Computational Physics I
Exercise 3.1: Diffusion, Entropy & the Arrow of Time.

PHYS 3500K

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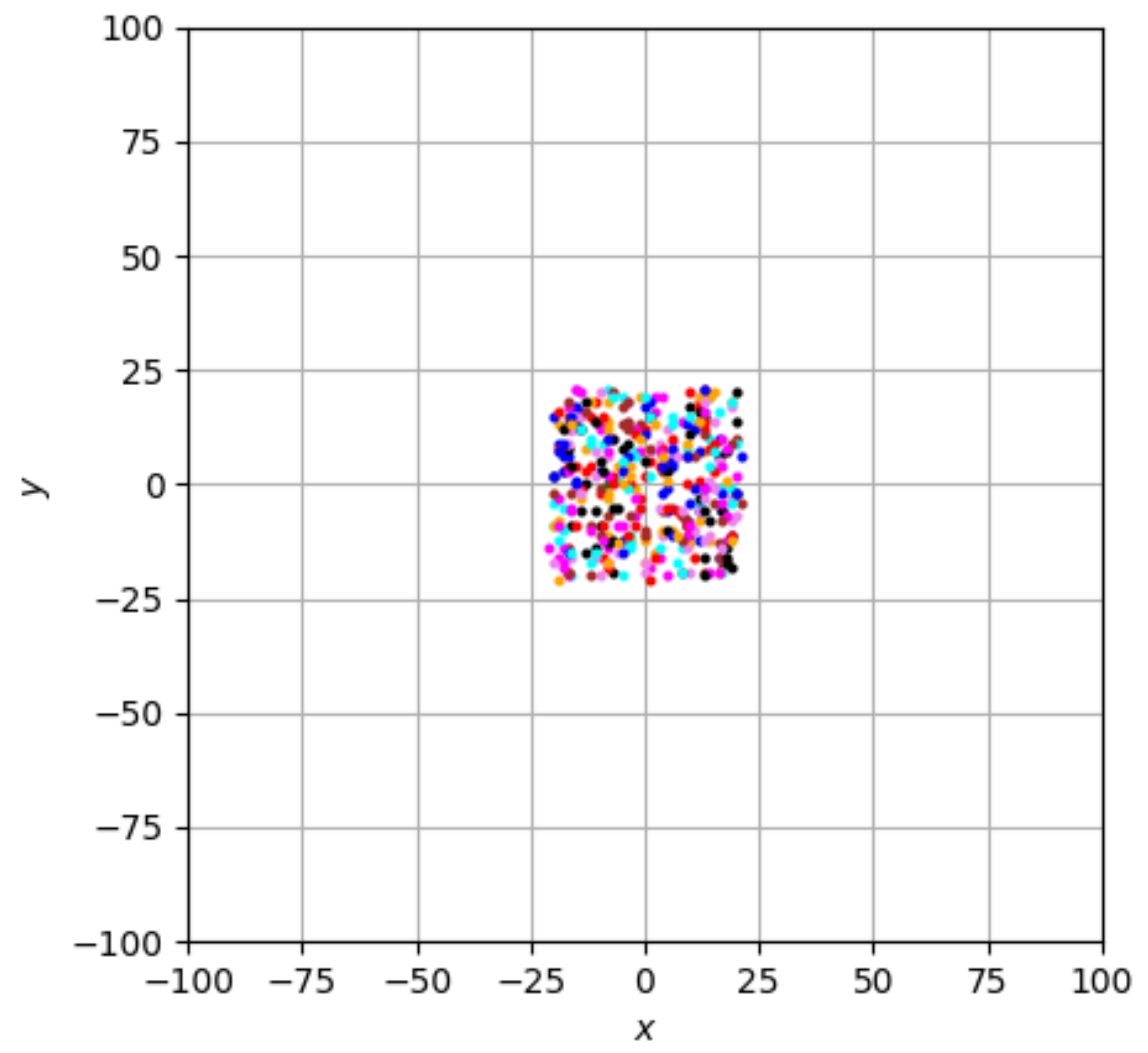
The Problem

- A typical "**stochastic**" problem is **diffusion**.
- **A stochastic system** = a system in which **randomness plays a central role**.
- An example of a problem in diffusion is that of a drop of cream, carefully placed at the center of a cup of black coffee.
- The white mass of cream will slowly spread to fill the cup, and eventually the coffee will take on a uniform brownish color.
- At the microscopic level: process would be described by a large number of "cream particles".
- Roughly speaking, each cream particle would perform a **random walk**.
- In this problem, we will **simulate this phenomenon**.

