Brownian motion simulation

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Introduction

Brownian motion is simulated in 2D using a system of 150 particles. Collisions between particles and between particles and boundaries are fully elastic.

Model equations

In order to update the positions of the particles the collision time between particles and between particles and boundaries needs to be determined. Collision times t_{ab} between particles are computed by:

$$t_{ab} = \frac{-\mathbf{r}_{ab} \cdot \mathbf{v}_{ab} - \sqrt{(\mathbf{r}_{ab} \cdot \mathbf{v}_{ab})^2 - \mathbf{v}_{ab} \cdot \mathbf{v}_{ab}(\mathbf{r}_{ab} \cdot \mathbf{r}_{ab} - (R_a + R_b)^2)}}{\mathbf{v}_{ab} \cdot \mathbf{v}_{ab}} \tag{1}$$

Where R_a is the radius of particle a, R_b is the radius of particle b, $\mathbf{r}_{ab}$ is the relative position $\mathbf{r}_a - \mathbf{r}_b$ with $\mathbf{r}_a$ the position of particle a and $\mathbf{r}_b$ the position of particle b and $\mathbf{v}_{ab}$ is the relative velocity $\mathbf{v}_a - \mathbf{v}_b$ with $\mathbf{v}_a$ the velocity of particle a and $\mathbf{v}_b$ the velocity of particle b:

$$\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b \tag{2}$$

$$\mathbf{v}_{ab} = \mathbf{v}_a - \mathbf{v}_b \tag{3}$$

Collision times t_c between particles and boundaries are computed by:

$$t_c = \frac{\mathbf{t} \cdot (\mathbf{w} - \mathbf{r}_i)}{\mathbf{t} \cdot \mathbf{v}_i} \tag{4}$$

Where $\mathbf{t}$ is the unit vector normal to the boundaries (and directed inward), $\mathbf{w}$ is the vector (w, w) with w the location of the boundaries (which in this work is taken to be ± 3), $\mathbf{r}_i$ is the position vector of particle i and $\mathbf{v}_i$ is the velocity vector of particle i.

The collision times between all particles and between all particles and boundaries are computed. Then, the minimum collision time is taken and used to update the particle positions.

Should the minimum collision time be between two particles the velocities $\mathbf{v}_a$ and $\mathbf{v}_b$ are updated as follows:

$$\mathbf{v}_a = \mathbf{v}_a - \frac{2m_b}{m_a + m_b} \cdot \mathbf{f} \tag{5}$$

$$\mathbf{v}_b = \mathbf{v}_b + \frac{2m_a}{m_a + m_b} \cdot \mathbf{f} \tag{6}$$

Where m_a is the mass of particle a, m_b is the mass of particle b and the quantity $\mathbf{f}$ is given by:

$$\mathbf{f} = \mathbf{n}((\mathbf{v}_a - \mathbf{v}_b) \cdot \mathbf{n}) \tag{7}$$

Where $\mathbf{n}$ is the unit vector normal to the contact point:

$$\mathbf{n} = \frac{(\mathbf{r}_a - \mathbf{r}_b)}{\sqrt{(\mathbf{r}_a - \mathbf{r}_b) \cdot (\mathbf{r}_a - \mathbf{r}_b)}} \tag{8}$$

Should the minimum collision time be between a particle and the boundary the velocities are simply reflected. For collisions with the upper or lower boundaries the reflection is defined by $f : \mathbb{R}^2 \to \mathbb{R}^2$:

$$f((v_x, v_y)) = (v_x, -v_y) \tag{9}$$

For collisions with the left or right boundaries the reflection is defined by $g : \mathbb{R}^2 \to \mathbb{R}^2$:

$$g((v_x, v_y)) = (-v_x, v_y) \tag{10}$$

Verification

Simulations showed that kinetic energy and momentum are conserved, indicating that the computation proceeds correctly.

Results

The mean squared displacement $d = x_c^2 + y_c^2$, with x_c the x coordinate and y_c the y coordinate, of the particle of interest is approximately proportional with time. A plot of the results is given in figure 1, where the mean squared displacement is plotted against time.

The number of particles in some given region between r and $r + \delta r$ observed in simulations at time t_f is compared with the number of particles in the same region predicted theoretically using the solution to the diffusion equation. A comparison is shown in figure 2.

