Stochastic differential equations with memory

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Abstract

We investigate the stochastic dynamics of persistent Brownian walkers through numerical simulations of overdamped Langevin equations with Ornstein-Uhlenbeck colored noise. We validate our numerical implementation by demonstrating perfect agreement with theoretical predictions for both the noise autocorrelation and the mean squared displacement of free particles across persistence times $\tau = 1, 10, 100$. We then examine the system's response to external perturbative forces, testing force magnitudes from $f = 0.001$ to $f = 1$ at $\tau = 10$. By extracting the mobility μ and diffusion coefficient D from long-time dynamics, we identify that forces with $f \leq 0.01$ maintain the fluctuation-dissipation relation $D = \mu k_B T$, characteristic of the linear response regime. For $f \geq 0.1$, the fluctuation-dissipation relation breaks down as diffusion increases without corresponding changes in mobility, and the system exhibits superdiffusive behavior, indicating non-equilibrium dynamics.

1 Introduction

The objective of this work is to investigate the stochastic dynamics of a random walker through numerical simulations, focusing on Langevin equations with non-Markovian noise. Our starting point is the overdamped Langevin equation:

$$\gamma \dot{\mathbf{r}}(t) = \mathbf{F}(\mathbf{r}) + \boldsymbol{\xi}(t) \tag{1}$$

where $\boldsymbol{\xi}$ represents a Gaussian stochastic force satisfying

$$\langle \boldsymbol{\xi} \rangle_n = \mathbf{0}, \quad \langle \xi_\alpha(t) \xi_\beta(t') \rangle_n = \Gamma(t - t') \delta_{\alpha\beta} \tag{2}$$

The subscript n indicates averaging over the noise distribution.

The presence of noise with temporal correlations introduces memory effects into the walker's dynamics. While memory can often be neglected when studying physical problems at scales much larger than those of interest, there are many situations where the noise correlation time is comparable to the characteristic timescales of the relevant dynamical variables. In such scenarios, particularly for systems with colored noise, memory effects must be explicitly incorporated. We illustrate this concept using a simple model system.

We examine N persistent Brownian walkers confined to a one-dimensional periodic domain of size L. Their motion is governed by the overdamped Langevin equations:

$$\gamma \dot{\mathbf{r}}_i(t) = \mathbf{F}_i + \boldsymbol{\xi}_i \tag{3}$$

$$\dot{\boldsymbol{\xi}}_i(t) = -\frac{\boldsymbol{\xi}_i}{\tau} + \sqrt{\frac{2D}{\tau^2}} \boldsymbol{\eta}_i(t) \tag{4}$$

Here, $\boldsymbol{\xi}_i$ represents non-Markovian colored noise, characterized by an Ornstein-Uhlenbeck process with persistence time τ. In contrast, $\boldsymbol{\eta}_i$ denotes standard Gaussian white noise with zero mean and unit variance. The colored noise introduces temporal persistence in the Brownian dynamics, reflected in its autocorrelation function:

$$\langle \xi_i(t) \xi_j(t') \rangle = \frac{D}{\tau} e^{-|t-t'|/\tau} \delta_{ij} \mathbf{1} \tag{5}$$

This model is commonly employed to describe self-propelled particles. It reduces to standard passive (equilibrium) Brownian motion in the limit $\tau \to 0$, where the colored noise correlation becomes instantaneous: $\langle \xi_i(t) \xi_j(t') \rangle \to 2D\delta(t - t')\delta_{ij}\mathbf{1}$ in the distributional sense. Throughout this work, we set $\gamma = 1$ without loss of generality.

