PC5 : Numerical Integration of Ordinary Differential Equations (Part III)

1 Introduction

The Petite Classe is divided into three parts. We will first continue the integration of two of the systems we have previously investigated, that is the Brusselator [10] and the van der Pol oscillator [12, 13, 7], switching to implicit high-order methods. The method we will focus on is the RADAU5, fully implicit method [8, 7]. Such methods are commonly used for several applications. For the RADAU5 method, we provide an appendix written in collaboration with Violaine Louvet for a school on numerical methods and scientific computing, which should help the students understand the subtleties of the method as well as of its implementation and use. It is also important to underline that the group of Hairer and Wanner at the University of Geneva[1] has transformed a class of method with a purely scientific interest into a class of very useful methods for applications. The second part of the PC is devoted to the integration of the Oregonator system of equations [5, 2, 9] derived in [4] from the Field, Koros and Noyes chemical mechanism [3]. It is another simplified system of equations modeling oscillations in chemical systems and for which we will illustrate the use of operator splitting techniques, in order to treat properly the stiffness of the resulting system. The final point is related to the resolution of system of ordinary differential equations issued from of semi-discretization in space of the heat equation. The use of stabilized Runge-Kutta explicit method, that is the ROCK4 method [7], will lead to a very efficient integration of the resulting dynamical system, which can be considered as mildly stiff.

2 Use of RADAU solver

The notebook proposed with this PC contains several implementation of the RADAU5 method of resolution based either on the "scipy" library or directly on the Fortran implementation of the original method by the authors. It includes time step adaptation based on a tolerance provided by the user.

2.1 Integration of Brusselator model

The dynamics of the oscillating reaction discovered by Belousov and Zhabotinsky [5, 2], can be modeled through the so-called Brusselator model [10] depending on two parameters:

$$\begin{cases} \mathrm{d}_t y_1 = 1 - (b+1)y_1 + a\, y_1^2 y_2 \\ \mathrm{d}_t y_2 = b\, y_1 - a\, y_1^2 y_2 \\ y_1(0) = y_1^0 \\ y_2(0) = y_2^0 \end{cases} \tag{1}$$

For the purpose of illustrating the concepts introduced in the course, we use $a = 1$, $b = 3$, $y_1^0 = 1.5$ and $y_2^0 = 3$. For that set of parameters, the dynamics admits a limit cycle as ω-limit set: after a short transition period of time, the behavior of the system becomes almost periodic.

2.1.1 Use the notebook in order to integrate the system with the RADAU5 method relying on the "scipy" library and investigate how many time step are used as a function of the tolerance.

[1] The website of E. Hairer contains a lot of useful information in the field `http://www.unige.ch/~hairer/`.

2.1.2 The notebook also includes other solvers, such as another RADAU5 solver based on a Fortran implementation called from the notebook, which is compiled, as well as a fixed time-step RK4 method, an adaptive RK4 embedded method studied during the previous PC and finally a DOPRI5 method[2]. Compare the methods in terms of computational cost and accuracy as a function of the tolerance.

2.1.3 Knowing the number of function calls necessary for the integration with this implicit methods, what is the amount of extra work conducted by implicit methods compared to the explicit methods.

2.1.4 For such a mildly stiff model, what would you conclude in terms of using an implicit method compared to an explicit method depending on the precision you want to achieve?

2.2 Integration of van der Pol oscillator model

We focus on the van der Pol oscillator [12, 13, 7]. We recall the form of the system for the sake of completeness written as:

$$\begin{cases} \mathrm{d}_t y_1 = \varepsilon^2 \left(y_2 - \dfrac{y_1^3}{3} + y_1 \right) \\ \mathrm{d}_t y_2 = -y_1, \end{cases} \tag{2}$$

where $\varepsilon \gg 1$ leads to a very stiff system.

2.2.1 Use the notebook in order to integrate the system with the method and investigate how many time steps are used as a function of the tolerance.

