Brownian motion simulation

Derek W. Harrison

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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 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 $f : \mathbb{R}^2 \rightarrow \mathbb{R}^2$:

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

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

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

Verification

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