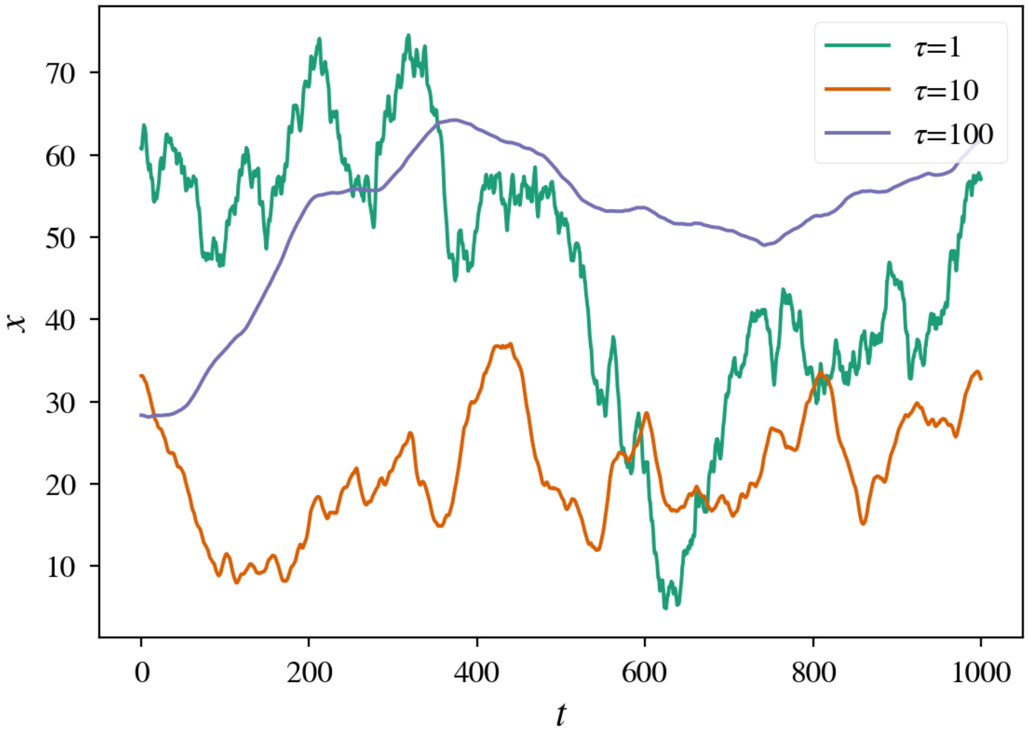

Figure 1: Trajectories of persistent Brownian walkers in a 1D segment of length $L = 100$, for three different relaxation time values $\tau = 1, 10, 100$. With parameter values $D = 1$, $\Delta t = \tau/100$, and a total simulation time of $t_{tot} = 1000$.

1.1 Euler-Mayurama discretization

To solve this system of stochastic differential equations numerically, we employ the Euler-Maruyama method, which extends the standard Euler method to stochastic systems. The discretization begins by dividing the time into intervals of size Δt and advancing the system using finite-difference approximations. At each time step, the colored noise $\boldsymbol{\xi}_i$ is updated according to:

$$\boldsymbol{\xi}_i(t + \Delta t) = \boldsymbol{\xi}_i(t) - \frac{\boldsymbol{\xi}_i(t)}{\tau}\Delta t + \sqrt{\frac{2D}{\tau^2}}\Delta \mathbf{W}_i \tag{6}$$

where $\Delta \mathbf{W}_i$ represents the Wiener process increment, drawn from a normal distribution with zero mean and variance Δt, i.e., $\Delta \mathbf{W}_i \sim \mathcal{N}(0, \Delta t \mathbf{1})$. Subsequently, the particle positions are updated using:

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + [\mathbf{F}_i + \boldsymbol{\xi}_i(t)]\, \Delta t \tag{7}$$

The time step Δt must be chosen sufficiently small to ensure numerical stability and accuracy, typically requiring $\Delta t \ll \tau$ to properly resolve the dynamics of the colored noise. Periodic boundary conditions are applied by taking positions modulo L. In Fig. 1 we plotted some typical trajectories for relaxation times $\tau = 1, 10, 100$.

In all of our simulations, we have used the following values for N, L and D. $N = 50$, balancing computational efficiency with statistical significance. $L = 100$, since we apply PBC this number is not that significant. And $D = 1$, a realistic diffusivity value that also simplifies the calculations.

More important are the integration time parameters Δt and t_{tot}, the time step and the total integration time. Since this problem has a characteristic timescale, we are not free to choose any value for these parameters, as it can alter the experiment results. In our simulations, we used a $\Delta t \leq \tau/100$, in order to have sufficient detail on the relaxation time of the random walker. On the other hand, the total time of our simulation was always at least 10 times the relaxation time, $t_{tot} \geq 10\tau$, so that we can observe the two regimes clearly.