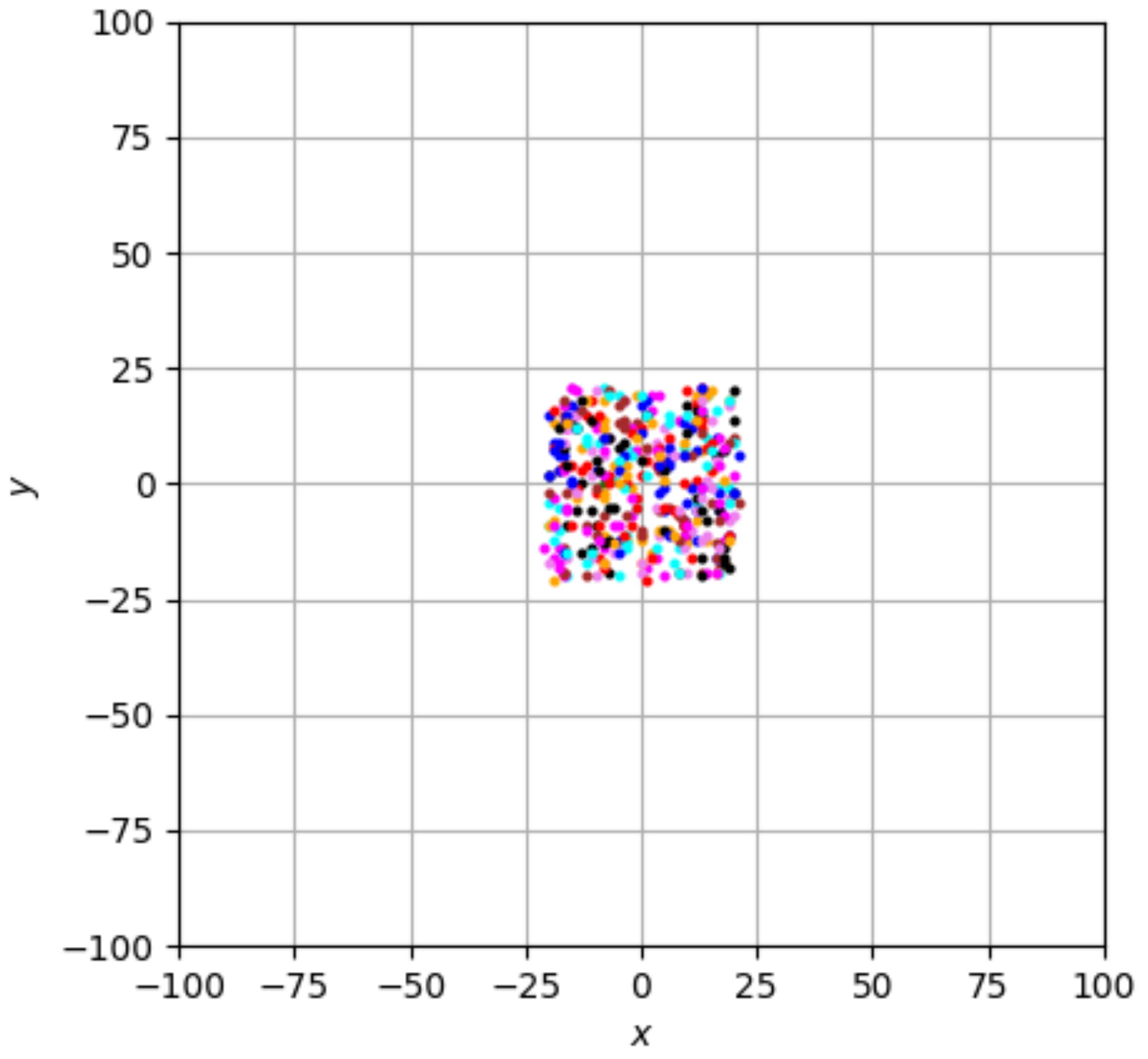
Setup

- The initial conditions: a cup of black coffee containing a drop of cream at its center.
- Consider a **two-dimensional cup**, with an **initial cream distribution in a square**.
- The cup has **rigid walls** at $x = \pm 100$ and $y = \pm 100$.
- We will consider $N = 400$ particles, starting in $x = \pm 20$ and $y = \pm 20$.
- Each particle will undergo **random walk motion on a grid**.

