PC9 : Hamiltonian systems and symplectic integrators

1 Introduction

The Petite Classe is divided into several parts. In the first part, we tackle some generic Hamiltonian systems, consisting in a particle in a double well potential as well as the bead on a hoop, for which we propose some standard integrators as well as symplectic integrators such as symplectic Euler as well as Störmer-Verlet scheme [9]. The objective of this first part, which has been investigated a bit in PC3, is to explain why the use of a dedicated integrator is important for conservative dynamical systems. In particular, the key issue is to show that even using high order Runge-Kutta methods, which are not symplectic, is not leading to a happy conclusion for long time integration of Hamiltonian systems. Furthermore, we want to highlight the impact of the order of the symplectic methods. The second part is dedicated to celestial mechanics, more precisely the solar system. In this case, the purpose is to use a series of symplectic methods and to investigate the accuracy of the solution, as well as to show that any use of non-symplectic integrator is a dead end. The use of high order composition methods is here essential in predicting the proper long time dynamics accurately. We also come back to the Arenstorf orbit [1, 2, 14], which we had already envisioned in the early parts of the course. The final part is related to the integration in time of a semi-discretized version of the Korteweg de Vries PDE (solitary water waves) [13, 10, 3, 5]. The idea is to combine a semi-discretization in space with time integrators in order to see to what extent we are able to capture solitary waves, which are homoclinc orbits of travelling wave type and which appear as a combination of a non-dispersive nonlinear term and a dispersive linear term.

2 Double well problem

In this first part of the PC, we consider the double-well problem, where a particle is place in a double-well potential, that is we investigate the dynamical system:

$$\mathrm{d}^2_{tt} q = -\partial_q U(q), \tag{1}$$

which can be also written

$$\mathrm{d}_t q = p, \quad \mathrm{d}_t p = -\partial_q U(q), \tag{2}$$

or

$$\mathrm{d}_t q = \partial_p \mathcal{H}(p,q), \quad \mathrm{d}_t p = -\partial_p \mathcal{H}(p,q), \quad \mathcal{H}(p,q) = \frac{1}{2} p^T\, p + U(q), \tag{3}$$

where q is the position of the particle in $\mathbb{R}$ and p its momentum and where $U(q) = (q^2-1)^2$ is the double-well potential energy. The Hamiltonian of the system is denoted $\mathcal{H}$ and is also the total energy of the system.

2.1 Show that we have the exact energy conservation in time through the previous dynamical system, that is $\mathcal{H}(p,q) = cst$.

2.2 Through the notebook, use various classical schemes (explicit and implicit Euler) in order to integrate the dynamics and explain what you observe in terms of energy conservation and qualitative dynamics.

2.3 Use the various symplectic schemes (symplectic Euler, Störmer-Verlet and Composition scheme optimized 8-15) in order to provide a solution in time. Plot the energy of the system and provide a synthesis of the comparison between the various resolution schemes.

3 Bead on a hoop

A circular wire hoop rotates with constant angular velocity ω about a vertical diameter. A small bead moves, with or without friction, along the hoop, where the dynamics of the bead is described through the θ angle. The equation of motion, using the standard notation in classical mechanics, can be shown to be [12]:

$$\ddot{\theta} = -\omega_c^2 \sin\theta + \omega^2 \sin\theta \, \cos\theta - \alpha\theta \tag{4}$$

with $\omega_c = \sqrt{g/R}$, where the gravity acceleration is denoted by g and the radius of the hoop is denoted R. The coefficient α is related to the friction in the system and can be idealized to be zero in the frictionless configuration.

In order to recast the system into our more mathematical notations, we introduce the following notation. Let $y_1 = \theta$ and $y_2 = \dot{\theta}$, its time derivative. Then, we can switch to a first order system of differential equations, when there is no friction:

$$\begin{cases} \mathrm{d}_t y_1 = y_2 \\ \mathrm{d}_t y_2 = \sin y_1 \, (\omega^2 \cos y_1 - \omega_c^2). \end{cases} \tag{5}$$

3.1 Show that there is an invariant for this dynamical system.

3.2 Based on what has been done during PC6 and relying on the notebook, integrate in time the system for various rotation velocities, using the various classical integrators. Explain what happens in terms of energy conservation.

