

Stochastic Simulation of Collision Detection Between Colloidal Particles

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Abstract

This report presents the implementation of a model that detects and treats collisions between particles undergoing a diffusive trajectory. The main motivation is to simulate the Brownian motion that particles undergo and account for the potential collision that may occur inbetween a time step, something a classical ballistic model fails to do. The collision event is determined via a probability calculated based on relative and final positions of the two particles. This project is intended to be a simulation of the first step of agglomeration and is to be paired with another model that simulates the second step: formation of a larger particle from two smaller particles.

I. INTRODUCTION

Collision detection is a popular physics and computational geometry problem that occurs in our daily lives, ranging from particles to pool balls to cars. Collision detection is applicable in computer graphics, computer simulations, and computational physics. The collisions of particles is the initial step in the process of agglomeration, the formation of larger particles upon collision and adhesion of two smaller particles [1]. Examples of agglomeration include formation of clouds, formation of bioaggregates in wastewater, and formation of planets. The collision step of agglomeration deals with particle-fluid interactions — particle-particle encounters and the time and location of their collision [1].

The motivation behind this project is to introduce a stochastic approach to simulate the collision step of agglomeration useful for situations where a numerical or analytical method does not exist. This approach considers the random and continuous of a particle's trajectory over a large time step and evaluates the probability of it interacting with another particle as well as both of their resulting trajectories. Provided that a collision occurs, the model then addresses when the collision occurs, where it takes place, and the resulting motion of the two particles.

II. RELATED WORK

A. Stochastic Approach

This project focuses on the model developed by Henry et al. in 2014 [1] which implements the model outlined in Mohaupt et al. in 2011 [2], a stochastic model to evaluate collisions between particles undergoing Brownian motion.

III. ALGORITHM IMPLEMENTATION

The following equations (Eq.(1), (2), (3), (4), (6), (5), (7)) are all derived by Henry et al. [1].

Particle motion

Particle motion is expressed by

$$X_p(t + \Delta t) = X_p(t) + B_x \sqrt{\Delta t} \xi_x \quad (1)$$

where X_p is the particle location, Δt is the time step of the simulation, B_x is the diffusion coefficient, and ξ_x is an independent vector of random variables sampled in a standard normal distribution. It is to be noted that this equation is valid only when $\Delta t \gg \tau_p$ where τ_p is the particle relaxation time. In this scenario, the fluid velocity is either at rest or disregarded and Eq. (1) is a simplified approach to particle motion. This simplified approach allows for a reasonable first step in building the simulation model.

Detection of collision

The next step is to determine if a collision occurs between a pair of particles given only their initial and final positions of the time step. This detection is determined stochastically and simulates the diffusive trajectories of the pair of particles as their paths follow random motion instead of straight lines. The formula to determine the probability of the collision is given by:

$$P_a^b(R_{ij}) = \frac{\exp\left(\frac{2R_{ij}(a+b-R_{ij})}{B_{x,ij}^2 \Delta t}\right) - 1}{\exp\left(\frac{2ab}{B_{x,ij}^2 \Delta t}\right) - 1} \quad (2)$$

where $R_{ij} = R_i + R_j$, a and b are the initial and final relative positions of the two particles, respectively, and $B_{x,ij}^2 = B_{x,i}^2 + B_{x,j}^2$. If a or b are less than the minimum threshold of R_{ij} , then the particles overlap at the beginning or end of the time step and therefore the collision probability is equal to 1. Afterwards, the collision between the pair of particles is then simulated by a Monte Carlo method such that given λ , a uniformly random sampled number between 0 and 1, if $P_a^b(R_{ij}) \geq \lambda$, the collision occurs. Otherwise, it does not.

Time of collision

Given that a collision has occurred, the cumulative distribution function for the collision time t_c is $F(q) = P_a^b(t_c < q | t_c < \Delta t)$ given by :

$$F(q) = \begin{cases} 0 & \text{if } q \leq 0 \\ \frac{1}{2} \left(1 - \frac{I_1 - I_2 - I_3 + I_4}{\exp\left(-\frac{(a+b-2R_{ij})^2}{2B_{x,ij}^2 \Delta t}\right) - \exp\left(-\frac{(a+b)^2}{2B_{x,ij}^2 \Delta t}\right)} \right) & 0 \leq q \leq \Delta t \\ 1 & \text{if } q \geq \Delta t \end{cases} \quad (3)$$