Discussion

Simulations show that the mean squared displacement d is approximately proportional with time. This implies that the probability density of the particle of interest can be given by:

$$\rho(r, t) = \frac{1}{4\pi D t} e^{-r^2/4Dt} \tag{11}$$

Where D is the diffusion coefficient and r the radial coordinate. Since the mean squared displacement is equal to the variance of equation (11):

$$d = \int_0^\infty \frac{1}{4\pi D t} e^{-r^2/4Dt} \cdot 2\pi r \cdot r^2 dr = 4Dt \tag{12}$$

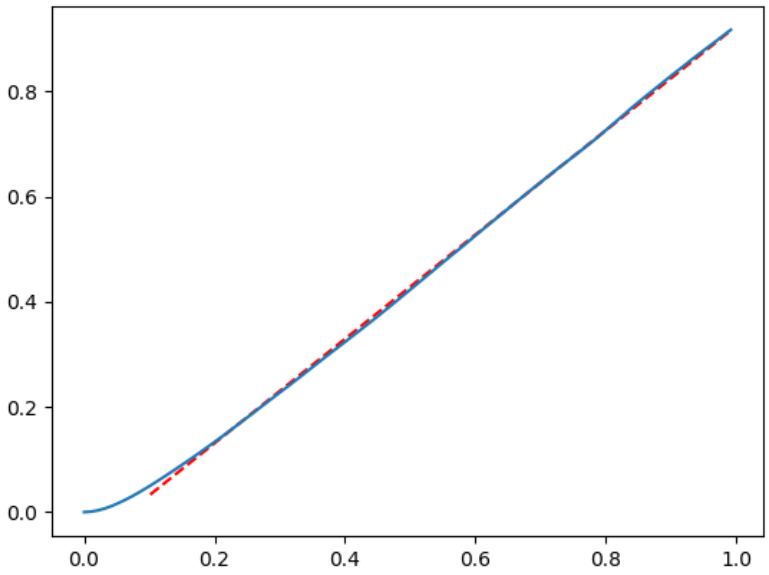

Figure 1: The mean squared displacement as a function of time.

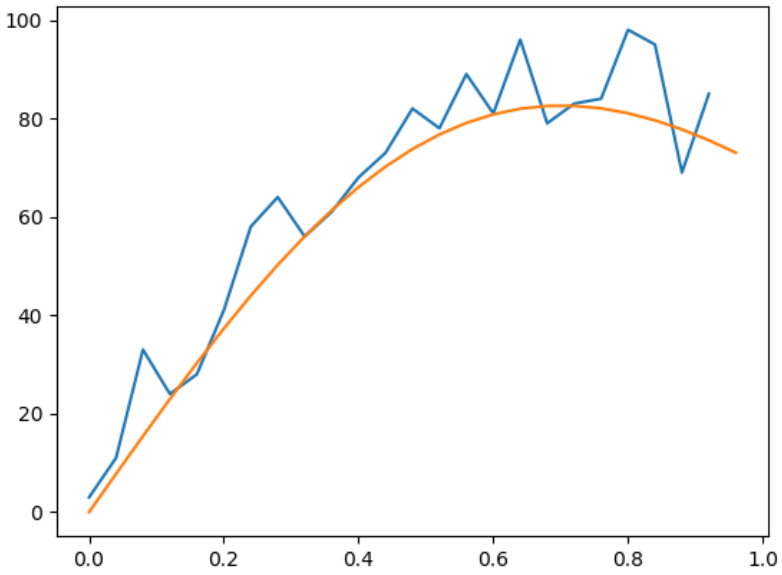

Figure 2: The blue line shows the computed number of particles within a given region between r and $r + \delta r$ vs the radial coordinate and the orange line shows the theoretical prediction of the number of particles within the same region.

The probability density function given by equation (11) is the solution to the transient diffusion equation:

$$\frac{\partial \rho}{\partial t} = \frac{D}{r}\frac{\partial}{\partial r}(r\frac{\partial \rho}{\partial r}) \tag{13}$$

With boundary conditions at time $t = 0$:

$$2\pi \int_0^\infty \rho(0,0) r dr = 1 \tag{14}$$

$$\rho(r,0) = 0 \tag{15}$$

For times $t > 0$ the following conditions apply:

$$\frac{\partial \rho(\infty, t)}{\partial r} = 0 \tag{16}$$

$$\frac{\partial \rho(0, t)}{\partial r} = 0 \tag{17}$$

The average motion of the particle of interest can therefore be described by the standard law of diffusion.

The number of particles within r and $r + \delta r$ can be estimated theoretically by:

$$\frac{1}{4\pi D t} e^{-r^2/4Dt} \cdot 2\pi r \delta r \tag{18}$$

Which can then be compared with the number of particles within r and $r + \delta r$ observed in simulations. A comparison between theoretical prediction and simulation is given in figure 2. The figure shows that, although there are oscillations, the number of particles within a given region predicted theoretically does not deviate much from the number of particles within a given region observed in simulations.