Numerical Simulation for Diffusion Processes

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1 Introduction

In this work we consider the framework of a diffusion process and try to compute the entropy of the system.

Given a Langevin equation

$$\dot{x} = \Phi(x) + \epsilon\xi(t)$$

the probability density $\rho(x,t)$ satisfy the Fokker Planck equation, and the entropy is given by:

$$S(t) = -\int \rho \log \rho dx$$

If $\Phi = Ax$ the density is Gaussian in d dimension.

For the entropy we can get an explicit result:

$$S = \frac{d}{2}\log(2\pi kT) + \frac{1}{2}\log(det(\Sigma^2)) \tag{1}$$

where d is the dimension of the system and Σ^2 is the covariance matrix.

Now, if we consider a system with a dumping force with constant γ and a force given by a potential $V(x)$ we get the Langevin equation:

$$\dot{x} = p$$

$$\dot{p} = -\gamma p - V'(x) + \epsilon\xi(t)$$

We have for $t \to \infty$ that the distribution $\rho(x,p,t)$ is the Maxwell-Boltzmann distribution:

$$\rho(x,p,\infty) = \frac{1}{Z}\exp(-\frac{H}{kT})$$

where we impose that

$$kT = \frac{\epsilon^2}{2\gamma}$$

In general the entropy $S(t)$ can be computed only numerically because not always has an analytical solution, but if we consider a system with an harmonic potential:

$$V(q) = \frac{m}{2}\omega^2 q^2$$

the solution is given by(3).

2 Numerical integration

Since the system is an Hamiltonian system, for the evolution of the system has been used a simplettic integrator of the form:

$$x_{n+1} = x_n + p_{n+1}dt$$

$$p_{n+1} = p_n - \gamma p_n dt - V'(x_n)dt + \xi_n\epsilon\sqrt{dt}$$

where we impose $m = 1$. Here the ξ_n are random variables with null mean and unitary variance.

2.1 Harmonic potential

First we consider an harmonic potential of the form:

$$V(x) = \frac{1}{2}\omega^2 x^2$$

So the simplettic integrator will be:

$$x_{n+1} = x_n + p_{n+1}dt$$

$$p_{n+1} = p_n - \gamma p_n dt - \omega^2 x_n dt + \xi_n \epsilon \sqrt{dt}$$

The evolution of system is implemented with a MonteCarlo simulation with N=10000 particles. So for each particle the coordinates x and the momenta p are given by the simplettic integrator at each time t

In the figure below we have the ditribution of the momenta and the distribution of the positions of the particles. The theoretical distributions are given by:

$$\rho(p,t) = \frac{1}{Z}e^{-\frac{H}{kT}}$$

$$\rho(x,t) = \frac{1}{Z}e^{-\frac{V(x)}{kT}}$$

with $Z = \int V(x)dx$ which is the partition function and $kT = \epsilon^2/2\gamma$. In the figure (1) we can see the evolution of the distribution of the momenta of the particles:

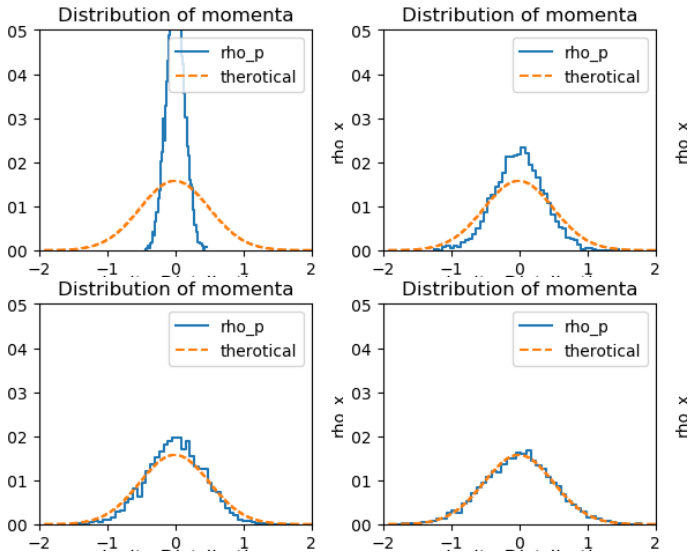

Figure 1: Distribution of the momenta at different times t for the system with an harmonic potential. Parameters: $\gamma = 0.7$, $\epsilon = 0.6$, $N = 10000$, $dt = 0.1$, $\omega = 1$

In the figure (2) we can see the evolution of the distribution of the momenta of the particles:

