PC7 : Spatially extended systems of equation Equilibria, traveling waves and Turing patterns

1 Introduction

The Petite Classe is divided into four parts. The first part is devoted to the thermal explosion, within the framework of the Frank-Kamenetskii theory in one space dimension [2], as well as its link with what we have seen in previous PCs (PC1 and 6). The second part is devoted to flames, deflagrations, modeled through a traveling wave self-similar solution, which leads us to the resolution of an ODE on the full real line [12], and to a heteroclinic orbit joining two equilibrium points at infinity. Such a case has been encountered and presented in the course for the Nagumo equation [3], for which there is an analytic solution. We only prove the existence of solution, whereas the stability of such solutions [4, 11], as well as the numerical resolution in the phase space through shooting methods is beyond the scope of the course [9]. The third part is devoted to the numerical simulation of traveling waves of semi-discretized in space systems of PDEs leading to the resolution of large systems of ODEs. We focus on the Nagumo reaction-diffusion equation, conduct numerical simulations and draw conclusions on the results. The last part is devoted to the simulation of a 1D Turing pattern, leading to the appearance of a stationary solution after the original slightly perturbed constant equilibrium state has lead to instability.

2 Thermal explosion - 1D problem

We consider inhomogeneous temperature and fuel mass fraction fields in space, which also depend on time. We consider a horizontal layer of height $2L$, homogeneous in the x and y directions as presented in the Figure in 2D, and inhomogeneous in space in the vertical z direction. The problem is then mono-dimensional and the system of interest is a PDE system of equations reading:

$$\partial_t Y - D\,\partial_{zz} Y = -B\, e^{-\frac{E}{RT}}\, Y, \tag{1}$$

$$\partial_t T - D\,\partial_{zz} T = (T_b - T_0)\, B\, e^{-\frac{E}{RT}}\, Y, \tag{2}$$

where ∂_{zz} denotes the second order partial differential in space in the z direction, and ∂_t is the time derivative. The following initial conditions are considered: $Y(0,z) = 1$ and $T(0,z) = T_0$, for all $z \in [0, 2L]$ as well as the boundary conditions $T(t,0) = T(t,2L) = T_0$ and $\partial_z Y(t,0) = \partial_z Y(t,2L) = 0$. It can be shown mathematically that there exists a unique C^∞ solution in time $z \in [0, 2L]$, $t \in [0, +\infty[$, at least for some proper set of coefficients, such that $Y(t,z) \in [0,1]$, $T(t,z) \in [T_0, T_b[$ and such that $z \to T(t,z)$ is concave for all $t \in [0, +\infty[$.

2.1 Link with 0D problem studied in the PC1

2.1.1 Write an equation on the average quantity $\overline{Y}(t) = \frac{1}{2L}\int_0^{2L} Y(t,z)\mathrm{d}z$ of Y on the interval $[0, 2L]$, as well as for $\overline{T}(t) = \frac{1}{2L}\int_0^{2L} T(t,z)\mathrm{d}z$ of T.
2.1.2 Using the boundary conditions, the sign of $T - T_0$, as well as the sign of the gradient of T at the boundaries $z = 0$ and $z = 2L$, evaluate the temperature and mass fraction fields in the limit $t \to +\infty$.
2.1.3 Make the link with the homogeneous model we have already studied, in particular in PC1.

2.2 Stationary solution as equilibria of the infinite dimensional dynamical system - qualitative analysis

2.2.1 We introduce a diffusion time $\tau_{\rm dif} = L^2/D$, as well as $\lambda = \tau_{\rm dif}/\tau_I$, for which we recall the expression

$$\tau_I = \frac{T_{FK}}{T_b - T_0}\frac{\exp(E/(RT_0))}{B}, \quad T_{FK} = \frac{RT_0^2}{E}.$$

Using the L as a spatial scale, $\xi = z/L$, $\tau = t/\tau_I$, and $\theta = (T-T_0)/T_{FK}$, $\epsilon = T_{FK}/(T_b-T_0)$, derive the non-dimensional form of the PDE on θ and Y, as well as using the Frank-Kamenetskii transform (large heat of reaction and activation energy):

$$\partial_\tau \theta - \frac{1}{\lambda}\partial_{\xi\xi}\theta = \exp(\theta)\, Y, \tag{3}$$

$$\partial_\tau Y - \frac{1}{\lambda}\partial_{\xi\xi}Y = -\epsilon\, \exp(\theta) Y. \tag{4}$$

