

# Order and Chaos in a 2D potential

## Numerical Methods and Simulation Project

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# 1 Introduction

The goal of this numerical project is to develop computational techniques for simulation and analysis of orbits under the influence of Hénon–Heiles potential. This potential represents a simplified dynamical system where particles can exhibit both regular and chaotic behavior depending on the total energy of the system. It was inspired by whether there was an analytical solution of the motion of stars moving in the potential of the galaxy. It was assumed such a potential had a symmetry axis, and so Hénon & Heiles (1964) investigated whether an axis symmetric potential admits a third isolating integral of motion.

Integrals of motion are the quantities that are conserved along the orbit, e.g. energy, angular momentum, etc. These integrals of motion act as constraints, limiting the regions of the phase space that the object can explore. For the galactic dynamics, as conveyed above it was assumed that the potential had a symmetry axis and was time-independent. The system is a 6-dimensional phase space  $(R, \theta, z, \dot{R}, \dot{\theta}, \dot{z})$ , therefore it has five independent conservative integrals of the motion (Hénon & Heiles 1964). Each of these integrals represent a hypersurface in the 6D phase space and the trajectory is the intersection of these. These integrals can be categorized into isolating or non-isolating.

The non-isolating integrals fill the whole phase space and give no restriction on the trajectory. Thus, one can say that non isolating integrals have no significance in determining the orbit. It can shown that at least 2 integrals in general are non isolating and at the time of writing of the paper two isolating integrals for the total energy and the angular momentum per unit mass of the star were known. Since, no analytical solution for the motion of the stars under the galactic potential was found it was assumed that the third integral is also non-isolating but the observations of orbits of stars near the sun as well as a number of numerical computations of orbits behaved as if there were three isolating integrals. Hénon–Heiles set to find any proof for the existence of this integral but not limiting themselves to the astronomical nature of the problem, they chose a potential that became to be known as Hénon–Heiles potential, to explore this question in a broader context.<sup>1</sup>

In this numerical project, we tested various numerical integrators like Euler method, 2<sup>nd</sup> order Runge–Kutta method (RK2) and 4<sup>th</sup> order Runge kutta method (RK4) to compute the orbits under a potential. We tested our integrators for a potential whose analytical solutions are known like the Kepler potential and make a comparison between the efficiency and accuracy of each of them. After validating our integrators, we used the RK4 method and apply it to the Hénon–Heiles potential to compute the Poincaré sections to visualize both chaotic and regular orbits. Finally, we applied the technique from Gottwald & Melbourne (2004), which is based on the slope of the distance in the phase space along an orbit to find whether an orbit is chaotic or regular and make comparison between the results obtained through two different techniques.

## 2 Numerical Integrators

In order to simulate the a system from a set of equations governing it and recover its trajectory, we use numerical integrators. As part of the project, we developed different numerical integrators as given below.

### 2.1 Euler Method

The Euler method is one of the simplest numerical techniques for solving ordinary differential equations (ODEs). It approximates the solution by stepping forward in small increments using the slope of the function at each point. It is a first order method.

For a first-order differential equation of the form:

$$\frac{dy}{dx} = f(x, y) \quad (2.1)$$

<sup>1</sup>see [https://jfuchs.hotell.kau.se/kurs/amek/prst/11\\_hehe.pdf](https://jfuchs.hotell.kau.se/kurs/amek/prst/11_hehe.pdf)

with  $y(x_0) = y_0$ . To estimate the values taken by  $y$ , we discretize the problem: let us consider a step size  $h$ , then for all  $n$ :

$$y_{n+1} = y_n + h \cdot f(x_n, y_n) \quad (2.2)$$

where  $x_n = x_0 + nh$  and  $y_n = y(x_0 + nh) = y(x_n)$

## 2.2 Second Order Runge–Kutta Method

The second-order Runge–Kutta method (RK2), also known as the midpoint method, is a numerical technique for solving ordinary differential equations (ODEs). It improves upon the Euler method by using an additional intermediate step to estimate the slope more accurately. It is a second order predictor-corrector method, the central idea behind these methods is to first make a guess (predictor step) about the solution at a future point and then refine this guess (corrector step) to achieve higher accuracy.

For the same differential equation (2.1), the RK2 method estimates the next value of  $y$  as follows:

**Initial slope.** Calculate the slope at the beginning of the interval using:

$$k_1 = f(x_n, y_n), \quad (2.3)$$

where  $k_1$  is the slope at the current point  $(x_n, y_n)$ .

**Midpoint slope.** Estimate the slope at the midpoint of the interval by predicting  $y$  at the midpoint:

$$k_2 = f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2} \cdot k_1\right), \quad (2.4)$$

where  $k_2$  is the slope at the midpoint.

**Update the solution.** Using  $k_2$  to compute the next value of  $y$ :

$$y_{n+1} = y_n + h \cdot k_2. \quad (2.5)$$

Here:

- $h$  is the step size,
- $k_1$  represents the slope at the start of the interval,
- $k_2$  refines the slope estimate using the midpoint value.

## 2.3 Fourth Order Runge–Kutta Method

Another numerical integration method belonging to the Runge–kutta family is RK4. As evident from the name, it is a fourth order method. In this method, the value of the function i.e.  $y$  at the next step is determined by using the present value plus the weighted average of the slopes at different points within the next full step, multiplied by the step size.

We take the same differential equation (2.1) apply the RK4 method as follows to get the next values of  $y$ :

$$\begin{aligned} k_1 &= f(x_n, y_n) & k_3 &= f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2} \cdot k_2\right) \\ k_2 &= f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2} \cdot k_1\right) & k_4 &= f(x_n + h, y_n + h \cdot k_3) \end{aligned} \quad (2.6)$$

These increments are combined to compute the next value of  $y$  as:

$$y_{n+1} = y_n + \frac{h}{6} (k_1 + 2k_2 + 2k_3 + k_4),$$

**Here:**

- $h$  is the step size,
- $k_1, k_2, k_3$ , and  $k_4$  are the slopes calculated at different points within the interval.

## 3 Kepler Potential

### 3.1 Main Equations

The Kepler problem refers to a special case of the two body problem, in which the two bodies are interacting through a central force which follows the inverse square law e.g. gravitational force (Strauch 2009). The potential associated with such a force is called the Kepler potential. We consider a gravitational two body problem with point masses to compare the accuracy of our integrators by comparing it with the analytical solutions of the problem as well. This potential is given by

$$V(R) = -\frac{Gm_1m_2}{R} \quad (3.1)$$

where  $G$  is the gravitational constant and  $m_1, m_2$  are the masses of the central body and the orbiting particle respectively. In our project, for the sake of simplicity and without the loss of generality, we set  $G = 1$  and  $m_1 = m_2 = 1$ . We use the Hamiltonian formulism to find the set of equations governing the motion and the Hamiltonian of the problem.

The Hamilton equations for a system, in general are:

$$\frac{dq}{dt} = \frac{\partial \mathcal{H}}{\partial p} \quad \frac{dp}{dt} = -\frac{\partial \mathcal{H}}{\partial q}. \quad (3.2)$$

where  $\mathcal{H}$  is the Hamiltonian of the system,  $q$  represents the generalized position vector and  $p$  is the conjugate momentum vector. The Hamiltonian, which is equal to the total energy for a conservative system like the Kepler problem is given as

$$\mathcal{H}(q, p) = T + V = \frac{1}{2}(u^2 + v^2) - \frac{1}{\sqrt{x^2 + y^2}} \quad (3.3)$$

therefore:

$$\begin{aligned} \frac{dx}{dt} &= \frac{\partial \mathcal{H}}{\partial u} = u & \frac{du}{dt} &= -\frac{\partial \mathcal{H}}{\partial x} = -\frac{x}{r^3} \\ \frac{dy}{dt} &= \frac{\partial \mathcal{H}}{\partial v} = v & \frac{dv}{dt} &= -\frac{\partial \mathcal{H}}{\partial y} = -\frac{y}{r^3} \end{aligned} \quad (3.4)$$

where  $r = \sqrt{x^2 + y^2}$ . We solve the equations (3.4) numerically using the methods described in section 2 to simulate the orbit for a given time span.

The main reason, we chose this potential is that its analytical solution is known, so that we can compare our numerical schemes with the analytical result. For the particle in circular orbit (our case), the radial distance  $r_0$  as well as the angular velocity  $\omega = \sqrt{u_0^2 + v_0^2}/r_0$  are both constant. The position and the velocities are functions of time  $t$  and are given parametrically by:

$$x(t) = r_0 \cos(\omega t) \quad y(t) = r_0 \sin(\omega t), \quad (3.5)$$

and

$$u(t) = -r_0\omega \sin(\omega t) \quad v(t) = r_0\omega \cos(\omega t).$$

These parametric equations yield a trajectory that is a perfect circle centered on the origin. The total energy of the system, which is constant over time is given by=

$$E = \frac{[u(t)]^2 + [v(t)]^2}{2} - \frac{1}{r_0}. \quad (3.6)$$

With this we have all the required equations to test the numerical schemes which has been done in the subsequent section.

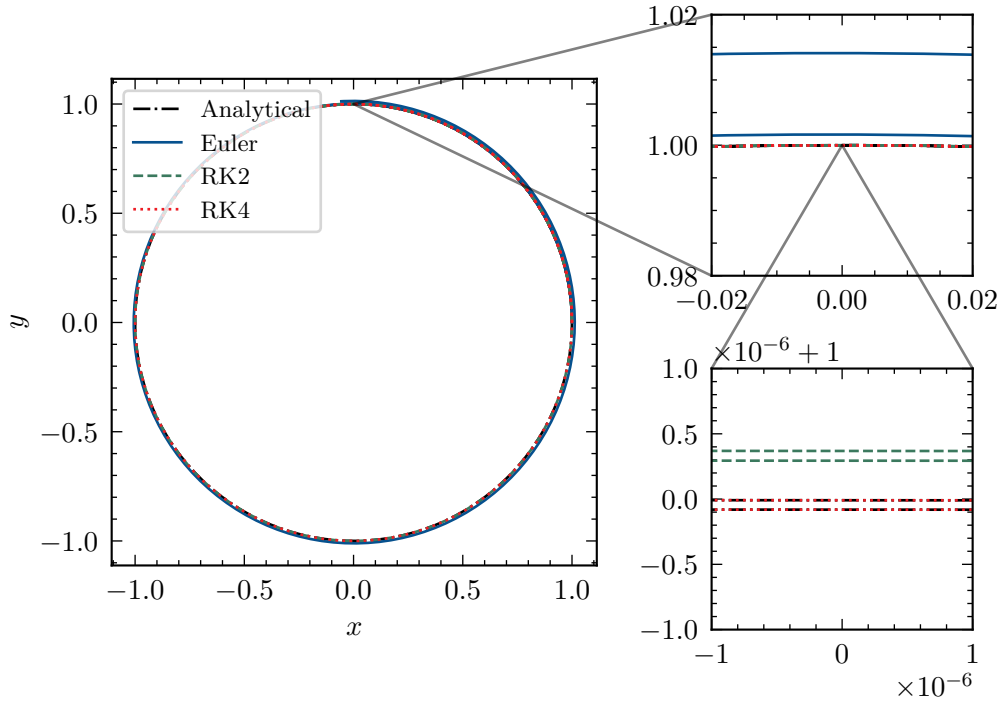


Figure 1: Global view of integrated orbits in a Kepler potential (left) and two zoomed panels (right). Three integrators are used: Euler (solid blue line), RK2 (dashed green line) and RK4 (dotted red line), and the analytical solution is also shown (black dashed-dotted line). The step size here is  $h = 0.001$ . The first zoom panel (top right) emphasizes the rapid deviation of the Euler method, with a first orbit start to deviate from the analytical solution already during the first orbit, and goes away even more during its second orbit. The second zoom panel (bottom right) emphasizes the deviation from the RK2 method. In this panel we also notice a deviation between the two analytical orbits, caused by the accumulation of machine error. The RK4 deviation cannot be noticed.

### 3.2 Accuracy of Numerical Integrators

In figure 1, we show the graphs obtained using the different integration as well as the evolution of the error with different step sizes for various integrators.

Even for such a small step size ( $h = 0.001$ ), the Euler method is already deviating significantly from the analytical trajectory. This behaviour is expected as the Euler method is just a first order method. Even though it appears that RK2 is as good as RK4, we show a zoomed in segment of the orbit to show that is not the case, even with such a small step RK4 is better than RK2. This difference is of the order of  $10^{-6}$  but as the integration time increases the error will increase, deviating significantly from the analytical path.

We show another plot for a higher step size in the figure 2. At such a step size, all the integrators are erroneous but it seems that RK4 is still able to reproduce the analytical orbit.

In the Keplerian problem the total energy of the body remains conserved, thus we present the error between the analytical energy value and the numerical value after the integration of the orbit with various integrators for different step sizes for same total integration time. As shown in the figure 3. One can now conclusively see that the RK4 integrator with the step size  $h = 0.001$  is an apt choice for our further analysis. With this step size we get an error nearly equal to the machine epsilon ( $\varepsilon \sim 10^{-16}$ ). In the graph, one can observe that unlike the other integrators the RK4 has comparatively more error at  $h < 0.001$  but we think it is just the artifact of the machine, RK4

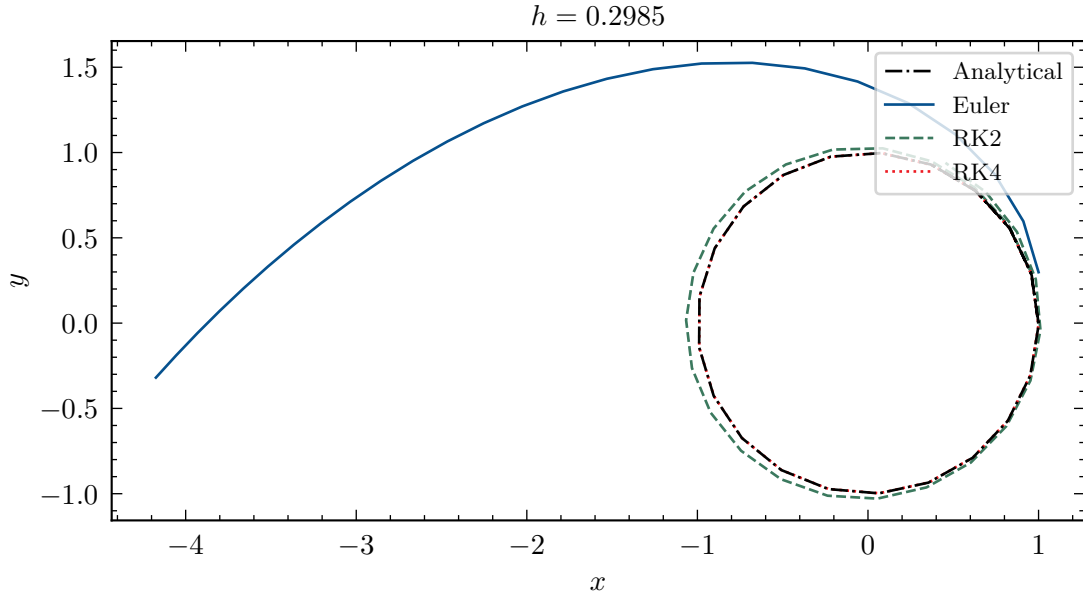


Figure 2: Integrated orbits in a Kepler potential. Three integrators are used: Euler (solid blue line), RK2 (dashed green line) and RK4 (dotted red line), and the analytical solution is also shown (black dashed-dotted line). The step size here is  $h = 0.2985$ . With this value very high for a step size, the Euler method can no longer produce relevant results, RK2 integrator starts to deviate from the analytical solution while the RK4 seems to produce results close enough from the analytical solution to be unnoticeable

starts to produce results that are more accurate than the machine epsilon, the numerical error is dominated by the limitations of floating-point precision in the system<sup>2</sup>.

