PC9 : Hamiltonian systems and symplectic integrators

1 Introduction

The Petite Classe is divided into several parts. In the first part, we warm up by studying the symplectic Euler schemes for a separable Hamiltonian. Then, we consider some generic one-dimensional Hamiltonian systems, consisting in a particle in a double well potential as well as the bead on a hoop, and study the behavior of several integration schemes. In particular, we highlight the differences between symplectic and non symplectic schemes for Hamiltonian systems. The final part is dedicated to celestial mechanics, which provide examples of higher-dimensional Hamiltonian systems. We study first the Sun-Jupiter-Saturn system, and then come back to the Arenstorf orbit [1, 2, 14] describing the motion of a satellite in the Earth-Moon system, which we had already encountered in the early parts of the course.

2 Basis symplectic schemes

We consider a Hamiltonian $\mathcal{H} : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ and the associated ODE

$$\begin{cases} p' = -\nabla_q \mathcal{H}(p, q) \\ q' = \nabla_p \mathcal{H}(p, q), \end{cases} \tag{1}$$

or equivalently

$$\begin{pmatrix} p \\ q \end{pmatrix}' = J \nabla H(p, q), \quad \text{where } J = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix}. \tag{2}$$

We recall that the two symplectic Euler schemes are given by

$$\begin{cases} p_{n+1} = p_n - h\nabla_q \mathcal{H}(p_{n+1}, q_n) \\ q_{n+1} = q_n + h\nabla_p \mathcal{H}(p_{n+1}, q_n) \end{cases} \quad \text{and} \quad \begin{cases} p_{n+1} = p_n - h\nabla_q \mathcal{H}(p_n, q_{n+1}) \\ q_{n+1} = q_n + h\nabla_p \mathcal{H}(p_n, q_{n+1}). \end{cases}$$

2.1 In this exercise, we assume that the Hamiltonian is separable, i.e. that $\mathcal{H}(p, q) = T(p)+U(q)$, where $T, U : \mathbb{R}^n \to \mathbb{R}$. Show that each symplectic Euler scheme can then be rewritten in an explicit form $(p_{n+1}, q_{n+1}) = \phi_h(p_n, q_n)$.
2.2 Compute $D\phi_h$ and check that

$$D\phi_h{}^T \; J \; D\phi_h = J.$$

2.3 From the previous question and the results seen in the course, what can you say about these two schemes, and in particular about an invariant for the schemes?
2.4 Still assuming that that $\mathcal{H}(p, q) = T(p) + U(q)$, how could you use Strang splitting to define another scheme for (1)? What is the name of the obtained scheme?

3 Double well problem

In this first experimental part of the PC, we consider the double-well problem, where a particle is placed in a double-well potential $U(q) = (q^2 - 1)^2$, where $q \in \mathbb{R}$ denotes the position of the particle. The corresponding dynamical system is given by

$$q'' = -\nabla U(q). \tag{3}$$

3.1 Introduce the momentum $p = q'$ (the particle is assumed to have mass 1) and rewrite the problem (3) as a system of two first order equations. Check that this system is Hamiltonian as in (1), with $\mathcal{H}(p, q) = \frac{1}{2}p^2 + U(q)$. What does this imply about the quantity $\mathcal{H}(p, q)$ as time evolves?

3.2 Assuming the initial datum is of the form $(q(0), q'(0)) = (q_0, 0)$, describe the different dynamics that should occur depending on q_0. Show the existence of a critical value $q_0^c = \pm\sqrt{2} \approx \pm 1.4142136$.

3.3 Using the notebook, investigate the behavior of the three order one schemes (explicit, implicit and symplectic Euler) for this system. Explain what you observe in terms of energy conservation and qualitative dynamics.

3.4 Investigate also the behavior of higher order symplectic scheme (Störmer-Verlet and Composition scheme optimized 8-15). What can be say about Hamiltonian conservation for this type of schemes?

3.5 Finally, compare also the symplectic composition scheme of order 8 with a RK scheme of order 8 (dopri853). How would you summarize the behavior of the various schemes that we tested on this example?

4 Bead on a hoop

We now go back to a system we have studied in PC6, which consists in a bead moving along a rotating hoop. We focus only on the friction-less case. We recall (see PC6 for more details) that the position of the bead is described by its angle θ with the downward vertical, whose behavior is governed by the following equation

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

where ω is the angular velocity of the hoop.

