

Simulate Mixing of Gas Molecules

Cheng Su

I. PROBLEM DESCRIPTION

Purpose of this project is to simulate the effect of collision of molecules in 3D using random walk in 2D. In particular, the random walk can be used to investigate how a quite ordered system, where one gas fills one half of a box, evolves through time to a more disordered system.

This physical process can be simulated by random walk inside a fixed area $A = [0, 1] * [0, 1]$. Initially, 10000 particles are placed at uniformly distributed random positions in area of $[0, 1/2] \times [0, 1]$. Then start the random walk and visualize the simulation during a long time and save as an animation.

II. BENCH-MARKING

Particle class is created to initialized the particle appearing at random position within area $[0, 1/2] \times [0, 1]$. It also allows particle to move in a random position(up, down, left, right) with the given step distance of 0.05.

Total duration of the simulation is 200, and visualized animation is done using matplotlib.FuncAnimation.

III. RESULT

Below are the results of simulation at $t = 0$, $t = 35$, and $t = 200$.

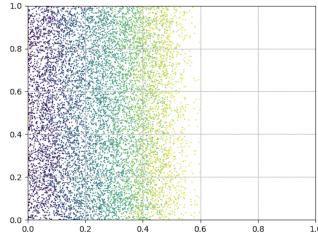


Fig. 1. particle positions at time 1

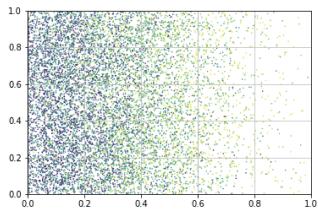


Fig. 2. particle positions at time 35

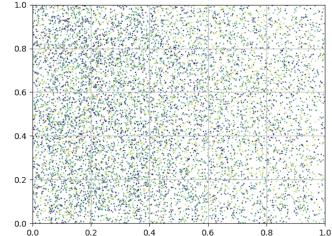


Fig. 3. particle positions at time 200

IV. DISCUSSION

From the result image, we can see that at $t = 0$ the color of popularized particles are of gradient, at $t = 35$ the particles start to move into initially empty space, at $t = 200$ the particles are uniformly distributed in the whole space. We can infer that eventually the system will evolve to a disordered system.