Computational Study of Conserved Quantities in the Kepler Problem Through First and Second Order Symplectic Integrators Using Sage Manifolds

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Abstract: A numerical integration of the Kepler Problem through Symplectic Euler and Storm-Verlet methods is presented. The integrated trajectories and conserved quantities were analyzed, it was found that both integrators give very good results completely in accordance with analytical predictions. A small analysis of possible perturbations was done, both in the Hamiltonian and the initial conditions, initial conditions were perturbed from below the minimal energy and in the Hamiltonian a relativistic correction was introduced to try to fit Mercury's orbit; for the former it was found that the integrator does not produce a well behaved orbit and for the latter that the numerical solution fits qualitatively the observations.

1 Introduction

Kepler's problems has been studied intensively since Newton and remains as one of the main examples for both central force and integrable systems. It is simple enough so that analytical solutions are possible [Lig73][GPS02], reasonably simple to interpret, and yet a computational study of its conserved quantities can not be done successfully using standard (i.e. non-symplectic) integrators, this is a sign that the N-body problem will also suffer from this inconveniences, making simulations of systems with many bodies that interact through gravity, as the Solar System, not only computationally expensive but also numerically complicated. Symplectic integrators, inspired in the formulation of classical mechanics in terms of symplectic geometry, appear as a great tool for making long term, stable simulations of problems where the preservation of conserved quantities is crucial for the computational model to reflect actual physics. Successfully applying them to the 1-body problem is a first indication that N-body systems can be successfully integrated, and in fact they already have as shown in [Yos93].

2 Theoretical Aspects

2.1 Hamiltonian Systems Background

Below we show some necessary definitions and constructions about the geometry of Hamiltonian Systems, we assume familiarity with concepts as flow, vector fields on manifolds and Poisson brackets. For a formal and technical treatment of symplectic geometry and Hamiltonian systems we refer the reader to [Lig73].

2.1.1 Association of functions with Hamiltonian vector fields in a symplectic manifold

Let $(\mathbb{T}^*\mathbb{Q}, \omega)$ be a simplectic manifold of dimension $2n$, with ω the symplectic form induced by the coordinates of $\mathbb{Q}$ and $f \in \mathcal{F}^\infty(M)$. The canonical 2-form allows us to associate vector fields with 1-forms in a way that is analog to how this is done in Riemannian manifolds via the use of a metric [see Fra11, page 43].

$$\omega = dq^\alpha \wedge dp_\alpha, \tag{1}$$

we define X_f as that vector field such that

$$\omega(X_f, \bullet) = df \tag{2}$$

If we now write both sides of equation (2) in canonical coordinates a coordinate expression for X_f can be found:

$$df = \frac{\partial f}{\partial q^\alpha} dq^\alpha + \frac{\partial f}{\partial p_\alpha} dp_\alpha \tag{3}$$

$$\omega(X_f, \bullet) = a_\alpha dq^\alpha - b_\alpha dp_\alpha \tag{4}$$

Where a_α, b_α are the components of X_f, substituting this equations into 2 it is found that:

$$a_\alpha = \frac{\partial f}{\partial q_\alpha} \tag{5}$$

$$b_\alpha = -\frac{\partial f}{\partial p_\alpha} \tag{6}$$

The above equations shows that it is indeed possible to identify functions with Hamiltonian vector fields using first and identification between vector fields and 1-forms as an intermediate step. This is based in the idea of musical isomorphisms in a symplectic geometry context [SBK19]. This point was crucial for the implementation of the code, as one a priori only knows the Hamiltonian and as far we knew *Sage Manifolds* does not give a standard way of constructing the associated vector fields but of calculating differentials, so it was necessary to implement our own routine that works for any differential form. [1]

[1] All our code can be found at `https://github.com/fvilladiego/Integradores_simplecticos`, it is commented and has many comments about the logic of the implementation.