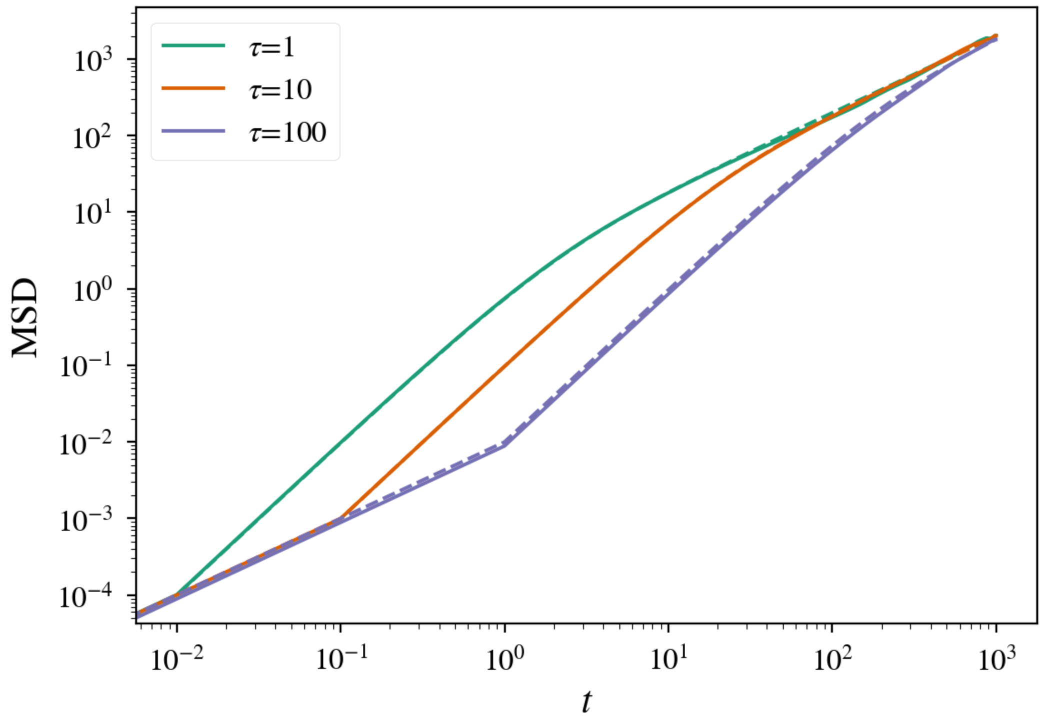

Figure 2: MSD as a function of time, in log-log scale. For $N = 50$ free persistent Brownian walkers in a 1D segment of length $L = 100$, for three different relaxation time values $\tau = 1, 10, 100$. Solid lines represent the numerical results obtained from simulations, while the dashed lines show the theoretical prediction. With parameter values $D = 1$, $\Delta t = \tau/100$, and a total simulation time of $t_{tot} = 1000$.

2 Mean square displacement of free particles

The mean square displacement, or MSD, is a way of quantifying how far do Brownian walkers wander away from where they started. And it is defined as

$$\mathrm{MSD}(t) = \frac{1}{N}\sum_i \langle (x_i(t) - x_i(0))^2 \rangle, \tag{8}$$

where $x_i(t)$ represents the position of the i-th particle at time t.

We compare this with the theoretical result of the mean square displacement for an Ornstein-Uhlenbeck process,

$$\mathrm{MSD}(t) = 2D(t + \tau(e^{-t/\tau} - 1)), \tag{9}$$

that we can easily see it reduces to normal diffusive behaviour, $\mathrm{MSD} = 2Dt$, in the limit where there is no memory in the process $\tau \to 0$.

We calculated the MSD for $N = 50$, free ($\mathbf{F} = 0$), persistent Brownian particles for different values of the relaxation time, $\tau = 1, 10, 100$ (Fig. 2), and we found complete agreement between our simulations and the theoretical prediction.

3 Decay of the correlation function

Next, we examine the temporal autocorrelation function of the colored noise. For the Ornstein-Uhlenbeck process described by Eq. 4, the theoretical autocorrelation function is given by:

$$C(t) = N^{-1}\sum_i \langle \xi_i(t)\xi_i(0) \rangle = \frac{D}{\tau} e^{-t/\tau} \tag{10}$$