## 4 Hénon–Heiles Potential

The potential chosen by the authors to be studied became known as the Hénon-Heiles potential. It is a two-dimensional potential which appears to be a harmonic potential with perturbative terms. It was chosen because of its three properties:

1. It is simple to solve analytically, making the computations easier;
2. It can give chaotic trajectories as well;
3. It represents a general class of potentials which behave in same way even when more perturbative terms are added.

The potential (shown in figure 4) is defined as:

$$V(x, y) = \frac{1}{2} \left( x^2 + y^2 + 2x^2y - \frac{2}{3}y^3 \right) \quad (4.1)$$

<sup>2</sup>see appendix A.

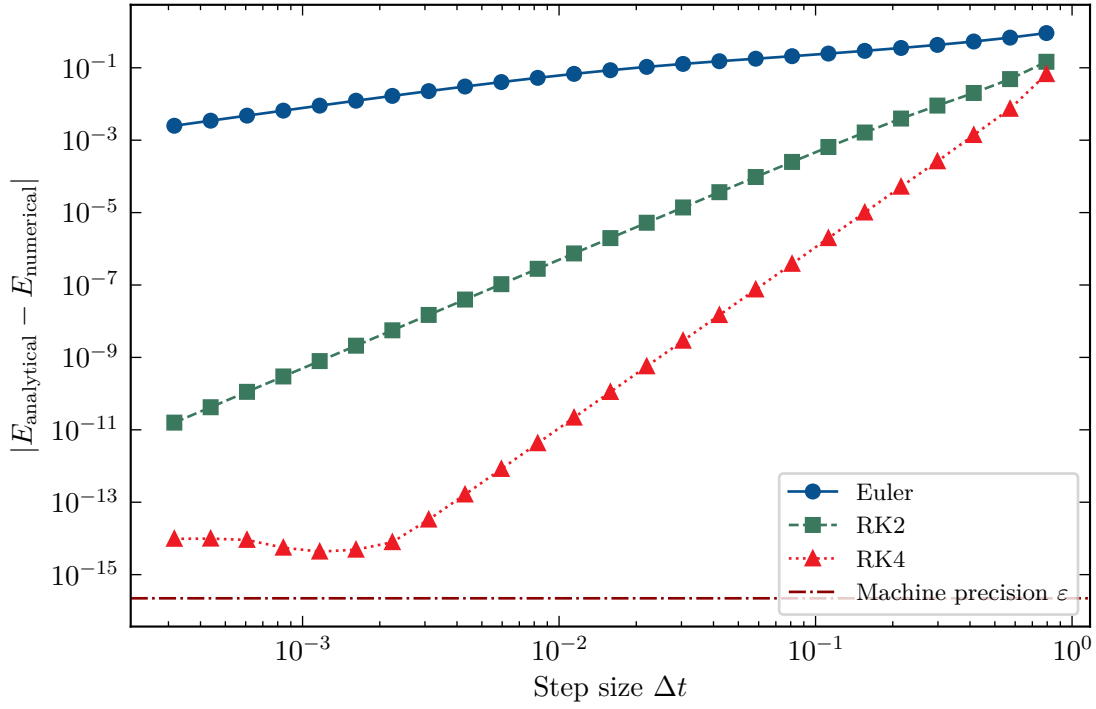


Figure 3: Difference between the analytical energy value and final numerical energy value for various step sizes. The machine precision correspond to the python `float` type precision.

#### 4.1 Equations of Motion

The motion of a particle in the Hénon–Heiles potential is governed by the equations of motion derived from the potential energy  $U(x, y)$ . The time evolution of the system is described by the following first-order differential equations:

$$\dot{x} = -\frac{\partial U}{\partial x} = -(x + 2xy) \quad \dot{y} = -\frac{\partial U}{\partial y} = -(x^2 - y^2 + y) \quad (4.2)$$

The equations of motion are integrated numerically using the RK4 method to compute the particle's trajectory, one such trajectory corresponding to  $E = 1/12$  with a step size of 0.001 has been provided in the figure 5.

#### 4.2 Initial Conditions

In their paper, [Hénon & Heiles \(1964\)](#) use  $x$  and  $y$  such that  $-1 \leq x \leq 1$  and  $-0.5 \leq y \leq 1$ <sup>3</sup>. We randomly sampled initial positions  $(x_0, y_0)$  in this range, according to the constraint that the potential energy of the particle must be less than the total energy of the particle i.e.  $U(x, y) < E$  to avoid leading to negative kinetic energies which is obviously unphysical.

The law of conservation of the energy for the system can be formulated as,

$$U(x, y) + \frac{1}{2}(u^2 + v^2) = E \quad (4.3)$$

This directly leads to  $U(x, y) \leq E$ . This constraint defines a bounded region in phase space where the particle's motion will be confined to a certain region otherwise the particle has enough energy

<sup>3</sup>These ranges were taken from the plot of the potential ([Hénon & Heiles 1964](#), figure 2).



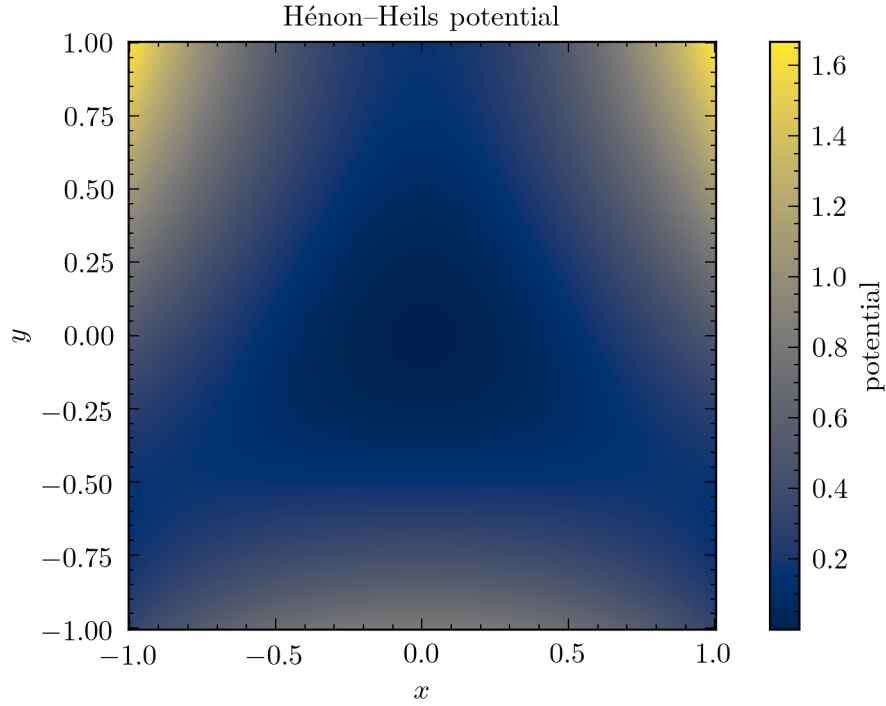


Figure 4: Hénon–Heiles potential in natural units, shown in real  $(x, y)$  space. The central blue part is attractive. There is also three “valleys” (top, bottom left and bottom right) that are also attractive, but that can drag particles away if their total energy is too high.

to escape the potential. Then, we generate  $N_{\text{part}} = 100$  particles of coordinates  $(x_0, y_0)$  in this region, and compute the norm of their velocity with:

$$\|\mathbf{v}_0\| = \sqrt{2[E - U(x_0, y_0)]} \quad (4.4)$$

and compute a  $u_0$  and  $v_0$  components (along the  $x$  and  $y$  axis respectively) by generating a random direction  $\theta_0 \in [0; 2\pi)$

$$u_0 = \sqrt{2[E - U(x_0, y_0)]} \cos(\theta_0) \quad v_0 = \sqrt{2[E - U(x_0, y_0)]} \sin(\theta_0) \quad (4.5)$$

This gives a set of initial conditions whose time evolution we can track in phase space to find nature of these orbits.

### 4.3 Chaotic orbits

The behavior of the particle under the potential is chaotic as well for higher energies. Figure 6 shows the one such chaotic trajectory. By varying the initial conditions and total energy, a wide range of orbits have been studied, from regular, periodic trajectories to chaotic ones, whose results will be discussed in the subsequent sections

### 4.4 Poincare Sections

In dynamical systems like ours, A Poincaré section (Poincaré 1893) is a method for visualizing the behavior of this dynamical system by taking a lower-dimensional “slice” through its phase space. It is created by sampling the trajectories of the system at regular intervals or whenever they intersect a predefined surface, known as the Poincaré surface of section. It reduces a continuous flow to a discrete-time mapping<sup>4</sup>. Mathematically, a Poincaré section is the set of points where a trajectory

<sup>4</sup>see [ocw.mit.edu/courses/12-006j-nonlinear-dynamics-chaos-fall-2022/mit12\\_006jf22\\_lec15-16.pdf](https://ocw.mit.edu/courses/12-006j-nonlinear-dynamics-chaos-fall-2022/mit12_006jf22_lec15-16.pdf)

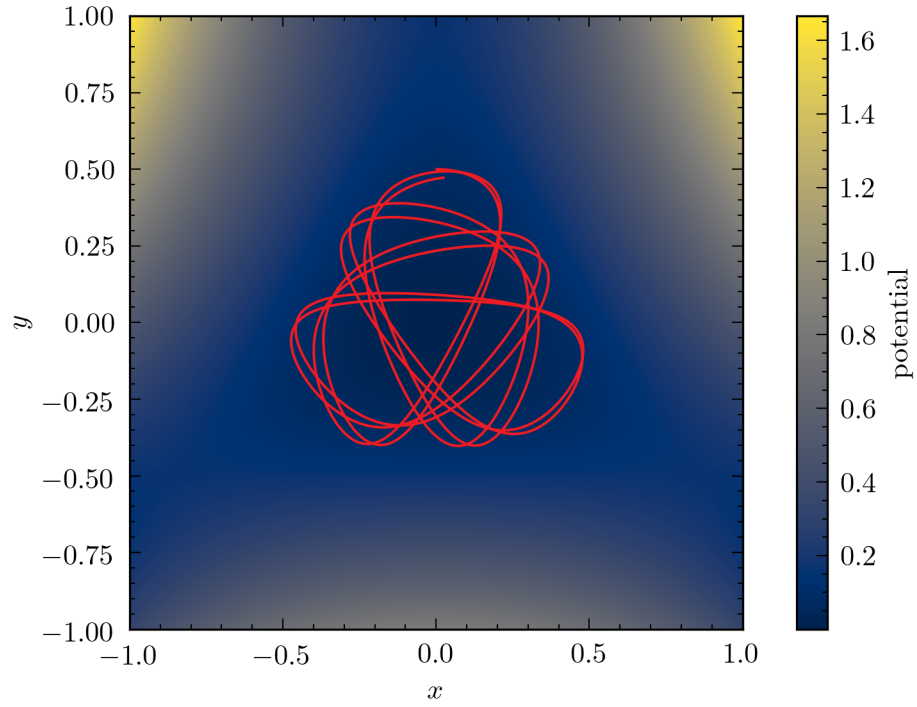


Figure 5: Trajectory of a particle under the influence of the Hénon-Heiles potential. The trefoil motion of the particle is ordered.

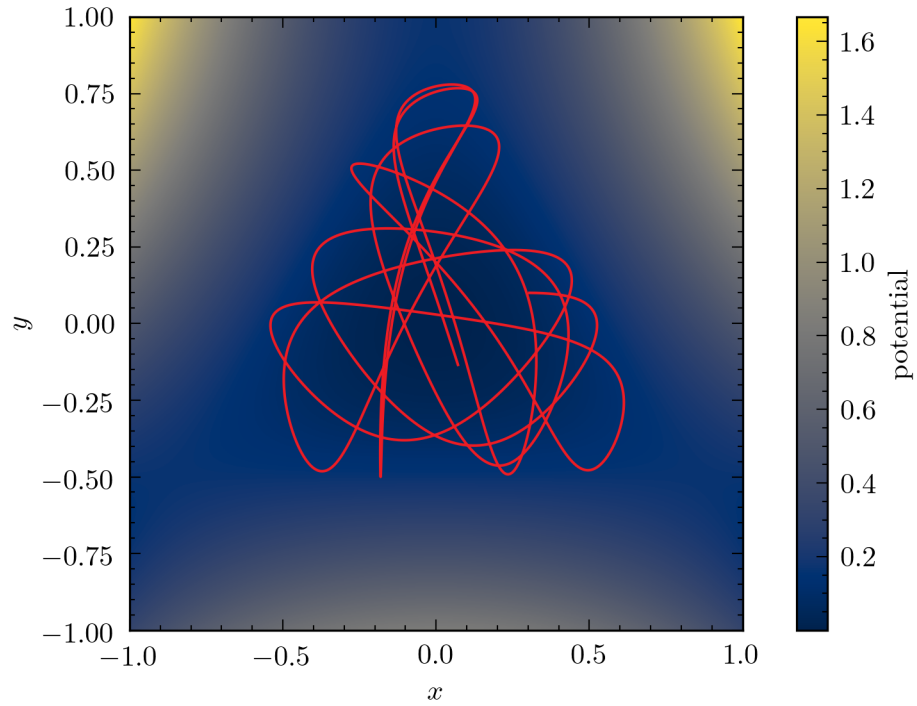


Figure 6: Chaotic trajectory of a particle under the influence of the Hénon-Heiles potential.

of a higher-dimensional system intersects a hypersurface in the phase space. By doing so, we reduce the dimensionality while still retaining the behavior of the system.