2.2.2 The notebook also includes other solvers, such as a RADAU5 solver in Fortran called from the notebook, which is compiled, as well as a fixed time-step RK4 method, an adaptive RK4 embedded method studied during the previous PC and finally a DOPRI5 method. Compare the methods in terms of computational cost and accuracy as a function of the tolerance.

2.2.3 When the stiffness of the system is becoming important, what can be said about the impact of the tolerance (based on a local error estimate) on the global error? Does this error build up as a function of time? Comment.

2.2.4 Depending of the stiffness of the problem related to ε, what would you conclude in terms of using an implicit method compared to an explicit method depending on the precision you want to achieve?

3 Operator splitting techniques for stiff ODEs

The operator splitting strategy for ODEs will be experimented on the Oregonator system of equations [3, 4, 5]. The system of ordinary differential equations reads:

$$\mathrm{d}_\tau y_1 = y_2 - y_1, \tag{3}$$

$$\epsilon\, \mathrm{d}_\tau y_2 = q\, y_3 - y_3\, y_2 + y_2(1 - y_2), \tag{4}$$

$$\mu\, \mathrm{d}_\tau y_3 = -q\, y_3 - y_3\, y_2 + f\, y_1, \tag{5}$$

with parameters

$$\epsilon = 10^{-2}, \quad \mu = 10^{-4} \text{ or } \mu = 10^{-6}, \quad f = 1, \qquad q = 2.10^{-4}. \tag{6}$$

In general $\mu \ll \epsilon \ll 1$ and $q \ll 1$. For the example, we take $y_1^0 = 0.5$, $y_2^0 = 0.001$ and $y_3^0 = 1200$.

[2] All these methods rely on a Python implementation.

3.1 Singular perturbation analysis and various forms of the system involving two operators

The purpose of this part is to exhibit two forms of the system (3-5) involving two non-linear operators where we have isolated the stiffest part of the system into one of the operators in order to treat numerically the two operators differently. In order to do so, we need to study the singular perturbation and analyze the fast and slow dynamics of the system, depending on the small parameter μ. Besides, the question is to identify to what extent one of the splitting is better reproducing the full dynamics and why.

3.1.1 Rewrite system (3-5) into the form:

$$\mathrm{d}_\tau \mathcal{U} = \mathcal{A}_1(\mathcal{U}) + \frac{1}{\mu}\mathcal{B}_1(\mathcal{U}) \tag{7}$$

where $\mathcal{U} = (y_1, y_2, y_3)^t$, where the main stiffness coming from the small parameter μ is isolated in the second operator $\mathcal{B}_1(\mathcal{U}) = (0, 0, ?)^t$, whereas the first operator only involves the not too stiff parts. Comment on the potential stiffness of the system and the ones of the two parts involved.

3.1.2 Show that in the limit $\mu \to 0$, the system of equations (3-5), through a singular perturbation analysis, is close to the slow dynamics governed by the new system :

$$\mathrm{d}_\tau \bar{y}_1 = \bar{y}_2 - \bar{y}_1, \tag{8}$$

$$\epsilon\, \mathrm{d}_\tau \bar{y}_2 = f\, \bar{y}_1 \frac{q - \bar{y}_2}{q + \bar{y}_2} + \bar{y}_2(1 - \bar{y}_2), \tag{9}$$

$$\bar{y}_3 = y_3^{eq}(\bar{y}_1, \bar{y}_2) = \frac{f\, \bar{y}_1}{q + \bar{y}_2}. \tag{10}$$

Propose an integration of the slow dynamics using the notebook, as well as the full dynamics and comment on the accuracy of the singular perturbation involving the small parameter μ (you can study in particular the period of the limit cycle for $\mu = 10^{-4}$ and for $\mu = 10^{-6}$). What is the approximate limit of μ for which the slow dynamics is a good approximation of the full dynamics?