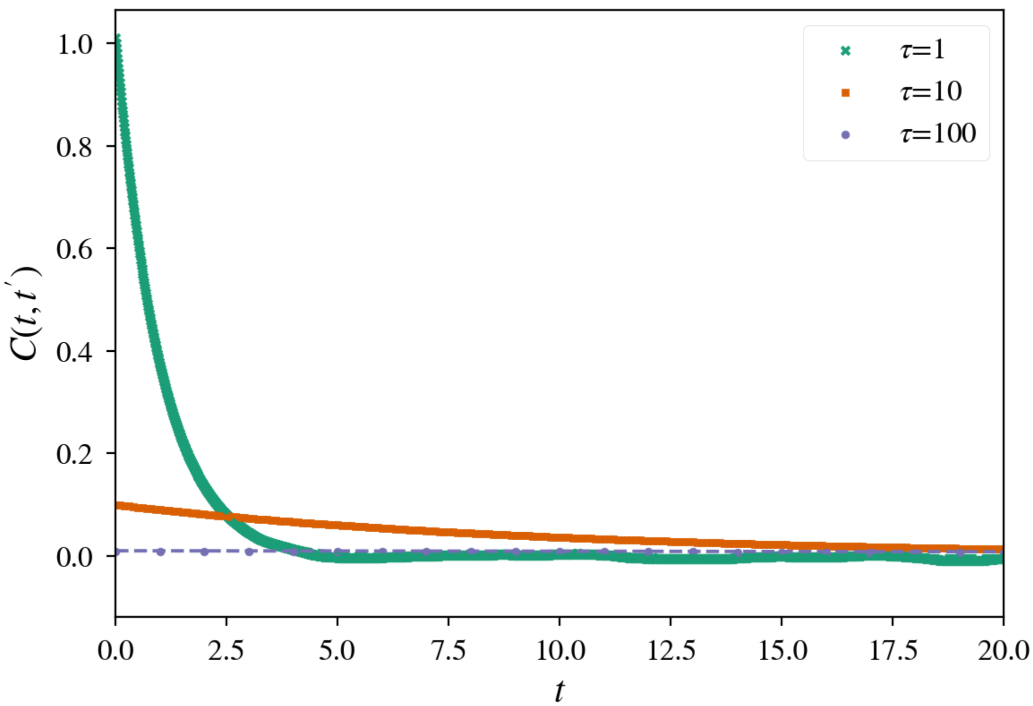

Figure 3: Temporal autocorrelation function of the colored noise for three different relaxation times, $\tau = 1, 10, 100$. Markers represent the numerical results obtained from simulations, while the dashed lines show the theoretical prediction. Parameters: $N = 50$ particles, $D = 1.0$, $\Delta t = \tau/100$, total simulation time $t_{tot} = 1000$.

We compute this correlation function from our simulations for three different values of the persistence time: $\tau = 1, 10, 100$. The results are shown in Fig. 3. For each value of τ, we observe the expected exponential decay with a characteristic timescale set by τ.

At short times ($t \ll \tau$), the autocorrelation remains close to its initial value $C(0) = D/\tau$, indicating strong temporal correlation in the noise. As time progresses beyond $t \sim \tau$, the correlation decays exponentially, demonstrating the loss of memory in the stochastic forcing. For larger values of τ, this decay occurs more slowly, reflecting the longer persistence time of the colored noise.

4 Response to perturbative forces

In this section, we study the effects of a constant force on the particles that we define as $\{_i = \epsilon_i f$, where $\epsilon_i = \pm 1$ with equal probability.

First, we plot the effect of this force on the MSD of the particles in Fig. 4, for different forces $f = 0, 0.001, 0.01, 0.1, 1$, and $\tau = 10$.

Next, we also plot the displacement in the force direction in Fig. 5. We define this displacement d_x as

$$d_x(t) = \frac{1}{N} \sum_i \epsilon_i \langle x_i(t) - x_i(0) \rangle, \tag{11}$$

and we also plot this quantity for different forces $f = 0, 0.001, 0.01, 0.1, 1$, and $\tau = 10$. Both the MSD and the displacement were averaged between 10 independent realizations.