One can interpret the behavior of the dynamics by visualizing the Poincaré maps. A periodic orbit can produce a single fixed point (if the period coincides with the return time of the section) or a finite set of points, a quasi-periodic dynamics will form smooth continuous closed loops and for the chaotic dynamics, the Poincaré section will appear scattered over a region of the section, there will be no simple repeating structure but if the chaos is deterministic the section can display some order but not simple curves (Cheb-Terrab & De Oliveira 1996).

In our study, we compute the Poincaré section by identifying the points where the particle's trajectory crosses the plane  $x = 0$  in phase space. At each crossing we record the  $y$ -coordinate and the velocity  $v_y$ , interpolating to ensure accuracy. Through this approach, we reduce the dimensionality, projecting the dynamics onto the  $y$ - $v_y$  plane. The figure 7 represents the recorded Poincaré sections.

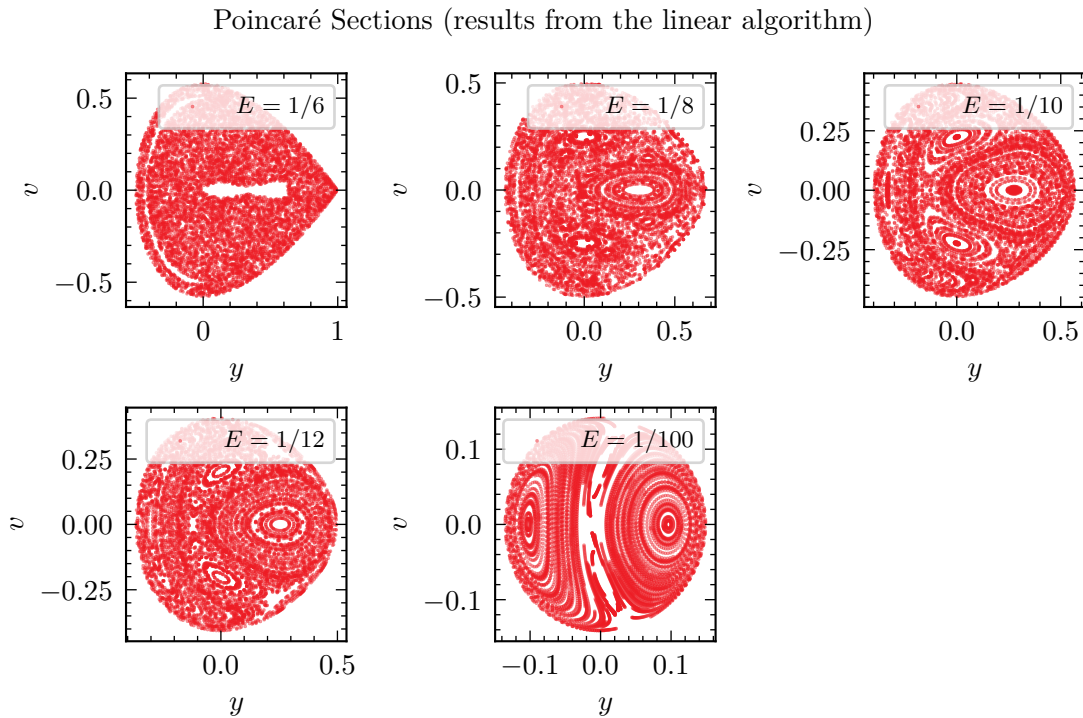


Figure 7: Poincaré sections of the Hénon-Heiles potential for energies  $E = 1/6, 1/8, 1/10, 1/12$  and  $1/100$

We can see that for the lower energy values the section has closed curves with all the points lying on the curves filling completely the available areas which shows that the particle has stable behavior but the Poincaré section for  $E = 1/8$  tells a different story, there are still closed curves in the various parts of the diagram (islands of stability) but it is evident these curves don't fill the whole area, there are a lot of isolated points through which one can not draw any curve, it represents a transition towards instability and chaotic dynamics. These apparently randomly distributed points fill the space between curves. As the energy is increased to  $E = 1/6$ , we see that the islands of stability are gone and there are just random points that appear to fill the whole phase space<sup>5</sup> i.e. ergodic behavior. The open circles (see figure 14) in the diagram for this energy correspond to a

<sup>5</sup>The outer line of all the diagrams is the limit given by  $U(0, y) + \dot{y}^2/2 = E$  for our chosen surface of  $x = 0$  in the phase space.

trajectory of new kind, intermediate between the closed curves and ergodic behavior. The particle is now totally in a chaotic regime, a drastic change from  $E = 1/12$  to  $1/6$ .

## 5 Chaos Analysis

In order to characterize the chaotic behavior of the Hénon-Heiles potential, we will use two different based, one based on the computation of the orbits and another based on the slope of the distance in the phase space along a single orbit.

### 5.1 Area Analysis

To study the transition in greater detail, we computed the proportion of the total allowable area in the  $(y, \dot{y})$  plane covered by curves for various values of  $E$ . The method used to determine whether a point  $P_i$  belongs to a curve or to an ergodic orbit involves a secondary initial point  $P'_i$ , taken very close to  $P_i$ , at a distance of  $10^{-7}$  in our case. For each point, a sequence of successive transforms, were calculated for both  $P_i$  and  $P'_i$ . If  $P_i$  and  $P'_i$  lie in a region occupied by curves, the distance  $P_i P'_i$  will increase slowly, approximately linearly, with the number of transforms  $i$ . Conversely, if  $P_i$  and  $P'_i$  are in the ergodic region, this distance will grow rapidly, roughly exponentially. To quantify this behavior, we compute the quantity :

$$\mu = \sum_{i=1}^{25} (\text{distance } P_i P'_i)^2 \quad (5.1)$$

The summation is over the last 25 states of the initial condition and perturbed initial condition. A point  $P_i$ , along with its transforms, was classified as belonging to the ergodic region if  $\mu > \mu_c$ , or to a curve if  $\mu \leq \mu_c$ , where  $\mu_c = 10^{-4}$  is a chosen constant. This criterion allowed for the distinction between regular and ergodic regions in phase space. As for the value of  $\mu_c$ , even though the authors suggest a cutoff of  $10^{-4}$ , we wanted to verify its behavior for various energies, figure 8 represents the  $\mu$  values for different initial conditions corresponding to various energies, the authors state that the  $\mu$  values range from  $10^{-12}$  to  $10^{+1}$  and our diagram is consistent with that, even from this plot it is evident that behavior is chaotic at high energies and stable at lower energies.

The results of the equation (5.1) have been given in the figure 9, as expected it complements all the findings so far both from  $\mu$  value calculation and Poincaré sections, there appears to be a critical energy ( $E = 0.09$ ) up to which the curves cover the whole area and as we go up, the area covered decreases rapidly going to zero at  $E \approx 0.167$ , any energy higher than this value means that the particle will eventually escape to infinity, hence it is called energy of escape, the phase space volume goes to infinity, consequently the area of our Poincaré section goes to infinity and relative area losses its meaning. Another important thing to state here is that the critical energy from Hénon & Heiles (1964) is  $E = 0.11$ , the method is very sensitive to initial conditions, total time of orbit integration, the  $\mu_c$  criteria, we believe these are the cause of discrepancy between but the overall behavior of the function is similar to the one recorded by authors.

### 5.2 Gottwald and Melbourne Scheme

The earlier method of chaos determination required computation of the orbits, which is computationally expensive. Melbourne and Gottwald suggested another method called the 0-1 test (Gottwald & Melbourne 2004) which is both independent of the dimensionality of the phase space as well as the underlying equations. It is based on the slope of the distance in phase space along an orbit. The input for this method is a time series data and the output is 0 or 1, depending on whether the dynamics is non-chaotic or chaotic. In this method, we consider an observable  $\phi(x)$ , it could be anyone from  $x, \dot{x}, y, \dot{y}$  or a combination of these. One has to then create a real valued function  $p(t)$  as follows:

$$\theta(t) = ct + \int_0^t \phi[x(s)] ds \quad p(t) = \int_0^t \phi[x(s)] \cos[\theta(s)] ds \quad (5.2)$$

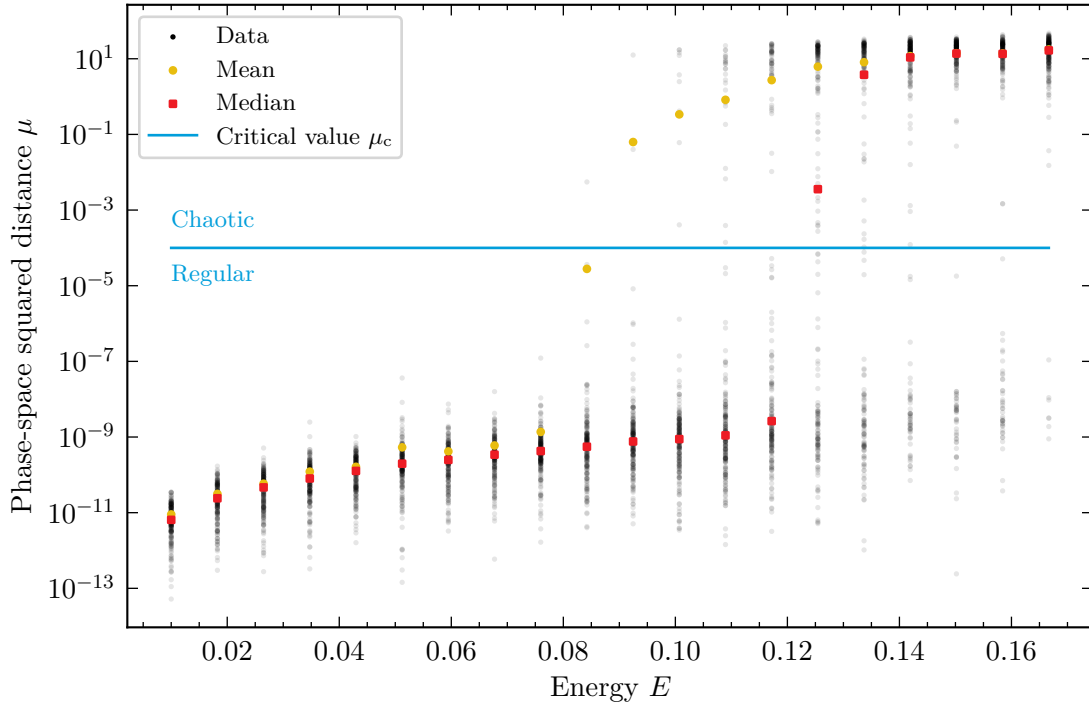


Figure 8: Behavior of  $\mu$  for various initial conditions for different total energies. Additionally, the mean (yellow circles) and median (red squares) values for each energy is plotted, and the critical value  $\mu_c$  is showed in light blue.

where  $c$  has to be chosen arbitrarily and must be greater than zero ( $c > 0$ ). The main observation is that if the system is non-chaotic,  $p(t)$  remains bounded, while for chaotic systems,  $p(t)$  behaves similarly to a Brownian motion. In the figure 10, one can see the exact behavior, for the energies less than the critical energy ( $E = 0.11$ )  $p(t)$  is bounded and for higher energies it behaves akin to the path under Brownian motion<sup>6</sup> (Kostykin et al. 2010). Thus, the former trajectories are regular while the latter ones are chaotic (Gottwald & Melbourne 2004).

To quantitatively analyze the behavior of  $p(t)$ , the mean-square displacement (MSD) has to be computed as:

$$M(t) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T (p(t + \tau) - p(\tau))^2 d\tau \quad (5.3)$$

The growth rate of MSD, defined as  $K = \lim_{t \rightarrow \infty} \log[M(t)] / \log(t)$  determines the nature of the system<sup>7</sup>:  $K = 0$  indicates non-chaotic behavior, while  $K = 1$  signifies chaos. The growth rate can be determined numerically using linear regression of  $\log[M(t)]$  versus  $\log(t)$ . Due to lack of time we were not able to rectify our MSD calculation function so we did not see the expected behavior of  $K$ , we have given the computed value of  $K$  for different energies in the table 1, we see the expected increase in the value of  $K$  as energy increases.

Energy	0.0100	0.0667	0.0833	0.1111	0.1250	0.1667
Chaos Indicator $K$	0.0003	0.0088	0.0145	0.0251	0.0423	0.0605

Table 1:  $K$  values for different energies.

<sup>6</sup>This behavior is represented significantly in the example shown in Appendix B.1.