3.3 Conduct the same types of simulations with the symplectic integrators and plot the evolution of the invariant versus time.

3.4 Conclude in terms of the influence of the symplectic integrators on the accuracy of the resolution of the dynamics.

4 Solar System - celestial mechanics

Following [8, 7], let us consider the Sun-Jupiter-Saturn system, where for simplicity we neglect the other bodies and influences in the solar system. Surprisingly, applying a standard numerical method yields a dramatically wrong solution, where one of the planets is ejected from its orbit. In contrast, a well chosen symplectic integrator with the same initial data yields the correct behavior. In 1687, Isaac Newton, inspired by the three laws of Kepler, proposes the universal law of gravitation, that all cosmic objects attract each other pairwise with equal forces (but in opposite directions) proportional to the product of their masses and inversely proportional to the square of the distance between them. It is this law that we will use to calculate the position of the planets. The gravitational force $\vec{F}_{S\to P}$ applied by a body S to a body P is given by the following formula:

$$\vec{F}_{S\to P} = -\vec{F}_{P\to S} = -\frac{G\, m_S\, m_P}{d^2}\vec{u}, \tag{6}$$

where G is the universal constant of gravitation, m_S , m_P are the masses of the bodies S and P, d is the (Euclidean) distance between S and P, and $\vec{u}$ is a vector with unit length in the direction from S to P .

We consider the Sun-Jupiter-Saturn system where we neglect the other planets and influences in the solar system. We represent the positions of these bodies by three functions of time, $q_i(t) \in \mathbb{R}^3$, $i \in 0, 1, 2$ where the index $i = 0$ corresponds to the Sun, $i = 1$ corresponds to Jupiter, and $i = 2$ corresponds to Saturn. The respective masses of the three bodies are denoted by m_i, $i \in 0, 1, 2$, while the universal constant of gravitation is denoted G. We also consider the momenta $p_i(t) \in \mathbb{R}^3$, $i \in 0, 1, 2$. Newton's second law of dynamics then reads

$$\mathrm{d}_t p_0 = \vec{F}_{Sa\to S} + \vec{F}_{J\to S}, \quad \mathrm{d}_t p_1 = \vec{F}_{S\to J} + \vec{F}_{Sa\to J}, \quad \mathrm{d}_t p_2 = \vec{F}_{S\to Sa} + \vec{F}_{J\to Sa}, \tag{7}$$

and we apply our numerical schemes to the above system of differential equations.

body	mass (relative to the Sun)	position (A.U.)	velocity (A.U./day)
Sun	$m_0 = 1.00000597682$ (sun + other planets)	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$
Jupiter	$m_1 = 9.54786104043\,10^{-4}$	$\begin{pmatrix} -3.5023653 \\ -3.8169847 \\ -1.5507963 \end{pmatrix}$	$\begin{pmatrix} +0.00565429 \\ -0.00412490 \\ -0.00190589 \end{pmatrix}$
Saturne	$m_2 = 2.85583733151\,10^{-4}$	$\begin{pmatrix} +9.0755314 \\ -3.0458353 \\ -1.6483708 \end{pmatrix}$	$\begin{pmatrix} +0.00168318 \\ +0.00483525 \\ +0.00192462 \end{pmatrix}$

We provide in Table 1 the positions and initial velocities for the Sun, Jupiter and Saturn at a given date (here September 5th 1994), expressed in astronomical units, based on the Earth-Sun distance (1 A.U. is about 150 million kilometers), and the time is in earth days.

Notice that these trajectories are almost in a plane, but they evolve in 3D. The Sun itself is slightly moving as well (this is by the way a common methodology to detect exoplanets), but we represent the trajectories with respect to the Sun, chosen as a reference, and located at the origin. Note that the code can be straightforwardly adapted to include additional planets of the solar system.

4.1 Using the classical integrators such as Euler (forward/backward), explain what happens to the dynamics of the problem. Explain what happens in terms of energy conservation.

