# Computational Physics: Project 2
# Brownian Motion

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## 1 Introduction

Brownian motion traditionally describes the random movement of particles suspended in a fluid resulting from collisions with fast-moving molecules. Here, we implement two modifications to this model. First, we consider inertial effects on the particle, usually neglected in environments with low Reynolds numbers. As described below, the particle's position is described by a 2nd order equation of motion driven by external white noise. Second, we allow the motion to occur in a confined one-dimensional environment that the particle can leave with some probability once it reaches the ends. The probability of leaving the domain or being reflected at the boundary is controlled by sampling simple probability distributions using both rejection sampling and the inverse CDF method. Our numerical study uses a stochastic Euler method, which is known to be appropriate for stochastic ODEs (SDEs from now on), and a naive implementation with white noise of the traditional Runge-Kutta (RK4) method for ODEs, which is known to not be appropriate in general for SDEs. A comparison of both results offers an interesting example where both approaches provide qualitatively similar results, even though it is known that one has to be careful to write an appropriate numerical implementation for noisy dynamics. We obtain from the stochastic Euler method that once the particle reaches one of the boundaries, it will most likely leave through that same boundary even if it doesn't get absorbed immediately. Although it is, in principle, allowed to be absorbed on the opposite side of the interval after being reflected, we compute histograms of the final position over multiple trajectories to show that this is unlikely. This is our key result. Finally, to validate our simulations, we show that we can recover standard results for the inertial Brownian particle in the limit where the boundary is infinitely far away from the starting position of the particle.

## 2 Inertial Brownian Particle

We consider a particle in one dimension with position $x(t)$ and velocity $v(t)$ at time $t$ described by the equation of motion,

$$m\ddot{x} = -\gamma\dot{x} + \sigma\eta \tag{1}$$

where $m$ is the mass of the particle, $\gamma$ the viscosity of the surrounding fluid, $\sigma = \sqrt{2D}$ where $D$ is the diffusion constant of the particle, and $\eta$ is delta-correlated white noise (i.e. $\langle\eta\rangle = 0$ and $\langle\eta(t)\eta(s)\rangle = \delta(t-s)$). This equation should be understood as a balance of forces between inertial forces (1st term), viscous forces (2nd term), and a rapidly fluctuating force (3rd term) coming from collisions of particles in the surrounding fluid with our main particle. Equivalently, it can be written as a system of 1st order equations,

$$\dot{x} = v \tag{2}$$

$$\dot{v} = -\frac{\gamma}{m}v + \frac{\sigma}{m}\eta \tag{3}$$

Usually, these two equations would be uncoupled, and one could solve for the velocity using the second equation first and then recover the positions later. However, since we envision stopping the dynamics when the particle hits the domain's boundary, there is an implicit boundary condition coupling $x$ and $v$. Hence, we discretize the two equations together. The stochastic Euler or Euler-Mayurama method gives,

$$x_{i+1} = x_i + v_i\Delta t \tag{4}$$

$$v_{i+1} = v_i - \frac{\gamma}{m}v_i\Delta t + \frac{\sigma}{m}\Delta \mathrm{W_n} \tag{5}$$

where $\Delta t$ is the time-step in the simulation and $\Delta \mathrm{W_n}$ are i.i.d normal random variables with zero mean and variance $\Delta t$. This is known to be the simplest numerical implementation of SDEs.

To impose the absorbing/reflecting boundary condition, we choose a value L and take as a domain $x \in [-\mathrm{L}, \mathrm{L}]$ and a value $p \in [0, 1]$. Whenever $x = \pm \mathrm{L}$, we choose a value $p^* \in [0, 1]$ and check if $p \leq p^*$. If so, we say the particle is absorbed and stop the simulation. Otherwise, we set $v_{i+1} = -v_i$, i.e. we force the particle to move in the opposite direction as an effective reflection and continue the simulation. We allow the dynamics to take place up a time T, i.e. $t \in [0, \mathrm{T}]$. To choose $p^*$, we sample from two possible probability distributions using rejection sampling (a Gaussian distribution) or inverse CDF sampling (an exponential distribution).