Moreover, from the long-time behavior of the mean displacement and MSD, we extract two fundamental transport coefficients: the mobility μ and the diffusion coefficient D, defined as:

$$\mu = \lim_{t \to \infty} \frac{d_x}{ft} \tag{12}$$

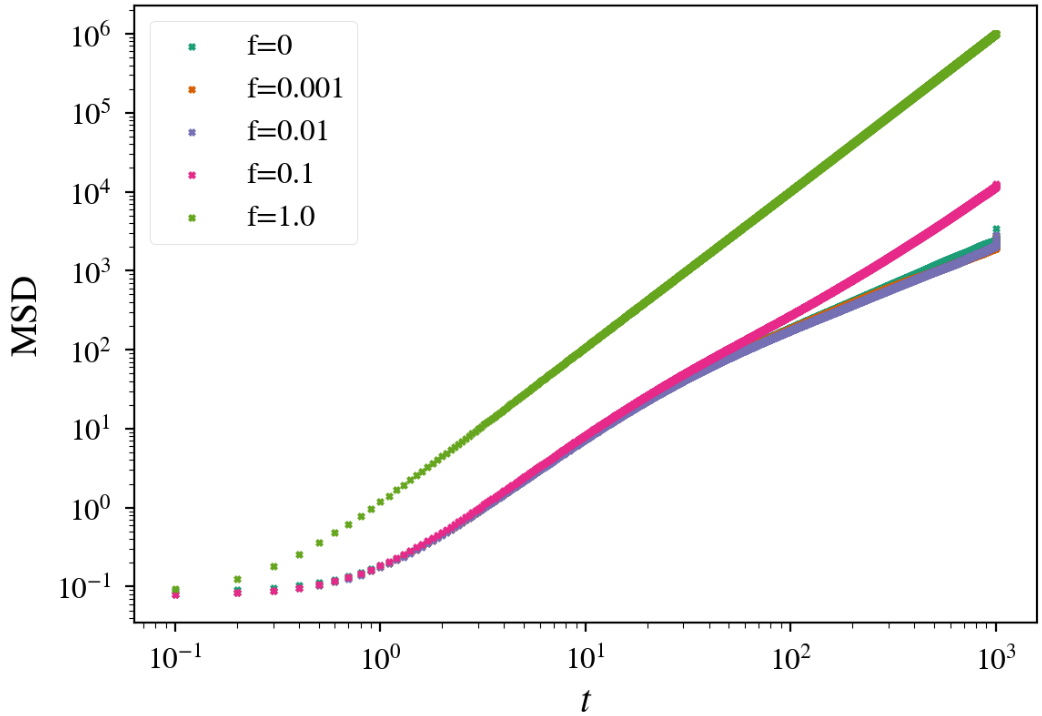

Figure 4: MSD as a function of time, in log-log scale. For Brownian particles under a constant force, with possible values $f = 0, 0.001, 0.01, 0.1, 1$, with relaxation time $\tau = 10$, averaged over 10 independent realizations. With parameter values $D = 1$, $\Delta t = 0.1$, $L = 100$, $N = 50$, and a total simulation time of $t_{tot} = 1000$.

and

$$D = \lim_{t\to\infty} \frac{\mathrm{MSD}(t)}{2t} \tag{13}$$

These quantities are obtained by performing linear fits to the displacement and MSD in the long-time regime (typically $t > 5\tau$). We compute μ and D for several values of the persistence time: $\tau = 0.5, 1, 2, 5, 10, 20, 50$, using a small force $f = 0.01$ to ensure operation within the linear response regime. The results are shown in Figs. 6 and 7.

As it can be seen, the diffusion coefficient increases monotonically with force magnitude f due to the stronger driving enhancing particle dispersion. For the smallest forces ($f = 0.001$), D approaches 1, recovering the input diffusivity from the stochastic noise term. The mobility displays consistent values when $f \geq 0.01$. However, for $f = 0.001$, the mobility measurements show large fluctuations.

5 Conclusions

In this work, we have successfully implemented and validated numerical simulations of persistent Brownian walkers governed by overdamped Langevin equations with Ornstein-Uhlenbeck colored noise. Our Euler-Maruyama integration scheme accurately reproduces the theoretical predictions for both the noise autocorrelation function and the mean squared displacement of free particles across a wide range of persistence times ($\tau = 1$ to 100).

Based on our simulations of the system's response to external forces, we can answer the question of when forces can be considered perturbative. Forces with magnitude $f \leq 0.01$ clearly operate within the linear response regime, as evidenced by the upholding of the Fluctuation-Dissipation relation $D = \mu k_B T$.

