

## Experiments with diffusion

### ***Diffusion applet***

To run the *Diffusion* applet, start MATLAB and type `Diffusion` at the prompt. The program simulates the random motion of  $M$  non-interacting particles on a grid. Each particle can only go up, down, left or right, with equal probability. All of the particles start their random walk from the origin, at the center of the box.

The plot on the left shows the position of all of the particles as time evolves. One of the particles is marked in blue, so that its random walk can easily be followed.

At the end of the simulation, the plot on the right shows the quantity  $\langle L^2 \rangle$  as a function of  $N$ . Here,  $L$  is the distance between a particle and the origin after  $N$  steps (or equivalently after a time  $T = N \delta t$ , where  $\delta t$  is fixed), and the brackets indicate averaging over all of the particles.

The sliders allow you to choose the number of particles,  $M$ , as well as the total number of steps,  $N_{max}$ . Click on the *Go* button to start the simulation. It will stop automatically after  $N_{max}$  steps.

### ***Two-dimensional random walk***

- Run the applet for different values of  $M$  and  $N_{max}$  and describe what happens.
- Based on the output of the simulations, relate  $\langle L^2 \rangle$  to  $N$  or equivalently  $T$ . Does this relationship depend on the value of  $M$ ? If so, in what way?
- Use the above to define a characteristic time scale and a dimensionless parameter involving time and space scales.

### ***One-dimensional random walk***

The purpose of this section is to explore the scaling properties of a one-dimensional random walk. If you know probability theory, you may want to study this process analytically. If not, the following describes a way of investigating these questions numerically. Assume that a walker walks along a line from the point  $x = 0$ , by taking random steps either to the left or to the right, with equal probability. The goal of the exercise is to figure out how far the walker has gone from the origin, on average, after  $N$  steps.

- A simple way to model a random walk
  - Take the convention that a step taken to the left from coordinate  $x$  leads to coordinate  $x-1$ , and that a step taken to the right leads to coordinate  $x+1$ .

- A random walk can therefore be represented by a sequence of numbers equal to either -1 or +1. For instance, -1, -1, -1, 1, would correspond to 3 steps to the left followed by 1 step to the right. The position at the end of such a walk would be  $-3+1 = -2$ .
- More generally, a walk of length  $N$  corresponds to an  $N$ -dimensional vector whose entries are either -1 or +1. The position at the end of the walk is equal to the sum of all of the entries.
- Use MATLAB to simulate a single random walk of  $N$  steps.
  - The function `X = rand(1,N)` returns a row vector  $X$  of length  $N$ , whose entries are random numbers uniformly distributed between 0 and 1.
  - Say we decide that if the random number generator returns a number between 0 and 0.5, this corresponds to a step taken by the walker to the left, and that a number between 0.5 and 1 corresponds to a step taken to the right.  
Typing `Y = (X > 0.5) - (X <= 0.5)` at the MATLAB prompt will return a vector of length  $N$  whose entries are equal to +1 when  $X$  is strictly larger than 0.5 and equal to -1 when  $X$  is less than equal to 0.5.
  - To obtain the position of the walker after  $N$  steps, one needs to take the sum of all of the entries of  $Y$ . This is accomplished by the MATLAB function `sum(Y)`.
- Create a short MATLAB script that simulates a single random walk. Run the simulation 10 times and record the position of the walker at the end of each random walk. For each simulation, the distance between the final position of the walker and the origin is equal to the absolute value of the final coordinate of the walker. Calculate the average of these distances.

Number of steps:  $N =$  \_\_\_\_\_ (choose a relatively large number, e.g. 100)

Simulation #	1	2	3	4	5	6	7	8	9	10
Final position										
Distance from origin										

Average distance from origin:  $\langle L \rangle =$  \_\_\_\_\_

- Modify your MATLAB script to calculate  $\langle L \rangle$  over 1000 simulations, instead of 10 as done above. Paste your script below.
- Then choose a few different values of  $N$  and plot the square of  $\langle L \rangle$  as a function of  $N$ . Paste your plot below. What do you observe? How does  $\langle L \rangle$  scale with  $N$ ?
- As for the two-dimensional random walk, define a dimensionless quantity involving  $\langle L \rangle$  and  $N$ . Compare the result to the dimensionless variable appearing in the heat equation. What does this suggest?