4.1 Rewrite the equation as a system of first order ODEs, find an invariant for the system, and show that it is Hamiltonian. *Hints: use $q = \theta$, $p = \theta'$, and notice that* (4) *has the same structure as* (3)*.*

4.2 Assuming the initial datum is of the form $(q(0), p(0)) = (0, p_0)$, $0 < p_0 \ll 1$, describe the two types of behavior that you expect to observe, depending on whether ω is small or large.

4.3 As in section 3, use the notebook to investigate the behavior of the various schemes proposed.

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

5 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. 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:

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

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 represent the positions of the Sun, Jupiter and Saturn 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, $i \in 0, 1, 2$. We also consider the momenta $p_i(t) = m_i q_i'(t) \in \mathbb{R}^3$, $i \in 0, 1, 2$. Newton's second law of dynamics then reads

$$p_0' = \vec{F}_{Sa\to S} + \vec{F}_{J\to S}, \quad p_1' = \vec{F}_{S\to J} + \vec{F}_{Sa\to J}, \quad p_2' = \vec{F}_{S\to Sa} + \vec{F}_{J\to Sa}.$$

We thus end up with a system of 6 equations (or more precisely 18, since each p_i and q_i belongs to $\mathbb{R}^3$):

$$\begin{cases} p_i' = -G\displaystyle\sum_{j\neq i} \frac{m_i m_j}{\|q_i - q_j\|^2}\frac{q_i - q_j}{\|q_i - q_j\|} \\ q_i' = \dfrac{1}{m_i} p_i \end{cases} \qquad i \in 0, 1, 2. \tag{5}$$

We provide in the table below the positions and 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.

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	$m_2 = 2.85583733151\,10^{-4}$	$\begin{pmatrix} +9.0755314 \\ -3.0458353 \\ -1.6483708 \end{pmatrix}$	$\begin{pmatrix} +0.00168318 \\ +0.00483525 \\ +0.00192462 \end{pmatrix}$

Our goal is to study the behavior of the system, with these initial conditions, using various numerical schemes. It will be easier to visualize trajectories in a plane, but notice that the vertical component is also changing with time. The Sun itself is slightly moving (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.

5.1 We introduce

$$q = \begin{pmatrix} q_0 \\ q_1 \\ q_2 \end{pmatrix}, \qquad p = \begin{pmatrix} p_0 \\ p_1 \\ p_2 \end{pmatrix}$$

and

$$\mathcal{H}(p,q) = \frac{1}{2}\left(\frac{\|p_0\|^2}{m_0} + \frac{\|p_1\|^2}{m_1} + \frac{\|p_2\|^2}{m_2}\right) - G\left(\frac{m_0 m_1}{\|q_0 - q_1\|} + \frac{m_0 m_2}{\|q_0 - q_2\|} + \frac{m_1 m_2}{\|q_1 - q_2\|}\right).$$

Check that (5) is of the form (1).

5.2 Use the various schemes proposed in the notebook to integrate the system for a *short time* (roughly one rotation or Saturn around the Sun), and comment the obtained results.

5.3 What happen if you integrate for a much longer time? Comment.

5.4 What are your conclusions regarding the influence of the symplectic integrators on the accuracy of the resolution of the dynamics for this system.

6 Arenstorf Orbits

Finally, we go back to the reduced three body problem and more precisely to the Arenstorf orbit that we have already studied in PC3. We recall that this model describes the motion of a satellite under the attraction of the moon and the earth, where we assumed 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 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.

As we have seen in PC3, to corresponding dynamical system is given by

$$\begin{array}{rcl} \mathrm{d}_t y_1 &=& y_3, \\ \mathrm{d}_t y_2 &=& y_4, \\ \mathrm{d}_t y_3 &=& y_1 + 2\,y_4 - (1-\mu)(y_1+\mu)/r_1^3 - \mu(y_1 - 1 + \mu)/r_2^3, \\ \mathrm{d}_t y_4 &=& y_2 - 2\,y_3 - (1-\mu)y_2/r_1^3 - \mu y_2/r_2^3, \end{array} \tag{6}$$

with $r_1 = ((y_1+\mu)^2 + y_2^2)^{1/2}$ and $((y_1 - 1 + \mu)^2 + y_2^2)^{1/2}$. In the sequel, it will be convenient to write

$$q = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \quad \text{and} \quad p = \begin{pmatrix} y_3 \\ y_4 \end{pmatrix}.$$

For well chosen initial values found by Arenstorf [1, 2], we obtain a periodic orbit.

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

In PC3, we showed that the quantity

$$\mathcal{H}(p,q) = \frac{1}{2}\|p\|^2 - \frac{1-\mu}{r_1} - \frac{\mu}{r_2} - \frac{1}{2}\|q\|^2,$$

is an invariant of the system (6).