For forces in the range $f \sim 0.1$, the Fluctuation-Dissipation relation breaks down, as diffusion grows without an increasing mobility μ. Non-linear effects appear also in the MSD representation,

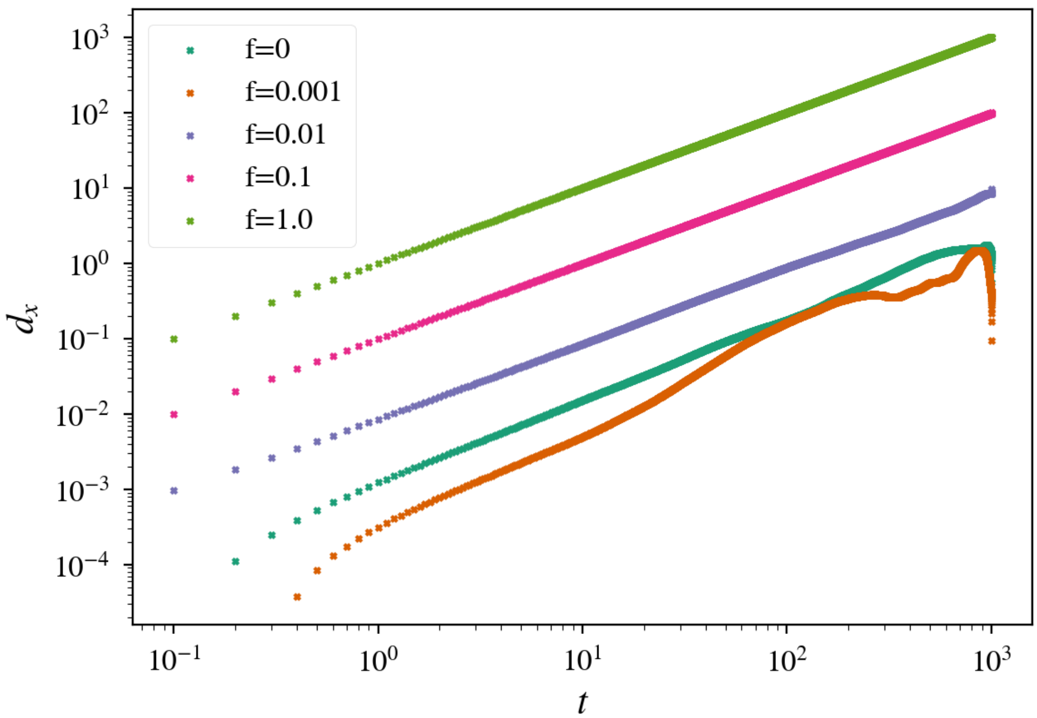

Figure 5: Displacement, as defined in Eq. 11, as a function of time, in log-log scale. For Brownian particles under a constant force, with possible values $f = 0, 0.001, 0.01, 0.1, 1$, with relaxation time $\tau = 10$, averaged over 10 independent realizations. With parameter values $D = 1$, $\Delta t = 0.1$, $L = 100$, $N = 50$, and a total simulation time of $t_{tot} = 1000$.

