MAP551 - PC9: Hamiltonian systems and symplectic integrators

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1 Double well problem

For a double-well problem where a particle is place in a double-well potential, we a dynamical system like :

$$\mathrm{d}_{tt}q = -\partial_q U(q)$$

To transfer the problem into a first order form :

$$\begin{cases} \mathrm{d}_t q = p \\ \mathrm{d}_t p = -\partial_q U(q) \end{cases}$$

Let us consider the quantity $\mathcal{H} = \frac{1}{2}p^T p + (q^2-1)^2$, and its derivative by time variable t can be written as :

$$\partial_t \mathcal{H} = p^T \times -\partial_q U(q) + \partial_q U(q) \times \mathrm{d}_t q = p^T \times (-\partial_q U(q) + \partial_q U(q)) = 0$$

Then $H(p,q) = cst$ through time.

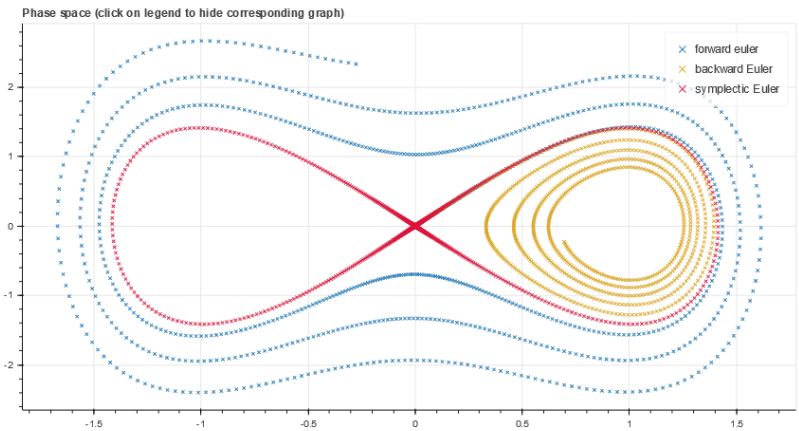

Figure 1 – Classical schemes and its phase space

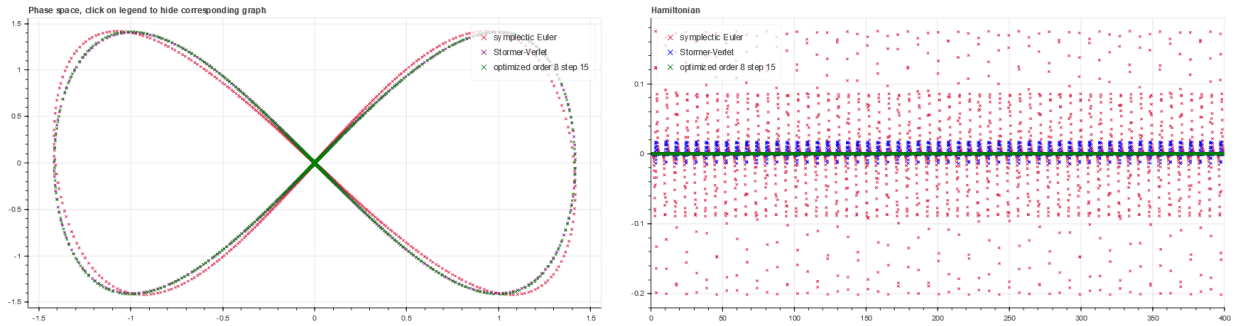

Figure 2 – Sympletic schemes and its phase space, energies

Through the figure 1, we can see that the **explicit Euler schema adds an residue energy to the system**, while the implicit Euler kills some energy due to the accumulated error.

Contrarily to the classical schemes, the energy generally conserves with some oscillation around the real conservative value (Figure 2). When we compare these three numerical method, **the symplectic Euler seems to have the most strong oscillation. And the optimized method with 8 order and 15 steps reduces the error into a level that far smaller than the other two**. Effectively, it respond quiet well to our insight since the higher order the method use, the smaller the error will be.

To fully demonstrate the advantage of a symplectic method, we compare the DOPRI853, which is almost the best numerical non-symplectic method to solve a dynamical system, and the optimized order 8 step 15 method.

