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 [11, 12, 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 for large times and 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.

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[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 [11, 12, 7]. We recall the form of the system for the sake of completeness written as:

$$\begin{cases} \mathrm{d}_t y_1 = y_2 \\ \mathrm{d}_t y_2 = \varepsilon \left(1 - y_1^2\right) y_2 - y_1, \end{cases} \tag{2}$$

with $\epsilon > 0$ and where the stiffness can be tuned through the ε parameter.

2.2.1 Use the notebook in order to integrate the system with the method and investigate how many time step 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:

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

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

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

$$\tag{6}$$

with paremeters

$$\epsilon = 10^{-2}, \quad \mu = 10^{-6}, \quad f = 1, \quad q = 2.10^{-4}. \tag{7}$$

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

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) involving two non-linear operators where we have isolated the stiffest part of the system into one of the operators in order to treat

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

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.

3.1.1 Rewrite system (3) into the form:

$$d_\tau \mathcal{U} = \mathcal{A}_1(\mathcal{U}) + \frac{1}{\mu}\mathcal{B}_1(\mathcal{U}) \tag{8}$$

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 $\mathcal{B}_1(\mathcal{U}) = (0, 0, \alpha)^t$, 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), through a singular perturbation analysis, is close to the slow dynamics governed by the new system :

$$d_\tau \bar{y}_1 = \bar{y}_2 - \bar{y}_1, \tag{9}$$

$$\epsilon \, d_\tau \bar{y}_2 = f \, \bar{y}_1 \frac{q - \bar{y}_2}{q + \bar{y}_2} + \bar{y}_2(1 - \bar{y}_2), \tag{10}$$

$$y_3 = y_3^{eq}(y_1, y_2) = \frac{f \, y_1}{q + y_2}. \tag{11}$$

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. What is the approximate limit of μ for which the slow dynamics is a good approximation of the full dynamics?

3.1.3 Propose another way of separating the system so that the slow dynamics is fully included into the first operator :

$$d_\tau \mathcal{U} = \mathcal{A}_2(\mathcal{U}) + \frac{1}{\mu}\mathcal{B}_2(\mathcal{U}) \tag{12}$$

where $\mathcal{A}_2(\mathcal{U}) = (y_2 - y_1, y_3^{eq}(y_1, y_2)(q - y_2) + y_2(1 - y_2), 0)^t$. To what extent can such a splitting isolate the stiffness in one of the operators? Does the reduced system lead to a less stiff set of ordinary differential equations for all values of μ? Comment.

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, integrate the previous system of equation using various splitting time steps and propose a synthesis of the results in terms of global error for the first (and usual) splitting strategy, in a range of μ (not too small) for which the singular perturbation analysis is not valid.

3.2.3 Investigate the order of the two classical splitting methods. Explain what you observe based on what we have proved in Class. For a range of too large μ, where the singular perturbation analysis is not valid and the reduced system is not a good approximation of the original system, how does the second splitting behave? What happens to the resolution of the dynamics of the full system? Conclude on the good way of splitting the original system and on the numerical strategy to be used.

3.2.4 Bonus - Play with the tolerances of both integrators and identify what is the limit of the chosen tolerance so that the errors involved in the sub-step integrators do not influence the splitting error.

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 PDE system of equations and to the presence of strong gradients in the solution.

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

$$\partial_t T - \partial_{xx}^2 T = 0, \tag{13}$$

with the proper non-dimensional setting so that the diffusion coefficient is one and with an initial condition to the Cauchy problem on $\mathbb{R}$, $T(x,0) = T_0(x) = 1/(2\sqrt{\pi t_0}) \exp(-x^2/(4t_0))$, $x \in \mathbb{R}$, that is the fundamental solution of the heat equation at a given time $t_0 > 0$.

For the sake of the numerical resolution of the heat equation, we focus on a given interval $I_a = [-a, a]$, $a > 0$, of $\mathbb{R}$ in order to conduct a numerical integration of the system. The I_a interval 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 $\Delta x = 2a/N$. Th exact solution at these points is given by $U(t) \in \mathbb{R}^{N+1}$, $\forall i \in [0, N]$, $U_i(t) = T(t, x_i)$.