3.1.3 Based on the previous question, the main drawback of the splitting proposed in (7) is that the part $\mathcal{A}_1$ corresponds to the dynamics of the slow system but with a fixed y_3, whereas y_3 is supposed to evolve on the slow manifold according to $y_3 \approx \frac{f\, y_1}{q+y_2}$. Propose another way of separating the system:

$$\mathrm{d}_\tau \mathcal{U} = \mathcal{A}_2(\mathcal{U}) + \mathcal{B}_2(\mathcal{U}) \tag{11}$$

in such a way that $\mathcal{A}_2$ still corresponds to the dynamics of the slow system, but now depends on y_1 and y_2 only. For which values of μ (close or far from the singular limit $\mu = 0$?) does this splitting seem adequate?

3.2 Integration of the system using operator splitting

3.2.1 Describe the four splitting formulae (Lie and Strang) during one time step and explain how the RADAU5 solver can then be used.

3.2.2 Using RADAU5 method and a very small tolerance, so that the only source of error is coming from the operator splitting, integrate the previous system of equation using various splitting time steps. Compare the behavior of the two splitting strategies, with $\mu = 10^{-4}$ where the singular perturbation analysis is not valid, and with $\mu = 10^{-6}$ where it is valid (isolate the dynamics of y_1 and y_2 on the one side, especially in terms of the period of the oscillations, and the dynamics of the fast variable y_3, on the other side)? What happens to the resolution of the dynamics of the full system? Discuss the pros and cons of each splitting strategy.

4 An ODE system derived from the semi-discretization in space of the heat equation

In the third part of the Petite Classe, we will tackle another source of stiffness, which can come from the semi-discretization in space of a partial differential equation (PDE).

We will derive a discretization through the method of lines (MOL) of the heat equation :

$$\begin{cases} \partial_t u(t,x) = \partial^2_{xx} u(t,x) & t \geq t_0 \\ u(t_0,x) = u_0(x), \end{cases} \tag{12}$$

with the proper non-dimensional setting so that the diffusion coefficient is one. We will study this equation both when x lies in $\mathbb{R}$, and when x lies on a bounded domain (say $I_a = [-a,a]$, $a > 0$). We recall that one must impose conditions *at infinity* in the first case, and at the boundary of the domain in the second case, otherwise there is no uniqueness of the solution[3]!

While both cases can be interesting to study, our numerical simulations based on a spatial discretization will only be able to handle bounded domains. That does not necessarily mean that problem on unbounded domains cannot be approximated numerically, but one must then chose the boundary conditions carefully, and always be aware that there will be errors associated to the reduction to a bounded domain, which are independent of the algorithm used for the numerical approximation.

Given an interval $I_a = [-a,a]$, $a > 0$, we now describe a method to conduct a numerical integration of the heat equation on this bounded domain, with homogeneous Neumann (or *no flux*) boundary conditions:

$$\begin{cases} \partial_t u(t,x) = \partial^2_{xx} u(t,x), & t \geq t_0,\ x \in]-a,a[\\ u(t_0,x) = u_0(x) & x \in [-a,a] \\ \partial_x u(t,-a) = 0 = \partial_x u(t,a) & t \geq t_0. \end{cases} \tag{13}$$

The interval I_a is subdivided into N equidistributed subinterval $(x_i)_{i\in[0,N]}$, $x_0 = -a$, $x_N = a$, so that the space discretization step if given by $\Delta x = 2a/N$. We denote by $U(t) \in \mathbb{R}^{N+1}$ the vector containing all the values $u(t,x_i)$, that is $U_i(t) = u(t,x_i)$ for all i in $\{0,1,\dots,N\}$.

In order to build an approximation of the solution, we will rely on a finite difference discretization of the Laplace operator : $\forall i \in \{0,1,\dots,N\}$, we use

$$\begin{aligned} \partial^2_{xx} u(t,x_i) &\approx \frac{1}{(\Delta x)^2}(u(t,x_i+\Delta x) - 2u(t,x_i) + u(t,x_i-\Delta x)) \\ &= \frac{1}{(\Delta x)^2}(U_{i+1}(t) - 2U_i(t) + U_{i-1}(t))(t). \end{aligned} \tag{14}$$