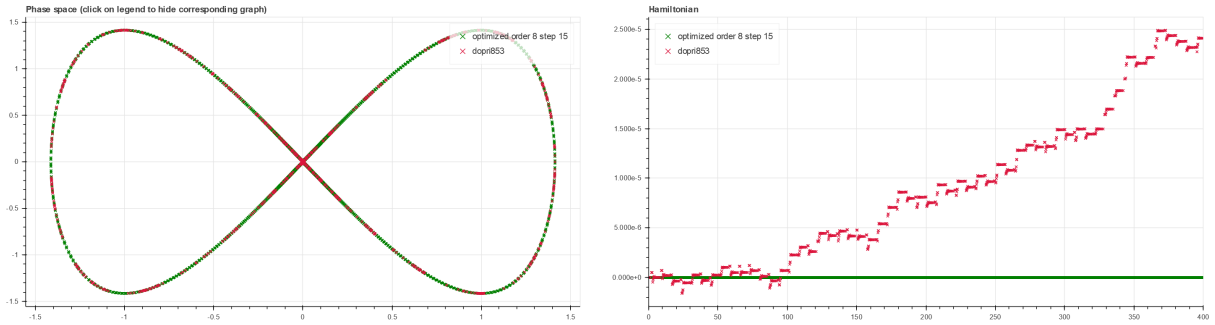

Figure 3 – DOPRI853 and Symplectic method

There is no doubt on the strong performance of DOPRI853, which has reduced the error into a magnitude around 10^{-5} within 400s (compared with Euler symplectic method, this can be considerably good). Yet, the error accumulate through time and it adds (because this is a explicit method) extra energy to the system. If we would like to study the evolution for a long time, that will be not acceptable.

2 Bead on a hoop

A "bead on a hoop" system is characterized by the equation :

$$\ddot{\theta} = -\omega_c^2 \sin\theta + \omega^2 \sin\theta \, \cos\theta$$

In order to recast the system into a more mathematical notations, we transform the system into a group of first order equations.

$$\begin{cases} \dot{y_1} = y_2 \\ \dot{y_2} = \sin y_1 \, (\omega^2 \cos y_1 - \omega_c^2) \end{cases}$$

where $y_1 = \theta$ and $y_2 = \dot{\theta}$

Let $\boxed{\mathcal{H} = \frac{1}{2}(-\omega^2 \sin^2 y_1 + y_2^2) - \omega_c^2 \cos y_1}$ And its derivative by time t is written :

$$\partial_t \mathcal{H} = -\omega^2 \sin y_1 \cos y_1 \mathrm{d}_t y_1 + y_2 \mathrm{d}_t y_2 + \omega_c^2 \sin y_1 \mathrm{d}_t y_1 = y_2 \sin y_1 (-\omega^2 \cos y_1 + \omega_c^2) + y_2 \sin y_1 (\omega^2 \cos y_1 - \omega_c^2) = 0$$

So the quantity $\mathcal{H}$ is conservative through time.

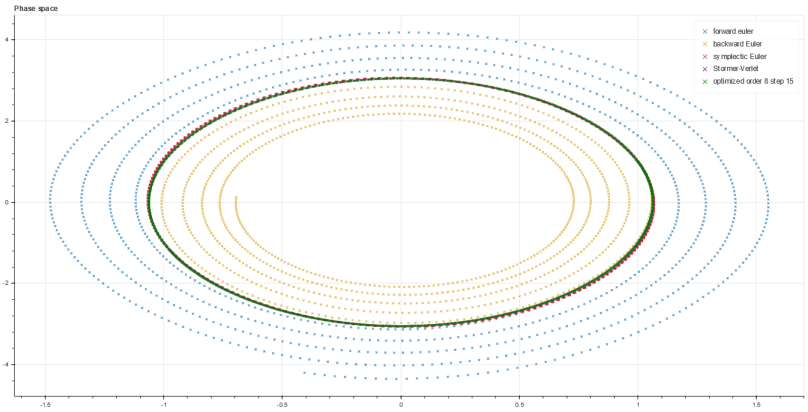

Figure 4 – Classical schemes and its phase plan

By inspecting the Figure 4, we can obtain the same conclusion as the double-well problem : **the explicit method increases the energy while the implicit scheme decrease the energy.**