2.1.2 Poisson brackets and dynamical variables evolution, a necessary and sufficient condition for time independent conserved quantities

One elementary result in Hamiltonian Mechanics is that the evolution of any dynamical variable G along a Hamiltonian flow can be written in terms of the Poisson bracket [JS00]

$$\{G, H\} = \frac{dG}{dt} - \frac{\partial G}{\partial t} \tag{7}$$

thus any conserved quantity must satisfy that:

$$\{G, H\} = 0 \tag{8}$$

This is a crucial idea in the integration of Hamiltonian systems, any numerical method that does not preserve Poisson's bracket is most likely doomed to not give well behaved conserved quantities, as it destroys the symplectic structure in which the systems lives, and conversely well behaviour is most likely to arise from structure preserving methods. Nevertheless this a rule of thumb rather than a general result, there are examples of non-symplectic methods that can give well behaved conserved quantities although usually they only work for low degrees, the interested reader is refereed to [Hai01][Mar]. With this idea the concept of *symplectormophism* is introduced.

2.1.3 Definition of Symplectomorphism

A diffeomorphism $f : \mathbb{M} \to \mathbb{M}'$ between two symplectic manifolds $(\mathbb{M}, \omega)$ and $(\mathbb{M}', \omega')$, is called a *symplectomorphism* if

$$f^*\omega' = \omega. \tag{9}$$

$$\omega'(df(V), df(W)) = \omega(V, W) \qquad \forall V, W \in \mathbb{M}_p$$

for arbitrary $p \in \mathbb{M}$. This is expressing that the diffeomorphism preserves the symplectic structure. [Abr+80][Mun]

2.2 Symplectic Integrators

2.2.1 Definition of Symplectic Integrator

A symplectic integrator is a smooth family of diffeomorphism on $\mathbb{M}$, $\Psi : \mathbb{M} \times \mathbb{R} \to \mathbb{M}$ such that $\Psi_{\Delta t}(\xi_0) := \Psi(\xi_0, \Delta t) \approx \xi(\Delta t; \xi_0)$ and when we hold Δt fixed, $\Psi_{\Delta t}$ is a symplectomorphism [Mun][Mar][Yos93]. The concept captured by the definition is that we are demanding step-wise preservation of the Poisson bracket, and this is what makes symplectic integrators symplectic. Notice it is not necessary to have a fixed time step method for it be symplectic.

2.3 Hamiltonian Splitting Method

The technique we focused on is called *Hamiltonian Splitting*[Mun][Yos93][Mar][DR05][Mar], it consists in approximating the flow of a given Hamiltonian by composing multiple simpler flows and it differs from the approach of variational methods (see for example [SG09]), as it focuses on approximating Hamilton's equations and in fact requires solving them for easier Hamiltonians. Consider a Hamiltonian H that can be written in some chart $(\mathbb{T}^*\mathbb{Q}, (q, p))$ as:

$$H(q, p) = H_T(p) + H_V(q) \tag{10}$$

this is the splitting part, in which the target Hamiltonian is separated into a part H_T that can be identified as solely kinetic energy and another one H_V that is identified as solely potential energy. The flows Ψ_{H_T} and Ψ_{H_V} generated by this Hamiltonians are supposed to be integrable so that closed expressions for them can be found, after they have been obtained one composes them to form a third flow (symplectomorphisms form a group so this new flow is also symplectic) that is expected to approximate the original flow:

$$\Psi_H^{\Delta t} = \prod_{i=0}^{n} \Psi_{c_i H_T}^{\Delta t} \circ \Psi_{d_i H_V}^{\Delta t} + O(t^{n+1}) \tag{11}$$

the value of the constants c_i, d_i is crucial for the order of the integrator, a lot of work was done during the 90's to obtain them for different orders [Yos93] and it is even to possible to construct arbitrary order integrators this way [Suz92]. Another interesting result is that this new flow is actually the exact solution of another Hamiltonian that is *close* to that one is trying to approximate [DF76][Yos93].

Theorem 2.1 *The symplectic mapping (11) exactly describes the time evolution of an associated Hamiltonian system , which is close to the original Hamiltonian (10) and has the expression of a formal power series in* Δt

$$\tilde{H} = H + \Delta t H_1 + \Delta t^2 H_2 + \Delta t^3 H_3 + ... \tag{12}$$

This theorem allows us to explain possible anomalous behaviour in the numerical results by looking at the higher order terms of the expansion.