<sup>7</sup>To avoid negative logarithms, the authors suggest to use  $\lim_{t \rightarrow \infty} \log[M(t) + 1] / \log(t)$

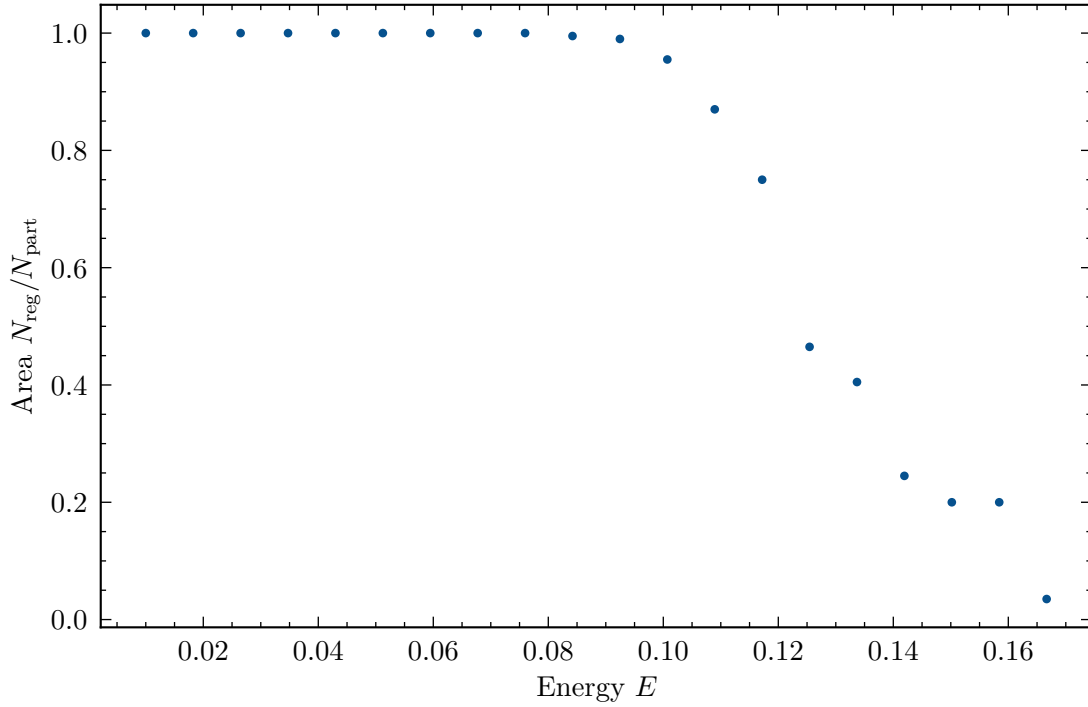


Figure 9: Relative area of the curves as function of energy.

## 6 Parallelization of the Code

In this section, we will focus on the problem of finding Poincaré sections: first, we generate  $N_{\text{part}} = 100$  particles, and integrate their trajectories in the Hénon-Heils potential for  $N_{\text{iter}} = 30\,000$  iterations (with a time-step  $h = 0.01$ ). Then, for each particle trajectory, we find two successive points on each sides of  $x = 0$ , and interpolate its position  $y$  and velocity  $v$  at  $x = 0$ .

The most computationally expensive part of the algorithm is the integration of the trajectories. In our first approach of this problem, the algorithm we made performed serial computations, therefore it was not very efficient, and quite long to run.

However, we designed our code to be easily improved by using Numpy arrays and its ability to perform data-based parallelism. Soon after, we made a new version of this algorithm to take advantages of vectorization.

To be able to quantify the improvement of the vectorization, we kept the two versions of the code, and wrote a script to test the wall clock time required to run each code. We also make sure to keep the same (realistic) conditions for the two runs. to get better statistics, the code is run for 5 times (with different total energy values), and we compute the mean wall clock time per iteration of the code. Only the integration and Poincaré section search are timed, the initialization and result writing parts are not counted. We performed two tests, on two different CPU: an 8-core Apple M1 3.2 GHz (1) and the **astromaster** 16-core Intel Xeon CPU E5-2609 v4, 1.70 GHz. (2) Our results are:

1. On Apple M1:
  - for the serial algorithm:  $t = (33.13 \pm 0.15)$  s per energy iteration;
  - for the parallel algorithm:  $t = (1.38 \pm 0.15)$  s per energy iteration.
2. On **astromaster**:

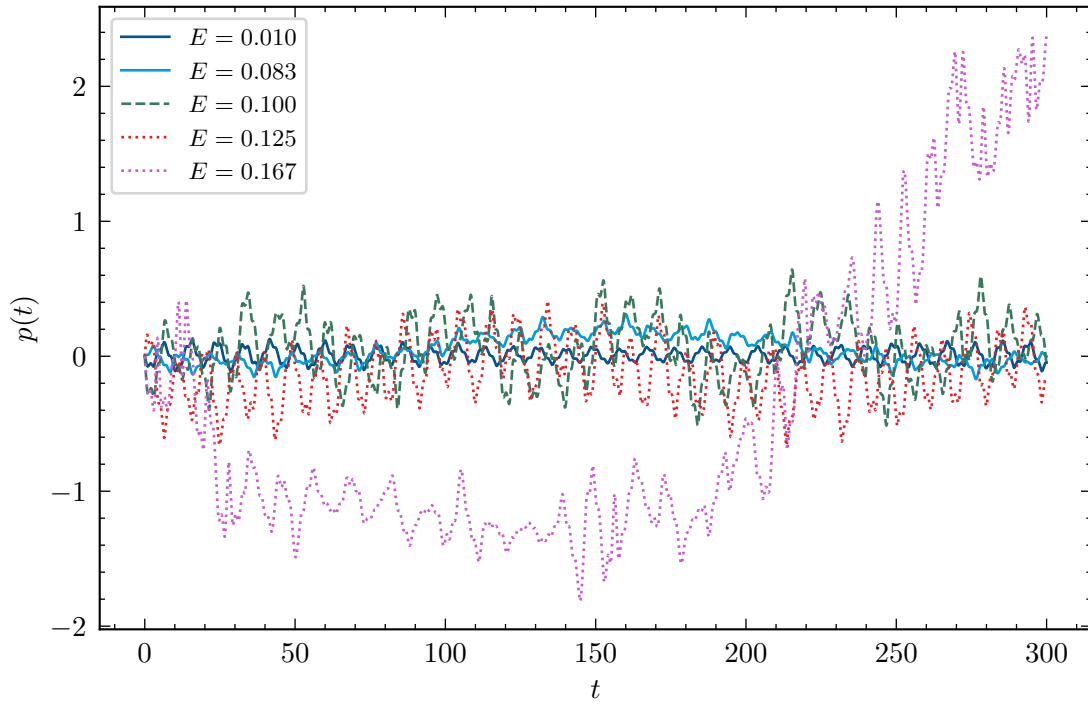


Figure 10: Behavior of  $p(t)$  for various energies. The orange trajectory  $E = 0.125$  is above the critical energy but here we see a bounded behavior because a significant portion of orbits are still regular, so a significant portion of initial conditions will yield bounded trajectories.

- for the serial algorithm:  $t = (123.9 \pm 2.8)$  s per energy iteration;
- for the parallel algorithm:  $t = (5.5 \pm 2.8)$  s per energy iteration.

The uncertainty correspond to the standard deviation. Using Numpy arrays reduced the time required to run the script by a factor 20–25 in both machines.

Another possibility for parallelization of the program would have been to implement a task-based parallelization, for instance by computing each of the energy iteration on one core (assuming there are at least five cores available). In this case, the time per energy iteration would stay roughly the same, but the total wall clock time would be divided by roughly a factor 5.

## 7 Conclusion

In this project, we studied the Hénon–Heiles potential by using numerical methods to understand the dynamics of a particle under this potential and the transition from regular to chaotic behavior. Before employing Runge–Kutta 4<sup>th</sup> order integrator on the Hénon–Heiles potential, we compared and tested the accuracy as well as the efficiency of the Euler method, RK2 and RK4 for the Kepler two body problem. After establishing that indeed RK4 is the best choice among them, we computed the trajectories of particles under this potential, one in regular regime and another in chaotic regime.

For analysis of overall behavior of the potential, we computed the Poincaré sections, for lower energy values the sections were smooth continuous loops, meaning the orbits were stable and for higher energies the section turned into a sea of chaos. There were also some energy values for which islands of stability were there but they did not fill the whole space, indicating that there is a critical energy separating the regular and chaotic dynamics. In order to find this energy, we plotted the area in the phase space plane covered by curves and found a critical energy of  $E = 0.09$

below which all the allowable area is covered by curves and above this it starts to decrease going to nearly 0 at  $E = 0.167$ , a totally chaotic behavior.

We also tried to verify our previous findings with the Melbourne-Gottwald 0–1 scheme based on the slope of distance in an orbit, we did find the behavior to be chaotic for energies above the critical energy, inferred by plotting  $p(t)$  as a function of integration time but were unable to reproduce nearly 0 or nearly 1 values for the growth rate of the mean square displacement as the method suggests, we believe there was some inaccuracy in the calculation of the mean square displacement, but nevertheless we saw an increase in the growth rate of MSD as energies increased, which is expected as  $p(t)$  is first bounded for lower energies and then shows Brownian motion-like behavior for higher energies.

Furthermore, to enhance the computational efficiency, we implemented vectorized parallelization technique and also discussed how it can be further improved. In nutshell, we demonstrated the chaotic as well as the regular dynamics of the particles under the Hénon-Heiles potential.

## References

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# Appendix

## A Evolution of the Energy Error

The fig.11 represents the error between the analytical value of energy and the numerical values of energy calculated using various integrators as the orbit evolves. All these computations were done for equal integration time, the behavior is as expected, with the RK4 being the most accurate one, but what is of interest is that for early orbit integration time, the error between the RK4 method and the analytical expression is less than machine error, so it means the floating point error can't reliably distinguish between two values, the error no longer represents the true physical or mathematical difference between results rather it is dominated by the limits of machine.

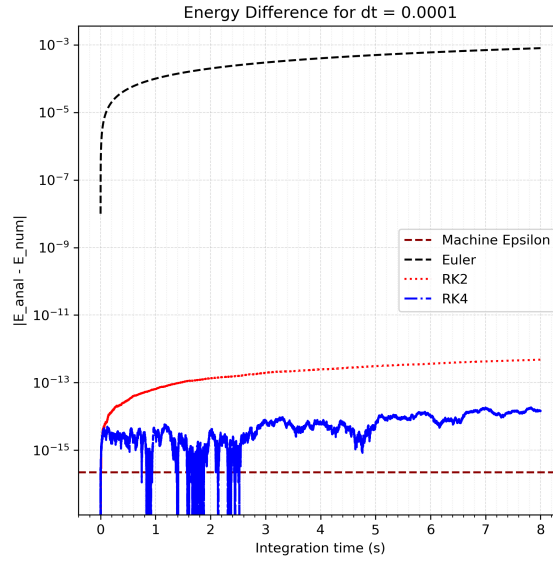


Figure 11: energy error evolution for  $dt = h = 0.0001$

We also calculated the computation time for all integrators for different time steps as given in figure 12, as expected the Euler method is the fastest, followed by RK2 and the RK4. RK4 is almost one order of magnitude slower than the Euler method but given that for  $dt = h = 0.001$  it is more than 4 orders of magnitude better than RK2 and 10 orders of magnitude better than the Euler method(see figure 3).

## B Linear Interpolation

Between two consecutive time steps, the particle might have cross  $x = 0$  between two time steps, in that case the exact crossing point is not explicitly recorded. To accurately determine the  $y$ -coordinate and  $v_y$ -velocity at the exact point where a trajectory crosses the plane  $x = 0$ , linear interpolation is used. The interpolated values are calculated as:

$$y_0 = y[i] + \frac{y[i+1] - y[i]}{x[i+1] - x[i]} \cdot (0 - x[i]),$$

$$v_0 = v[i] + \frac{v[i+1] - v[i]}{x[i+1] - x[i]} \cdot (0 - x[i]).$$

Linear interpolation is valid as the time step is very small  $dt = h = 0.001$  and the particle's motion is nearly linear in this interval.

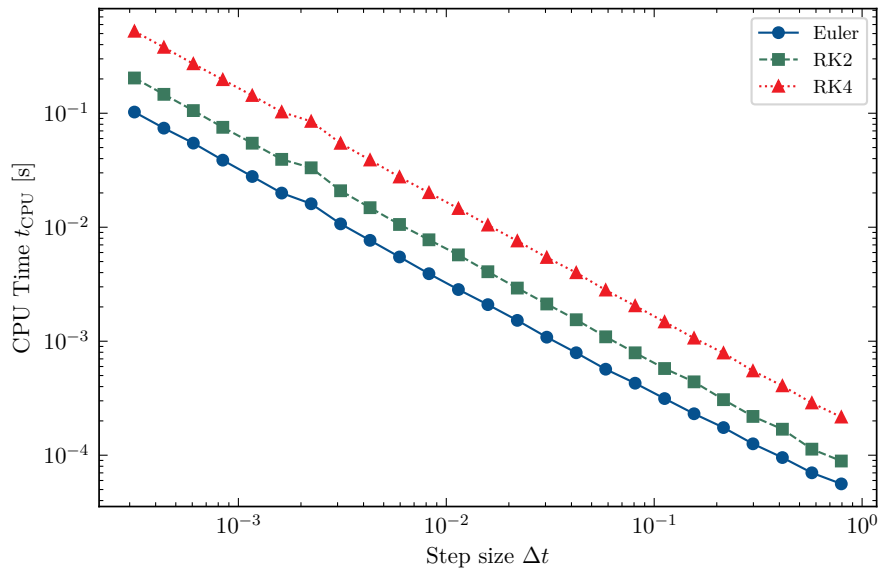


Figure 12: Computation time for various time steps for Euler, RK2 and RK4 scheme

## B.1 Melbourne-Gottwald 0–1 test

Here, we present another example of the behavior of  $p(t)$ , we can clearly see the Brownian motion like behavior of the function above critical energy.

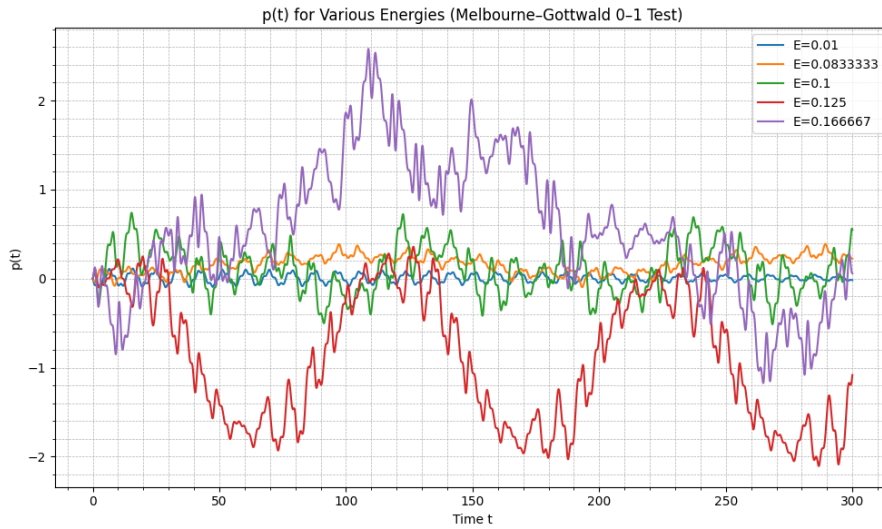


Figure 13: Behavior of  $p(t)$  for various energies

## B.2 Poincaré Sections

Figure 14 and 15 present a magnified view of the Poincaré sections for various energies in order to see the features of the phase space that are not evident explicitly in the main diagram included in the report.