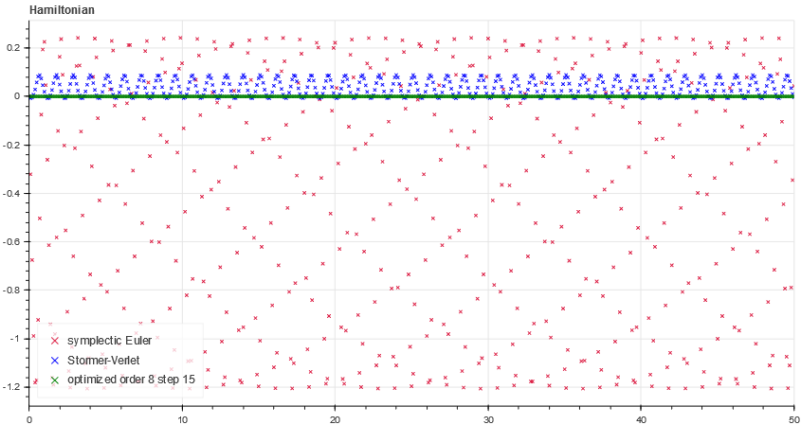

Figure 5 – "Invariant" by different symplectic methods

Again, to bring what has been demonstrated by Figure 5, the higher order the method is of, the smaller the error turns out to be, with symplectic Euler having a strong oscillation and optimized method having the smallest error.

The symplectic integrators is extremely helpful when we try to solve a conservative system, since the methods themselves try to conserve a certain quantity during the resolution. Although the conservative quantity may not be the exact one, it is no more far from it if we reduce the size of time steps. As a result, the symplectic method is ideal for a conservative dynamic problem.

3 Solar System - celestial mechanics

By conducting the same numerical manipulation, we get several numerical strategy to solve the system.

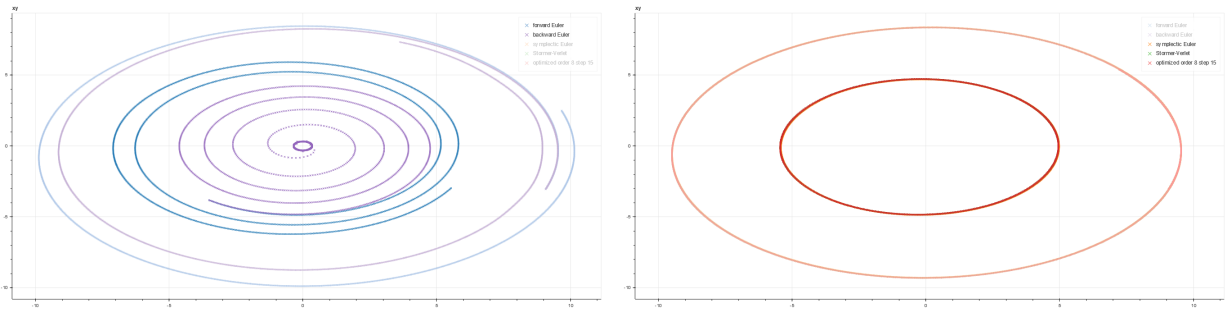

Figure 6 – Phase plane for classical Euler and symplectic methods

It comes as no surprise that the explicit Euler increases the system energy while the implicit one turns to an energy vanishing dilemma. (Hopefully the numerical solution is wrong, or else we will all extinct by the heat of the sun or in the darkness without the sun.)

And the symplectic methods feed us with a more satisfying result where all planet remains on their orbits.

If we look at the energy of system, all symplectic methods conserves the energy with a potential oscillation.

If we narrow the time step, the error becomes smaller as well. Take the Stormer-Verlet method for example, we study the influence of time step on the error. **If we consider the norm 2 for the error, it is a function of order $\frac{1}{2}$ of time step. That is, when reduce the time step size by 100, the norm of the error becomes 10 times smaller.**

From Figure 7 and Figure 8, we can see the symplectic method helps us to integrate a conservative system without being driven to a complete error by the accumulated residue.

4 Arenstorf Orbits

In PC3 we have supposed RK schemes as a quasi-exact solution for a short term evolution. Yet, if we integrate through 10 periods... (Figure 9)

Let $H(t, \mathcal{Y}) = 1/2(y_3^2 + y_4^2 - y_1^2 - y_2^2) - \frac{1-\mu}{r_1} - \frac{\mu}{r_2}$. Then, we set $\mathcal{Y} = (y_1, y_2, y_3, y_4)^t$, therefore,

$$\partial_{\mathcal{Y}} H = (-2y_1 + \frac{\mu(y_1 - 1 + \mu)}{r_2^3} + \frac{(1-\mu)(y_1+\mu)}{r_1^3}, -2y_2 + \frac{\mu y_2}{r_2^3} + \frac{(1-\mu)y_2}{r_1^3}, y_3, y_4)^t$$

$$\partial_{\mathcal{Y}} H = (2y_4 - \mathrm{d}_t y_3, -2y_3 - \mathrm{d}_t y_4, \mathrm{d}_t y_1, \mathrm{d}_t y_2)^t$$