2.3.1 Symplectic Euler and Stormer-Verlet Integrators

The integrators considered can be constructed by compositions of the form (11). The Symplectic Euler (here abbreviated as SE) is first order and defined as[Mun][DR05][Yos93]:

$$\Psi_{SE} = \Psi_{H_T}^{\Delta t} \circ \Psi_{H_V}^{\Delta t}. \tag{13}$$

While the Storm-Verlet (here abbreviated as SV) is second order and defined as [Mun][Yos93]

$$\Psi_{SV}^{\Delta t} = \Psi_{\frac{1}{2}H_V}^{\Delta t} \circ \Psi_{H_T}^{\Delta t} \circ \Psi_{\frac{1}{2}H_V}^{\Delta t}. \tag{14}$$

2.4 Symplectic Geometry Formulation of the Kepler Problem

Let $\mathbb{Q} = \mathbb{R}^3/\vec{0}$, consider the symplectic manifold $(\mathbb{T}^*\mathbb{Q}, \omega)$ with ω the canonical 2-form and the Hamiltonian[2]

$$H(q,p) = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) - \frac{GMm}{\sqrt{x^2+y^2+z^2}} \tag{15}$$

with $G, M, m \in \mathbb{R}^+$, find the Hamiltonian flow. The problem can be non-dimenzionalized if we use as units of time the period of the circular orbit, distance in perimeters of the circular orbit and energy in 2 times the energy of the circular orbit, this results can be found in [GPS02]. The units chosen for energy imply that any physically significant state has an energy of -0.5. Notice that different values of the angular momentum produce different values of reference, making the results for different L non commensurable. The main results of the Kepler problem can be found in [GPS02][JS00][Lig73].

[2]For a coordinate independent approach see [Lig73]

3 Results

The initial conditions used for the integrator were $(x_0, y_0, z_0, p_{x0}, p_{y0}, p_{z0}) = (1, 0, 0, 0, 1.3, 0)$, corresponding to an energy of $E = -0.155$, for which the theory gives closed trajectories, and $L = 1.3$. As stated in the previous section, these quantities must be conserved. Figures 1 and 2 show the calculated trajectories for both methods.

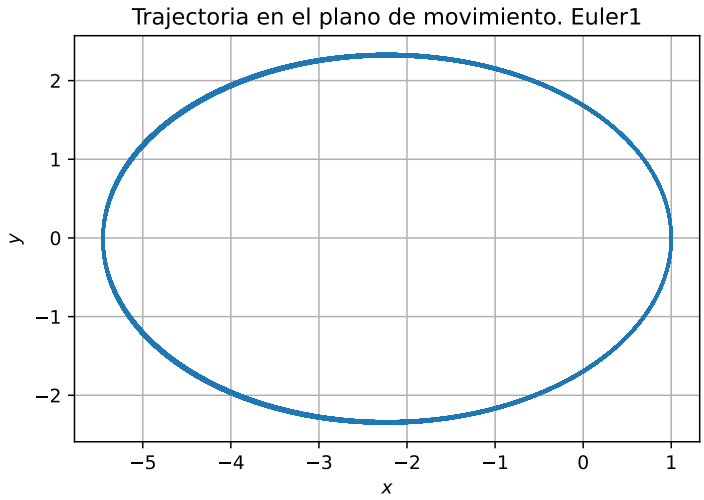

Figure 1: Calculated trajectories using Symplectic Euler method.