Poincaré Sections (results from the parallel algorithm)

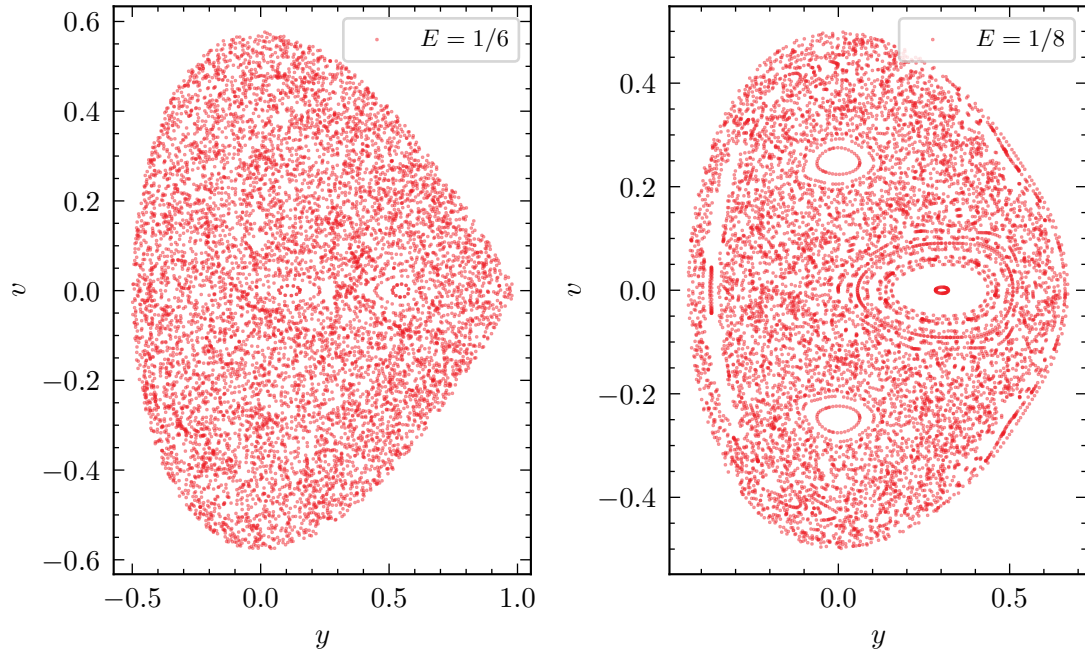


Figure 14: Poincaré section for  $E = \frac{1}{6}, \frac{1}{8}$

Poincaré Sections (results from the parallel algorithm)

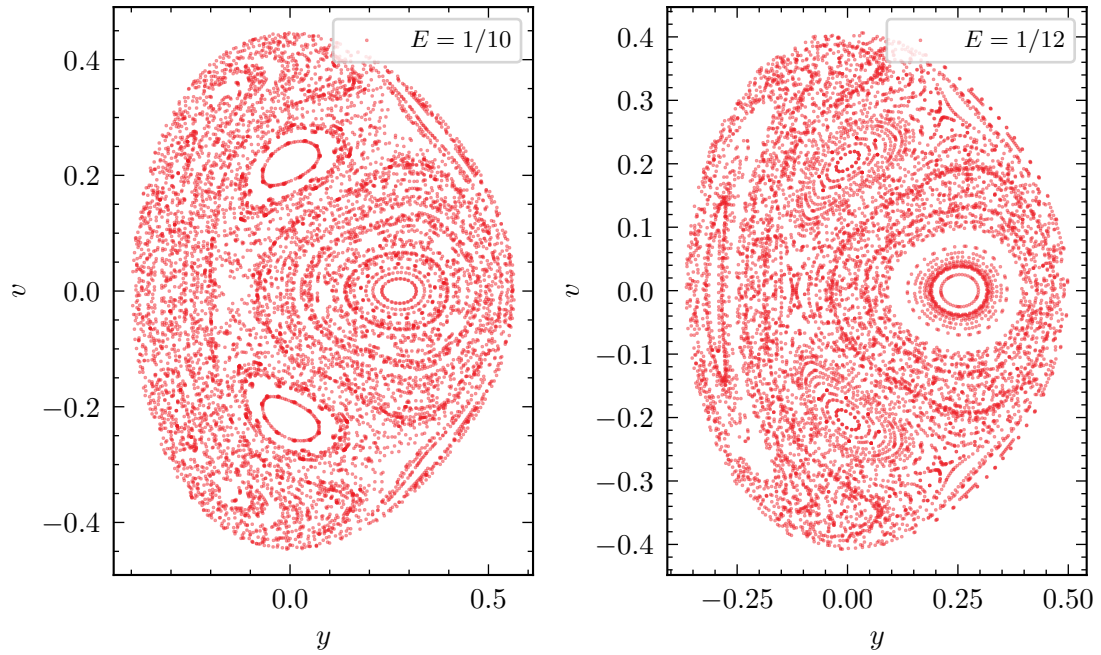


Figure 15: Poincaré section for  $E = \frac{1}{10}, \frac{1}{12}$

## C Listings

The listings of the codes are provided here. However, the source code is also available on [Github](https://github.com/Yael-II/MSc2-Project-Chaos)<sup>8</sup> (with installing and usage instructions).

### C.1 Library Files

file: `energies.py`

```
1  #!/usr/bin/env python
2  """
3  Energies
4
5  Compute energies (kinetic or total)
6
7  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
8  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
9                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
10 @ Date: 2025-01-01
11
12 Licence:
13 Order and Chaos in a 2D potential
14 Copyright (C) 2025 Yael Moussouni (yael.moussouni@etu.unistra.fr)
15                  Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
16
17 energies.py
18 Copyright (C) 2025 Yael Moussouni (yael.moussouni@etu.unistra.fr)
19                  Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
20
21 This program is free software: you can redistribute it and/or modify
22 it under the terms of the GNU General Public License as published by
23 the Free Software Foundation; either version 3 of the License, or
24 (at your option) any later version.
25
26 This program is distributed in the hope that it will be useful,
27 but WITHOUT ANY WARRANTY; without even the implied warranty of
28 MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
29 GNU General Public License for more details.
30
31 You should have received a copy of the GNU General Public License
32 along with this program. If not, see https://www.gnu.org/licenses/.
33 """
34
35 import numpy as np
36
37 def kinetic(W: np.ndarray) -> np.ndarray:
38     """Computes the kinetic energy.
39     @param
40         - W: Phase-space vectors
41     @returns
42         - T: Kinetic energy
43     """
44     U = W[1,0]
45     V = W[1,1]
46     # If U or V is not an array (or a list), but rather a scalar, then we
47     # create a list of one element so that it can work either way
48     if np.ndim(U) == 0: U = np.array([U])
49     if np.ndim(V) == 0: V = np.array([V])
50
51     return (U**2 + V**2)/2
52
53 def total(W: np.ndarray,
54           potential,
55           kinetic = kinetic) -> np.ndarray:
56     return potential(W) + kinetic(W)
```

<sup>8</sup><https://github.com/Yael-II/MSc2-Project-Chaos>

file: initial\_conditions.py

```
1  #!/usr/bin/env python
2  """
3  Initial Conditions
4
5  Generate initial conditions depending on different criteria
6
7  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
8  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
9                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
10 @ Date: 2025-01-01
11
12 Licence:
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15                Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
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17 initial_conditions.py
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20
21 This program is free software: you can redistribute it and/or modify
22 it under the terms of the GNU General Public License as published by
23 the Free Software Foundation; either version 3 of the License, or
24 (at your option) any later version.
25
26 This program is distributed in the hope that it will be useful,
27 but WITHOUT ANY WARRANTY; without even the implied warranty of
28 MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
29 GNU General Public License for more details.
30
31 You should have received a copy of the GNU General Public License
32 along with this program. If not, see https://www.gnu.org/licenses/.
33 """
34
35 import numpy as np
36 import matplotlib.pyplot as plt
37 POS_MIN = -1
38 POS_MAX = +1
39 VEL_MIN = -1
40 VEL_MAX = +1
41 N_PART = 1
42
43 def mesh_grid(N: int = N_PART,
44              xmin: float = POS_MIN,
45              xmax: float = POS_MAX,
46              ymin: float = POS_MIN,
47              ymax: float = POS_MAX) -> np.ndarray:
48     """Generates a set of regularly sampled particles with no velocity
49     @ params:
50         - N: number of particles
51         - xmin: minimum value for position x
52         - xmax: maximum value for position x
53         - ymin: minimum value for position y
54         - ymax: maximum value for position y
55     @ returns:
56         - W: phase-space vector
57     """
58     X = np.linspace(xmin, xmax, N)
59     Y = np.linspace(ymin, ymax, N)
60     X,Y = np.meshgrid(X,Y, indexing="ij")
61     return np.array([X,Y])
62
63 def one_part(x0: float = 0,
64             y0: float = 0,
65             u0: float = 0,
66             v0: float = 0) -> np.ndarray:
67     """Generates a particle at position (x0, y0)
68     with velocities (u0,v0)
69     @ params:
```

```

70         - N: number of particles
71         - x0: initial position x
72         - y0: initial position y
73         - u0: initial velocity u
74         - v0: initial velocity v
75     @ returns:
76         - W: phase-space vector
77     """
78     X = x0
79     Y = y0
80     U = u0
81     V = v0
82     return np.array([[X,Y], [U,V]])
83
84 def n_energy_part(potential,
85                  N: int = N_PART,
86                  E: float = 0,
87                  xmin: float = -1,
88                  xmax: float = +1,
89                  ymin: float = -0.5,
90                  ymax: float = +1):
91     """Generates N particles with an energy E in a potential.
92     @ params:
93         - potential: gravitational potential
94         - N: number of particles
95         - E: total energy
96         - xmin: minimum value for position x
97         - xmax: maximum value for position x
98         - ymin: minimum value for position y
99         - ymax: maximum value for position y
100     @ returns:
101         - W: an array of all the positions and velocities.
102     """
103     X = []
104     Y = []
105     POT = []
106     U = []
107     V = []
108     while len(X) < N:
109         x = np.random.random()*(xmax-xmin)+xmin
110         y = np.random.random()*(ymax-ymin)+ymin
111         w = np.array([x, y])
112         pot = potential(w, position_only=True)[0]
113         if pot <= E:
114             X.append(x)
115             Y.append(y)
116             POT.append(pot)
117     X = np.array(X)
118     Y = np.array(Y)
119     POT = np.array(POT)
120     U = np.zeros_like(X)
121     V = np.zeros_like(Y)
122     C = np.sqrt(2 * (E - POT))
123     THETA = np.random.random(N)*2*np.pi
124     U = C*np.cos(THETA)
125     V = C*np.sin(THETA)
126     return np.array([[X, Y], [U, V]])
127
128 def n_energy_2part(potential,
129                   N: int = N_PART,
130                   E: float = 0,
131                   sep: float = 1e-7,
132                   xmin: float = -1,
133                   xmax: float = +1,
134                   ymin: float = -0.5,
135                   ymax: float = +1):
136     """Generate a sample of 2N particles with the energy E in a potential in
137     two sets: one "normal" set (see n_energy_part), and a slightly shifted set
138     with a separation sep.
139     @ params:

```

```
140     - potential: gravitational potential
141     - N: number of particles
142     - E: total energy
143     - sep: the separation between the two sets
144     - xmin: minimum value for position x
145     - xmax: maximum value for position x
146     - ymin: minimum value for position y
147     - ymax: maximum value for position y
148 @ returns:
149     - (W1, W2): the two arrays of all the positions and velocities for
150       each set.
151 """
152 W_1 = n_energy_part(potential, N, E)
153 W_2 = np.zeros_like(W_1)
154 alpha = np.random.uniform(0, 2*np.pi, N)
155 W_2[0, 0] = W_1[0, 0] + sep*np.cos(alpha)
156 W_2[0, 1] = W_1[0, 1] + sep*np.sin(alpha)
157 W_2[1, 0] = W_1[1, 0]
158 W_2[1, 1] = W_1[1, 1]
159 return (W_1, W_2)
```

