PC3 : Numerical Integration of Ordinary Differential Equations (Part I)

1 Introduction

The Petite Classe is divided into three parts. First we investigate the importance of the Lipschitz property of the vector field on the numerical scheme and numerical integration of the system of equations. For that purpose, we consider a tailored example, for which the Lipschitz property is not satisfied, in a framework close to the one of the example given in the Course, for which we know that uniqueness is not achieved. We study the influence of the multiplicity of solution on the numerical solutions. Then, since we want to focus on dissipative systems, we investigate the resolution, using the methods described in the Course, of a simple example issued from celestial mechanics and inspired from the work of R.F. Arenstorf [1, 2] also studied in Ernst Hairer and Gerhard Wanner [5]. The purpose of this part is to check if the classical Runge-Kutta schemes are well-suited in order to resolve conservative systems. We then switch to dissipative systems and come back to the notions we have presented during the course for a toy problem known as the Curtiss-Hirschfelder equation [4, 5], for which we can change the stiffness as well as the time integration step. The purpose is here to get a precise idea about the influence of the concepts of stability / accuracy / order, and their response to the presence of stiffness.

2 Numerical integration in the framework of application of Peano's theorem

2.1 Study of the ODE

Consider the dynamical system on the function $u(t) \in \mathbb{R}$:

$$\mathrm{d}_t u = f(t,u), \qquad u(0) = 0. \tag{1}$$

with

$$f(t,u) = 4\Big(\operatorname{sign}(u)\sqrt{|u|} + \max\left(0, t - \frac{|u|}{t}\right)\cos\left(\frac{\pi \log(t)}{\log 2}\right)\Big), \qquad t \neq 0, \tag{2}$$

and

$$f(t,u) = 4\Big(\operatorname{sign}(u)\sqrt{|u|}\Big), \qquad t = 0. \tag{3}$$

2.1.1 Explain how and why the previous function does not fall into the framework of the Cauchy-Lipschitz theorem but falls into the framework of the Peano theorem.

2.1.2 Let Δt denote the time step we are going to use for an explicit Euler method in order to solve the previous equations. We assume that $\Delta t = 2^{-i}$, where i is an integer such that $i \geq 1$. Evaluate $f(\Delta t, 0)$, as well as $f(t,y)$ for $|y| \geq t^2$ and explain how the function has been constructed by identifying several regions in the (y,t) half-plane.

2.1.3 Show that when $u(0) \neq 0$, we fall again within the framework of Cauchy-Lipschitz theorem and build various trajectories in the (t,x) plane using a converged numerical solution.

2.2 Numerical integration

2.1.3 By integrating equation (1-2) using an Euler method with time step $\Delta t = 2^{-i}$, with even i, propose a conjecture about the function of t, toward which the numerical solution is converging.

2.1.4 By integrating equation (1-2) using an Euler method with time step $\Delta t = 2^{-i}$, with odd i, propose a conjecture about the function of t, toward which the numerical solution is converging.

2.1.4 Propose a conclusion based on the results of the previous two questions on the necessity for the original ordinary differential equation to admit a unique solution. Is the framework of the Peano theorem adequate for numerical simulations ?

3 Conservative System and Euler integration methods

We consider a reduced three body problem consisting in the motion of a satellite in the framework of the attraction of the moon and the earth [1, 2, 7, 3, 6]. For the purpose of the exercise, we assume that the earth-moon system is in circular rotation at constant speed in a planar motion with the center of mass 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. Thus, we can neglect the impact of the mas of the satellite on the dynamics of 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 :

$$\epsilon\, \mathrm{d}_t^2 Y = \frac{\epsilon(1-\mu)}{||A-Y||^2}\, \frac{A-Y}{||A-Y||} + \frac{\epsilon\mu}{||B-Y||^2}\, \frac{B-Y}{||B-Y||}. \tag{4}$$

In order to eliminate the factor e^{it} in $A = -\mu\, e^{it}$ and $B = (1-\mu)e^{it}$, 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 reads :

$$\mathrm{d}_t^2 y + 2\, i\, \mathrm{d}_t y - y = (1-\mu)\, \frac{-\mu - y}{||\mu + y||^3} + \mu\, \frac{1-\mu-y}{||1-\mu-y||^3}. \tag{5}$$

Introducing the real and imaginary parts of y and then switching to a first order system of differential equations, using $r_1 = \sqrt{(y_1+\mu)^2 + y_2^2}$ and $r_2 = \sqrt{(y_1 - 1 + \mu)^2 + y_2^2}$, we obtain :

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

Let us emphasize that the resulting system is still Hamiltonian, but does not have the canonical structure we have studied during the course for classical mechanics but has a so-called noncanonical Hamiltonian structure (see [6] and the course on symplectic methods for conservative systems).

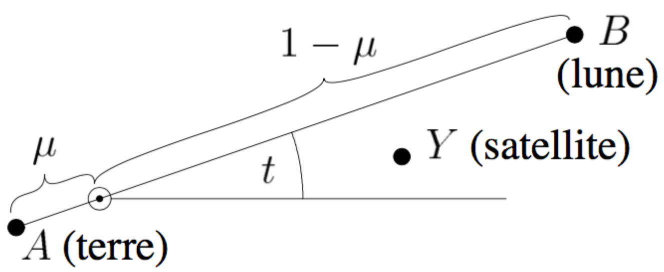

FIGURE 1 – Motion of a satellite in the rotating earth-moon gravity system.