In order to build an approximation of the solution, we will rely on a finite difference discretization of the Laplace, $\forall i \in [1, N-1]$, we use:

$$\partial_{xx}^2 T(t, x_i) \approx \frac{1}{(\Delta x)^2}(U_{i+1} - 2U_i + U_{i-1})(t) \tag{14}$$

We also have to set up boundary conditions, which we will take as Neumann boundary conditions

$$\begin{cases} \partial_{xx}^2 T(t, x_0) \approx \dfrac{1}{(\Delta x)^2}(U_1 - U_0) \\[2ex] \partial_{xx}^2 T(t, x_N) \approx \dfrac{1}{(\Delta x)^2}(-U_N + U_{N-1}) \end{cases}$$

From there, it si easy to show that an approximate solution, $\widetilde{U}$, is solution of the linear system of ordinary differential equations

$$\mathrm{d}_t \widetilde{U} = A_N \widetilde{U}, \tag{15}$$

with

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

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

The point is here to identify the source of stiffness, first in the original equation (14) and then in its semi-discretized version (15).

4.1.1 What is the dynamics of a single Fourier mode through the heat equation? How does it relate to the frequency? Explain how the stiffness of the problem can be found in the Fourier transform of the initial data. Focusing on the chosen initial condition, connect the stiffness to the time t_0.

4.1.2 Knowing that the spectrum of A_N is given by $\lambda_m = -4\sin^2(m\pi/(2(N+1)))$, $m = 0, 1 \ldots, N$, describe how the stiffness is related to the discretization step (or to N). Knowing that the largest eigenvalues are related to the high frequency in the initial solution explain how stiff the system can be.

4.2 Integration of the dynamics for a given space discretization

We discretize the space interval $[-2, 2]$ with 2000 points, and we will start with the function $T_0(x) = 1/(2\sqrt{\pi t_0}) \exp(-x^2/(4t_0))$ discretized on the proposed grid, with various t_0 (the one proposed in the notebook is 0.0001 with a final time of integration of 0.01), which will set up the stiffness of the solution. The size of the domain is related to the final time of integration since we use Neumann

boundary conditions and the dynamics of the solution at the boundary points should remain, for comparison purposes, almost non-varying and close to 0.

4.2.1 Compare the solution with ROCK4 to the exact solution as a function of the tolerance. Explain what happens when the tolerance is getting small enough.
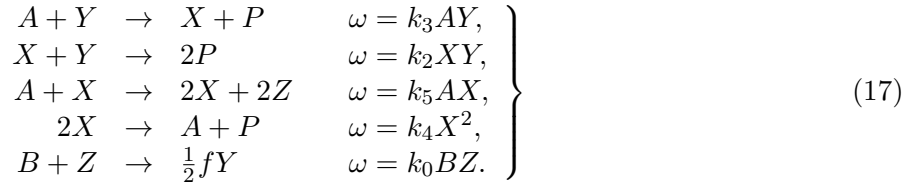
4.2.2 What happens when you compare the solution to a semi-exact solution obtained from an integration with a very fine tolerance using the RADAU5 method?

4.2.3 Depending on the initial condition t_0, that is for various stiffness levels, explain the choice by ROCK of the time steps and their evolution with time.

4.2.4 In terms of computational cost, that is the number of function evaluation here, comment on the the advantages of a solution using the ROCK4 method compared to the RADAU5 method.

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 :

$$
\left.
\begin{array}{rcll}
A + Y & \to & X + P & \omega = k_3 AY, \\
X + Y & \to & 2P & \omega = k_2 XY, \\
A + X & \to & 2X + 2Z & \omega = k_5 AX, \\
2X & \to & A + P & \omega = k_4 X^2, \\
B + Z & \to & \frac{1}{2} f Y & \omega = k_0 BZ.
\end{array}
\right\}
\tag{17}
$$

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

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

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

Using

$$
y_1 = Z/Z_0, \qquad y_2 = X/X_0, \qquad y_3 = Y/Y_0, \qquad \tau = t/T_0, \tag{18}
$$

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 :

$$
\mathrm{d}_\tau y_1 = y_2 - y_1, \tag{19}
$$

$$
\epsilon \, \mathrm{d}_\tau y_2 = q \, y_3 - y_3 \, y_2 + y_2(1 - y_2), \tag{20}
$$

$$
\mu \, \mathrm{d}_\tau y_3 = -q \, y_3 - y_3 \, y_2 + f \, y_1, \tag{21}
$$

$$
\tag{22}
$$

with paremeters

$$
\epsilon = 10^{-2}, \quad \mu = 10^{-6}, \quad f = 3, \qquad q = 2.10^{-4}. \tag{23}
$$

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

$$
\epsilon = k_0 B/k_5 A, \qquad \mu = 2k_0 k_4 B/k_2 k_5 A, \qquad q = 2k_3 k_4/k_2 k_5. \tag{24}
$$

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.

References

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