The equations for $i = 0$ and $i = N$ involve U_{-1} and U_{N+1}, which are not defined, but will be fixed thanks to the boundary condition. At the discrete level, taking a centered difference to approximate the first order derivative, the homogeneous Neumann boundary conditions amounts to imposing

$$\frac{u(t,x_0-\Delta x) - u(t,x_0+\Delta x)}{2\Delta x} = 0 = \frac{u(t,x_N-\Delta x) - u(t,x_N+\Delta x)}{2\Delta x} \quad \forall\ t \geq 0.$$

or equivalently

$$U_{-1}(t) = U_1(t) \text{ and } U_{N+1}(t) = U_{N-1}(t) \quad \forall\ t \geq 0.$$

Putting everything together, we can get an approximation $\widetilde{U}$ of U by solving the following system of ordinary differential equations

$$\begin{cases} \mathrm{d}_t \widetilde{U} = A_N\, \widetilde{U} \\ \widetilde{U}(t_0) = (u_0(x_0),\dots,u_0(x_N))^t, \end{cases} \tag{15}$$

[3]We will give examples of this in the case of a bounded domain. For the unbounded case, we refer to the work of Tychonoff [11]

with

$$A_N = \frac{1}{(\Delta x)^2} \begin{pmatrix} -2 & 2 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ & & \ddots & \ddots & \ddots & \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 2 & -2 \end{pmatrix}. \tag{16}$$

4.1 Properties of the original system of PDEs and of the discretized one

The main point here is to identify the source of stiffness, first in the original equation (13) and then in its semi-discretized version (15).

4.1.1 Assuming that the initial data u_0 can be written

$$u_0(x) = \sum_{m=0}^{\infty} a_m^0 \cos\left(m \frac{x+a}{2a}\pi\right),$$

give an explicit solution of (13) of the form

$$u(t,x) = \sum_{m=0}^{\infty} a_m(t) \cos\left(m \frac{x+a}{2a}\pi\right).$$

Connect possible sharp transition in the solution for small times with the Fourier decomposition of u_0.

4.1.2 Find all the $\lambda \in [-4, 0]$ such that there exist $(v_n)_{0 \le n \le N}$ satisfying

$$\begin{cases} v_{n+1} - (2+\lambda)v_n + v_{n-1} = 0 \qquad n = 0, \dots, N \\ v_{-1} = v_1 \text{ and } v_{N+1} = v_{N-1}. \end{cases}$$

Conclude that the spectrum of A_N is given by $\lambda_m = -\frac{N^2}{a^2} \sin^2\left(\frac{m\pi}{2N}\right)$, $m = 0, 1 \dots, N$.

4.1.3 Describe how the stiffness of (15) is related to the discretization step (or to N). Compare the eigenvalues λ_m of A_N with the $N+1$ first eigenvalues of the continuous Laplacian on $[-a, a]$ with Neumann boundary conditions.

4.2 Integration of the dynamics for a given space discretization

We discretize the space interval $[-2, 2]$ with 401 points (i.e. $N = 400$), and consider two different initial conditions:

$$u_{0,1}(x) = \cos\frac{\pi x}{2} \qquad \text{and} \qquad u_{0,2}(x) = \mathbb{1}_{x>0} - \mathbb{1}_{x<0}. \tag{17}$$

4.2.1 For the initial data $u_{0,1}$, integrate the solution from $t_0 = 0$ up to $t = 0.1$, using the RK45 method and the ROCK4 method. Compare the computational cost of the two methods, and explain why one is better adapted than the other for this problem.

4.2.2 For both initial data $u_{0,1}$ and $u_{0,2}$, integrate the solution using the ROCK4 method from $t_0 = 0$ up to $t = 0.5$, and have a precise look at how the time step is adapted. What happens when you refine the spatial disretization (i.e. when you increase N)? Describe and explain the similarities and the differences in the two cases.

4.2.3 For the initial data $u_{0,1}$, integrate the solution from $t_0 = 0$ up to $t = 1$, using the ROCK4 method and the RADAU5 method. Compare the computational cost of the two methods. What happens when you refine the spatial disretization (i.e. when you increase N)? Even if RADAU5 is faster on this problem, can you think of other similar problems where ROCK4 might be more advantageous?