6.2 Show that (6) is not exactly of the form (2), but rather writes

$$\begin{pmatrix} p \\ q \end{pmatrix}' = \tilde{J}\nabla H(p,q), \quad \text{where } \tilde{J} = \begin{pmatrix} R & -I_2 \\ I_2 & 0 \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix}. \tag{7}$$

This non-canonical Hamiltonian structure means we have to adapt our symplectic schemes. We are going to use Scovel's method [11], which will replace the Störmer-Verlet scheme as our *building block* to obtain higher order schemes, but first we rewrite (7) as

$$\begin{cases} p' = Rp - \nabla U(q) \\ q' = p, \end{cases}$$

where $U(q) = -\frac{1-\mu}{r_1} - \frac{\mu}{r_2} - \frac{1}{2}\|q\|^2$ is the "potential" energy. Scovel's scheme writes

$$\begin{cases} p_{n+(1/2,0)} = p_n - \dfrac{h}{2}\nabla U(q_n) \\ q_{n+(1/2,0)} = q_n \end{cases}$$

$$\begin{cases} p_{n+(1/2,1)} = e^{hR} p_{n+(1/2,0)} \\ q_{n+(1/2,1)} = q_{n+(1/2,0)} + R^{-1}\left(e^{hR} - I_2\right) p_{n+(1/2,0)} \end{cases}$$

$$\begin{cases} p_{n+1} = p_{n+(1/2,1)} - \dfrac{h}{2}\nabla U(q_{n+(1/2,1)}) \\ q_{n+1} = q_{n+(1/2,1)} \end{cases}$$

6.3 Interpret this scheme as a splitting scheme.

6.4 Integrate the system with all the schemes proposed in the notebook. Can you stay on the periodic orbit for 1 period? 3 periods? 5 periods? Comment on the behavior of the various schemes.

References

[1] R. F. Arenstorf. Periodic solutions of the restricted three-body problem representing analytic continuations of Keplerian elliptic motions. *American Journal of Mathematics*, 85:27–35, 1963.

[2] R. F. Arenstorf. Periodic solutions of the restricted three-body problem representing analytic continuations of Keplerian elliptic motions. *NASA-TN-D-1859 Technical Report*, pages 1–17, 1963.

[3] J. Boussinesq. Théorie de l'intumescence liquide appelée onde solitaire ou de translation, se propageant dans un canal rectangulaire. *C. R. Acad. Sci. Paris*, 72:755–759, 1871.

[4] R. K. Bullough. "The wave" "par excellence", the solitary progressive great wave of equilibrium of the fluid: an early history of the solitary wave. In *Solitons (Tiruchirapalli, 1987)*, Springer Ser. Nonlinear Dynam., pages 7–42. Springer, Berlin, 1988.

[5] O. Darrigol. The spirited horse, the engineer, and the mathematician: water waves in nineteenth-century hydrodynamics. *Archive for History of Exact Sciences*, 58(1):21–95, 2003.

[6] J. de Frutos and J.M. Sanz-Serna. Accuracy and conservation properties in numerical integration: The case of the Korteweg-de Vries equation. *Numer. Math.*, 75(4):421–445, 1997.

[7] S. Fiorelli Vilmart and G. Vilmart. Les planètes tournent-elles rond ? *Revue scientifique Interstices (éditée par INRIA)*, 2013.

[8] S. Fiorelli Vilmart and G. Vilmart. Computing the long term evolution of the solar system with geometric numerical integrators. *Snapshots of modern mathematics from Oberwolfach, 2017.*, pages 1–16, 2017.

[9] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration.* Springer-Verlag, Berlin, 2nd edition, 2006. Structure-Preserving Algorithms for Ordinary Differential Equations.

[10] D.J. Korteweg and G. de Vries. On the change of form of long waves advancing in a rectangular canal, and on a new type of long stationary waves. *Phil. Mag.*, 39(5):442–443, 1895.

[11] B. Leimkuhler and S. Reich. *Simulating Hamiltonian dynamics*, volume 14 of *Cambridge Monographs on Applied and Computational Mathematics*. Cambridge University Press, Cambridge, 2004.

[12] L. A. Raviola, M. E. Véliz, H.D. Salomone, N. A. Olivieri, and E.E. Rodríguez. The bead on a rotating hoop revisited: an unexpected resonance. *European Journal of Physics*, 38:015005, 2016.

[13] J.S. Russel. Report on waves. *York 1844 BA reports*, pages 311–390, 1845.

[14] V. Szebehely. *Theory of Orbits*. Academic Press, New York and London, 1967. The restricted problem of three bodies.