If we make the same assumption as before and neglect the fuel consumption, that is $Y \equiv 1$, we get an independent equation on θ:

$$\partial_\tau \theta - \frac{1}{\lambda}\partial_{\xi\xi}\theta = \exp(\theta). \tag{5}$$

2.2.2 Provide an analytical expression of the stationary temperature profile $\theta^{\rm st}(\xi)$ of (5) (hint : remark the existence of a first integral of $\theta^{\rm st}$ in ξ, multiplying by the derivative of the profile. Use the symmetry and the concave character of the solution in order to characterize $\mathrm{d}_\xi \theta^{\rm st}$ at $\xi = 1$ in the center of the layer. The second integration can be conducted using the proper change of variable $\phi^2 = \exp(\theta^{\rm st}(1)) - \exp(\theta^{\rm st})$ leading to an equation of the type

$$\Psi(\theta_m^{\rm st}) = \sqrt{\lambda/2}, \tag{6}$$

making the link between λ and the maximum temperature $\theta_m^{\rm st}$ at the center.

2.2.3 Plot the function Ψ; show that it admits a maximum as well as a related critical parameter $\sqrt{\lambda_{\rm cr}/2} = \Psi^{\max}$. Deduce that there are three scenarios on the existence or not of stationary temperature profiles depending on $\lambda < \lambda_{\rm cr}$, $\lambda = \lambda_{\rm cr}$ or $\lambda > \lambda_{\rm cr}$.

2.2.4 When $\lambda < \lambda_{\rm cr}$, how many profiles do you think there are? Referring to the last PC, propose a conjecture on their stability.

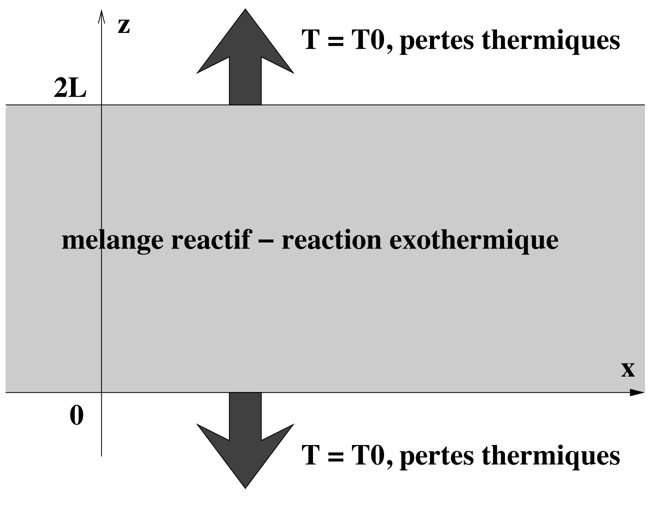

Figure 1: Schematic diagram of the configuration in the (x, z) plane.

2.3 Numerical resolution of the semi-discretized in space problem

2.3.1 Semi-discretize the two sets of PDEs on θ and Y on the one side $(3-4)$ and purely on θ on the other side (5) using a central second order finite difference approximation as already done previously. Explain what is the form of the system of ODEs resulting from the semi-discretization in space.

2.3.2 Starting from an initial profil $\theta \equiv 0$ for the single equation on θ neglecting the fuel consumption, and for $\lambda < \lambda_{\mathrm{cr}}$, describe the dynamics of the system as well as the final state towards which the dynamics is converging. Check that it is coherent with the analytic solution obtained previously. You will use the ROCK4 or RADAU5 solvers provided in the notebook in order to conduct the integration in time of the system.

2.3.3 Taking into account the fuel consumption, and taking any positive Y profile at $t=0$, which has the same average as $Y \equiv 1$, show that the diffusion of the fuel mass fraction is so quick that its initial spatial distribution has no influence on the dynamics of the problem for $\lambda < \lambda_{\mathrm{cr}}$, and even in the neighborhood of the critical λ parameter (check $\lambda = 0.9$ for example).

2.3.4 Propose a synthesis of the results in connection with the original problem of PC1 and with the analytical results obtained above.

3 Study of Combustion waves

One way of modeling combustion fronts or deflagration fronts is to consider systems of reaction-diffusion equations, modeling the coupling between a diffusive process and a reaction one, and to prove that they admit “traveling waves” solution, which are self-similar spatial profiles traveling at constant speed. The combustion process is once again described through a system of partial differential equations on the fuel mass fraction and the temperature, with a non linear monotone positive function of T, which will be clarified later

$$\begin{cases} \partial_t Y - D\,\partial_{xx} Y = -B\,\widetilde{\psi}(T)\,Y, \\ \partial_t T - D\,\partial_{xx} T = (T_b - T_0)\,B\,\widetilde{\psi}(T)\,Y, \end{cases} \tag{7}$$

for $Y \in [0,1]$ and $T \in [T_0, T_b]$. The notation are similar to the thermal explosion problem and, for simplicity, we assume the same diffusion coefficients for mass and temperature (unit Lewis number).