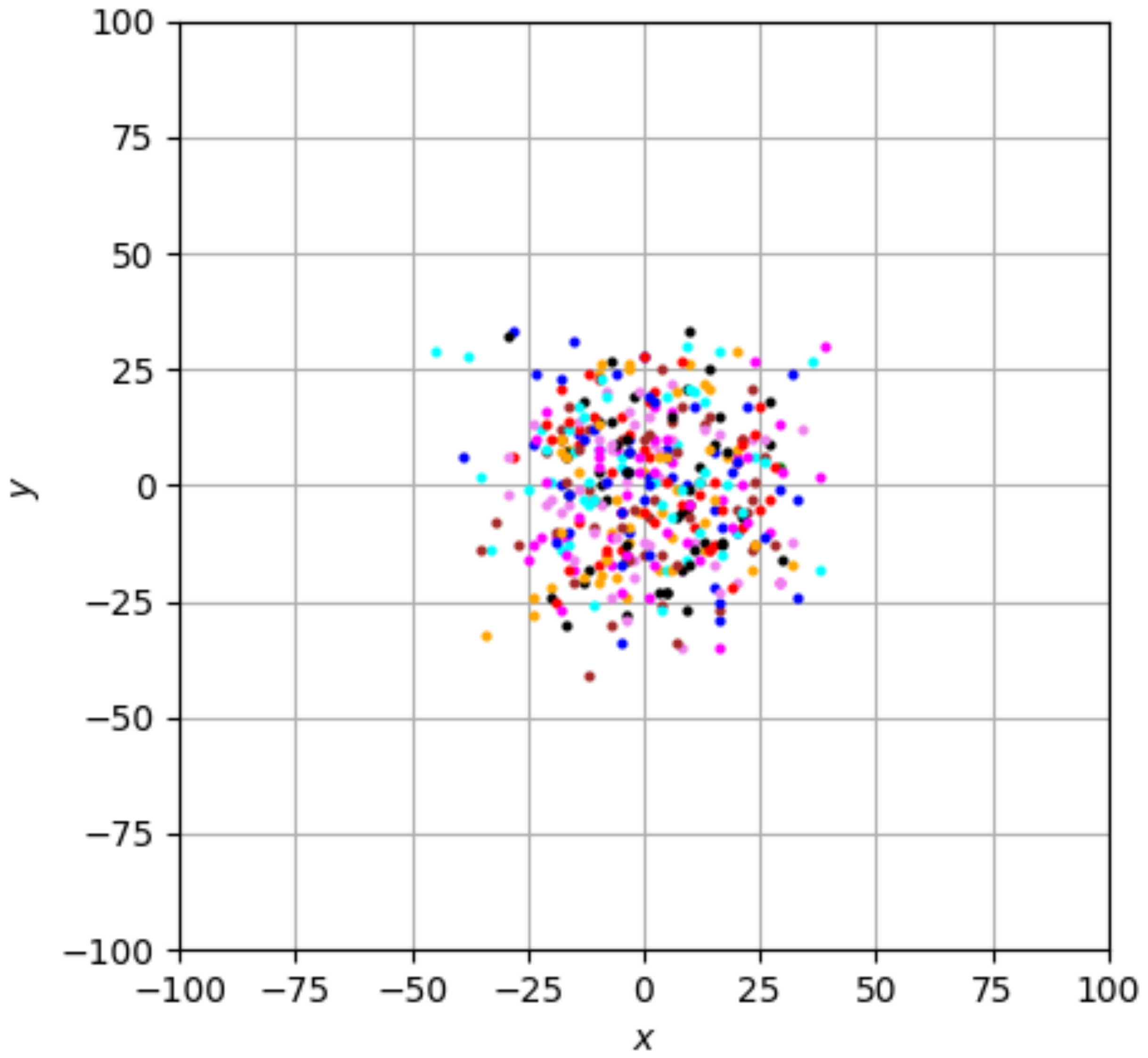
[Note that colors have no meaning!]