file: integrator.py

```
1  #!/usr/bin/env python
2  """
3  Integrator
4
5  Integrate differential equations.
6
7  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
8  @ Institution:  Universite de Strasbourg, CNRS, Observatoire astronomique
9                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
10 @ Date: 2025-01-01
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15                  Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
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19                  Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
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22 it under the terms of the GNU General Public License as published by
23 the Free Software Foundation; either version 3 of the License, or
24 (at your option) any later version.
25
26 This program is distributed in the hope that it will be useful,
27 but WITHOUT ANY WARRANTY; without even the implied warranty of
28 MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
29 GNU General Public License for more details.
30
31 You should have received a copy of the GNU General Public License
32 along with this program. If not, see https://www.gnu.org/licenses/.
33
34 """
35 import numpy as np
36
37 def euler(t0: float,
38          W0: np.ndarray,
39          h: float,
40          n: int,
41          func):
42     """Euler method adapted for state vector [[x, y], [u, v]]
43     @ params
44         - t0: initial time value
45         - W0: initial state vector [[x, y], [u, v]]
46         - h: step size (time step)
47         - n: number of steps
48         - func: RHS of differential equation
49     @returns:
50         - t, W: time and state (solution) arrays
51     """
52     time = np.zeros(n)
53     W = np.zeros((n,) + np.shape(W0))
54
55     t = t0
56     w = W0
57     for i in range(n):
58         k1 = func(t, w)
59         w = w + h*k1
60         t = t + h
61
62         time[i] = t
63         W[i] = w
64     return time, W
65
66 def rk2(t0: float,
67        W0: np.ndarray,
68        h: float,
69        n: int,
```



```
70     func):
71     """RK2 method adapted for state vector [[x, y], [u, v]]
72     @ params
73         - t0: initial time value
74         - W0: initial state vector [[x, y], [u, v]]
75         - h: step size (time step)
76         - n: number of steps
77         - func: RHS of differential equation
78     @returns:
79         - t, W: time and state (solution) arrays
80     """
81     time = np.zeros(n)
82     W = np.zeros((n,) + np.shape(W0))
83
84     t = t0
85     w = W0
86     for i in range(n):
87         k1 = func(t, w)
88         k2 = func(t + h/2, w + h/2*k1)
89
90         w = w + h*k2
91         t = t + h
92
93         time[i] = t
94         W[i] = w
95     return time, W
96
97 def rk4(t0: float,
98        W0: np.ndarray,
99        h: float,
100        n: int,
101        func):
102     """RK4 method adapted for state vector [[x, y], [u, v]]
103     @ params
104         - t0: initial time
105         - W0: initial state vector [[x, y], [u, v]]
106         - h: step size (time step)
107         - n: number of steps
108         - func: RHS of differential equation
109     @returns:
110         - t, W: time and state (solution) arrays
111     """
112     time = np.zeros(n)
113     W = np.zeros((n,) + np.shape(W0))
114     # to accommodate the state vector
115     t = t0
116     w = W0
117     for i in range(n):
118         k1 = func(t, w)
119         k2 = func(t + h/2, w + h/2*k1)
120         k3 = func(t + h/2, w + h/2*k2)
121         k4 = func(t + h, w + h*k3)
122
123         w = w + h*(k1/6 + k2/3 + k3/3 + k4/6)
124         t = t + h
125
126         time[i] = t
127         W[i] = w
128     return time, W
129
130 def integrator_type(t0, W0, h, n, func, integrator):
131     return integrator(t0, W0, h, n, func)
132
133 def kepler_analytical(t0: float,
134                      W0: np.ndarray,
135                      h: float,
136                      n: int):
137     """Computes the evolution from the Kepler potential derivative
138     @ params
139         - t0: initial time value
```

```
140     - W0: initial state vector [[x, y], [u, v]]
141     - h: step size (time step)
142     - n: number of steps
143 @returns:
144     - t, W: time and state (solution) arrays
145 """
146 X0 = W0[0, 0]
147 Y0 = W0[0, 1]
148 U0 = W0[1, 0]
149 V0 = W0[1, 1]
150
151 time = np.arange(t0, t0 + n*h, h)
152 W = np.zeros((n,) + np.shape(W0))
153
154 R0 = np.sqrt(X0**2 + Y0**2)
155 Omega0 = np.sqrt(U0**2 + V0**2)/R0
156
157 X = R0 * np.cos(Omega0 * time)
158 Y = R0 * np.sin(Omega0 * time)
159 U = -R0 * Omega0 * np.sin(Omega0 * time)
160 V = R0 * Omega0 * np.cos(Omega0 * time)
161
162 W = np.array([[X, Y], [U, V]])
163 W = np.swapaxes(W, 0, 2)
164 W = np.swapaxes(W, 1, 2)
165 return time, W
```

file: poincare\_sections.py

```
1  #!/usr/bin/env python
2  """
3  Poincare Sections
4
5  Computes the Poincare Sections
6
7  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
8  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
9                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
10 @ Date: 2025-01-01
11
12 Licence:
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14 Copyright (C) 2025 Yael Moussouni (yael.moussouni@etu.unistra.fr)
15                Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
16
17 poincare_sections.py
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19                Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
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33 """
34
35 import numpy as np
36 def pcs_find(pos_x, pos_y, vel_x, vel_y):
37     """Find Poincare sections (PCS; x = 0)
38     @ params:
39         - pos_x: position along the x axis
40         - pos_y: position along the y axis
41         - pos_x: velocity along the x axis
42         - pos_y: velocity along the y axis
43     @ returns: (tuple)
44         - pcs_pos_y: position of the points in the PCS along the y axis
45         - pcs_vel_y: velocity of the points in the PCS along the y axis
46     """
47     if np.ndim(pos_x) == 1:
48         pos_x = np.array([pos_x])
49         pos_y = np.array([pos_y])
50         vel_x = np.array([vel_x])
51         vel_y = np.array([vel_y])
52     pcs_pos_y = []
53     pcs_vel_y = []
54     for j in range(len(pos_x[0])): # for each particle
55         i = 0
56         x = pos_x[:,j]
57         y = pos_y[:,j]
58         u = vel_x[:,j]
59         v = vel_y[:,j]
60         while i < len(x) - 1:
61             if x[i] * x[i+1] < 0:
62                 y0 = y[i] \
63                     + (y[i+1] - y[i])/(x[i+1] - x[i]) \
64                     * (0 - x[i])
65                 v0 = v[i] \
66                     + (v[i+1] - v[i])/(x[i+1] - x[i]) \
67                     * (0 - x[i])
68                 pcs_pos_y.append(y0)
69                 pcs_vel_y.append(v0)
```

```
70         i += 1
71     return pcs_pos_y, pcs_vel_y
72
73 def pcs_find_legacy(pos_x, pos_y, vel_x, vel_y):
74     """DEPRECIATED - DO NOT USE
75     Depreciated legacy function that should not be used
76     """
77     if np.ndim(pos_x) == 1:
78         pos_x = np.array([pos_x])
79         pos_y = np.array([pos_y])
80         vel_x = np.array([vel_x])
81         vel_y = np.array([vel_y])
82     pcs_pos_y = []
83     pcs_vel_y = []
84     for j in range(len(pos_x)): # for each particle
85         i = 0
86         x = pos_x[j]
87         y = pos_y[j]
88         u = vel_x[j]
89         v = vel_y[j]
90         while i < len(x) - 1:
91             if x[i] * x[i+1] < 0:
92                 y0 = y[i] \
93                     + (y[i+1] - y[i])/(x[i+1] - x[i]) \
94                     * (0 - x[i])
95                 v0 = v[i] \
96                     + (v[i+1] - v[i])/(x[i+1] - x[i]) \
97                     * (0 - x[i])
98                 pcs_pos_y.append(y0)
99                 pcs_vel_y.append(v0)
100             i += 1
101     return pcs_pos_y, pcs_vel_y
```

file: potentials.py

```
1  #!/usr/bin/env python
2  """
3  Potentials
4
5  Functions of the different potentials (and their derivatives for the evolution)
6
7  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
8  @ Institution:  Universite de Strasbourg, CNRS, Observatoire astronomique
9                 de Strasbourg, UMR 7550, F-67000 Strasbourg, France
10 @ Date: 2025-01-01
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16
17 potentials.py
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19                 Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
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33
34 """
35
36 import numpy as np
37
38 MAX_VAL = 1e3
39
40 def kepler_potential(W_grid: np.ndarray,
41                     position_only: bool = False) -> np.ndarray:
42     """Computes the Kepler potential:  $V(R) = -G*m_1*m_2/R$ 
43     (assuming  $G = 1$ ,  $m_1 = 1$ ,  $m_2 = 1$ )
44     assuming the point mass at  $(x = 0, y = 0)$ .
45     @params:
46         - W: Phase-space vector
47         - position_only: True if W is np.array([X, Y])
48     @returns:
49         - computed potential
50     """
51     if position_only:
52         X = W_grid[0]
53         Y = W_grid[1]
54     else:
55         X = W_grid[0,0]
56         Y = W_grid[0,1]
57     # If X or Y is not an array (or a list), but rather a scalar, then we
58     # create a list of one element so that it can work either way
59     if np.ndim(X) == 0: X = np.array([X])
60     if np.ndim(Y) == 0: Y = np.array([Y])
61     R = np.sqrt(X**2 + Y**2)
62     return -1/R
63
64 def kepler_evolution(t: np.ndarray, W: np.ndarray):
65     """Computes the evolution from the Kepler potential derivative
66     @params
67         - t: Time (not used)
68         - W: Phase space vector
69     &returns
```

```
70         - dot W: Time derivative of the phase space vector
71     """
72     X = W[0, 0]
73     Y = W[0, 1]
74     U = W[1, 0]
75     V = W[1, 1]
76     R = np.sqrt(X**2 + Y**2)
77     DX = U
78     DY = V
79     DU = -X/R**3
80     DV = -Y/R**3
81     return np.array([[DX, DY], [DU, DV]])
82
83 def hh_potential(W_grid: np.ndarray,
84                 position_only=False) -> np.ndarray:
85     """Computes the Henon-Heiles potential.
86     @params:
87         - W: Phase-space vector
88         - position_only: True if W is np.array([X, Y])
89     @returns:
90         - POT: Potential
91     """
92     if position_only:
93         X = W_grid[0]
94         Y = W_grid[1]
95     else:
96         X = W_grid[0, 0]
97         Y = W_grid[0, 1]
98
99     # If X or Y is not an array (or a list), but rather a scalar, then we
100    # create a list of one element so that it can work either way
101    if np.ndim(X) == 0: X = np.array([X])
102    if np.ndim(Y) == 0: Y = np.array([Y])
103
104    POT = (X**2 + Y**2 + 2*X**2*Y - 2*Y**3/3)/2
105    return POT
106
107 def hh_evolution(t: np.ndarray, W: np.ndarray):
108     """Computes the evolution from the HH potential derivative
109     @params
110         - t: Time (not used)
111         - W: Phase space vector
112     @returns
113         - dot W: Time derivative of the phase space vector
114     """
115     X = W[0, 0]
116     Y = W[0, 1]
117     U = W[1, 0]
118     V = W[1, 1]
119     DX = U
120     DY = V
121     DU = -(2*X*Y + X)
122     DV = -(X**2 - Y**2 + Y)
123     return np.array([[DX, DY], [DU, DV]])
```

## C.2 Main Files

file: main\_area.py

```
1  #!/usr/bin/env python
2  """
3  Main: Compute Relative Area
4
5  Computes the relative area covered bu the curves for different energies, to
6  study ordered and chaotic regimes.
7
8  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
9  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
10                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
11  @ Date: 2025-01-01
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17
18  main_area.py
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30  GNU General Public License for more details.
31
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33  along with this program. If not, see https://www.gnu.org/licenses/.
34
35  """
36  import numpy as np
37  from scipy.optimize import curve_fit
38
39  import potentials as pot
40  import energies as ene
41  import integrator as itg
42  import initial_conditions as init
43  import poincare_sections as pcs
44
45  OUT_DIR = "./Output/"
46  FILENAME_PREFIX = "phase_separation_"
47  EXTENSION = ".csv"
48  DEFAULT_N_iter = int(1e5)
49  DEFAULT_N_part = 200
50  DEFAULT_h = 0.005
51  E_all = np.linspace(1/100, 1/6, 20)
52
53  def compute_mu(E: float,
54                N_iter: int = DEFAULT_N_iter,
55                N_part: int = DEFAULT_N_part,
56                h: float = DEFAULT_h) -> tuple:
57      """
58      Computes the phase-space squared distances for particles of given energy E.
59      @params:
60          - E: the total energy of each particles
61          - N_iter: the number of iteration
62          - N_part: the number of particles
63          - h: integration steps
64      @returns:
65          - mu: phase-space squared distance
66      """
67      W_1, W_2 = init.n_energy_2part(pot.hh_potential, N_part, E)
```

```
68     t_1, positions_1 = itg.rk4(0, W_1, h, N_iter, pot.hh_evolution)
69     x_1 = positions_1[:, 0, 0]
70     y_1 = positions_1[:, 0, 1]
71     u_1 = positions_1[:, 1, 0]
72     v_1 = positions_1[:, 1, 1]
73
74     t_2, positions_2 = itg.rk4(0, W_2, h, N_iter, pot.hh_evolution)
75     x_2 = positions_2[:, 0, 0]
76     y_2 = positions_2[:, 0, 1]
77     u_2 = positions_2[:, 1, 0]
78     v_2 = positions_2[:, 1, 1]
79     dist_sq = (x_2[-25:] - x_1[-25:])**2 \
80               + (y_2[-25:] - y_1[-25:])**2 \
81               + (u_2[-25:] - u_1[-25:])**2 \
82               + (v_2[-25:] - v_1[-25:])**2
83
84     mu = np.sum(dist_sq, axis=0)
85     return mu
86
87 if __name__ == "__main__":
88     mu_all = []
89     for i in range(len(E_all)):
90         mu = compute_mu(E_all[i])
91         filename = OUT_DIR + FILENAME_PREFIX \
92                 + str(i) + EXTENSION
93         np.savetxt(filename, mu)
```



file: main\_poincare\_sections\_linear.py

```
1  #!/usr/bin/env python
2  """
3  Main: Computes Poincare Sections (Linear Algorithm)
4
5  Computes the Poincare Sections with a linear algorithm
6  (i.e. no parallel computing).
7
8  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
9  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
10                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
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17
18  main_poincare_sections_linear.py
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20                Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
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33  along with this program. If not, see https://www.gnu.org/licenses/.
34
35  """
36  import numpy as np
37
38  import potentials as pot
39  import integrator as itg
40  import initial_conditions as init
41  import poincare_sections as pcs
42
43  # Parameters
44  OUT_DIR = "./Output/"
45  FILENAME_PREFIX = "poincare_sections_linear_"
46  EXTENSION = ".csv"
47  DEFAULT_N_iter = 30000
48  DEFAULT_N_part = 100
49  DEFAULT_h = 0.01
50  E_all = np.array([1/100, 1/12, 1/10, 1/8, 1/6])
51
52  text_E = ["1/100", "1/12", "1/10", "1/8", "1/6"]
53
54  def compute_poincare_sections_linear(E: float,
55                                     N_iter: int = DEFAULT_N_iter,
56                                     N_part: int = DEFAULT_N_part,
57                                     h: float = DEFAULT_h) -> tuple:
58
59     """
60     Computes the Poincare sections for a given energy E.
61     @params:
62         - E: the total energy of each particles
63         - N_iter: the number of iteration
64         - N_part: the number of particles
65         - h: integration steps
66     @returns:
67         - y_section, v_section: arrays containing the y and v coordinates of
68           the Poincare sections
69     """
70     W_all_part = init.n_energy_part(pot.hh_potential, N_part, E)
```

```
70     y_section = []
71     v_section = []
72     for i in range(N_part):
73         W_part = W_all_part[:, :, i]
74
75         # Perform integration
76         t_part, coord_part = itg.rk4(0, W_part, h, N_iter, pot.hh_evolution)
77
78         # Extract positions and velocities
79         x_part = coord_part[:, 0, 0]
80         y_part = coord_part[:, 0, 1]
81         u_part = coord_part[:, 1, 0]
82         v_part = coord_part[:, 1, 1]
83
84         # Find Poincare section points for the current initial condition
85         y_pcs, v_pcs = pcs.pcs_find_legacy(x_part, y_part, u_part, v_part)
86         # The legacy is important here, the algorithm is the same but the
87         # data format is different...
88
89         # Append the current Poincare section points to the overall lists
90         y_section += y_pcs
91         v_section += v_pcs
92     return y_section, v_section
93
94 if __name__ == "__main__":
95     y_section_all = []
96     v_section_all = []
97     for i in range(len(E_all)):
98         y_section, v_section = compute_poincare_sections_linear(E_all[i])
99         section = np.array([y_section, v_section])
100         filename = OUT_DIR + FILENAME_PREFIX \
101             + str(text_E[i][2:]) + EXTENSION
102         np.savetxt(filename, section)
```