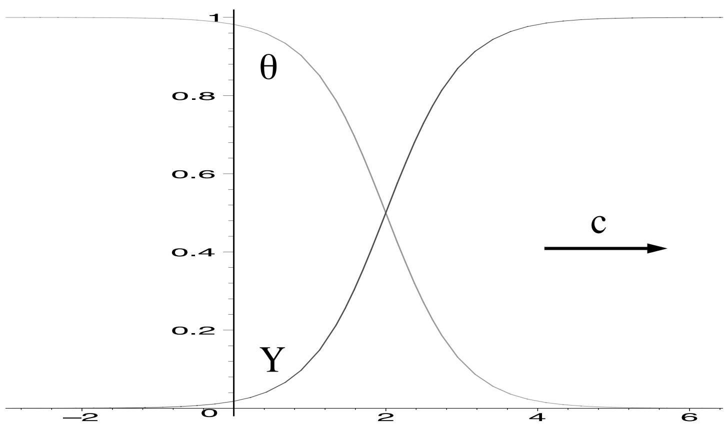

Figure 2: Traveling wave representing a deflagration front.

3.1 Traveling waves

We are looking for self-similar profiles $\phi(y)$ and $\theta(y)$, $y \in \mathbb{R}$ as well as a velocity of the wave c (c is part of the unknowns of the problem), such that $y = x - ct$, $Y(t,x) = \phi(y)$ and $T(t,x) = \theta(y)(T_b - T_0) + T_0$ are solutions of the previous system (7). The special character of this problem is that we have to impose boundaries at infinity: $\lim_{y\to+\infty} \phi(y) = 1$, $\lim_{y\to-\infty} \phi(y) = 0$ and $\lim_{y\to+\infty} \theta(y) = 0$, $\lim_{y\to-\infty} \theta(y) = 1$. The unburnt gases are then on the "$+\infty$" side and the burnt gases on the "$-\infty$" one. We suppose that $\theta(y) \in]0,1[$ and $\phi(y) \in]0,1[$. The flame is moving from the burnt gases toward the unburnt gases at the unknown velocity c (Figure 2).

3.1.1 First, setting a positive velocity c, write the system of ODEs satisfied by the two functions $\phi(y)$ and $\theta(y)$.

3.1.2 We note $\mathcal{H} = \phi + \theta$. Show that if we have a traveling wave, this quantity is constant. It does not depend on space nor time (Hint: solve the differential equation satisfied by $\mathcal{H}$ and use the conditions at infinity).

3.1.3 Show that the problem can be reduced to an equation on $\theta(y)$

$$c\,\theta' + D\,\theta'' + \psi(\theta) = 0, \tag{8}$$

and give an explicit expression for the non-linearity ψ.

3.1.4 We assume that equation (8) on θ admits a smooth C^2 solution. Show that his solution is monotone in y (hint : convexity).

We make a few assumption on the non-linear source term ψ so that we can prove existence and uniqueness of the wave profile and of the velocity c. We assume that there exists $\eta \in]0,1[$, $\psi(\theta) = 0$ for $\theta \in [0,\eta[$, and $\psi(\theta) > 0$ for $\theta \in [\eta, 1[$, as well as $\psi(1) = 0$, $\mathrm{d}_\theta\psi(1) = \gamma$, with $\gamma < 0$ and finite. Such a function is represented in Figure 3. The existence of the traveling wave will rely on the the study of two first order differential equations in the phase plane (θ, θ') and, for the sake of simplicity, we will assume $D = 1$.

3.1.5 We introduce $\widetilde{p} = \theta' = \mathrm{d}_y\theta$, the derivative of θ. Write the first order system of ODEs on $(\theta(y), \widetilde{p}(y))$. The plane $(\theta, \widetilde{p})$ is called the phase plane.

3.1.6 Show that we can reformulate the system in the phase plane (θ, p) with $p \geq 0$ and $\theta \in [0,1]$

$$p\,\mathrm{d}_\theta p = c\,p - \psi(\theta), \tag{9}$$

with $p(\theta(y)) = -\widetilde{p}(y)$ and the boundary conditions $p(\theta = 0) = p(\theta = 1) = 0$, the solution of which allows to connect the the two stationary states $(0,0)$ et $(1,0)$ as presented in Figure 4.