4.2 Relying on the notebook, integrate in time the system for various symplectic integrators. Plot the evolution of the gravitational energy versus time and comment the results as a function of discretization time.

4.3 Conclude in terms of the influence of the symplectic integrators on the accuracy of the resolution of the dynamics.

5 Arenstorf Orbits

We consider a reduced three body problem consisting of the motion of a satellite in the framework of the attraction of the moon and the earth. For the purpose of the exercise, we assume that the system earth-moon is in circular rotation at constant speed in a planar motion with the mass center of gravity located at the origin and that the mass of the satellite ϵ is small enough compared the mass of the earth $1-\mu$ and the mass of the moon μ to so that we can neglect its impact on the earth-moon system. We also assume that the motion of the satellite is governed by the attraction of the two bodies earth and moon through the Newton gravitation law.

The motion of the satellite in the complex plane satisfies the equation:

$$\epsilon\, \mathrm{d}_t^2 Y = \frac{\epsilon(1-\mu)}{||A-Y||^2}\,\frac{A-Y}{||A-Y||} + \frac{\epsilon\mu}{||B-Y||^2}\,\frac{B-Y}{||B-Y||}. \tag{8}$$

In order to eliminate the factor e^{it} in $A = -\mu\, e^{it}$ and $A = (1-\mu)e^{it}$, we introduce the variable $y = e^{-it}\,Y = y_1 + i\,y_2$. In this new referential the earth and the moon are motionless. We have $Y = e^{it}y$ and $\mathrm{d}_t^2 Y = -e^{it}y + 2\,i\,e^{it}\mathrm{d}_t y + e^{it}\mathrm{d}_t^2 y$ and the equation of motion thus read:

$$\mathrm{d}_t^2 y + 2\,i\,\mathrm{d}_t y - y = (1-\mu)\,\frac{-\mu-y}{||\mu+y||^3} + \mu\,\frac{1-\mu-y}{||1-\mu-y||^3}. \tag{9}$$

Introducing the real and imaginary parts of y and then switching to a first order system of differential equations, we obtain:

$$\begin{aligned}
\mathrm{d}_t y_1 &= y_3, \\
\mathrm{d}_t y_2 &= y_4, \\
\mathrm{d}_t y_3 &= y_1 + 2\,y_4 - (1-\mu)(y_1+\mu)/r_1^3 - \mu(y_1 - 1 + \mu)/r_2^3, \\
\mathrm{d}_t y_4 &= y_2 - 2\,y_3 - (1-\mu)y_2/r_1^3 - \mu y_2/r_2^3,
\end{aligned} \tag{10}$$

with $r_1 = ((y_1+\mu)^2 + y_2^2)^{1/2}$ and $((y_1 - 1 + \mu)^2 + y_2^2)^{1/2}$.

For the initial values, we have chosen:

$$y_1(0) = 0.994, \quad y_2(0) = 0, \quad y_3(0) = 0, \quad y_4(0) = -2.00158510637908252240537862224. \tag{11}$$

The motion of the satellite is on a periodic orbit with period $T = 17.0652165601579625588917206249$.

5.1 Remind the reader about what has been done in PC3 (conservative_system.ipynb) using standard Runge-Kutta schemes.

We will then show that the previous system [1, 2], even if it is a restricted three-body problem [14], has a symplectic structure [11] but it is not the canonical Hamiltonian structure.

5.2 Show that the previous system can be recast into the following form

$$\mathrm{d}_t \mathcal{Y} = J\, \partial_{\mathcal{Y}} H(t, \mathcal{Y}), \tag{12}$$

with

$$J = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & R \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix}, \tag{13}$$

$$H(t, \mathcal{Y}) = E^{\text{cin}}(p) + E^{\text{pot}}(q), \quad q = (y_1, y_2)^t \quad p = (y_3, y_4)^t, \quad \mathcal{Y} = (q^t, p^t)^t, \tag{14}$$

$$E^{\text{cin}}(p) = \frac{1}{2}\left(y_3^2 + y_4^2\right) = \frac{1}{2}||p||^2, \quad E^{\text{pot}}(q) = -\frac{y_1^2 + y_2^2}{2} - \frac{1-\mu}{r_1} - \frac{\mu}{r_2}. \tag{15}$$

