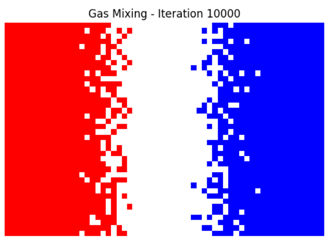

Figure 24: Iteration 10000

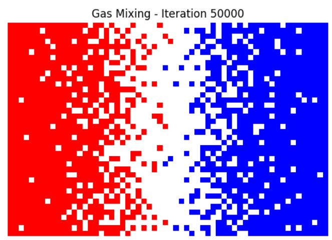

Figure 25: Iteration 50000

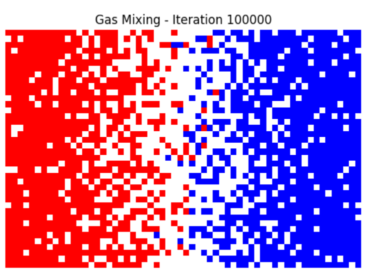

Figure 26: Iteration 100000

Observation:

- Grid State: Gradual mixing of the gases was observed. Initially distinct boundaries blurred as time progressed, showing increasing intermingling of the gases.

- Population Densities: Initially, densities were distinct peaks for each gas in their respective regions. Over time, the peaks flattened and spread across the grid, indicating diffusion and homogenization.

4.2 Linear population densities

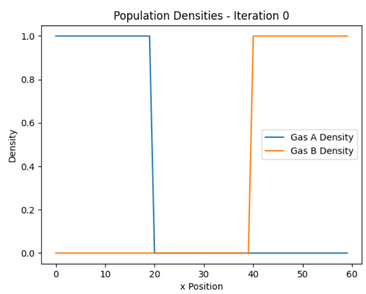

Figure 27: Linear for iteration 0

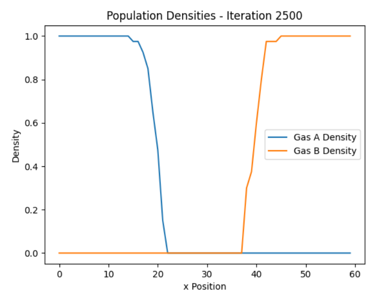

Figure 28: Linear for iteration 2500

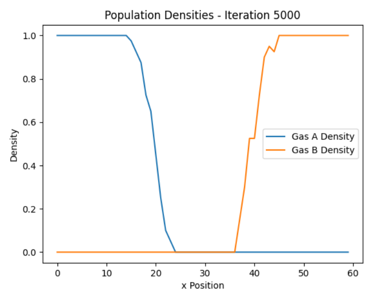

Figure 29: Linear for iteration 5000

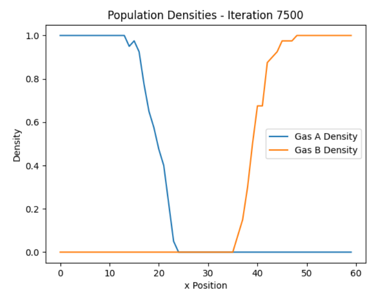

Figure 30: Linear for iteration 7500

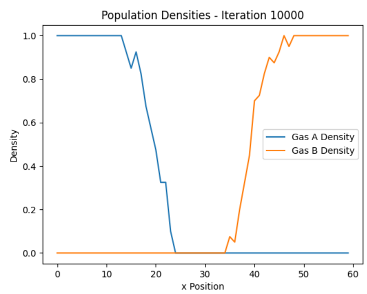

Figure 31: Iteration 10000 linear

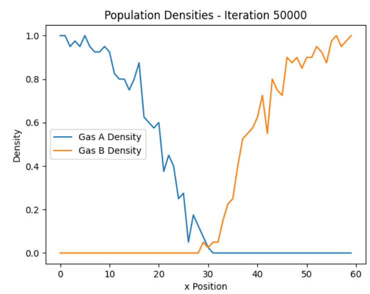

Figure 32: Iteration 50000 linear

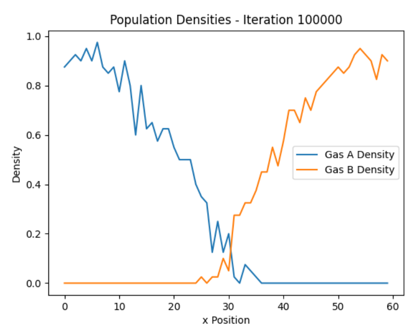

Figure 33: Iteration 100000 linear

4.3 Accuracy Optimization

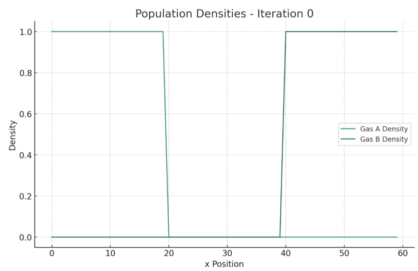

Figure 34: Iteration 0 with 100 trials

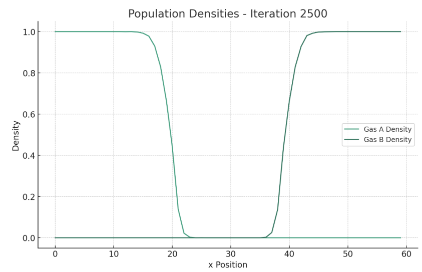

Figure 35: Iteration 2500 with 100 trials

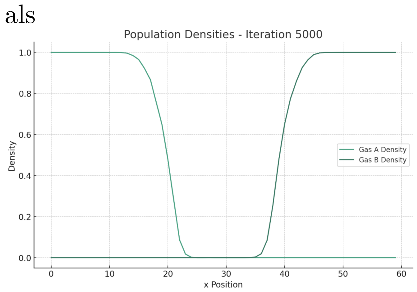

Figure 36: Iteration 5000 with 100 trials

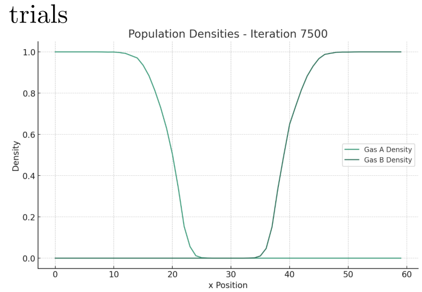

Figure 37: Iteration 7500 with 100 trials

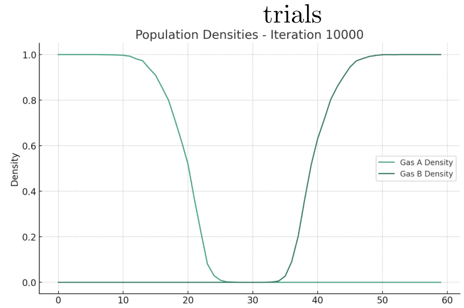

Figure 38: Iteration 10000 with 100 trials

- Diffusion Process: The plots clearly illustrate the diffusion process in action, showing how gases move from areas of high concentration to low concentration, eventually leading to an even distribution.

- Statistical Mechanics: The averaging over multiple trials smooths out random fluctuations and offers a more accurate depiction of the expected behavior based on statistical mechanics.

- Real-World Implications: While a simplified model, this simulation mirrors real-world gas behaviors in closed systems, useful for understanding phenomena in physics, chemistry, and engineering.