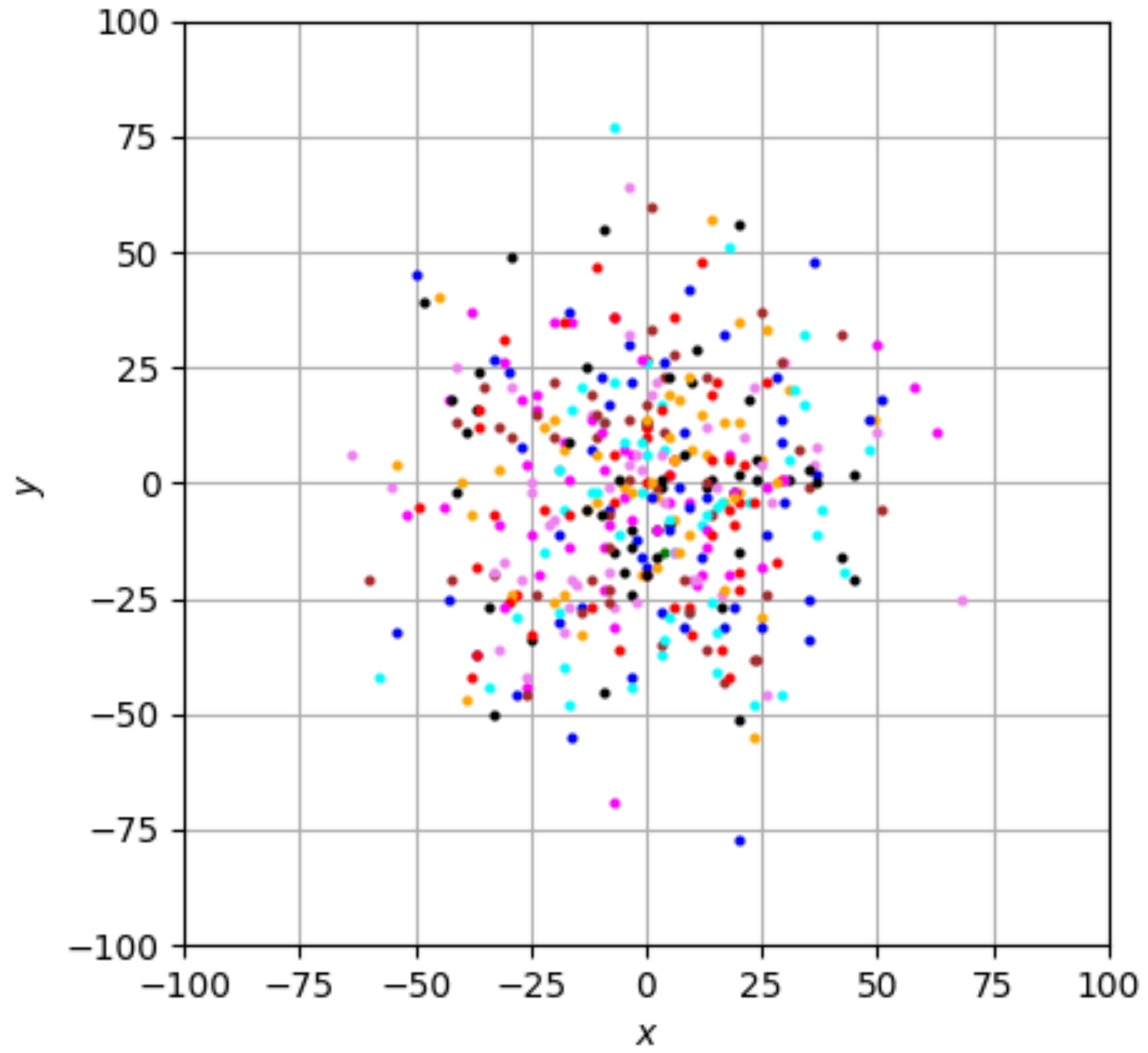
Diffusion