Lastly, we consider the limit where $\mathrm{L} \to \infty$ to validate our results. Numerically, we implement this limit by taking $\mathrm{L} >> 1$ since the starting position of the particle will be $x(0) = 0$. In this regime, we can drop the boundary condition and let the particle run over the whole space $\mathbb{R}$. Hence, equations (2-3) uncouple. As our first validation check, notice that the average value (over realizations of the noise) of the velocity follows an exponential decay,

$$\langle v \rangle = v(0) e^{-\frac{\gamma}{m} t} \tag{6}$$

where $v(0)$ is the initial velocity. Hence, we expect the trajectories for the velocity to be exponentially decaying with some fluctuations when the particle cannot reach the boundary. As our second check, it is well known that the velocities relax to an equilibrium state where the probability density, $\rho(v)$, is given by statistical mechanics [reference],

$$\rho(v) \propto e^{-\beta \frac{m v^2}{2}} \tag{7}$$

The histogram of velocities should converge to the Boltzmann distribution (7) as the boundary is moved to infinity. As our third, and final check, we can check in our simulations that the Mean Square Displacement (MSD) follows the predict behavior, namely MSD $\propto t$ for short times and MSD $\propto \sqrt{t}$ for long times, where the appropriate timescale to compare against is the relaxation time of the system.

# 3 Results

We run the simulation for 100 iterations, with $1,000,000$ time steps each, using the following parameters:

- Initial position and velocity $(x_0, v_0)$: $(0.01, 50.0)$
- Length of interval $(L)$: $200,000$
- Friction coefficient $(\gamma)$: 0.5
- Mass $(m)$: 1.0
- Noise amplitude $(\sigma)$: 1.5

Figure (1) presents representative trajectories of the position and velocity over time and shows how most trajectories make it as far as possible from their initial position since the boundary sits effectively at infinity, $\mathrm{L} = 200,000 >> 1$.

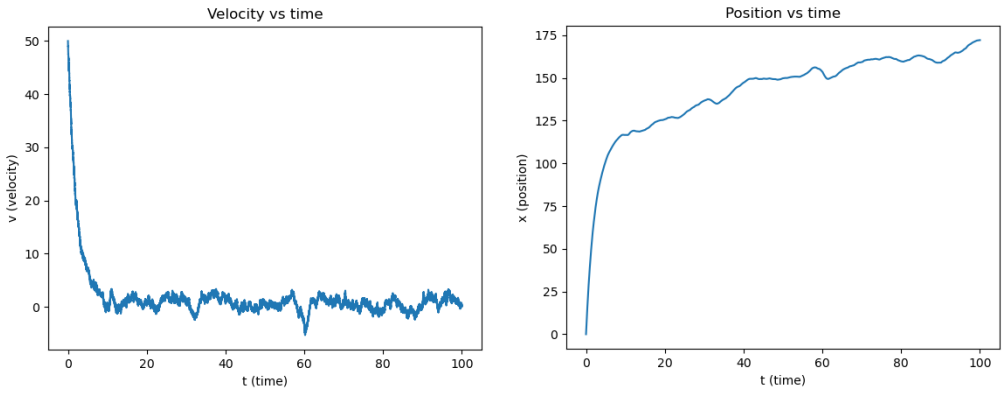


Figure 1: Trajectory

Figure (2) shows a comparison between the two methods, the stochastic Euler and the naively implemented Runge-Kutta (RK4) method. We remark that the stochastic Euler method is the appropriate one for SDEs. Nevertheless, the naive implementation of the Runge-Kutta, where we use the same formulation as for deterministic ODEs, does follow the trend.

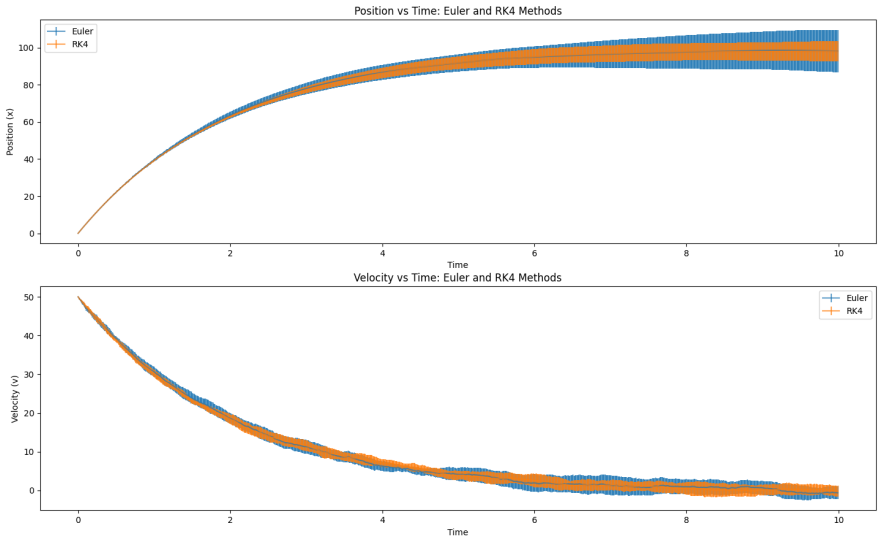


Figure 2: Euler and RK4 Method

Figure (3)is a histogram showing the probability distribution of positions for a Brownian particle, displaying a highly skewed, asymmetric distribution with peak probabilities occurring around x=150-160. The