with

$$\begin{cases} I_1 = \exp\left(-\frac{(a+b-2R_{ij})^2}{2B_{x,ij}^2\Delta t}\right) \operatorname{erf}\left(\frac{a-R_{ij}}{B_{X,ij}\sqrt{2}}\sqrt{\frac{1}{q}-\frac{1}{\Delta t}} - \frac{b-R_{ij}}{B_{x,ij}\sqrt{2}\Delta t\sqrt{\frac{1}{q}-\frac{1}{\Delta t}}}\right) \\ I_2 = \exp\left(-\frac{(a-b)^2}{2B_{x,ij}^2\Delta t}\right) \operatorname{erfc}\left(\frac{a-R_{ij}}{B_{X,ij}\sqrt{2}}\sqrt{\frac{1}{q}-\frac{1}{\Delta t}} + \frac{b-R_{ij}}{B_{x,ij}\sqrt{2}\Delta t\sqrt{\frac{1}{q}-\frac{1}{\Delta t}}}\right) \\ I_3 = \exp\left(-\frac{(a+b)^2}{2B_{x,ij}^2\Delta t}\right) \operatorname{erf}\left(\frac{a-R_{ij}}{B_{X,ij}\sqrt{2}}\sqrt{\frac{1}{q}-\frac{1}{\Delta t}} - \frac{b+R_{ij}}{B_{x,ij}\sqrt{2}\Delta t\sqrt{\frac{1}{q}-\frac{1}{\Delta t}}}\right) \\ I_4 = \exp\left(-\frac{(a-b-2R_{ij})^2}{2B_{x,ij}^2\Delta t}\right) \operatorname{erfc}\left(\frac{a-R_{ij}}{B_{X,ij}\sqrt{2}}\sqrt{\frac{1}{q}-\frac{1}{\Delta t}} + \frac{b+R_{ij}}{B_{x,ij}\sqrt{2}\Delta t\sqrt{\frac{1}{q}-\frac{1}{\Delta t}}}\right) \end{cases} \quad (4)$$

Location of collision

The location of where the two particles collide is dependent on the barycentre (centre of gravity) X_g of the collision. The barycentre also follows a Brownian motion with diffusion coefficient $B_{x,g}$ equal to

$$B_{x,g}^2 = \left(\frac{m_{p,i}B_{x,i}}{m_{p,i} + m_{p,j}}\right)^2 + \left(\frac{m_{p,j}B_{x,j}}{m_{p,i} + m_{p,j}}\right)^2 \quad (5)$$

Then X_c , the location of the collision, is given by a sample from the normal distribution:

$$X_{c,\alpha} = \mathcal{N}(X_{M,\alpha}, \sigma_M^2) \quad (6)$$

where mean $X_M = X_g(t) + [X_g(t + \Delta t) - X_g(t)]t_c/\Delta t$ and variance $\sigma_M^2 = B_{x,g}^2 t_c(\Delta t - t_c)/\Delta t$.

Modified particle motion

Provided a collision has occurred, the positions of each of the two particles involved at the end of the time step must be calculated and updated.

$$X_{p,i}(t + \Delta t) = X_{p,i}(t + t_c) + B_{x,i}\sqrt{\Delta t - t_c}\xi'_x \quad (7)$$

where ξ'_x is another vector of independent random variables sampled in a standard normal distribution. Note that the position of only one particle is updated. The second particle, according to Henry et al., does not need to be updated [1].

Model

The algorithm used to detect and treat particle collisions is described in [1] and shown schematically in Fig. 1. For each time step, to summarize, Eq. (1) is first used to calculate the motion of N particles in a three-dimensional space. Next, for each pair of particles, the probability of a collision occurring is calculated using Eq. (2). Then, the collision probabilities are ranked in decreasing order and are each treated. The collision time is found via Eq. (3) and subsequently, the collision location via Eq. (6). Finally, the particle positions are modified via Eq. (7). After each collision is treated, we advance the time step by Δt .