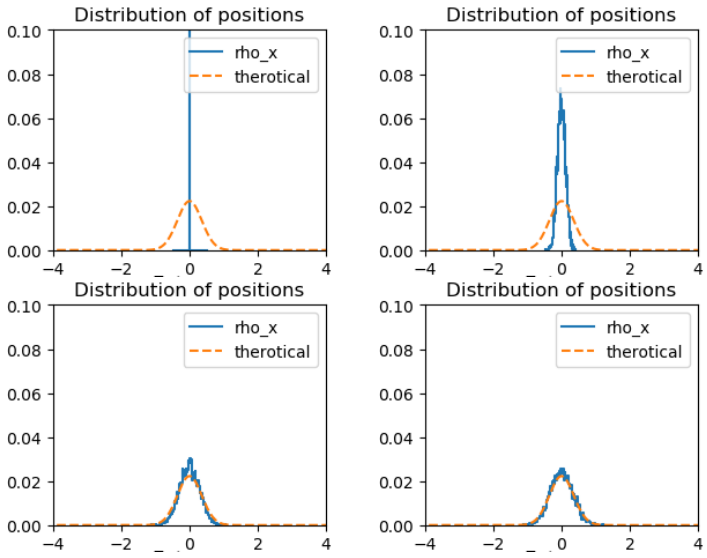

Figure 2: Distribution of the positions at different times t. Parameters: $\gamma = 0.7$, $\epsilon = 0.6$, $N = 10000$, $dt = 0.1$, $\omega = 1$

2.2 Double well potential

Then we consider a potential of the form:

$$V(x) = (x^2 - ax)(x^2 + bx)$$

where $a, b > 0$. So the simplettic integrator will be:

$$x_{n+1} = x_n + p_{n+1}dt$$

$$p_{n+1} = p_n - \gamma p_n dt - (4x_n^3 + 3bx_n^2 - 3ax_n^2 - 2abx_n)dt + \xi_n \epsilon \sqrt{dt}$$

Also in this case the evolution of system is implemented with a MonteCarlo simulation with N=10000 particles. So for each particle the coordinates x and the momenta p are given by the simplettic integrator at each time t

In the figure (3) we can see the evolution of the distribution of the momenta of the particles:

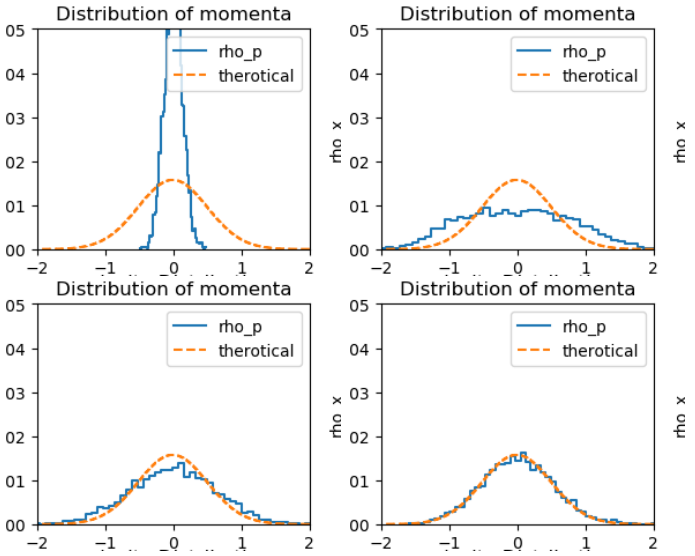

Figure 3: Distribution of the momenta at different times t for the system with a double well potential. Parameters: $\gamma = 0.7$, $\epsilon = 0.6$, $N = 10000$, $dt = 0.1$, $a = 1.7$, $b = 1.7$

In the figure (4) we can see the evolution of the distribution of the momenta of the particles:

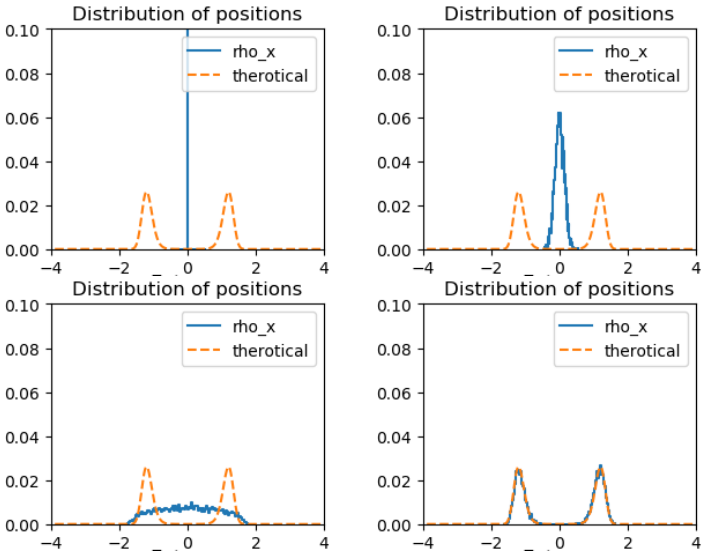

Figure 4: Distribution of the positions at different times t for the system with a double well potential. Parameters: $\gamma = 0.7$, $\epsilon = 0.6$, $N = 10000$, $dt = 0.1$, $a = 1.7$, $b = 1.7$

From this figures we can see that the distribution of the momenta is the same of the distribution of the momenta in the case of the harmonic potential. This is so beacuse the distribution $\rho(p, t)$ is independent from the potential $V(x)$! But if we look at the distribution of the positions, we can see that the majority of the particles lay near the two minimums of the double well potential.