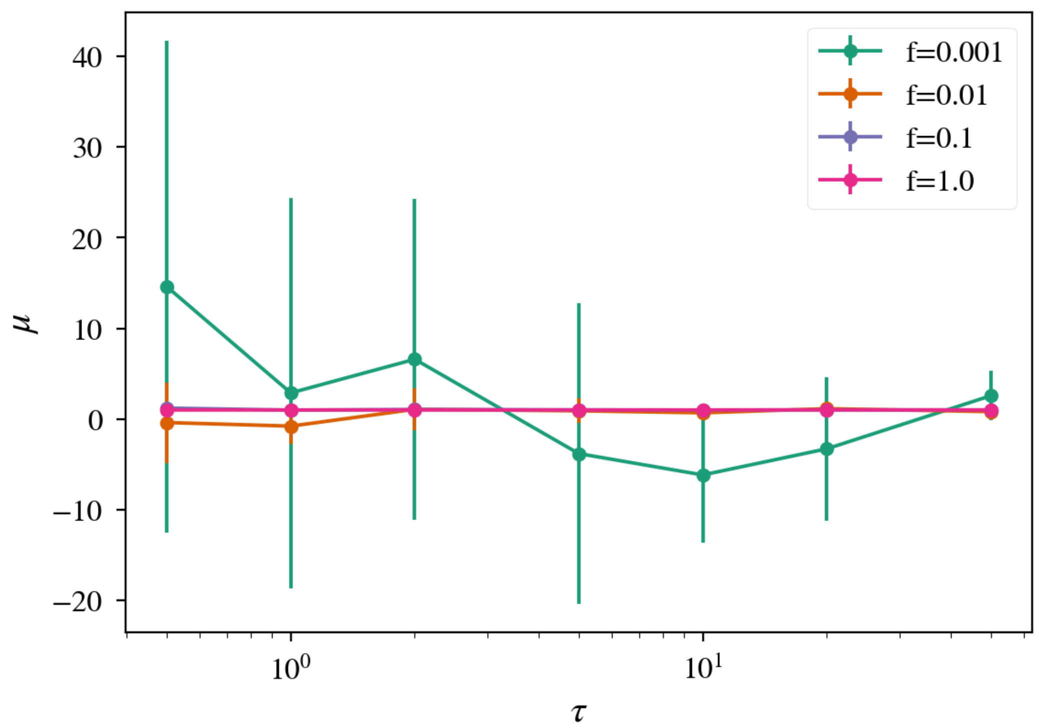

Figure 6: Mobility μ as a function of relaxation time τ. Error bars represent standard deviations over 10 independent realizations. Parameters: $f = 0.001, 0.01, 0.1, 1$, $N = 50$, $\gamma = 1$, $D_{\text{input}} = 1.0$, $\Delta t = \tau/100$, $t_{tot} = 100\tau$.

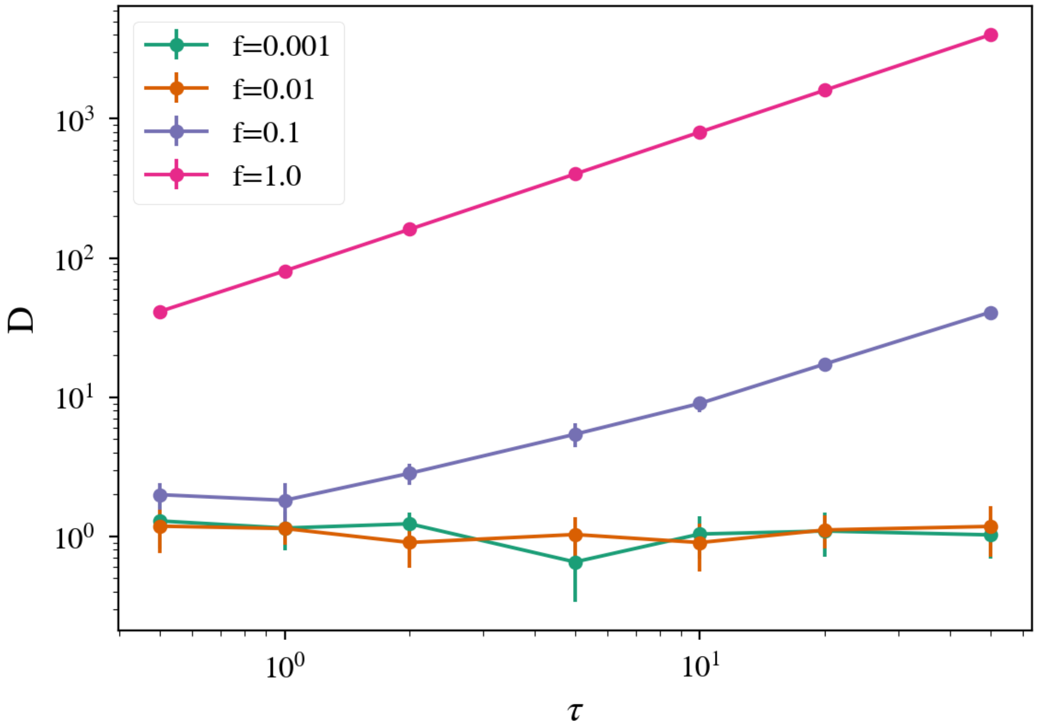

Figure 7: Diffusion coefficient D as a function of τ. Error bars represent standard deviations over 10 independent realizations. Parameters: $f = 0.001, 0.01, 0.1, 1$, $N = 50$, $\gamma = 1$, $D_{\text{input}} = 1.0$, $\Delta t = \tau/100$, $t_{tot} = 100\tau$.

where for $f \geq 0.1$, the system is firmly in the superdiffusive regime, as the force is large enough to drive the system out of equilibrium.

A Code availability

Code is available in the following GitHub repository Project 2 Francesc Bagur