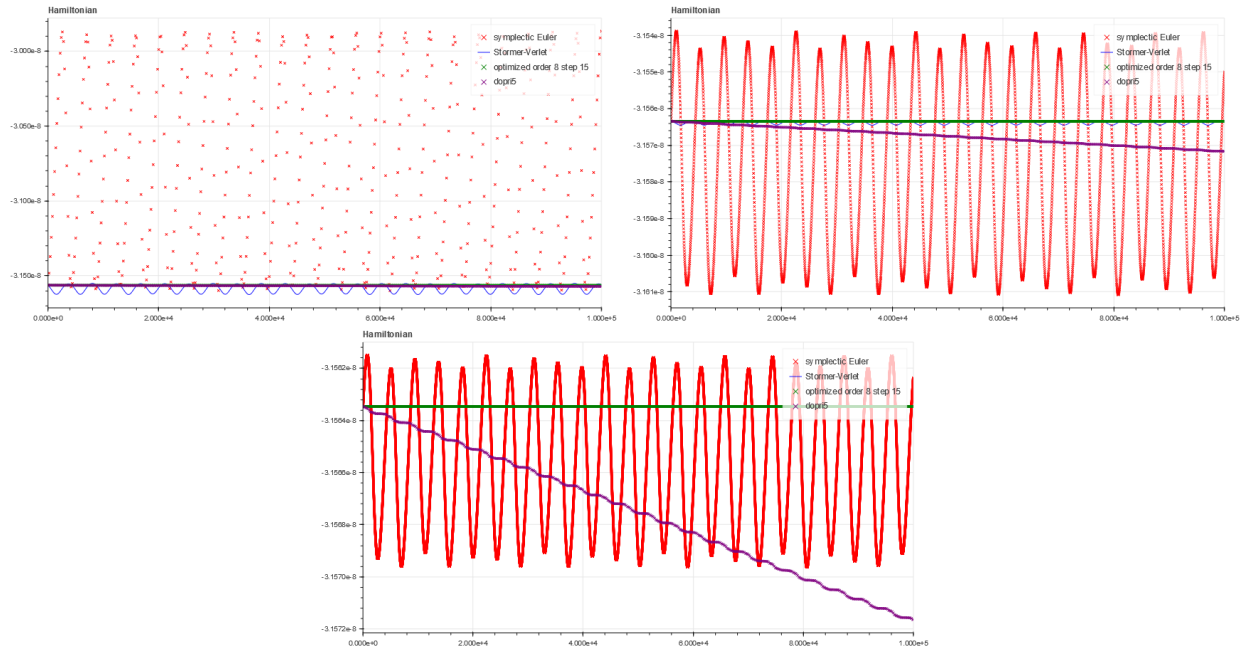

Figure 7 – Energy for different symplectic methods, 1-time step =200.0, 2-time step = 20, 3-time step=2.0

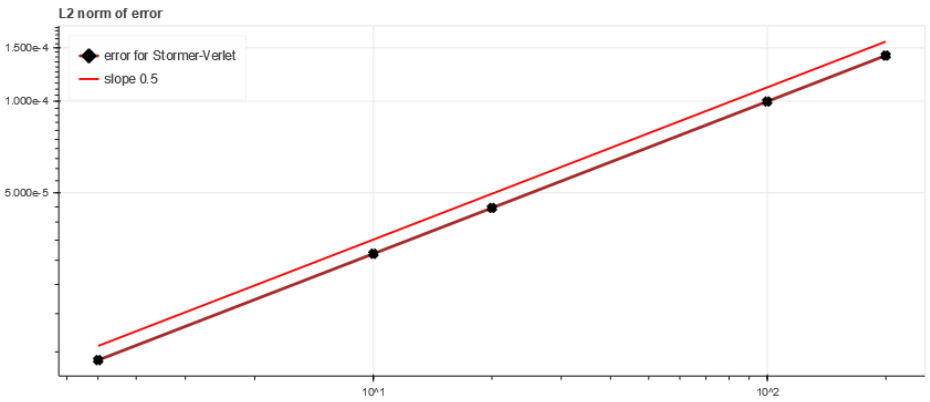

Figure 8 – Norm L^2 for energy as a function of time step for Stormer-Verlet method