3 Entropy

To compute the entropy of the system one has to calculate:

$$S(t) = -\int \rho \log \rho dx \tag{2}$$

So we need firstly to find the distribution $\rho(x, p, t)$. To find the distribution $\rho(x, p, t)$ for each time we compute the normalized histogram in the phase space for all the particles at each time t.

3.1 Entropy for the system with harmonic potential

In the case of an harmonic potential the entropy can be found in analytical way and in particular we know that $S(t)$ is a monotonic function always increasing, reaching an asymptotic value of :

$$S = \frac{d}{2}\log(2\pi kT) + \frac{1}{2}\log(det(\Sigma^2)) \tag{3}$$

where d is the dimension of the system and Σ^2 is the covariance matrix.

Once we have found the distribution $\rho(x, p, t)$ we can compute the integral(2). In the figure(5) we can see the evolution of the entropy of the system in the case of the harmonic potential.

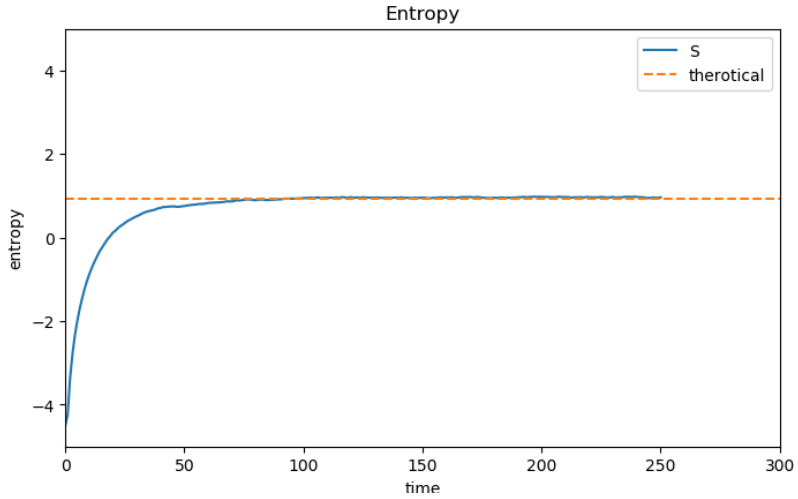

Figure 5: Evolution of the entropy of the system. We can see that $S(t)$ tends to the theoretical value of (3).

3.2 Entropy for the system with a double well potential

In the case of a system of a double well potential we don't have an analytical solution but we can however compute the integral(2). In the figure(6) we can see

the evolution of the entropy, and we can see that $S(t)$ is no more monotonically increasing but reaches a maximum and then decrease since reaches asymptotically the theoretical value of the entropy for the system with the harmonic potential!

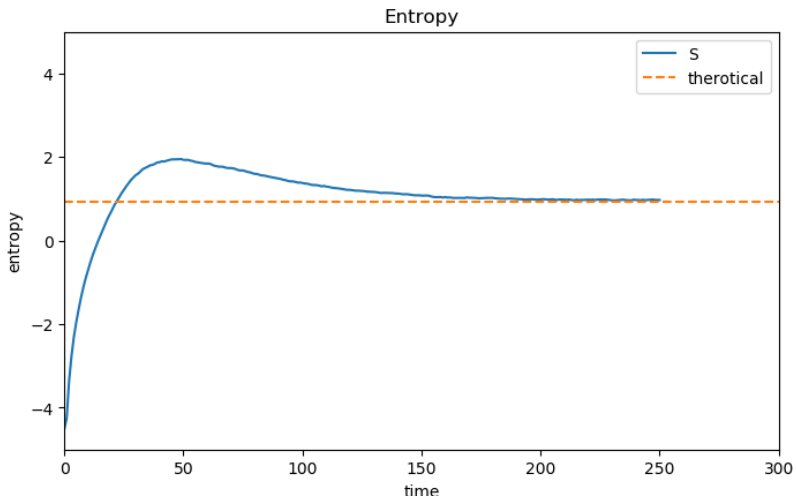

Figure 6: Evolution of the entropy of the system. We can see that $S(t)$ tends to the theoretical value of (3).

4 Conclusions

So in conclusion, we can see that using a MonteCarlo simulation and a simplettic integrator we can reach the theoretical results of a diffusion process. Moreover,we can find the entropy of the system and also we can compute numerically the value of the entropy even if we don't have an analytical solution.