NOSE HOOVER OSCILLATOR

Anuran Pal — 16MS152

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Abstract

The Nose Hoover thermostat is a deterministic algorithm for constant-temperature molecular dynamics simulations. It was originally developed by Nose and was improved further by Hoover. The Nose Hoover thermostat has been commonly used as one of the most accurate and efficient methods for constant-temperature molecular dynamics simulations. The aim is to generate a Gaussian distribution of velocity such that it acts as a physical gas at a given temperature. This system will have an average energy but it will fluctuate with time i.e. a non-uniformly conservative system.

Theory

The Nose Hoover Oscillator can be imagined as a block attached to a spring, but the damping is dependent on the surrounding temperature. Let us denote **T** as the temperature of the surrounding, $\boldsymbol{\zeta}$ be the feedback term due to the temperature and $\boldsymbol{\epsilon}$ denote the feedback constant.
Then the energy of the system will be:

$$E = \frac{1}{2}(q^2 + p^2 + \zeta^2) \tag{1}$$

and ζ will be governed by:

$$\frac{dE}{dt} = -\epsilon\zeta T \tag{2}$$

Thus, the equation of simple harmonic oscillator in the temperature dependent damping will be:

$$\frac{dq}{dt} = p \tag{3}$$

$$\frac{dp}{dt} = -q - \epsilon\zeta p \tag{4}$$

$$\frac{d\zeta}{dt} = \epsilon(p^2 - T) \tag{5}$$

Changing some variables and scaling some parameters we get the Nose Hoover Oscillator equation that we are going to numerically analyze in the next section.

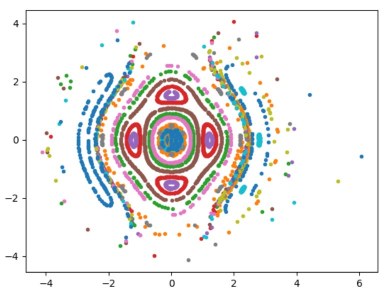
$$\dot{x} = y;\ \dot{y} = -x - zy;\ \dot{z} = b(y^2 - 1) \tag{6}$$

The numerical solution of the Nose Hoover Oscillator shows that it has conserved trajectories, but it does not have any fixed points.

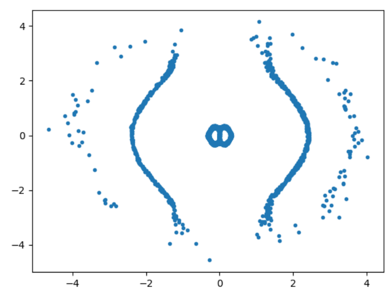
Numerical Simulation for few values of b

In the following section I have tried to plot the trajectories for the following **b** values 1, 2, 4, 20 and have tried to seperate out the possible conserved trajectories from the sea of chaotic trajectories.
I have selected these b values because it might give us an insight as to how the conserved structures change with change in b.
The analysis has been done in the following manner:
X-Y cross section of the trajectories with stable orbit.
X-Y cross-section of the trajectories with chaotic orbit.
3D plot of the stable structures.

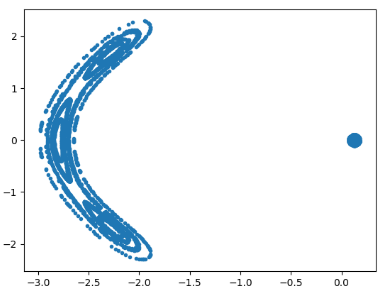
b=1.0



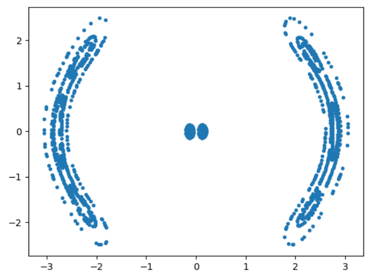
(a) Cross-section for some random initial conditions



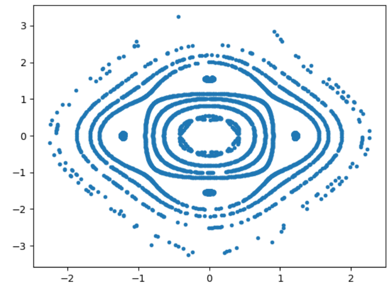
(b) Cross-section of the chaotic region



(a) Family of stable toroids

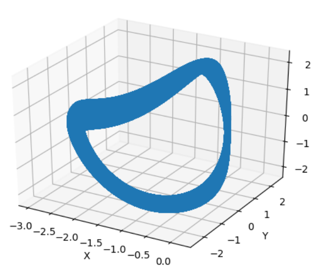


(b) Symmetrical family of stable toroids

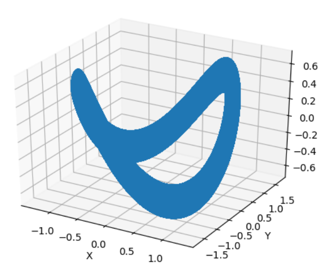


(c) Central family of toroids

Figure 1: X-Y Cross-section of the stable trajectories. We can see that **there are Three families of coexisting toroids such that the two peripheral toroids are intertwined with each other**.