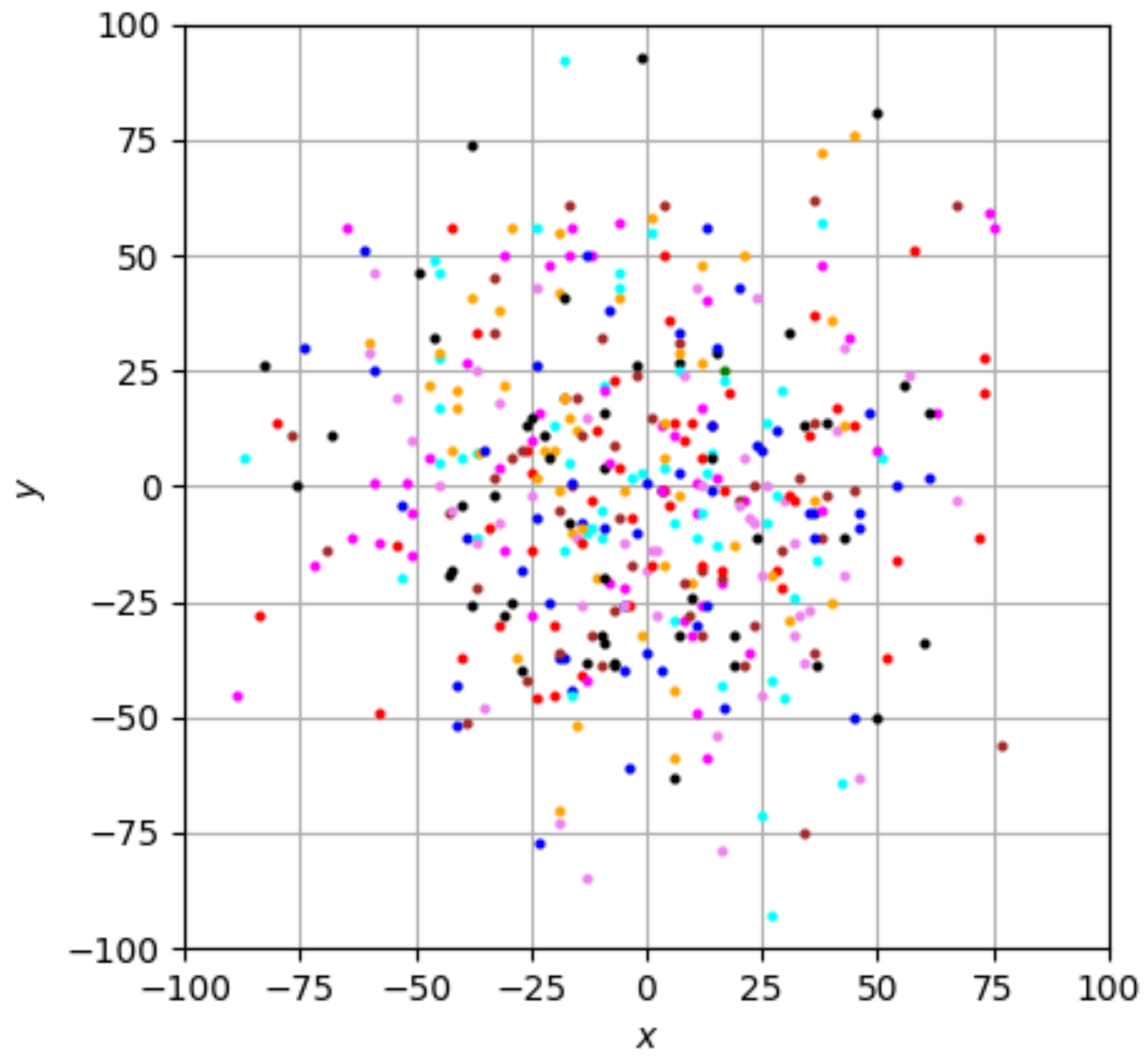
After 250 random moves on the grid:



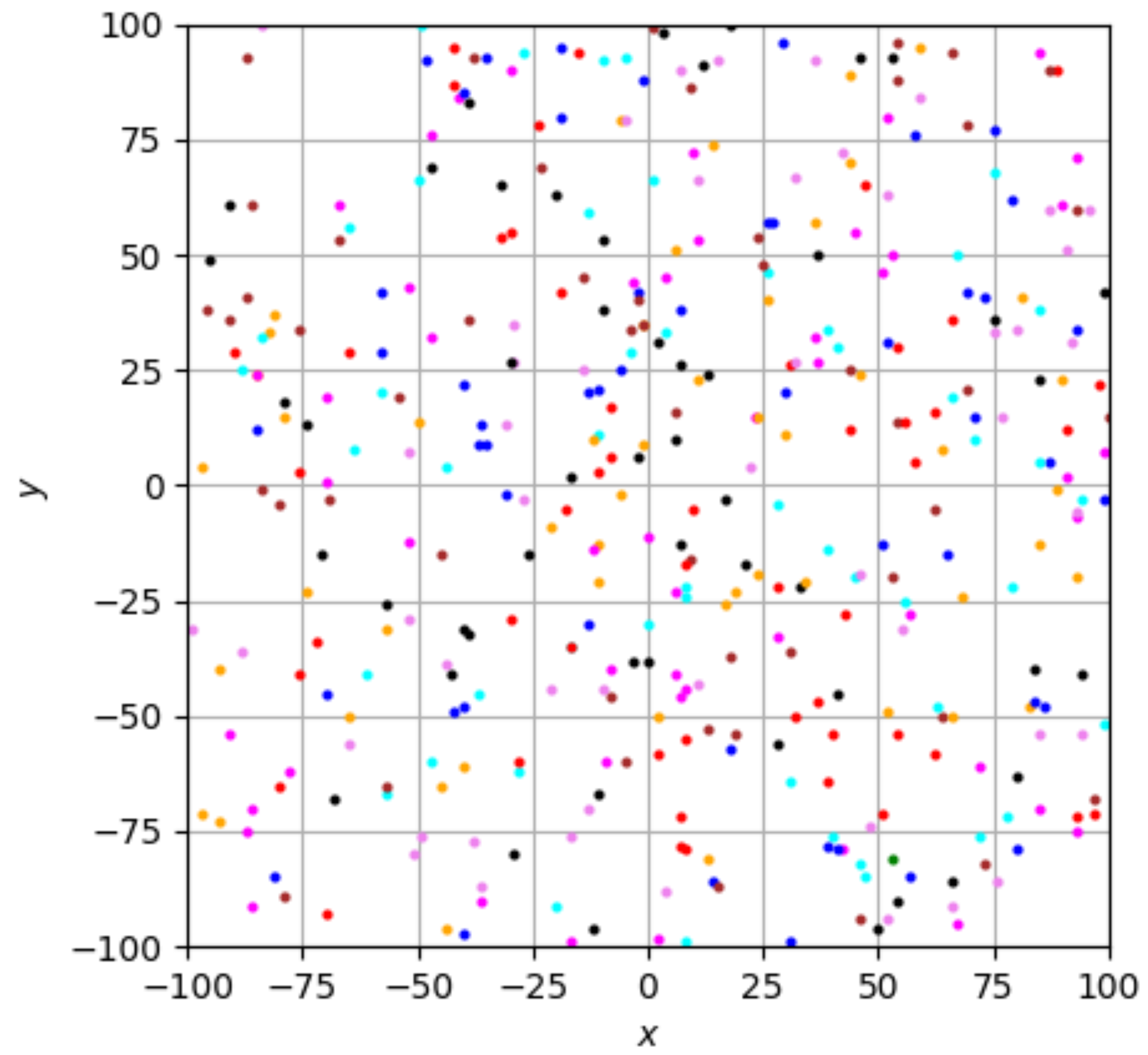
After 1000 random moves on the grid:



After 2000 random moves on the grid:



After 10000 random moves on the grid:



Entropy

- We want to relate this example to the second law of thermodynamics.
- We will do this through the entropy of the **system = roughly, the measure of the amount of disorder.**
- The **second law of thermodynamics states that the entropy of an isolated system either stays the same or increases with time**.
- Here, **"time" is represented by the number of steps taken by the walkers**. Initially, the walkers (i.e. cream particles) are in a low-entropy state, concentrated in the drop. They then diffuse into a higher-entropy state, filling the cup.
- To calculate the entropy, we will split the cup up in a square grid (not the same one that the walkers are moving on) and calculate the entropy via:
- $S = k_B \ln \Omega$ where in this case: $\Omega = \dfrac{N!}{\prod_{i=1} n_i!}$, where the N is the total number of cream particles, and the product is over the number of "cells" in the square grid defined above.
- $k_B = 1.38 \times 10 - 24 \text{ m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$ is the Boltzmann constant.

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Stirling's Approximation

- The entropy can be $S = k_B \ln \Omega$ where in this case: $\Omega = \frac{N!}{\prod_{i=1} n_i!}$, where the N is the total number of cream particles, and the product is over the number of "cells" in the square grid defined above.

- To calculate the logarithms of factorials, we can use **Stirling's approximation**:

$$\ln(x!) = x \ln x - x + \frac{1}{2} \ln(2\pi x) + \mathcal{O}(1/x)$$

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See the text in Exercise 3.1 for more details!