4.3 Back to the heat equation on $\mathbb{R}$

4.3.1 Check that the so-called fundemantal solution of the heat equation, given by

$$u_{funda}(t,x) = \frac{1}{2\sqrt{\pi t}} \exp\left(\frac{-x^2}{4t}\right) \qquad t>0,\, x\in\mathbb{R} \tag{18}$$

satisfies $\partial_t u(t,x) = \partial^2_{xx} u(t,x)$. For any $t_0 > 0$, what is then the solution of (12) with $u_0(x) = u_{funda}(t_0,x)$?

4.3.2 We again discretize the space interval $[-2,2]$, but this time with 2001 points (i.e. $N = 2000$), and consider $t_0 = 10^{-5}$ and the initial condition

$$u_0(x) = u_{funda}(t_0,x) = \frac{1}{2\sqrt{\pi t_0}} \exp\left(\frac{-x^2}{4t_0}\right). \tag{19}$$

Compute an approximate solution up to $t = 0.01$, with the RADAU5 method and a tolerance of 10^{-4}, and compare it both with the fundamental solution, and with a quasi exact solution. Comment what happens in term of the two errors, when you take a tolerance of 10^{-6} instead. Comment what happens in term of the error with respect to the fundamental solution, when you integrate longer (say up to $t = 0.1$).

Appendix : Oregonator model

In nonlinear chemical dynamics, the Oregonator system of equations [5, 2, 9] is derived in [4] from the Field, Koros and Noyes chemical mechanism [3]. It is a model that is a stiffer than the Brusselator model and can lead to chemical chaos. We start from a chemical mechanism with proper molar production rates :

$$\left.\begin{array}{rcll} A+Y & \to & X+P & \omega = k_3 AY, \\ X+Y & \to & 2P & \omega = k_2 XY, \\ A+X & \to & 2X+2Z & \omega = k_5 AX, \\ 2X & \to & A+P & \omega = k_4 X^2, \\ B+Z & \to & \frac{1}{2} fY & \omega = k_0 BZ. \end{array}\right\} \tag{20}$$

The concentrations of A and B are maintained contant, and the dynamics of the system is given by

$$\begin{aligned} \mathrm{d}_t X &= k_3 AY - k_2 XY + k_5 AX - 2k_4 X^2, \\ \mathrm{d}_t Y &= -k_3 AY - k_2 XY + \frac{1}{2} f k_0 BZ, \\ \mathrm{d}_t Z &= 2k_5 AX - k_0 BZ. \end{aligned}$$

where the f parameter is a given stoichiometric constant of order unity.

Using

$$y_1 = Z/Z_0, \qquad y_2 = X/X_0, \qquad y_3 = Y/Y_0, \qquad \tau = t/T_0, \tag{21}$$

and

$$X_0 = k_5 A/2k_4, \quad Y_0 = k_5 A/k_2, \quad Z_0 = (k_5 A)^2/k_4 k_0 B, \quad T_0 = 1/k_0 B,$$

we can finally recast the system into the final form :

$$\mathrm{d}_\tau y_1 = y_2 - y_1, \tag{22}$$

$$\epsilon\, \mathrm{d}_\tau y_2 = q\, y_3 - y_3\, y_2 + y_2(1-y_2), \tag{23}$$

$$\mu\, \mathrm{d}_\tau y_3 = -q\, y_3 - y_3\, y_2 + f\, y_1, \tag{24}$$

$$\tag{25}$$

with paremeters

$$\epsilon = 10^{-2}, \quad \mu = 10^{-6}, \quad f = 3, \qquad q = 2.10^{-4}. \tag{26}$$

In general $\mu \ll \epsilon \ll 1$ and $q \ll 1$. with

$$\epsilon = k_0 B/k_5 A, \qquad \mu = 2k_0 k_4 B/k_2 k_5 A, \qquad q = 2k_3 k_4/k_2 k_5. \tag{27}$$

We refer to [6, 7, 1] for several integration of such a system of equation and to [5] for the derivation of the system and the relation to chemical components and mechanism.

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