For the initial values, we have chosen [5] :

$$y_1(0) = 0.994, \quad y_2(0) = 0, \quad y_3(0) = 0, \quad y_4(0) = -2.00158510637908252240537862224. \tag{7}$$

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

3.1 Provide the derivation from equation (5) of the system of first order differential equations. The system is conservative ; provide the expression of one invariant quantity of the system and interpret the invariant as an energy, which is the sum of a two potential energies (gravitational and entrainment) and a kinetic energy. Using the notebook, describe the dynamics of the system in time and provide a quasi-exact solution for one period, that is a solution with a fine enough time integration using RK45 solver from Scipy library with fine tolerance and time adaptation, so that we retrieve the periodic character of the system.

3.2 We switch to the numerical simulation of the trajectories of the system using forward and backward Euler methods. Describe the obtained trajectories for various levels of discretization. Plot the evolution of the invariant quantity of the system for several values of the time step. What is happening ? Can we envision simulating the long-time behavior of the system with such an approach ?

3.3 We come back to the RK45 solver of the Scipy library in order to integrate the system, as for the quasi-exact solution. Does the use of such a very refined version of the adaptive Runge-Kutta method (RK45 uses a Dormand and Prince method [5]) yield a proper solution to this problem for long-time dynamics (integrate for a longer time) ? Comment. Check what precision we need on the invariant so that the solution remains relatively periodic during a couple of periods.

4 Stability, order and accuracy for non-stiff and stiff equations

Initially introduced in the paper by Curtiss and Hirschfelder [4, 5], we consider the following problem

$$\begin{cases} \mathrm{d}_t u(t) = k\,(\cos(t) - u(t)), & k > 1 \\ u(t_0) = u_0 \end{cases} \tag{8}$$

which is a non-autonomous ordinary differential equation (ODE), where the stiffness can be tuned through the k parameter.

4.1 Stiffness ?

4.1.1 Show that the exact solution of (8) is given by

$$u(t) = \frac{k}{k^2+1}\Big(k\cos(t) + \sin(t)\Big) + c_0\, e^{-k\,t}, \quad c_0 = \left(u_0 - \frac{k}{k^2+1}\Big(k\cos(t_0) + \sin(t_0)\Big)\right) e^{k\,t_0}. \tag{9}$$

We will assume that $t_0 = 0$ in the following.

4.1.2 Describe the behavior of the exact solution when $k >> 1$ and identify two regions. Justify the fact that the equation yield some level of “stiffness” in its dynamics.

4.1.3 What happens if the initial data is taken as $u_0 = \frac{k^2}{k^2+1}$, which is approximatively 1 if k is large enough ? Is the equation stiff, even if k is large ? Conclude on the fact that the stiffness of an ODE or a system of ODE can have several origins, which will be described in the framework of the present example.

4.2 Explicit Euler

Several schemes will be considered in order to solve (8), among which the Euler explicit scheme presented in class :

$$\begin{cases} U^0 = u_0 \\ U^{n+1} = U^n + \Delta t\, f(t^n, U^n), \quad \Delta t = t^{n+1} - t^n. \end{cases}$$

In the following, the questions will be answered first in the configuration where the initial data is taken as $u_0 = 2$, and then we will come back to the case where $u_0 = \frac{k^2}{k^2+1}$.

4.2.1 For a given level of stiffness, for example $k = 50$, describe the three regimes that you observe for the numerical solution when $u_0 = 2$. Can you identify the limits of the three regimes in terms of the discretization step ?

4.2.2 Make the link with the definition of stability of the scheme.

4.2.3 Describe the behavior of the error as a function of the time step. Plot the diagram of the log of the error (in various norms l^2, l^1 and l^∞) as a function of the log of the time step. Does it match the expected order ?

4.2.4 What is the influence of the stiffness on the error ? When the stiffness becomes sufficiently important ($k = 160$ or 200 for example), what happens in the order diagram ? Comment on the notion of order. When the stiffness increases, even if we stay in the domain of stability of the method, what do we have to do in order to maintain a similar level of error ?

4.2.5 We now envision the configuration where $u_0 = \frac{k^2}{k^2+1}$. Go again through the previous four questions with this new initial condition. What happens ? Propose a precise description of what is going on and justify your answer with Figures. Does the constant in front of the main term of the error depend on the initial condition ? Is the equation still stiff in this case ?

4.2.6 Conclude on the advantages and limits of the proposed scheme, making the link with the stiffness of the equation.

4.3 Implicit Euler

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$$\begin{cases} U^0 = u_0 \\ U^{n+1} = U^n + \Delta t \; f(t^{n+1}, U^{n+1}). \end{cases}$$

In the following, the questions will be answered first in the configuration where the initial data is taken as $u_0 = 2$, and then we will come back to the case where $u_0 = \frac{k^2}{k^2+1}$.

4.2.1 Describe the influence of the stiffness on the behavior of the approximate solution for a given discretization. Make the link with the definition of stability of the scheme.

4.2.2 In order to reach a given level of error in the stiff regime (you will do that for several k), what is the discretization step you need to take ? How does it compare with the discretization step in the explicit scheme ? Does stability imply accuracy ? justify your answer with illustrations. For a given level of accuracy, is it still interesting to use an implicit scheme ?

4.2.3 Describe the behavior of the error as a function of the time step. Plot the diagram of the log of the error (in various norms l^2, l^1 and l^∞) as a function of the log of the time step. Does it match the expected order ? Compare the influence of the stiffness on the error constant and order with what happened in the explicit case.

4.2.5 We now envision the configuration where $u_0 = \frac{k^2}{k^2+1}$. Go again through the previous questions with this new initial condition. What happens ? Propose a precise description of what is going on and justify your answer with Figures. Does the constant in front of the main term of the error depend on the initial condition ?

4.2.6 Conclude on the advantages and limits of the proposed scheme, making the link with the stiffness of the equation.

Références

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