Sorbonne Université, Master 1 Mathématiques et applications 2022–2023
4MA106 Foundations of numerical methods

Programming classes project

Marks. The marking policy is described on the moodle page of the course. The marking of the programming classes project is based on two criteria:

- report: clarity
- code: correctness, readability, algorithmics.

The project is **individual**, but you are of course authorised to discuss about the different exercices and to ask questions.

Code. The code has to be sent in form of one or more files, and can be written in Scilab or Python 3. The code must be fully functional: we have to be able to run it and visualise the results of the exercices.

Report. Write a report, to be returned in `.pdf`, commenting the results of the exercices and answering the different questions asked.

Deadline. The name of **every** file must begin by `SURNAME name`. The different files (code+report) have to be sent via the moodle page not later than **08/11/2022**.

The project subject has several independent parts. It is not important to do everything, the project evaluation will be more oriented on the quality of your work rather than the quantity. For all questions, you can write at:

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1 Fisher-Kolmogorov-Petrovski-Piskunov equation.

We consider a space region, filled with two chemical species, A, B. These species react according to the equation:

$$A + B \to 2A. \tag{1}$$

We denote $u(x,t)$ the proportion of particles of the specie A in a certain point x of the space, at a certain time t. The proportion of particles B is henceforth $1 - u(x,t)$. We remark here that $0 \leq u(x,t) \leq 1$. At initial time we have a certain concentration $u_0(x)$ of the particles A. The goal is to describe how this concentration is going to evolve in time.
To this end, we observe that u evolve as a consequence of two mechanisms:

1. Diffusion: the particles of the specie A tend to move from regions of high concentration towards regions of low concentration.

2. Chemical reaction: in every point x, the proportion of particle A tend to increase with a rate proportional to $u(1-u)$

The deterministic limit of these two mechanisms lead to a partial differential equation describing the space-time behaviour of u. Let $\nu \in \mathbb{R}^+$ the diffusion coefficient, let $\gamma \in \mathbb{R}^+$ be the reaction rate. We have:

$$\partial_t u = \nu \Delta u + \gamma u(1-u). \tag{2}$$

It is the so called Fisher-Kolmogorov-Petrovski-Piskunov (FKPP) equation, and it is a very important example of reaction-diffusion equation.

2 Finite differences discretisation.

Let $\overline{\Omega} = [0,1]$ be the spatial domain and $t \in [0, 1.0]$, the time. We consider the following boundary conditions: $u(0,t) = u(1,t) = 0 \ \forall t \in [0, 1.0]$. The diffusion coefficient is $\nu = 0.01$ and the reaction rate is $\gamma = 10$. The initial condition is:

$$u(x,0) = 0.25 \sin(\pi x) \exp(-20(x-0.5)^2).$$

The FKPP equation reads:

$$\begin{cases} \partial_t u = \nu \partial_x^2 u + \gamma u(1-u) \\ u(0,t) = u(1,t) = 0 \\ u(x,0) = 0.25 \sin(\pi x) \exp(-20(x-0.5)^2) \end{cases} \tag{3}$$

We introduce the time discretisation: we subdivide the time interval $[0,1]$ in $N_t + 1$ points and we define $\Delta t = \frac{1}{N_t}$. We will denote $u^{(n)}(x)$ the approximation of the solution $\overline{u}^{(n)} = u(x, t_n)$.

1. Write the discretised equation when using the implicit Euler method. In particular, write the problem in the form: $\mathcal{F}(u^{(n+1)}) = u^{(n)}$. We remark that it is a non-linear problem. In order to overcome the complexity of its solution, and the computational burden, we study an alternative way to perform the time discretisation.

2. We consider the following scheme:

$$\frac{u^{(n+1)} - u^{(n)}}{\Delta t} = \nu \partial_x^2 u^{(n+1)} + \gamma u^{(n+1)} - \gamma u^{(n)} u^{(n+1)}. \tag{4}$$

Let us remark that we have introduced a semi-implicit discretisation of the quadratic term. As a consequence, the problem is now linear in $u^{(n+1)}$.

Exercice 1 We discretise the problem (4) in space by using centred finite differences. To this end, we consider $N_x + 2$ points $\{x_i\}_{0 \leq i \leq N+1}$ where $x_i = ih,\ i = 0, \ldots, N_x + 1$ and $h = 1/(N_x+1)$. We will denote $U_h^{(n+1)}$ the vector whose components are $u_i^{(n+1)}$, the numerical approximation of the solution $u(x_i, t_{n+1})$, which is gathered into the vector $\overline{U}_h^{(n+1)}$.

1. Derive the expression of the numerical method we will use in order to compute $u_i^{(n+1)} \approx \overline{u}(x_i, t_{n+1})$. Show that the scheme can be written as follows:

$$\left[A + B(U_h^{(n)})\right] U_h^{(n+1)} = U_h^{(n)} + F, \tag{5}$$

where $A, B \in \mathbb{R}^{N_x \times N_x}$ are square matrices and $F \in \mathbb{R}^{N_x}$ is a vector.

2. Code a function whose inputs are: $N, U_h^{(n)}$ and outputs A, B, F.

3. Solve numerically the problem.

4. We have to study the convergence properties of the scheme. First, let us choose as a reference (fine) solution the one we obtain by using $N_x = 10^3$ et $N_t = 10^3$. Let us put the values of the reference solution in a vector $\bar{U}_n$. Study the convergence by considering simulations with smaller values of N_x, N_t. Plot the curves when considering the errors:

$$\varepsilon^{(2)}_{\Delta t, \Delta x} = \max_{n \geq 0} \ \left(\ \| U^n_{\Delta x} - \bar{U}^n_{\Delta x} \|_{2,\Delta} \ \right), \tag{6}$$

$$\varepsilon^{(2)}_{\Delta t, \Delta x} = \max_{n \geq 0} \ \left(\ \| U^n_{\Delta x} - \bar{U}^n_{\Delta x} \|_{\infty,\Delta} \ \right), \tag{7}$$

Be careful to choose N_x, N_t in such a way that the points of the coarse discretisations are also points of the fine reference discretisation in order to easily compare the solutions.

Exercice 2 Strang splitting is a way to decompose a problem solution into multiple stages, in which we consider only a part of an equation at a time. This way of discretising in time a problem, when applied to the present case, leads to:

$$\begin{aligned} \frac{u^{(n+1/3)} - u^{(n)}}{\Delta t/2} &= \nu \partial_x^2 u^{(n+1/3)}, \\ \frac{u^{(n+2/3)} - u^{(n+1/3)}}{\Delta t} &= \gamma u^{(n+2/3)}(1 - u^{(n+2/3)}), \\ \frac{u^{(n+1)} - u^{(n+2/3)}}{\Delta t/2} &= \nu \partial_x^2 u^{(n+1)}. \end{aligned} \tag{8}$$

Practically speaking, we perform a diffusion for a half step, followed by a reaction step, followed by a diffusion for a half step. Remark that, when performing the reaction step, this is a pointwise update, as there are no differential operators involved. As a consequence, considering an implicit Euler scheme for this non-linear problem does not involve a prohibitive computational cost. Write the problem satisfied by $u^{(n+1/3)}, u^{(n+2/3)}, u^{(n+1)}$.

1. Write the numerical scheme when considering a finite differences discretisation in space.
2. Code the method. Write two functions, one to solve the diffusion step, one to solve the reaction step. When performing the reaction step, discuss which of the two solutions of the second degree equation originating from the implicit Euler method we have to choose.
3. Study the convergence as done in the previous exercice.

General remark: Write synthetically what are the observations you do when solving the problems and their results. Which method would you choose and why?