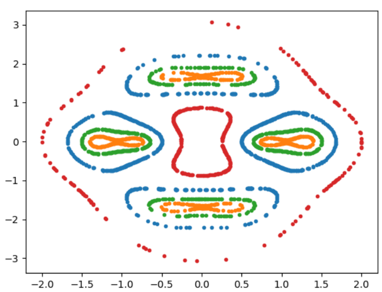


(a) This is responsible for Fig 2(a), **a symmetrical pair is present** such that these two are intertwined to form Fig 2(b)

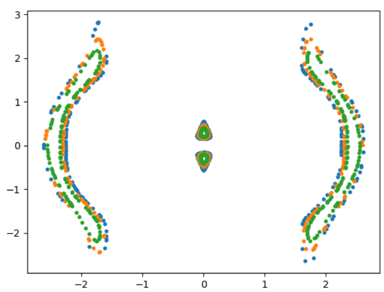


(b) 3D figure of a member of the central family of toroids which create Fig 2(c)

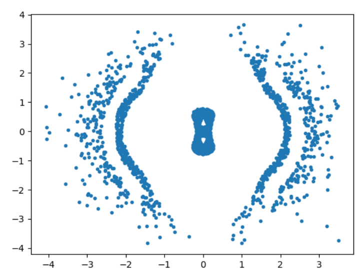
b=2.0



(a) Cross-section of stable trajectories of the family of central toroids

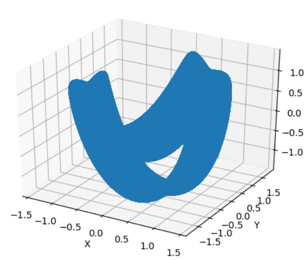


(b) Cross-section of stable trajectories due to the two peripheral trajectories.

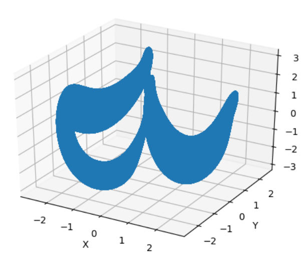


(c) The chaotic sea.

Figure 2: **Note that the chaotic sea seperates the inner toroid from the outer toroid**



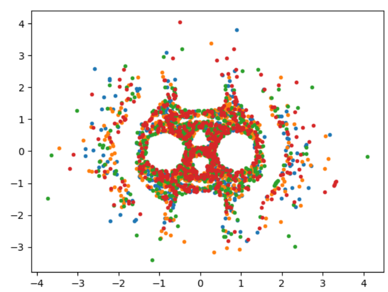
(a) 3D plot of the inner toroid



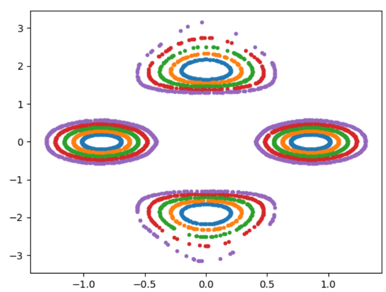
(b) 3D plot of the external toroid.

Figure 3: **Note in these two figures that the two peripheral toroids have joined.**

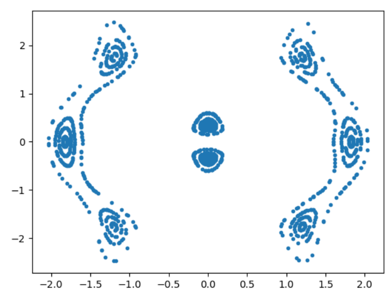
b=4.0



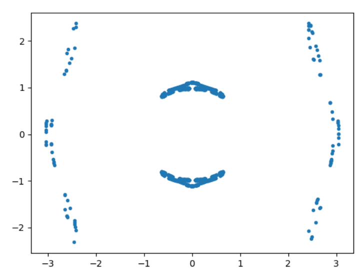
(a) Cross-section of the chaotic sea; Note: In the inner chaotic cross-section **there is a new region unaffected by chaos**



(a) Cross-section of stable trajectories of the family of central toroids

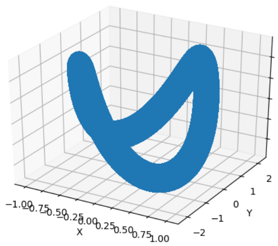


(b) Cross-section of stable trajectories due to the peripheral toroids.