3.1.7 We first look for $\alpha = \mathrm{d}_\theta p(1)$, the slope of the solution close to the point $(1,0)$. Using a Taylor expansion and assuming that $p = \alpha(1-\theta)$ and $\psi(\theta) = \gamma(1-\theta)$, with $\gamma = \mathrm{d}_\theta\psi(1)$, since p satisfies (9), determine α as a function of c and γ.

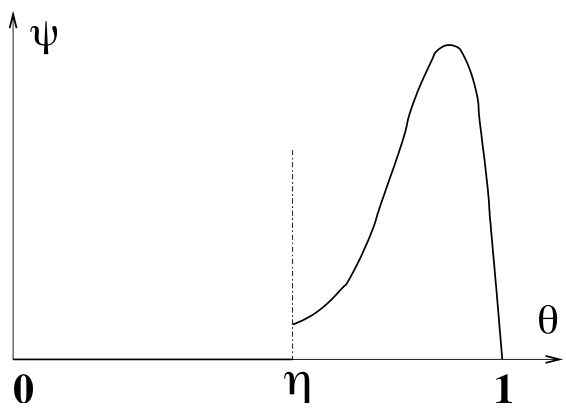

Figure 3: Structure of the non-linearity - cold boundary difficulty resolution.

3.1.8 We focus on the interval $\theta \in [\eta, 1]$. For each given velocity c, one can find a profile $p(\theta)$ satisfying (9)? Show that the solution in this interval is a decreasing function of c, provide the expression of this solution $\bar{p}$ for $c = 0$ as well as the value of $\bar{p}(\eta)$ as a function of $I = \int_0^1 \psi(\theta)\mathrm{d}\theta$.

3.1.9 Solve for the solution in the interval $\theta \in [0, \eta[$. What is the direction of variation of the solution on $[0, \eta[$ as a function of c? Prove the existence of a velocity c_0 such that there exist a continuous integral curve in the phase plane joining $(0, 0)$ and $(1, 0)$. This solution is denoted $p_0(\theta)$.

3.2 BONUS: Flame speed and its limit

The purpose of this final subsection is to evaluate the flame speed and deduce its limit in the case $\eta \to 1$ with fixed I. We first try to obtain some bounds on the flame speed as a function of η.

3.2.1 Prove that $c_0 = p_0(\eta)/\eta$.

3.2.2 Show that $p_0(\eta) \leq \sqrt{2I}$.

3.2.3 In order to obtain a lower bound, use the solution $\underline{p}$, of the ODE :

$$\mathrm{d}_\theta \underline{p} = c_0 - \psi(\theta)/\bar{p}(\theta)$$

on $\theta \in [\eta, 1]$ with $\underline{p}(1) = 0$. Show that in this interval $\underline{p}(\theta) \leq p_0(\theta)$.

3.2.4 Deduce from the previous question that :

$$\frac{\sqrt{2I}}{\eta} - c_0 \frac{1-\eta}{\eta} \leq c_0 \leq \frac{\sqrt{2I}}{\eta},$$

which gives a bound on the flame speed as a function of η.

3.2.5 Assuming that I remains constant as a function of η, and that only the non-linearity ψ is changed, can you describe the velocity of the flame as $\eta \to 1$? What can be said on the reaction rate? as well as the temperature profile? Does the temperature profile remain smooth? Plot it.

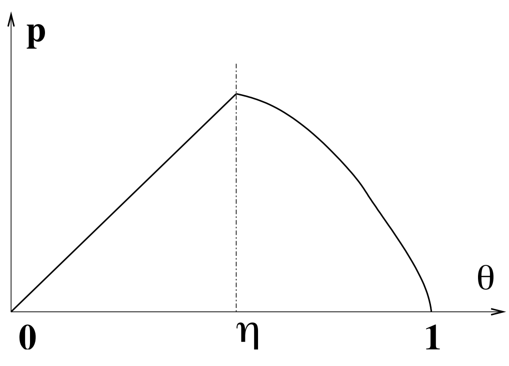

Figure 4: Phase space resolution of the wave profile.