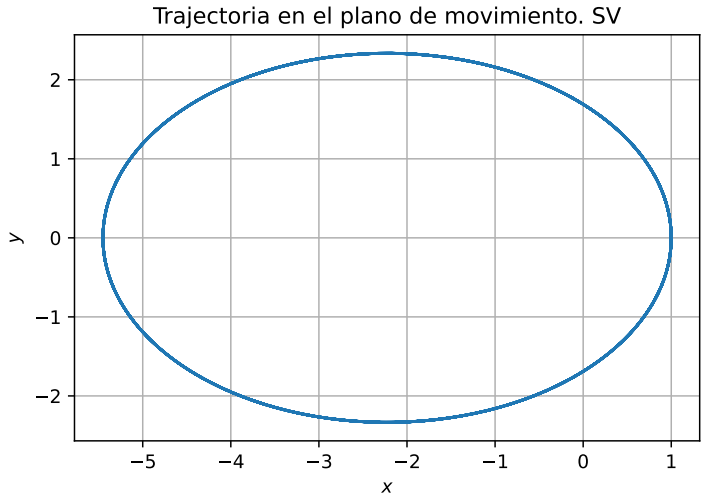

Figure 2: Calculated trajectories using Stormer-Verlet method.

Calculated trajectories have an almost identical shape, but Stormer-Verlet (SV) trajectories are cleaner in points different to $y = 0$.
Figures 3 and 4 show L as function of the parameter t. Fluctuations are of the order of 1×10^{-13}, which means that the behaviour obtained can be attributed to computational noise, and both integrators maintained the initial value of L.
Finally figures 5 and 6 show the kinetic(T), potential(V) and total energy for each step. As expected, total energy is kept constant throughout all the movement for both methods. Energy fluctuations are be attributed to a phase shift between kinetic and potential energy, as observed in [DR05] in the integration of an harmonic oscillator. However no

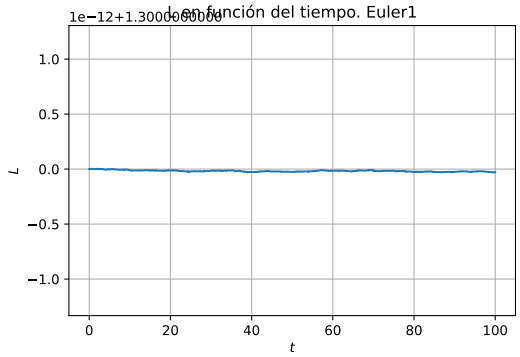

Figure 3: L as function of t for SE method.

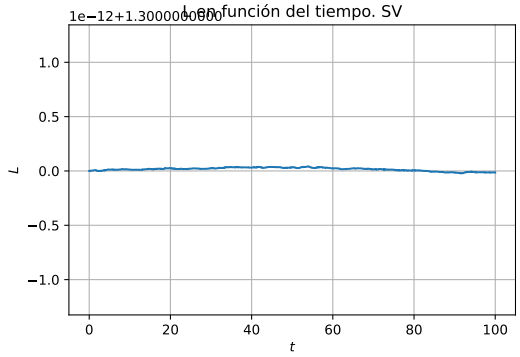

Figure 4: L as function of t for SV method.

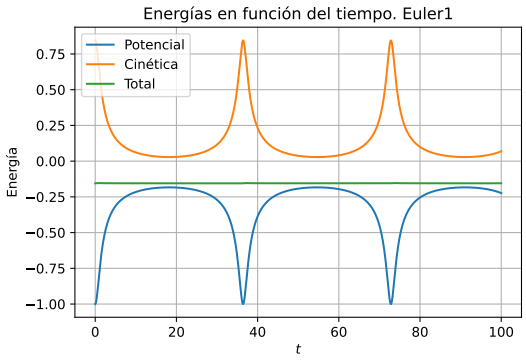

Figure 5: Energies for the SE method

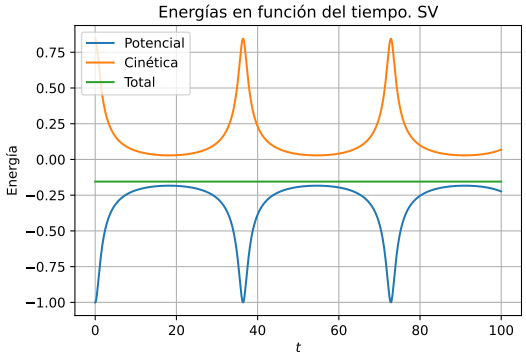

Figure 6: Energies for the SV method.