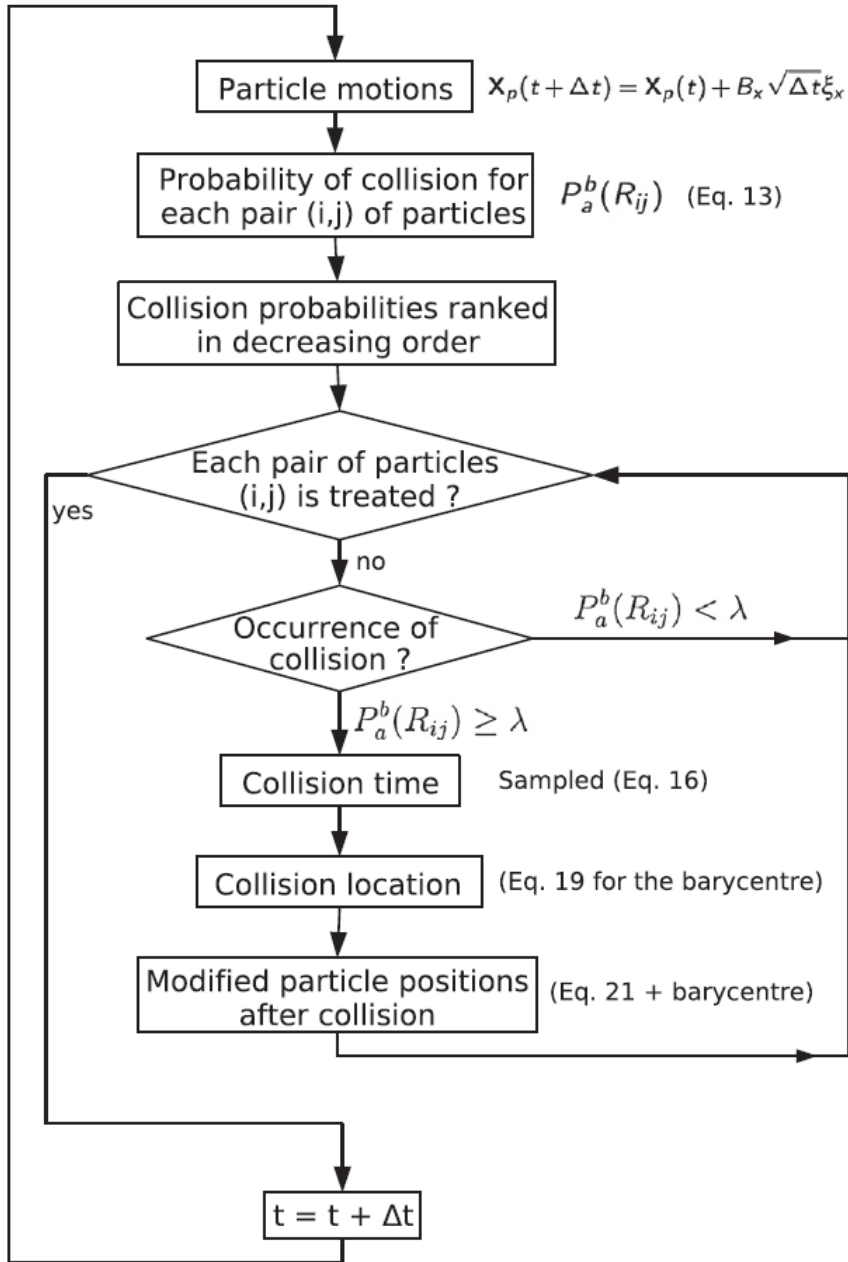


Fig. 1. Flowchart for algorithm of detecting and treating particle collisions.

The model was then implemented in MATLAB. Subsequent diagrams were produced in MATLAB.

IV. RESULTS AND DISCUSSION

Fig.2 show an example of the Brownian path a single particle undergoes.

Fig. 3 shows an example of a simulation involving three particles. Graphed are the position paths of the three particles.