distribution's shape deviates from the expected Gaussian (normal) distribution typically associated with Brownian motion, suggesting this might be a snapshot at a specific time rather than an ensemble average over many times. Nevertheless, particles are biased towards one direction due to their initial velocity. Even if they were to reach the boundary at $x = \mathrm{L}$ of the domain and be reflected, this distribution shows that they would keep bouncing back against the same boundary until they get absorbed.

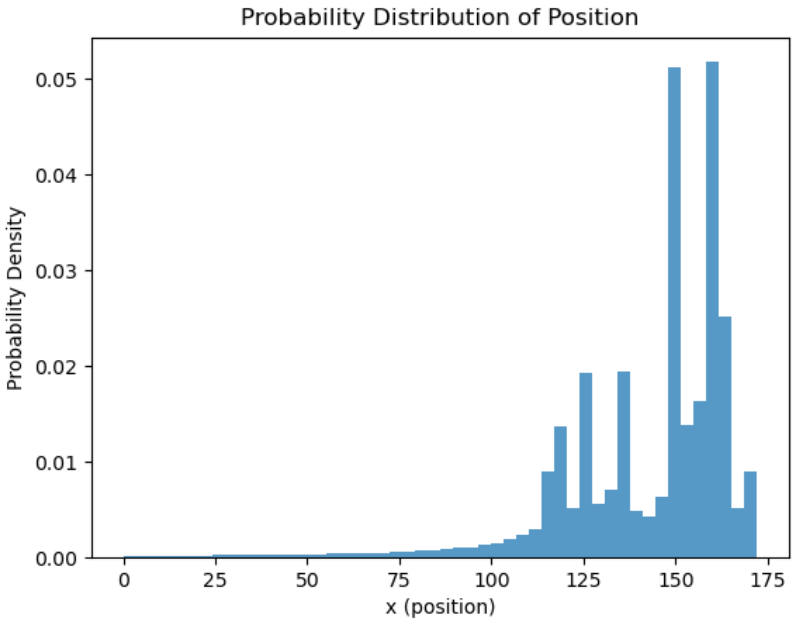


Figure 3: Distribution

## 3.1 Validation

The saturation around what seems to be a steady state in the velocity in Figure (1) suggests that we should be able to validate our numerics in this regime. Indeed, figure (4) corroborates that the average velocity, $\langle v(t) \rangle$, saturates around an exponential decay in the long-time regime for a representative curve while the velocity distribution shows a Boltzmann distribution, as expected from reaching equilibrium.