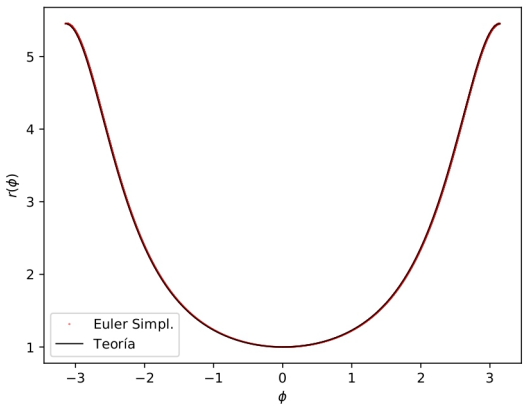

Figure 7: $r(\phi)$ for transition map obtained from SE solution compared to the analytical relation between r and θ.

shift was observed in figures 5 and 6, at least in the scale of T and V.

The symmetries of any central force problem suggest that a spherical chart makes use of conserved quantities to reduce the dimensionality of the problem. However the Hamiltonian in this chart cannot be expressed as in equation 10. Nevertheless by means of a transition map between both charts solutions can be obtained in the spherical chart.

Let $(U_\alpha, \varphi_\alpha)$ be the cartesian chart and (U_β, φ_β) the spherical, both on manifold M.

$$\begin{aligned} &\tau_{\alpha,\beta} : \varphi_\alpha(U_\alpha \cap U_\beta) \to \varphi_\beta(U_\alpha \cap U_\beta) \\ &\tau_{\alpha,\beta} = \varphi_\beta \circ \varphi_\alpha^{-1} \end{aligned} \tag{16}$$

A well known relation for the Kepler problem is $r(\phi) = \frac{L^2}{1+e\cos\phi}$, were the eccentricity of the orbit is $e = \sqrt{1+2EL^2}$. Figure 7 shows SE results compared with the analytic solution. The integrator not only produces closed orbits preserving energy and angular momentum, but also these orbits follow with great precision the analytical solutions.
By means of the transition map introduced in equation 16, a lot is gained in the visualization of the Kepler problem. Equation 17 corresponds to the projection of the Hamiltonian vector field in the spherical chart, in the base $\{\frac{\partial}{\partial r}, \frac{\partial}{\partial P_r}\}$.

$$\mathbf{X_r} = P_r \frac{\partial}{\partial r} + \left(\frac{P_\phi^2}{r^3} - \frac{1}{r^2} \right) \frac{\partial}{\partial P_r} \tag{17}$$

Equation 17 can be used to represent the flows calculated by the integrators, as P_ϕ is kept constant and coordinates r and P_r may be represented in a plane.
Figure 17 shows that the flow obtained by the integrator follows the path given by the vector field lines. Although the flow corresponds to another vector field, it approximates very well the integral curves of the given Hamiltonian vector field, and thus the solution to the problem.

An interesting application to the formalism considered in this work is introducing a perturbation term in the Hamiltonian, associated with considering a relativistic interaction between both bodies. As shown by [Ali19], the perturbed Hamiltonian may be written in its adimensionalized form as in equation 18.

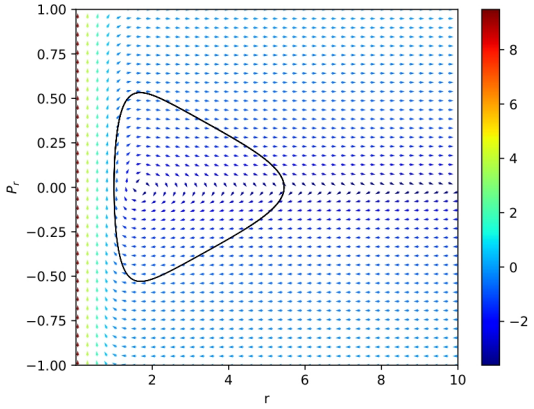

Figure 8: SE method flow over the projection of the Hamiltonian vector field in the base $\{\frac{\partial}{\partial r}, \frac{\partial}{\partial P_r}\}$.