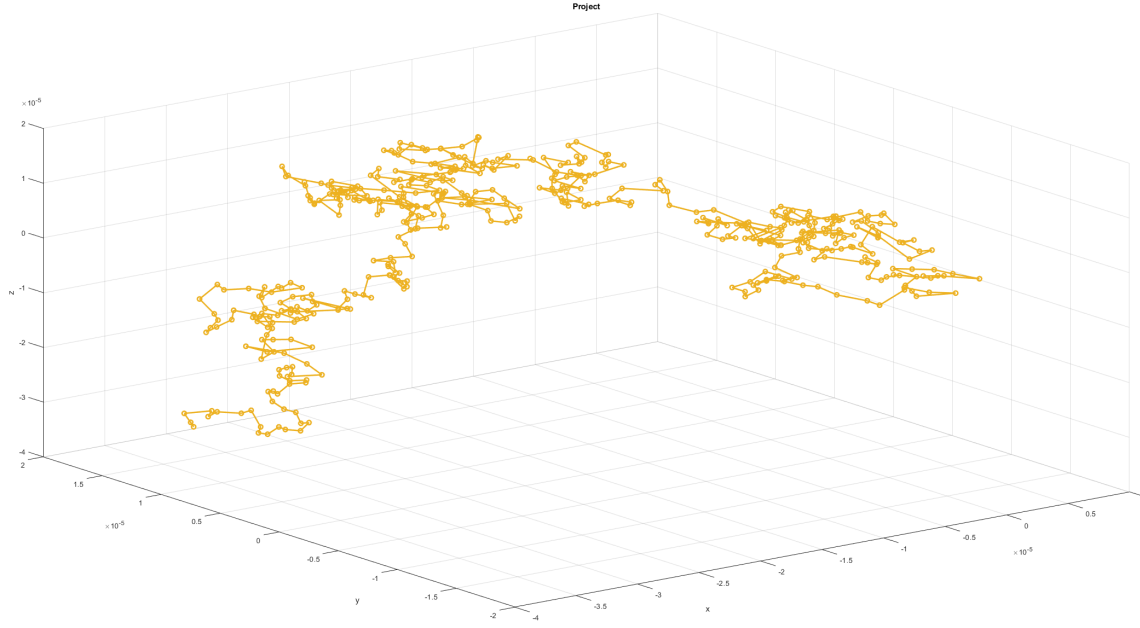


Fig. 2. Diagram of a singular particle Brownian motion path with radius $R = 10^{-6}m$, $\Delta t = 10^{-4}s$, and $B_x = 10^{-4}m \cdot s^{-1/2}$

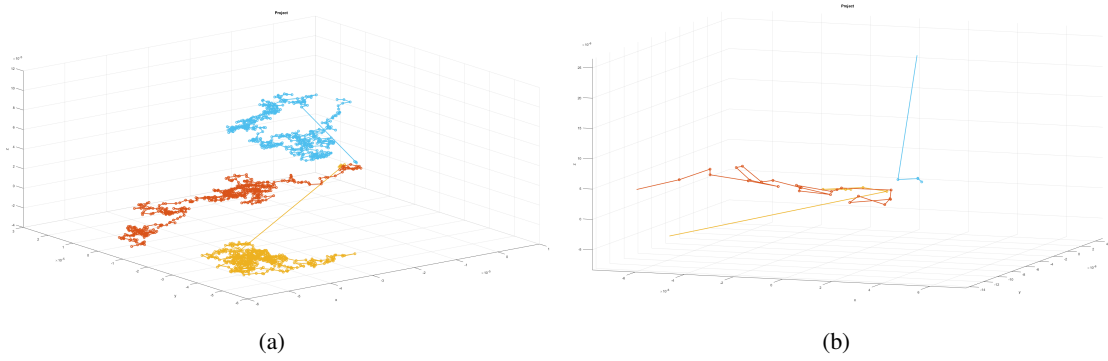


Fig. 3. (a) Position graphs of simulation of three particles with radius $R = 10^{-6}m$, $\Delta t = 10^{-4}s$, and $B_x = 10^{-4}m \cdot s^{-1/2}$ (b) Close-up image of the two collisions occurring in the simulation

Future Improvements

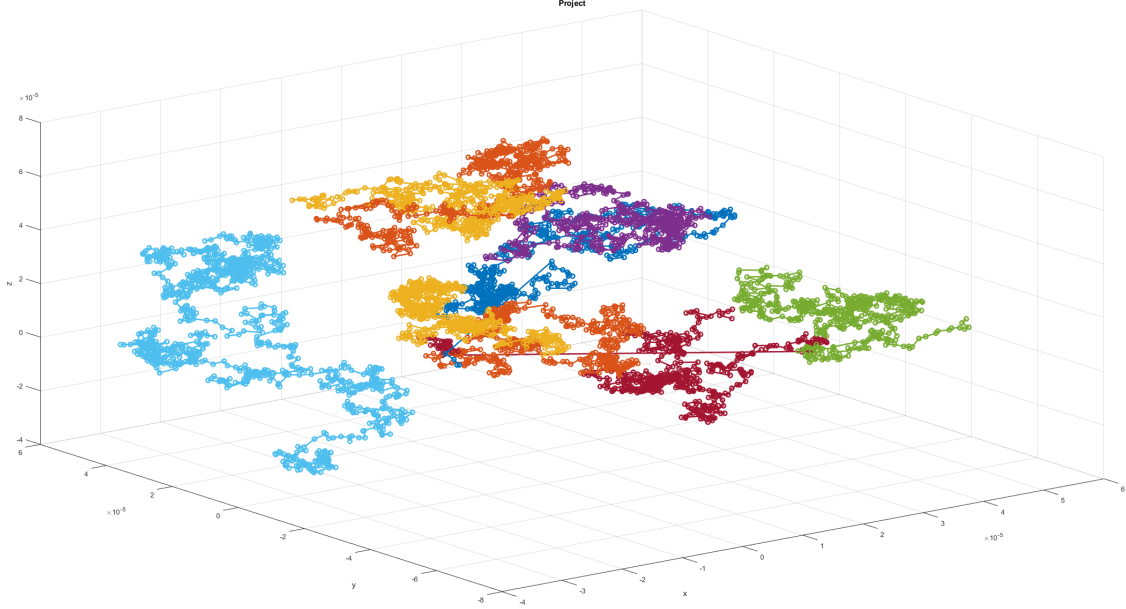


Fig. 4. Diagram of ten particles' motions with radius $R = 10^{-6}m$, $\Delta t = 10^{-4}s$, and $B_x = 10^{-4}m \cdot s^{-1/2}$

Fig. 4 shows the simulation of ten particles under 500 timesteps for a total time of 0.05s. Two collisions occur.