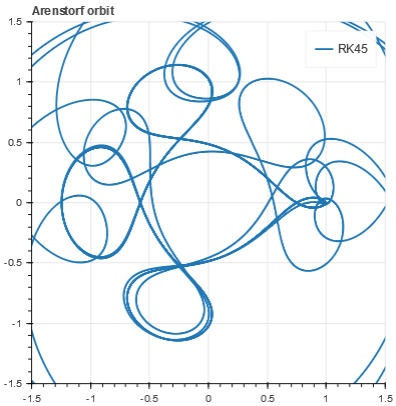

Figure 9 – RK schemes

And

$$J = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 2 \\ 0 & -1 & -2 & 0 \end{bmatrix}$$

So $J\partial_{\mathcal{Y}} H$ equals to $(\mathrm{d}_t y_1, \mathrm{d}_t y_2, 2y_4 - \mathrm{d}_t y_3 + 2\mathrm{d}_t y_2, 2y_4 - \mathrm{d}_t y_3 - 2\mathrm{d}_t y_1) = \mathrm{d}_t \mathcal{Y}$,

As for the notation of "splitting", we can see that for (q^{n+1}, p^{n+1}), knowing the value of (q^n, p^n), the computation during one time step can be completely separated. Therefore, we have split the part "position" and another "velocity".

Already, the splitting leads us to a explicit method since the (q^{n+1}, p^{n+1}) can be obtained from (q^n, p^n). And by splitting the equations we re-obtained a canonical symplectic strategy.

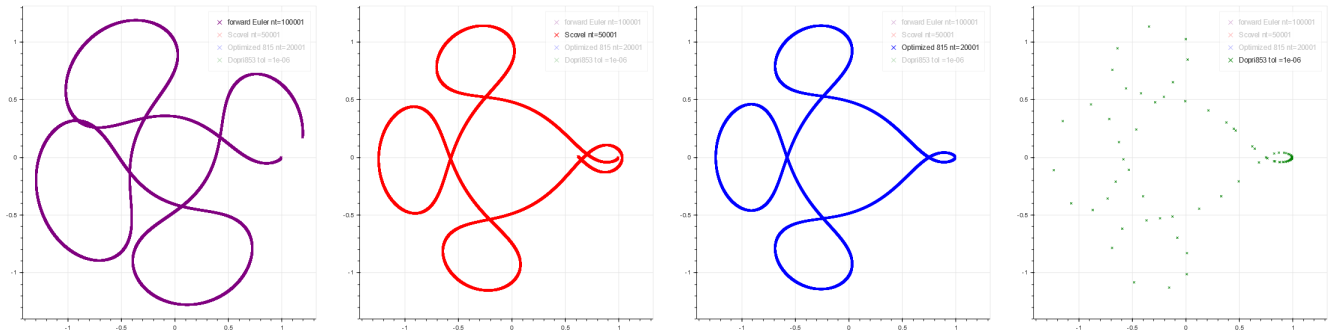

Figure 10 – Trajectory through time for different methods during $t \in [0, 18]$

We integrated in time the system with different method. Even for one period with number of time steps equal to 50001, the Scovel resolution appears some derivation from the real solution. That is because when the satellite approaches the Moon, the distance between the moon and itself becomes so small that $1/r$ becomes very large, leading the system becoming extremely rigid. And the splitting can be tricky while time step is not small enough. And still, we can be satisfied by the resolutions by optimized 814 and dopri853.

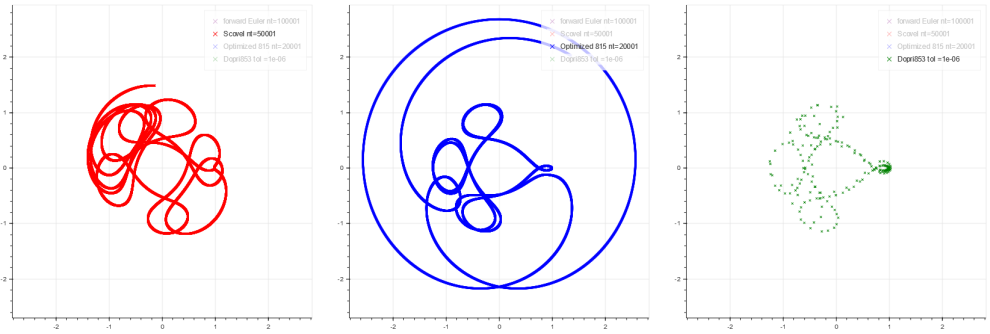

Figure 11 – Trajectory through time for different methods during $t \in [0, 3 \times 18]$

However when we integrate for three periods(Figure 11), the resolutions are no more acceptable with the same number of time steps (the time step becomes three time larger though). But the dopri853 seems to have done a good job.