The purpose of this part is to use an equivalent scheme as the Störmer-Verlet scheme (splitting method) designed for canonical Hamiltonian systems, but in the present case of a non-canonical Hamiltonian system of ODEs. This scheme is called Scovel's method [11]:

$$\begin{aligned} q^{n+1/2} &= q^n, & p^{n+1/2} &= p^n - \tfrac{\Delta t}{2} \partial_q E^{\text{pot}}(q^n) \\ q^* &= q^{n+1/2} + F(\Delta t)\, p^{n+1/2}, & p^* &= \exp(\Delta t\, R)\, p^{n+1/2}, \\ q^{n+1} &= q^*, & p^{n+1} &= p^* - \tfrac{\Delta t}{2} \partial_q E^{\text{pot}}(q^{n+1}) \end{aligned} \tag{16}$$

where $F(t)p_0 = \int_0^t \exp(s\, R) p_0 \mathrm{d}s$.

5.3 Explain, from the previous definition of the scheme (or referring to [11]), why the scheme can be characterized as a splitting scheme.

5.4 Integrate in time the system for various time steps and explain what is the influence of the symplectic integrators (Scovel's method and related optimized 815 composition method). Does it succeed in producing a coherent result for a one period solution? How does it compare to the other schemes you have used.

5.5 Conduct the same types of simulations with the symplectic integrators but on longer time integration (3 periods). Provide a synthesis of what is going on.

6 Korteweg de Vries equation

The final part is related to the integration in time of a semi-discretized version of the Korteweg de Vries PDE (solitary water waves) [13, 10, 3, 4, 5]. The KdV equation is a PDE, which combines a non-linear non-dispersive and a linear dispersive terms, which can interact in such a way as to produce, solitons also called solitary waves. Such waves have remarkable properties and have been a fascinating subject of research initiated by John Scott Russell[1], who clearly, beyond the controversy with Airy and Stokes [4, 5] resolved by Rayleigh, understood many features of such solitary waves, 130 years before a sound mathematical theory was built.

The PDE reads:

$$\partial_t u + 6u\,\partial_x u + \partial^3_{xxx} u = 0, \tag{17}$$

where the 6 factor is purely there for the sake of simplifying the integration. It wan be shown that this PDE admits special types of traveling wave solutions called solitary waves or solitons $u(t,x) = z(x - ct) = z(\xi)$, where z satisfies the ODE:

$$-c\,\mathrm{d}_\xi z + 6z\,\partial_\xi z + \partial^3_{\xi\xi\xi} z = 0, \tag{18}$$

for which there exists an analytical solution:

$$z(\xi) = \frac{c}{2}\cosh^{-2}\left(\frac{\sqrt{c}}{2}\xi\right), \tag{19}$$

where it is clear that the amplitude of the wave is strongly connected to its speed of propagation.

The key point is also that there are invariants for this equation, as well as for the solitary wave [6]. The idea of this part is to combine a semi-discretization in space with a symplectic time integrator in order to see to what extent we are able to capture solitary waves, which are homoclinc orbits of travelling wave type.

References

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[1] "I was observing the motion of a boat which was rapidly drawn along a narrow channel by a pair of horses, when the boat suddenly stopped - not so the mass of water in the channel which it had put in motion; it accumulated round the prow of the vessel in a state of violent agitation, then suddenly leaving it behind, rolled forward with great velocity, assuming the form of a large solitary elevation, a rounded, smooth and well-defined heap of water, which continued its course along the channel apparently without change of form or diminution of speed. I followed it on horseback, and overtook it still rolling on at a rate of some eight or nine miles an hour, preserving its original figure some thirty feet long and a foot to a foot and a half in height. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel. Such, in the month of August 1834, was my first chance interview with that singular and beautiful phenomenon which I have called the Wave of Translation." [13]

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