file: main\_poincare\_sections\_parallel.py

```
1 #!/usr/bin/env python
2  """
3  Main: Computes Poincare Sections (Parallel Algorithm)
4
5  Computes the Poincare Sections with a parallel algorithm (with Numpy)
6
7  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
8  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
9                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
10 @ Date: 2025-01-01
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17 main_poincare_sections_parallel.py
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32 along with this program. If not, see https://www.gnu.org/licenses/.
33
34 """
35 import numpy as np
36
37 import potentials as pot
38 import integrator as itg
39 import initial_conditions as init
40 import poincare_sections as pcs
41
42 # Parameters
43 OUT_DIR = "./Output/"
44 FILENAME_PREFIX = "poincare_sections_parallel_"
45 EXTENSION = ".csv"
46 DEFAULT_N_iter = 30000
47 DEFAULT_N_part = 100
48 DEFAULT_h = 0.01
49 E_all = np.array([1/100, 1/12, 1/10, 1/8, 1/6])
50
51 text_E = ["1/100", "1/12", "1/10", "1/8", "1/6"]
52
53 def compute_poincare_sections_numpy(E: float,
54                                   N_iter: int = DEFAULT_N_iter,
55                                   N_part: int = DEFAULT_N_part,
56                                   h: float = DEFAULT_h) -> tuple:
57     """
58     Computes the Poincare sections for a given energy E.
59     @params:
60         - E: the total energy of each particles
61         - N_iter: the number of iteration
62         - N_part: the number of particles
63         - h: integration steps
64     @returns:
65         - y_section, v_section: arrays containing the y and v coordinates of
66           the Poincare sections
67     """
68     W_part = init.n_energy_part(pot.hh_potential, N_part, E)
69     y_section = []
```

```
70     v_section = []
71
72     # Perform integration
73     t_part, coord_part = itg.rk4(0, W_part, h, N_iter, pot.hh_evolution)
74
75     # Extract positions and velocities
76     x_part = coord_part[:, 0, 0]
77     y_part = coord_part[:, 0, 1]
78     u_part = coord_part[:, 1, 0]
79     v_part = coord_part[:, 1, 1]
80
81     # Find Poincare section points for the current initial condition
82     y_section, v_section = pcs.pcs_find(x_part, y_part, u_part, v_part)
83     return y_section, v_section
84
85 if __name__ == "__main__":
86     y_section_all = []
87     v_section_all = []
88     for i in range(len(E_all)):
89         y_section, v_section = compute_poincare_sections_numpy(E_all[i])
90         section = np.array([y_section, v_section])
91         filename = OUT_DIR + FILENAME_PREFIX\
92             + str(text_E[i][2:]) + EXTENSION
93         np.savetxt(filename, section)
```

### C.3 Plot Files

file: plot\_area.py

```
1  #!/usr/bin/env python
2  """
3  Plot: Area
4
5  Plots areas
6
7  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
8  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
9                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
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32 along with this program. If not, see https://www.gnu.org/licenses/.
33
34 """
35 import os
36 import numpy as np
37 import matplotlib.pyplot as plt
38
39 if "YII_1" in plt.style.available: plt.style.use("YII_1")
40
41 OUT_DIR = "./Output/"
42 FILENAME_PREFIX = "phase_separation_"
43 EXTENSION = ".csv"
44
45 def plot_area(filelist: list, mu_c = 1e-4) -> int:
46     """
47     Plot all the Poincare sections in the file list.
48     @params:
49         - filelist: the list of files in the output directory, with the format
50           "poincare_sections_{linear, parallel}_{1/E}.csv"
51         - title: title of the figure
52     @returns:
53         - 0.
54     """
55     orderlist = np.argsort([(int(file
56                             .replace(FILENAME_PREFIX, "")
57                             .replace(EXTENSION, "")))
58                             for file in filelist])
59     filelist = np.array(filelist)[orderlist]
60     N = len(filelist)
61     E = np.linspace(1/100, 1/6, N)
62     mu = []
63     for filename in filelist:
64         with open(OUT_DIR + filename) as file:
65             data = file.readlines()
66             data = [np.float64(d.replace("\n", "")) for d in data]
67             mu.append(data)
```

```
68 mu = np.array(mu)
69
70 fig, ax = plt.subplots(1)
71 ax.scatter([], [], s=1, color="k", label="Data")
72 for i in range(len(mu)):
73     Y = mu[i]
74     ax.scatter([E[i]]*len(Y), Y, s=1, color="k", alpha=0.1)
75 ax.scatter(E, np.mean(mu, axis=1), s=5,
76            color="C1", marker="o", label="Mean")
77 ax.scatter(E, np.median(mu, axis=1), s=5,
78            color="C3", marker="s", label="Median")
79 ax.plot(E, [mu_c]*len(E),
80         color="C5", label="Critical value  $\mu_c$ ")
81 ax.text(0.01, 1e-5, "Regular", va="bottom", ha="left", color="C5")
82 ax.text(0.01, 1e-3, "Chaotic", va="top", ha="left", color="C5")
83 ax.set_xlabel("Energy  $E$ ")
84 ax.set_ylabel("Phase-space squared distance  $\mu$ ")
85 ax.set_yscale("log")
86 ax.legend()
87 fig.savefig("Figs/mu.pdf")
88
89 fig, ax = plt.subplots(1)
90 N_reg = np.count_nonzero(mu < mu_c, axis=1)
91 N = np.shape(mu)[1]
92 Area = N_reg / N
93 ax.scatter(E, Area, s=5, color="C0")
94 ax.set_xlabel("Energy  $E$ ")
95 ax.set_ylabel("Area  $N_{\text{reg}}/N_{\text{part}}$ ")
96 fig.savefig("Figs/area.pdf")
97 return 0
98
99 filelist = [f for f in os.listdir(OUT_DIR) if FILENAME_PREFIX in f]
100 plot_area(filelist)
101 plt.show()
```

file: plot\_poincare\_sections.py

```
1 #!/usr/bin/env python
2  """
3  Plot: Poincare Sections (Linear and Parallel)
4
5  Plots the Poincare sections for different energies, computed either with linear
6  or parallel algorithms.
7
8  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
9  @ Institution:  Universite de Strasbourg, CNRS, Observatoire astronomique
10                 de Strasbourg, UMR 7550, F-67000 Strasbourg, France
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17
18  plot_poincare_sections.py
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33  along with this program. If not, see https://www.gnu.org/licenses/.
34
35  """
36  import os
37  import numpy as np
38  import matplotlib.pyplot as plt
39
40  if "YII_1" in plt.style.available: plt.style.use("YII_1")
41
42  OUT_DIR = "./Output/"
43  FILENAME_PREFIX = "poincare_sections_"
44  EXTENSION = ".csv"
45
46  def plot_poincare_sections(filelist: list, title: str = "") -> int:
47      """
48      Plot all the Poincare sections in the file list.
49      @params:
50          - filelist: the list of files in the output directory, with the format
51                    "poincare_sections_{linear, parallel}_{1/E}.csv"
52          - title: title of the figure
53      @returns:
54          - 0.
55      """
56      orderlist = np.argsort([(int(file
57                               .replace(FILENAME_PREFIX, "")
58                               .replace(EXTENSION, "")
59                               .replace("linear_", "")
60                               .replace("parallel_", "")))
61                             for file in filelist])
62      filelist = np.array(filelist)[orderlist]
63      N = len(filelist)
64      fig, axs = plt.subplot_mosaic("ABC\nDEF")
65      axs = list(axs.values())
66      fig.suptitle(title)
67      for i in range(N):
68          ax = axs[i]
69          filename = filelist[i]
```

```
70     inv_E = (filename
71              .replace(FILENAME_PREFIX, "")
72              .replace(EXTENSION, "")
73              .replace("linear_", "")
74              .replace("parallel_", ""))
75     data = np.loadtxt(OUT_DIR + filename)
76     y_section = data[0]
77     v_section = data[1]
78     ax.scatter(y_section, v_section,
79               s=.1, color="C3", marker=".", alpha=0.5,
80               label="$E = 1/{ }\$".format(inv_E))
81     ax.set_xlabel("$y$")
82     ax.set_ylabel("$v$")
83     ax.legend(loc="upper right")
84     while i < N:
85         i += 1
86         axs[i].axis('off')
87         if "linear" in title: kind = "linear"
88         elif "parallel" in title: kind = "parallel"
89         else: kind = "error"
90         fig.savefig("Figs/pcs_{ }\pdf".format(kind))
91         return 0
92     print("\033[32m"
93           + "[P]arallel or [L]inear algorithm result, or [B]oth?"
94           + "\033[0m")
95     answer = input("\033[32m" + "> " + "\033[0m").upper()
96
97     if answer == "P":
98         FILENAME_PREFIX += "parallel_"
99     elif answer == "L":
100         FILENAME_PREFIX += "linear_"
101
102     filelist = [fname for fname in os.listdir(OUT_DIR) if FILENAME_PREFIX in fname]
103
104     if answer in ["L", "B"]:
105         filelist_linear = [fname for fname in filelist if "linear_" in fname]
106         plot_poincare_sections(filelist_linear,
107                               title=("Poincare Sections "
108                                     "(results from the linear algorithm)"))
109     if answer in ["P", "B"]:
110         filelist_parallel = [fname for fname in filelist if "parallel_" in fname]
111         plot_poincare_sections(filelist_parallel,
112                               title=("Poincare Sections "
113                                     "(results from the parallel algorithm)"))
114
115     plt.show()
```



## C.4 Test Files

file: test\_evolution.py

```
1  #!/usr/bin/env python
2  """
3  Test: Evolution
4
5  Evolve a particle with a given energy in a potential and show the result path
6  followed by the particle in a given time.
7
8  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
9  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
10                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
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17
18  test_evolution.py
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31
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33  along with this program. If not, see https://www.gnu.org/licenses/.
34
35  """
36
37  import numpy as np
38  import matplotlib.pyplot as plt
39  import potentials as pot
40  import energies as ene
41  import integrator as itg
42  import initial_conditions as init
43  import poincare_sections as pcs
44
45  if "YII_1" in plt.style.available: plt.style.use("YII_1")
46  # Loading matplotlib style...
47
48  # Constants
49  N_grid = 5000
50  h = 0.01
51  N_inter = 5000
52  eps = 1e-2
53
54  x_0 = 0.0
55  y_0 = 0.5
56  E = 0.125
57
58  # Main
59  if __name__ == "__main__":
60      W_part = init.one_part(x_0, y_0, 0, 0)
61      POT = pot.hh_potential(W_part)[0]
62      u_0 = np.sqrt(2 * (E - POT))
63      v_0 = 0.0
64
65      W_part[1,0] = u_0
66      W_part[1,1] = v_0
67
```

```
68     pos_t, positions = itg.rk4(0, W_part, h, N_inter, pot.hh_evolution)
69
70     pos_x = positions[:,0,0]
71     pos_y = positions[:,0,1]
72     vel_x = positions[:,1,0]
73     vel_y = positions[:,1,1]
74
75     W_grid = init.mesh_grid(N_grid)
76     X_grid = W_grid[0]
77     Y_grid = W_grid[1]
78     potential = pot.hh_potential(W_grid, position_only=True)
79
80     fig, ax = plt.subplots(1)
81
82     pcm = ax.pcolormesh(X_grid, Y_grid, potential)
83     line = ax.plot(pos_x, pos_y, color="C3")
84     fig.colorbar(pcm, label="potential")
85
86     ax.set_xlabel("$x$")
87     ax.set_ylabel("$y$")
88     ax.set_aspect("equal")
89
90     plt.savefig("Figs/evolution.png")
91
92     plt.show(block=True)
```

file: test\_evolution\_chaotic.py

```
1  #!/usr/bin/env python
2  """
3  Test: Evolution
4
5  Evolve a particle with a given energy in a potential and show the result path
6  followed by the particle in a given time.
7
8  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
9  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
10                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
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34
35  """
36
37  import numpy as np
38  import matplotlib.pyplot as plt
39  import potentials as pot
40  import energies as ene
41  import integrator as itg
42  import initial_conditions as init
43  import poincare_sections as pcs
44
45  if "YII_1" in plt.style.available: plt.style.use("YII_1")
46  # Loading matplotlib style...
47
48  # Constants
49  N_grid = 5000
50  h = 0.01
51  N_inter = 5000
52  eps = 1e-2
53
54  x_0 = 0.3
55  y_0 = 0.1
56  E = 1/6
57
58  # Main
59  if __name__ == "__main__":
60      W_part = init.one_part(x_0, y_0, 0, 0)
61      POT = pot.hh_potential(W_part)[0]
62      u_0 = np.sqrt(2 * (E - POT))
63      v_0 = 0.0
64
65      W_part[1,0] = u_0
66      W_part[1,1] = v_0
67
68      pos_t, positions = itg.rk4(0, W_part, h, N_inter, pot.hh_evolution)
69
```

```
70 pos_x = positions[:,0,0]
71 pos_y = positions[:,0,1]
72 vel_x = positions[:,1,0]
73 vel_y = positions[:,1,1]
74
75 W_grid = init.mesh_grid(N_grid)
76 X_grid = W_grid[0]
77 Y_grid = W_grid[1]
78 potential = pot.hh_potential(W_grid, position_only=True)
79
80 fig, ax = plt.subplots(1)
81
82 pcm = ax.pcolormesh(X_grid, Y_grid, potential)
83 line = ax.plot(pos_x, pos_y, color="C3")
84 fig.colorbar(pcm, label="potential")
85
86 ax.set_xlabel("$x$")
87 ax.set_ylabel("$y$")
88 ax.set_aspect("equal")
89
90 plt.savefig("Figs/evolution_chaotic.png")
91
92 plt.show(block=True)
```