Fig. 5 shows the computation time of the MATLAB implementation. The computation time almost scales linearly with the total number of timesteps used. Further improvements to efficiency can be made. Currently, a naive algorithm is used to check every particle against every other particle. This results in $O(n^2)$ cost.

One limitation of plotting the position paths of each particle is that it is difficult to verify whether the collision calculated and drawn is correct. It is evident when a collision occurs (Fig. 3 (b)), however, the implementation offers no way of seeing where the original final position was calculated to be.

Furthermore, MATLAB does not support arbitrary CDFs, making computing the collision time with Eq. (3) impossible. The collision time was instead computed as $t_c = \lambda \Delta t$ where λ is a random number sampled uniformly between 0 and 1.

No. of Particles	# of Timesteps	Total Time (s)	Total Computation Time (s)
10	10 ⁴	1	0.31
10	10 ⁵	10	2.83
10	10 ⁶	100	25.78
10	10 ⁷	1000	249.82

Fig. 5. Computation time of different number of maximum time steps

Limitations

One limitation that this model faces is that it is only able to assess a single collision per pair of particles for each time step. One solution that Henry et al. suggests in [1] to account for the possibility of multiple collisions between the same pair of particles in a single time step is to introduce sub-time steps. The algorithm would be modified to recalculate the collision probability with other pairs in the remaining time after the initial collision has occurred.

Another next step is that the model is only valid for a time step Δt where it is much larger than τ_p (i.e. $\Delta t \simeq 100\tau_p$). In scenarios where this constraint is not present, Eq. (1) is no longer valid to calculate a particle's motion. Instead, the following equation has been suggested to be used instead:

$$\begin{cases} X_p(t + \Delta t) = X_p(t) + U_p(t)\tau_p(1 - e^{-\Delta t/\tau_p}) + U_s(t)[\Delta t - \tau_p(1 - e^{-\Delta t/\tau_p})] \\ \quad + B_v\tau_p\sqrt{\Delta t - 2\tau_p\frac{(1-e^{-\Delta t/\tau_p})}{(1+e^{-\Delta t/\tau_p})}} + B_v\tau_p^2\frac{(1-e^{-\Delta t/\tau_p})^2}{\sqrt{2\tau_p(1-e^{-2\Delta t/\tau_p})}}\xi_u \\ U_p(t + \Delta t) = U_p(t)e^{-\Delta t/\tau_p} + U_s(t)e^{-\Delta t/\tau_p} + B_v\sqrt{\frac{\tau_p}{2}(1 - e^{-2\Delta t/\tau_p})}\xi_u \end{cases} \quad (8)$$

where U_p is the particle's velocity, U_s is the fluid velocity, and ξ_u and ξ_v are independent vectors of random variables sampled in a standard normal distribution. Furthermore, the collision probability step would have to be modified to account for the initial and final relative velocities.

V. CONCLUSION

This project implements the stochastic method to detect and treat diffusive particle collisions described in Henry et al.'s paper [1]. The project outlines the limitations of classical models that do not account for potential collisions between time steps and accounts for the entire diffusive and relative trajectories of these particles. The results obtained showcase the Brownian motion paths of the particles in the simulation and their collisions, if any.

This method is a beginning step and leaves the door open to further advancements and improvements mentioned in the 'Limitations' section. It presents the first step of agglomeration and is to be coupled with the second step of formation of larger particles.

REFERENCES

- [1] Christophe Henry, Jean-Pierre Minier, Mikaël Mohaupt, Christophe Profeta, Jacek Pozorski, and Anne Tanière, “A stochastic approach for the simulation of collisions between colloidal particles at large time steps,” *International Journal of Multiphase Flow*, vol. 61, pp. 94–107, 2014.
- [2] M. Mohaupt, J.-P. Minier, and A. Tanière, “A new approach for the detection of particle interactions for large-inertia and colloidal particles in a turbulent flow,” *International Journal of Multiphase Flow*, vol. 37, no. 7, pp. 746–755, 2011.