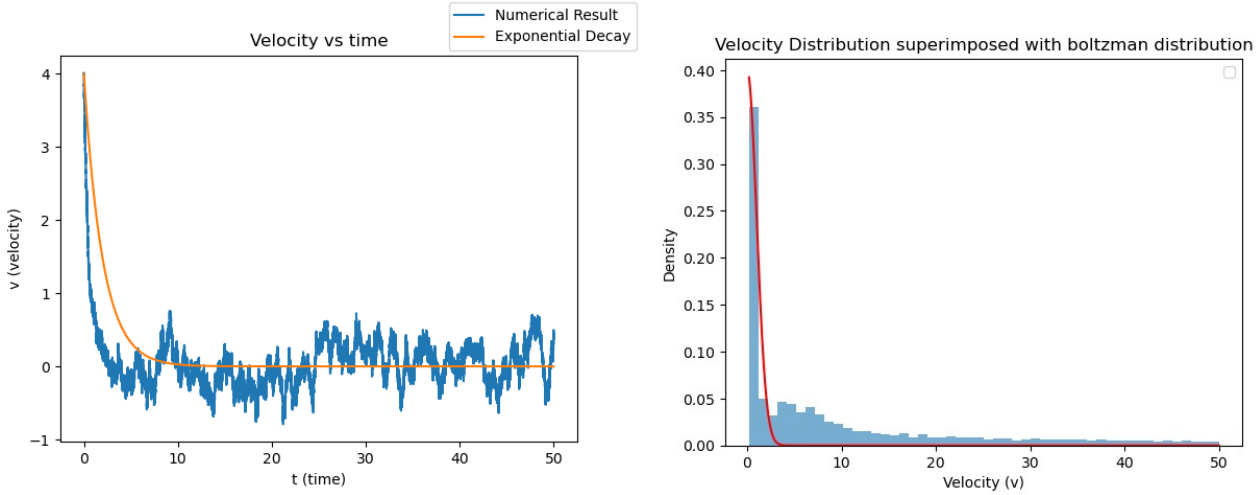


Figure 4: Velocity and Velocity distribution

In addition, we compute the mean square displacement, a classical object characterizing Brownian motion. Figure (5) shows the results of numerical simulations (blue curve) with a linear fit (red dashed line) superimposed for reference. It is well known that the MSD of Brownian motion with inertia is linear in time early on and goes

as $\sqrt{t}$ for long times, with the first regime controlled by the initial momentum of the particle and the second by diffusive motion controlled by the Einstein relation in 1D, $\langle x(t) \rangle = 2Dt$ where D is the diffusion constant [reference]. These two regimes are easily identified in figure (5), where the crossover seems to be around $t = 20$. Hence, the plot clearly demonstrates the three key characteristics of the MSD of Brownian motion with inertia.

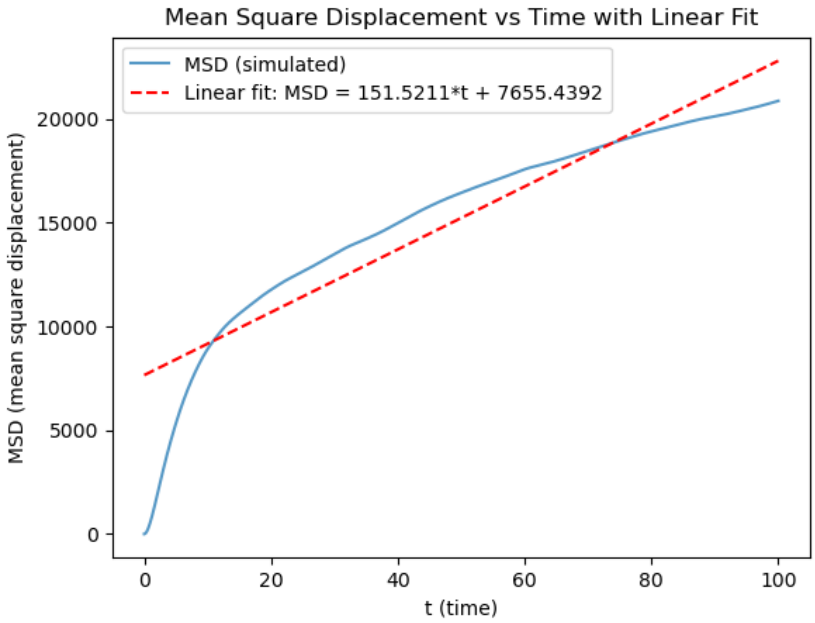


Figure 5: Caption

## 3.2 Errors

To study diverse sources of error in our simulations, we computed 1) the numerical error over time, 2) the statistical error over time, 3) the finite precision error over time, and 4) the statistical error as a function of the number of simulations. Figure (6) shows our results.

The numerical error is a plot of the difference of numerical error calculated for the stochastic Euler method and Runge-Kutta (RK4) method. We infer from the graph that the RK4 method is more accurate as the difference goes negative in the plot since we are plotting *Euler error - RK4 error*.

The growth shown in the plot of the statistical error is exactly what we would expect for Brownian motion since the standard deviation grows linearly in time, and the statistical error typically grows proportional to the standard deviation. Indeed, when plotted against time, we expect quadratic growth approximately. Moreover, the initial flat region suggests good numerical stability at small time scales, effective initial sampling, and minimal statistical variations early in the simulation. Finally, the accelerating growth is consistent with Brownian motion since as time increases, the random walks have more opportunity to diverge.

The finite precision error over time is shown on a logarithmic scale along the vertical axis. The increasing error over time is expected in Brownian motion because the process is inherently random and chaotic, accumulating small numerical and rounding errors over time. The stabilization fo error at later times is also expected because there is typically a maximum bound on the possible total accumulated error in stable numerical schemes. Hence, additional time steps don't need to lead to worse precision beyond a certain point.