4 Simulation of traveling waves: Nagumo

4.1 Traveling waves of Nagumo type

In their original paper [4], the authors introduced a model describing the propagation of a virus through a reaction-diffusion PDE, and the first rigorous analysis of a stable traveling wave solution of a nonlinear reaction-diffusion equation. This equation, also called the Fisher equation was at the origin of several studies in the field and is related to a nonlinearity of monostable character [11]. Here we rather focus on a bistable case, with a cubic nonlinear term of as a limit of Nagumo type [3]:

$$\partial_t u - D\,\partial_x^2 u = k\,u^2(1-u), \tag{10}$$

for which we have presented a resolution during the course. We consider a 1D discretization with $N+1$ points on a $[-70,70]$ region with homogeneous Neumann boundary conditions, for which we have negligible spatial discretization errors with respect to the ones coming from the numerical time integration.
The description of the dimensionless model and the structure of the exact solution can be found in [3], where a change of variable

$$\tau = kt, \qquad r = (k/D)^{1/2}x, \tag{11}$$

allows to characterize the velocity of the wavefront:

$$c \propto (Dk)^{1/2}, \tag{12}$$

whereas the sharpness of the wave profile is measured by

$$\mathrm{d}_x u|_{\max} \propto (k/D)^{1/2}. \tag{13}$$

In the case of $D = 1$ and $k = 1$, the velocity of the self-similar traveling wave is $c = 1/\sqrt{2}$ in (12) and the maximum gradient value reaches $1/\sqrt{32}$ in (13). The key point of this illustration is that the velocity of the traveling wave is proportional to $(k\,D)^{1/2}$, whereas the maximum gradient is proportional to $(k/D)^{1/2}$. Hence, we consider the case $kD = 1$, for which one may obtain steeper gradients with the same speed of propagation. The resolution of the semi-discretized version of the PDE in space is conducted using a combination of operator splitting with Strang formula, and of ROCK4 and RADAU5 for the various sub-steps dedicated to respectively diffusion and source.

4.1.1 Explain how the stiffness of the system of equation is related to the two coefficients k and D.

4.1.1 Propose a simulation, where the initial condition is taken as the exact traveling wave solution (without boundary condition nor space discretization), for a time interval of $[0,50]$. In order to conduct a analysis of the splitting error, to what profile do you compare your simulation? Explain why you will have to propose a very fine simulation of the full coupled dynamics using RADAU5 for the whole system versus comparing to the exact solution of the original PDE on the full real line.

4.1.3 Evaluate the wave speed and wave profile in the phase space compared to the exact one, for several splitting time steps, whereas the evaluation through ROCK4 and RADAU5 of the various sub-steps are resolved with a small tolerance, so as to obtain a pure splitting error. Conduct this experiment for $D = 1$ and $k = 1$ and for $D = 0.1$ and $k = 10$. What is the influence of stiffness on the results?

4.1.4 Conclude on the ability of the proposed strategy to resolve the wave.

5 Simulation of Turing pattern in 1D

In this section, we focus on the simulation of Turing patterns [10, 1, 6] using the Lengyel-Epstein model [5] and use an article where some simulation were performed some time ago [7].

The system of reaction diffusion is the following one:

$$\begin{cases} \partial_t u = D_u\, \partial_x^2 u + f(u,v), \qquad f(u,v) = a - u - \dfrac{4\,u\,v}{1+u^2}, \\ \partial_t v = \delta \left[D_v\, \partial_x^2 v + g(u,v) \right], \qquad g(u,v) = b \left(u - \frac{u\,v}{1+u^2} \right), \end{cases} \tag{14}$$

where $x \in \Omega \subset \mathbb{R}$, $D_u = 1$, $D_v = 1.5$, $\delta = 8$, and where a and b remain the control parameters.
4.3.1 Conduct and analysis of the source term and identify the only equilibrium when the diffusion in not present as a function of a. Study the stability of such a state in terms of a and b and show that there can be a Hopf bifurcation for some values of b as a function of a.

4.3.2 Investigate the critical value of b_T such that, for a given a, we have a stable equilibrium in the previous question and the development of a Turing pattern (instability of the equilibrium with diffusion) and provide the interval of b we can work with in order to get a Turing pattern.

4.3.3 We take $a = 30$ and $b = 2.8$. Identify the eigenvalue related to the instability and plot the stability curve as a function of n^2. What is the most amplified mode, knowing that we work on a domain $[0, L]$, $L = 50$? Conduct a numerical simulation by taking a perturbed initial solution of the equilibrium state and observe the evolution with time of the solution. Propose an analysis of the results. You will use the notebook first with a time integration on a smaller interval in order to observe the initial dynamics (with a 1000 points and time of integration of 160). Moreover, once the initial dynamics has been observed, take an integration time ten times larger in order to see if the dynamics converges toward a stationary state. Identify the integer such that $n_*^2 L/2\pi$ is the most amplified mode and check that this mode is the one emerging from the simulation. Make the link with what is commonly know as the "stripes" pattern [6, 8, 5].

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