At last, let us look at the Hamilton of the system. For the symplectic method, the variation of the energy is so violent that the numerical solution might be terrible (and which have been observed by its phase plane.) The dopri853 works just fine.

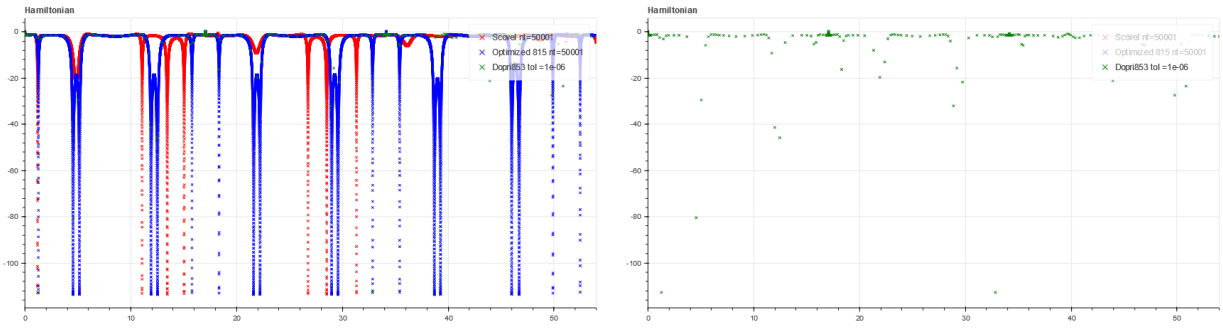

Figure 12 – Hamilton through time for different methods

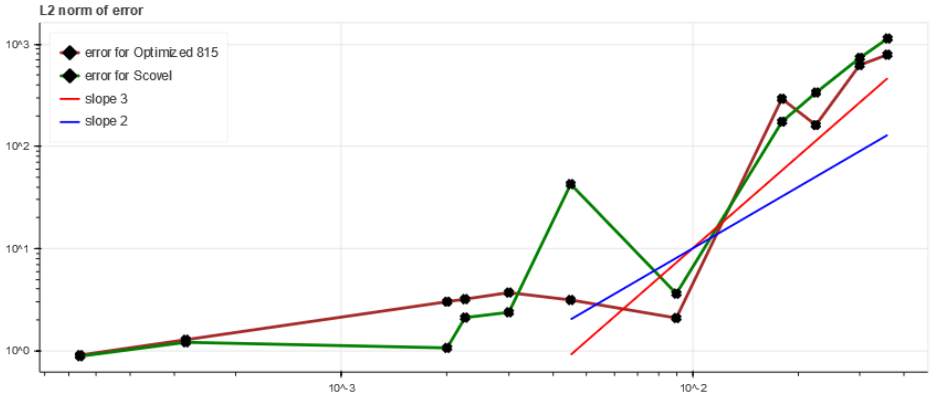

Figure 13 – Hamilton order for different time steps, using symplectic resolution

From Figure 13, we see that the norm of Hamilton tends to be zero (Yes!) when time step is becoming smaller. But the convergence order is not that obvious and the error converge to zero with oscillations.

Conclusion, we have seen the advantage by using symplectic method when we are dealing with a conservative system. It conserves a certain "energy" which is not far from the real first integral. This propriety can be extremely helpful to prevent the deviation of trajectory from accumulated error.

But, an obvious disadvantage of symplectic methods is that we can not optimize time step according to the stiffness of system. Being characterized by a conservative Hamiltonian for each time step, a variation of length of time step will just betray the basic principle of symplectic resolution. This non-adaptable time step shall be considerably time consuming. It is exactly the case of Arenstrof orbits, where DOPRI853 (that can change the length of time step) with a reasonable tolerance, solves faster and better than optimized-815.

Consequently, if the system is dissipative, the choice of integrator would be obvious.

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