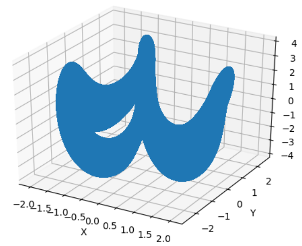


(c) **The new developing stable structure**

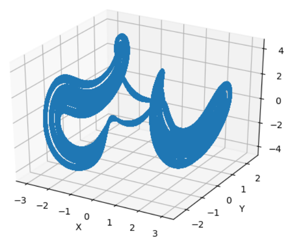
Figure 4: Figure 5(c) is a new stable structure that is developing in the system.



(a) Member of the inner family of toroids.



(b) Member of the outer family of toroids

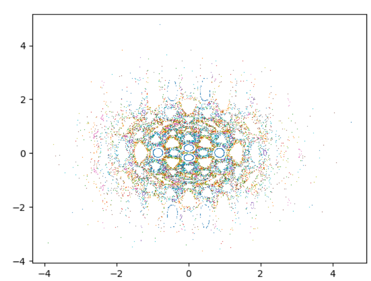


(c) **3D plot of the new stable structure.**

Figure 5: The developing new stable structure is similar to the outer family of toroids. Thus **there could have been a bifurcation at the peripheral toroid at b less than 4.**

Thus, the system becomes more complicated as the value of b increases.

b=20.0



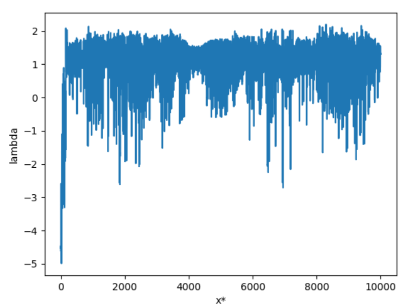
(a) The plot has been done with small points to show the intricacy of the system. Cross-section of trajectories of random few initial points.

Lyapunov Exponent

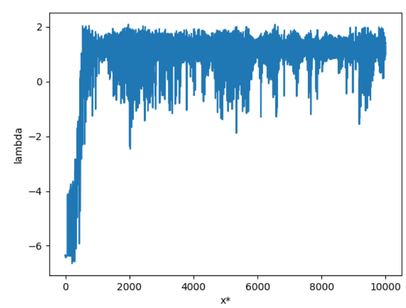
I have used two different metric to calculate the lyapunov exponent. They are as follows:
Two points are taken close to each other; then they are iterated once and the distance is stored. Before the next iteration another point is taken close to the original trajectory. This process is continued till the exponent reaches a constant value.
The other method was taught in the class by Professor Subhasis Sinha which involves the computation of M matrix:

$$\lambda = \frac{1}{2t}(\lambda_{max}(M^T M)) \tag{7}$$

where λ_{max} denotes the largest eigenvalue and M is $\frac{\delta x(t_i)}{\delta x(0)}$.
Both of the methods gives us a positive value for the lyapunov exponent which is close to 1 for trajectories inside a stable toroid as well as in the chaotic sea.



(a) Lyapunov exponent for a trajectory in the chaotic sea for b=1



(b) Lyapunov exponent for a trajectory in the central torus familyfor b=1

Figure 6: Thus the lyapunov exponent reaches a positive value approximately 1 in both the cases; implies the seperation of nearby trajectories gradually increase.

Conclusion

With the limited understanding of Chaos that we have it is not possible to analyze the system in further details. But from the analysis we did till now we have realized that **there exists stable toroidal structures like islands amidst a sea of chaos. With change in the parameter b the toroidal structures undergo bifurcation and give rise to new toroidal structures which are also stable and are separated by the chaotic sea from other toroidal structures.**

A bifurcation occurs within b = 1 to 2 where the intertwined symmetric peripheral toroidal structures join and become a single toroidal stable family.
Another **bifurcation occurs near 4, where the peripheral toroidal family gives birth to a new stable toroidal structure.**

References

Harmonic Oscillator with Non-linear damping; J.C. Sprott, W.G. Hoover, 2017.
Class notes of PH4104 : Non Linear Dynamics.
Nose Hoover Thermostats; Karl Gross, Brian Shi, Lora Weiss, 2013.
Wikipedia.