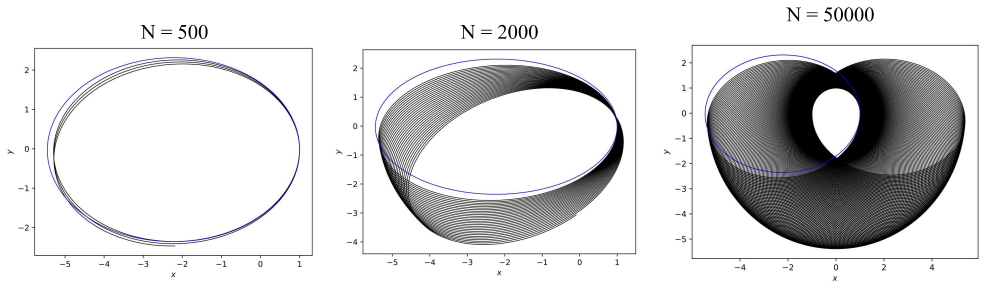

Figure 9: Orbits with relativistic perturbation for N steps plotted with unperturbed solution.

$$H(r, P_r, P_\phi) = \frac{1}{2}\left(P_r^2 + \frac{P_\phi^2}{r^2}\right) - \frac{1}{r} - \alpha\frac{P_\phi^2}{r^3} \tag{18}$$

Historically this additional term causes an anomaly, most present in Mercury's orbit around the Sun, that classical mechanics could not explain and later served as an empirical observation of Einstein theory of general relativity. For the computations calculated, $\alpha \simeq 2.2482 \times 10^{-3}$.

Identical initial conditions are given for the perturbed and unperturbed Hamiltonian. The difference in energy is of the order of the perturbation term. Results for different steps are shown in figure 9.
Orbits precess around the origin for certain angle, but the main orbit shape is close to the original one.

Another perturbation that can be studied is considering non physically valid initial conditions-those whose energy is less than the circular orbit energy value. Mathematically these initial conditions should not have any drawback on the solution. Figures 10 and 11 show the obtained solution with certain number of steps.
Clearly the solutions presented by the integrator in 10 do not go along with previous plots, as the initial conditions are not physical. The limit value is presented in 11, which

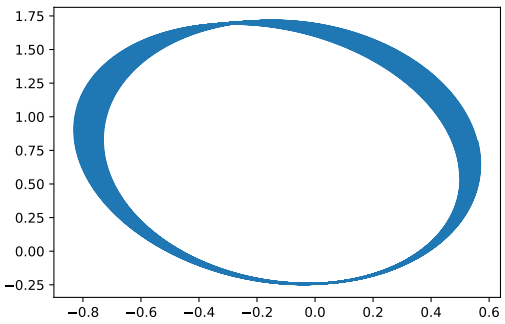

Figure 10: $N = 30000$ with $E = -0.50075$

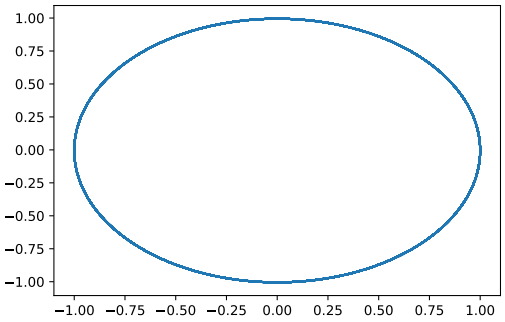

Figure 11: $N = 30000$ with $E = -0.5$

is a perfectly valid physical solution and thus the integrator behaves as expected for large steps.

4 Conclusions

Symplectic integrators show great advantages over traditional ones, by working with the conserved quantities of a problem. Specially when considering longer integration times symplectic integrators demonstrate their capabilities. Variations found in conserved quantities were considerably small.

Transition maps between charts allow for greater visualization of a problem's solution. In this paper this was shown by plotting the integral curves of the method and how they naturally approximate the flow of the original hamiltonian.

The formalism developed in this work can be applied to different perturbation cases, offering a direct computation method to calculate trajectories without the need of approximations. On the other hand, initial conditions close but below the minimum value of energy allowed were considered, exhibiting a break in the solutions. The integrator failed to compute these initial conditions because they did not correspond to a physical value on the manifold.

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