file: test\_initial\_E.py

```
1  #!/usr/bin/env python
2  """
3  Test: Initial Conditions With a Given Energy
4
5  Sample random particles with the same given energy in a valid coordinates range.
6
7  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
8  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
9                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
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32 along with this program. If not, see https://www.gnu.org/licenses/.
33
34 """
35 import numpy as np
36 import matplotlib.pyplot as plt
37
38 import potentials as pot
39 import energies as ene
40 import integrator as itg
41 import initial_conditions as init
42 import poincare_sections as pcs
43
44 if "YII_1" in plt.style.available: plt.style.use("YII_1")
45 # Loading matplotlib style...
46 # parameters
47 N_grid = 1000
48 N_inter = 30000
49 N_part = 100
50 E = 1/12
51 h = 0.01
52
53 if __name__ == "__main__":
54     # Initial conditions
55     W_grid = init.mesh_grid(N_grid, xmin=-1, xmax=1, ymin=-1, ymax=1)
56     X_grid = W_grid[0]
57     Y_grid = W_grid[1]
58     potential = pot.hh_potential(W_grid, position_only=True)
59     pot_valid = np.ma.masked_where(potential > E, potential)
60
61     W_all_part = init.n_energy_part(pot.hh_potential, N_part, E)
62
63     # Plot
64     fig, ax = plt.subplots(1)
65
66     pcm = ax.pcolormesh(X_grid, Y_grid, pot_valid, vmin = 0)
67     sct = ax.scatter(W_all_part[0, 0], W_all_part[0, 1], s=1, color="C3")
68     fig.colorbar(pcm, label="potential")
69     ax.set_title("$E = {:.2f}$".format(E))
```

```
70     ax.set_xlabel("$x$")
71     ax.set_ylabel("$y$")
72     ax.set_aspect("equal")
73
74     fig.savefig("Figs/initial_E.png")
75
76     plt.show(block=True)
```

file: test\_integrators.py

```
1  """
2  Test: Integrators
3
4  Demonstrating Keplerian 2-body orbits using various integrators,
5  and comparing accuracy and runtime over a range of step sizes.
6
7  @ Author: Moussouni, Yael (MSc student) & Bhat, Junaid Ramzan (MSc student)
8  @ Institution: Universite de Strasbourg, CNRS, Observatoire astronomique
9                de Strasbourg, UMR 7550, F-67000 Strasbourg, France
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28 GNU General Public License for more details.
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30 You should have received a copy of the GNU General Public License
31 along with this program. If not, see https://www.gnu.org/licenses/.
32 """
33
34 import numpy as np
35 import matplotlib.pyplot as plt
36 import time
37
38 import integrator as itg
39 import initial_conditions as init
40 import potentials as pot
41 import energies as ene
42
43 from matplotlib.patches import ConnectionPatch
44
45 if "YII_1" in plt.style.available: plt.style.use("YII_1")
46
47 # -----
48 # 1. Setup & global parameters
49 # -----
50 t0 = 0.0
51 T_final = 8.0
52 W0 = init.one_part(1, 0, 0, 1) # [x, y, vx, vy]
53
54 h_range = np.logspace(-3.5, -0.1, 25)
55 h_range = np.append(h_range, 0.001)
56
57 # For plotting lines/colors
58 methods = [
59     ("Euler", itg.euler, 'o--', 'C0'),
60     ("RK2", itg.rk2, 's--', 'C2'),
61     ("RK4", itg.rk4, '^--', 'C3')
62 ]
63 colors = {'Analytical': 'k',
64          'Euler': 'C0',
65          'RK2': 'C2',
66          'RK4': 'C3'}
67
68 # Compute machine epsilon
69 eps = 1.0
```

```
70 while 1.0 + eps/2 > 1.0:
71     eps /= 2.0
72 print(f"Machine epsilon: {eps}")
73
74 # Arrays to store final energy errors & times
75 err_euler, err_rk2, err_rk4 = [], [], []
76 time_euler, time_rk2, time_rk4 = [], [], []
77
78 # -----
79 # 2. Main loop over step sizes h in h_range
80 # -----
81
82 fig, ax = plt.subplots(1)
83
84 for h in h_range:
85     ax.cla()
86     N = int(T_final / h)
87
88     # Analytical solution
89     t_ana, W_ana = itg.kepler_analytical(t0, W0, h, N)
90     W_ana_E = np.swapaxes(W_ana, 0, 2)
91     W_ana_E = np.swapaxes(W_ana_E, 0, 1)
92     E_analytical_final = ene.total(W_ana_E, pot.kepler_potential)
93
94     # Numerical integrators + timing
95     all_solutions = {}
96     for (label, method, *_), store_err, store_t in zip(
97         methods,
98         [err_euler, err_rk2, err_rk4],
99         [time_euler, time_rk2, time_rk4]
100     ):
101         start_time = time.time()
102         t_num, W_num = itg.integrator_type(t0, W0, h, N, pot.kepler_evolution,
103             method)
104         elapsed = time.time() - start_time
105
106         store_t.append(elapsed)
107
108         # Final energy error
109         W_num_E = np.swapaxes(W_num, 0, 2)
110         W_num_E = np.swapaxes(W_num_E, 0, 1)
111         E_numerical_final = ene.total(W_num_E, pot.kepler_potential)
112         store_err.append(np.max(abs(E_analytical_final - E_numerical_final)))
113
114         all_solutions[label] = W_num
115
116     # Orbit plot (optional, can comment out if too many figures)
117     eu_vals = all_solutions["Euler"]
118     rk2_vals = all_solutions["RK2"]
119     rk4_vals = all_solutions["RK4"]
120
121     ax.plot(W_ana[:, 0, 0],
122             W_ana[:, 0, 1],
123             "-",
124             color=colors['Analytical'],
125             label="Analytical",
126             zorder=4)
127     ax.plot(eu_vals[:, 0, 0],
128             eu_vals[:, 0, 1],
129             "-",
130             color=colors['Euler'],
131             label="Euler")
132     ax.plot(rk2_vals[:, 0, 0],
133             rk2_vals[:, 0, 1],
134             "--",
135             color=colors['RK2'],
136             label="RK2")
137     ax.plot(rk4_vals[:, 0, 0],
138             rk4_vals[:, 0, 1],
```



```

139         ":",
140         color=colors['RK4'],
141         label="RK4")
142
143     ax.set_title("$\\Var{t} = {:.4f}$".format(h))
144     ax.set_xlabel("$x$")
145     ax.set_ylabel("$y$")
146     ax.set_aspect("equal")
147     ax.legend(loc="upper right")
148     fig.tight_layout()
149     fig.savefig("Figs/orbit_dt_{:.4f}.pdf".format(h))
150
151     if h == h_range[-1]:
152         mosaic = ("AB\n"
153                  "AC")
154         fig, axs = plt.subplot_mosaic(mosaic)
155         axs = list(axs.values())
156         for i in [0,1,2]:
157             axs[i].plot(W_ana[:, 0, 0],
158                        W_ana[:, 0, 1],
159                        "-",
160                        color=colors['Analytical'],
161                        label="Analytical")
162             axs[i].plot(eu_vals[:, 0, 0],
163                        eu_vals[:, 0, 1],
164                        "-",
165                        color=colors['Euler'],
166                        label="Euler")
167             axs[i].plot(rk2_vals[:, 0, 0],
168                        rk2_vals[:, 0, 1],
169                        "--",
170                        color=colors['RK2'],
171                        label="RK2")
172             axs[i].plot(rk4_vals[:, 0, 0],
173                        rk4_vals[:, 0, 1],
174                        ":",
175                        color=colors['RK4'],
176                        label="RK4")
177
178             axs[i].set_aspect("equal")
179
180         #fig.suptitle("$\\Var{t} = {:.4f}$".format(h))
181         axs[0].set_xlabel("$x$")
182         axs[0].set_ylabel("$y$")
183         axs[0].legend(loc="upper left")
184
185         win_1 = 0.02
186         axs[1].set_xlim(0 - win_1, 0 + win_1)
187         axs[1].set_ylim(1 - win_1, 1 + win_1)
188         #axs[0].indicate_inset_zoom(axs[1], lw=1)
189         win_2 = 1e-6
190         axs[2].set_xlim(0 - win_2, 0 + win_2)
191         axs[2].set_ylim(1 - win_2, 1 + win_2)
192         #axs[1].indicate_inset_zoom(axs[2], lw=1)
193
194         ln1 = ConnectionPatch(xyA=(0,1), xyB=(0-win_1,1+win_1),
195                              coordsA="data", coordsB="data",
196                              axesA=axs[0], axesB=axs[1],
197                              color="k", lw=1, alpha=0.5)
198         ln2 = ConnectionPatch(xyA=(0,1), xyB=(0-win_1,1-win_1),
199                              coordsA="data", coordsB="data",
200                              axesA=axs[0], axesB=axs[1],
201                              color="k", lw=1, alpha=0.5)
202         fig.add_artist(ln1)
203         fig.add_artist(ln2)
204
205         ln3 = ConnectionPatch(xyA=(0,1), xyB=(0-win_2,1+win_2),
206                              coordsA="data", coordsB="data",
207                              axesA=axs[1], axesB=axs[2],
208                              color="k", lw=1, alpha=0.5)

```

```

209         ln4 = ConnectionPatch(xyA=(0,1), xyB=(0+win_2,1+win_2),
210                               coordsA="data", coordsB="data",
211                               axesA=axes[1], axesB=axes[2],
212                               color="k", lw=1, alpha=0.5)
213     fig.add_artist(ln3)
214     fig.add_artist(ln4)
215     #fig.tight_layout()
216     fig.savefig("Figs/orbit_dt.pdf")
217
218
219
220 # -----
221 # 3. Summary Plots: CPU time and final energy error (Log-Log)
222 # -----
223
224 # --- Step size vs. CPU Time (Log-Log) ---
225 fig, ax = plt.subplots()
226 ax.plot(h_range[:-1], time_euler[:-1], 'o-', color='C0', label="Euler")
227 ax.plot(h_range[:-1], time_rk2[:-1], 's--', color='C2', label="RK2")
228 ax.plot(h_range[:-1], time_rk4[:-1], '^:', color='C3', label="RK4")
229
230 ax.set_xscale("log")
231 ax.set_yscale("log")
232
233 ax.set_xlabel("Step size  $h$ ")
234 ax.set_ylabel("CPU Time  $t_{\text{CPU}}$  in units of s")
235 #ax.minorticks_on()
236 #ax.grid(True, which="major", linestyle="--", linewidth=0.5, alpha=0.7)
237 #ax.grid(True, which="minor", linestyle=":", linewidth=0.5, alpha=0.5)
238 ax.legend(loc="best")
239 fig.tight_layout()
240 fig.savefig("Figs/dt_vs_cpu_time_loglog.pdf")
241
242 # --- Step size vs. Final Energy Error (Log-Log) ---
243 fig, ax = plt.subplots()
244
245 ax.plot(h_range[:-1], err_euler[:-1], 'o-', color='C0', label="Euler")
246 ax.plot(h_range[:-1], err_rk2[:-1], 's--', color='C2', label="RK2")
247 ax.plot(h_range[:-1], err_rk4[:-1], '^:', color='C3', label="RK4")
248
249 ax.set_xscale("log")
250 ax.set_yscale("log")
251 # Machine Epsilon line (horizontal)
252 ax.axhline(eps, color='darkred', ls='-.',
253            label='Machine precision  $\epsilon$ ')
254
255 ax.set_xlabel("Step size  $h$ ")
256 ax.set_ylabel(" $|\epsilon_{\text{analytical}} - \epsilon_{\text{numerical}}|$ ")
257 #ax.minorticks_on()
258 #ax.grid(True, which="major", linestyle="--", linewidth=0.5, alpha=0.7)
259 #ax.grid(True, which="minor", linestyle=":", linewidth=0.5, alpha=0.5)
260
261 # Ensure 'Machine Epsilon' is in legend
262 """
263 handles, labels = ax.get_legend_handles_labels()
264 if 'Machine Epsilon' not in labels:
265     import matplotlib.lines as mlines
266     h_me = mlines.Line2D([], [], color='darkred', ls='--', label='Machine Epsilon')
267     handles.append(h_me)
268     labels.append('Machine Epsilon')
269 ax.legend(handles, labels, loc="best", fontsize=12)
270 """
271 ax.legend()
272 fig.tight_layout()
273 fig.savefig("Figs/timestep_vs_final_energy_error_loglog1.pdf")
274 plt.show()

```

file: test\_potentials.py

```
1  #!/usr/bin/env python
2  """
3  Test: Potential
4
5  Draw the Kepler potential and the Henon--Heils potential
6
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11
12 Licence:
13 Order and Chaos in a 2D potential
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15                  Bhat, Junaid Ramzan (junaid-ramzan.bhat@etu.unistra.fr)
16
17 test_potentials.py
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20
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25
26 This program is distributed in the hope that it will be useful,
27 but WITHOUT ANY WARRANTY; without even the implied warranty of
28 MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
29 GNU General Public License for more details.
30
31 You should have received a copy of the GNU General Public License
32 along with this program. If not, see https://www.gnu.org/licenses/.
33 """
34 import numpy as np
35 import matplotlib.pyplot as plt
36
37 import potentials as pot
38 import initial_conditions as init
39
40 if "YII_1" in plt.style.available: plt.style.use("YII_1")
41 # Loading matplotlib style...
42
43 W = init.mesh_grid(300)
44
45 def kepler(W):
46     """Plots the Kepler potential"""
47     X = W[0]
48     Y = W[1]
49     POT = pot.kepler_potential(W, position_only=True)
50     fig, ax = plt.subplots(1)
51     ax.set_title("Kepler potential")
52     pcm = ax.pcolormesh(X, Y, POT)
53     fig.colorbar(pcm, label="potential")
54     ax.set_aspect("equal")
55     ax.set_xlabel("$x$")
56     ax.set_ylabel("$y$")
57
58     fig.savefig("Figs/pot_kepler.png")
59     return 0
60
61 def hh(W):
62     """Plots the Henon--Heils potential"""
63     X = W[0]
64     Y = W[1]
65     POT = pot.hh_potential(W, position_only=True)
66     fig, ax = plt.subplots(1)
67     ax.set_title("Henon--Heils potential")
68     pcm = ax.pcolormesh(X, Y, POT)
69     fig.colorbar(pcm, label="potential")
```

```
70     ax.set_aspect("equal")
71     ax.set_xlabel("$x$")
72     ax.set_ylabel("$y$")
73
74     fig.savefig("Figs/pot_hh.png")
75     return 0
76
77 if __name__ == "__main__":
78     kepler(W)
79     hh(W)
80
81     plt.show(block=True)
```