The statistical error demonstrates characteristic scaling behavior according to the central limit theorem, namely $error \propto \frac{1}{\sqrt{N}}$ where $N$ is the number of simulations.

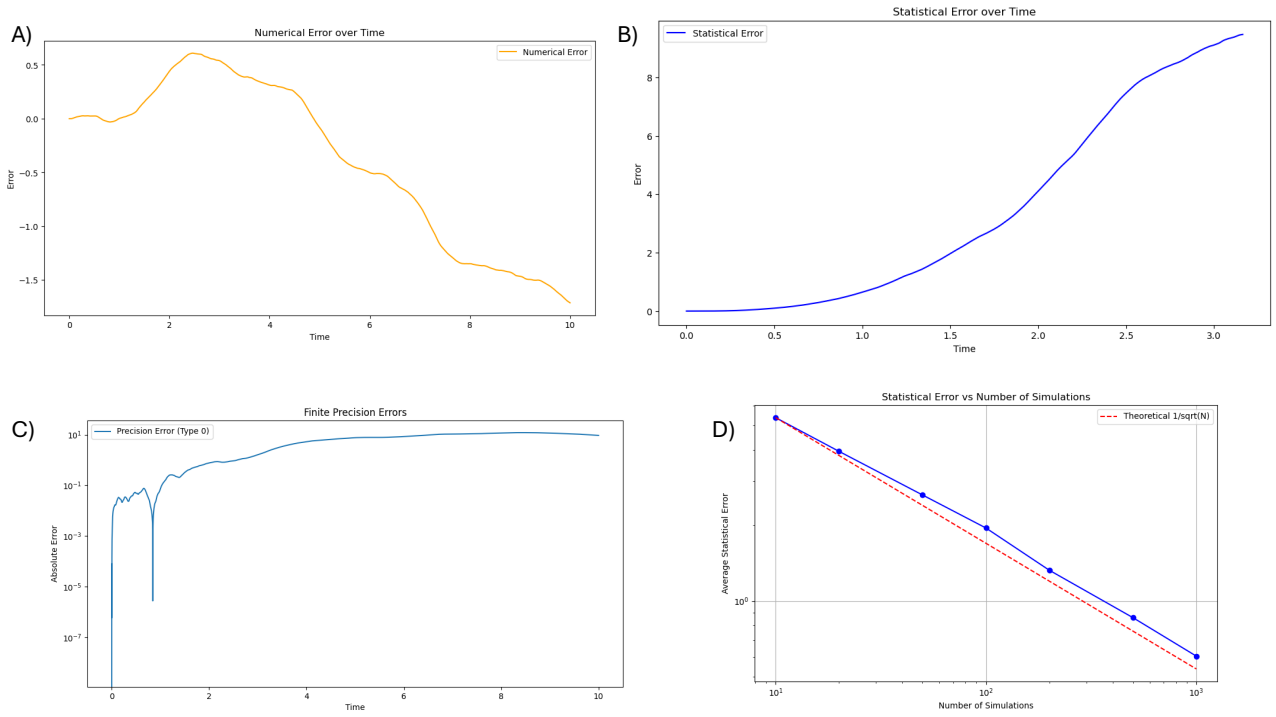


Figure 6: Error Analysis

### 3.3 Computational Complexity

We also present a simple theoretical analysis of the computational complexity of our methods for simulating Brownian motion.

The stochastic Euler method performs one single evaluation per time step, leading to a theoretical complexity of $\mathcal{O}(\mathrm{N})$ where N is the number of time steps. In each step one 1) updates position and velocity of the particle, 2) use a random number generator for the stochastic terms, and 3) checks boundary conditions.

On the other hand, the RK4 method requires four evaluations per time step, resulting in a theoretical complexity of $\mathcal{O}(\mathrm{N})$.

## 4 Conclusion

The study of Brownian motion using numerical simulations provides insight into the random behavior of particles. The Euler and RK4 methods yielded consistent results, while the sampling techniques demonstrated effective ways to obtain distributions from random processes. Future work may involve exploring other numerical methods and their efficiencies in simulating complex stochastic systems.

## 5 References


- Kloeden, P. E., & Platen, E. (1992). *Numerical Solution of Stochastic Differential Equations*. Springer.
- Oksendal, B. (2003). *Stochastic Differential Equations: An Introduction with Applications*. Springer.