MAP551 - PC7: Spatially extended systems of equation Equilibria, traveling waves and Turing patterns

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1 Thermal explosion

We consider the PDE system of equations reading :

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

1.1 Link with 0D problem

As the variable Y and T are both bounded, so we have no worry about the intergrability when we apply the Fubini theorem.

$$\begin{aligned}\partial_t \bar{Y} &= \frac{1}{2L}\int_0^{2L} D\partial_{zz}Y - B\, e^{-\frac{E}{RT}} Y \mathrm{d}z \\ &= -\frac{B}{2L}\int_0^{2L} e^{-\frac{E}{RT}} Y \mathrm{d}z \\ \partial_t \bar{T} &= \frac{1}{2L}\int_0^{2L} D\partial_{zz}T + (T_b - T_0)B\, e^{-\frac{E}{RT}} Y \mathrm{d}z \\ &= \frac{D}{2L}[\partial_z T]_0^{2L} + \frac{(T_b - T_0)B}{2L}\int_0^{2L} e^{-\frac{E}{RT}} Y \mathrm{d}z\end{aligned}$$

As we know, $T > T_0$, $T(t,z)$ is a concave function for all $t \in [0, +\infty]$, then $\partial_z T(t,0) > 0 \quad \partial_z T(t,2L) < 0$. $\partial_t \bar{Y} = -\frac{B}{2L}\int_0^{2L} e^{-\frac{E}{RT}} Y \mathrm{d}z \leq -B\, e^{-\frac{E}{RT_0}}$. The function $\bar{Y}$ decrease and smaller than $\bar{Y}_0 \exp(-B\exp(\frac{E}{RT_0}) \times t) \to 0$. Meanwhile, Y is of $\mathcal{C}^\infty$, therefore, when $\bar{Y} \xrightarrow{t\to\infty} 0 \Longrightarrow Y \xrightarrow{t\to\infty} 0$. As for $\bar{T}$, it tends to $\frac{D}{2L}[\partial_z T]_0^{2L} < 0$. And T is bounded, therefore, $\bar{T} \to T_\infty$. With the boundary condition we will obtain that $T \xrightarrow{t\to\infty} T_0$. **2.1.1-2.1.2**

When we look at the homogeneous model from PC1, we see that the mass fraction decrease as well, but the temperature stabilized around T_b, here, because of the non-homogeneous propriety, the term $\partial_{zz} Y$ and the boundary condition will dissipate the internal heat and stablize around T_0. **2.1.3**

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

We introduce

$$\tau_I = \frac{T_{FK}}{T_b - T_0}\frac{\exp(E/(RT))}{B}, \quad T_{FK} = \frac{RT_0^2}{E}, \quad \xi = \frac{z}{L}, \quad \tau = t/\tau_I, \quad \lambda = \tau_{diff}/\tau_I, \quad \tau_{diff} = \frac{L^2}{D}$$

$$\begin{aligned}
\frac{1}{\tau_I}\partial_\tau Y - \frac{1}{\tau_{diff}}\partial_{\xi\xi}Y &= -B\, e^{-\frac{E}{RT}}Y, \\
\partial_\tau Y - \frac{1}{\lambda}\partial_{\xi\xi}Y &= -B\tau_I\, e^{-\frac{E}{RT}}Y \\
\partial_\tau Y - \frac{1}{\lambda}\partial_{\xi\xi}Y &= -\epsilon\exp(-\frac{E}{RT} + \frac{E}{RT_0}))Y \\
&\boxed{\partial_\tau Y - \tfrac{1}{\lambda}\partial_{\xi\xi}Y = -\epsilon\exp(\theta\tfrac{T_0}{T})Y} \\
\partial_t T - D\partial_{zz}T &= (T_b - T_0)B\, e^{-\frac{E}{RT}}Y \\
\partial_\tau T - \partial_{\xi\xi}T &= (T_b - T_0)B\, e^{-\frac{E}{RT}}Y \\
\partial_\tau \theta - \partial_{\xi\xi}\theta &= (T_b - T_0)\lambda/T_{FK}B\, e^{-\frac{E}{RT}}Y \\
\partial_\tau \theta - \partial_{\xi\xi}\theta &= e^{(-\frac{E}{RT}+\frac{E}{RT_0})}Y \\
&\boxed{\partial_\tau \theta - \partial_{\xi\xi}\theta = \exp(\theta\tfrac{T_0}{T})Y}
\end{aligned}$$

If we suppose that $Y \equiv 1$, we will have the formulae **2.2.1** :

$$\boxed{\partial_\tau\theta - \partial_{\xi\xi}\theta = \exp(\theta)}$$

We look for the solution that is not dependent on time.

$$-\frac{1}{\lambda}\partial_{\xi\xi}\theta = \exp(\theta)$$

Note here $\theta' = \partial_\xi\theta$

$$\begin{aligned}
-\frac{1}{\lambda}\theta''\theta' &= \exp(\theta)\theta' \\
\frac{1}{2\lambda}\theta'^2 + \exp(\theta) &= \frac{1}{2\lambda}\theta^{st}(1)'^2 + \exp(\theta^{st}(1))
\end{aligned}$$

As the system is symmetric with the line $z = L$ ($\xi = 1$), so the derivative $\mathrm{d}_\xi\theta^{st}(1) = 0$. We substitute the variable with $\phi^2 = \exp(\theta^{st}(1)) - \exp(\theta^{st}(\xi))$. Therefore, $\mathrm{d}_\xi(\phi^2) = 2\phi\mathrm{d}_\xi\phi = -\exp(\theta^{st})\mathrm{d}_\xi\theta = (\phi^2 - \exp(\theta^{st}(1)))\mathrm{d}_\xi\theta$. $\phi = 0$ only at the center $\xi = 1$. At the same time, we have $\theta(1) = \theta^{st}_m$, $\phi(1) = 0$ and $\phi(0) = \sqrt{\exp(\theta(1)) - 1}$.

$$\begin{aligned}
2\phi\mathrm{d}_\xi\phi &= (\phi^2 - \exp(\theta^{st}(1)))\phi \times \sqrt{2\lambda} \\
\frac{\mathrm{d}_\xi\phi}{(\phi^2 - \exp(\theta^{st}(1)))} &= \sqrt{\lambda/2}
\end{aligned}$$

After solving the equation and use the boundary condition, we have an equation about $\theta(1)$

$$\sqrt{\frac{\lambda}{2}} = \frac{1}{2}\exp(-\frac{\theta_m^{st}}{2})\ln\left(\frac{\exp(\frac{\theta_m^{st}}{2}) + \sqrt{\exp(\theta_m^{st}) - 1}}{\exp(\frac{\theta_m^{st}}{2}) - \sqrt{\exp(\theta_m^{st}) - 1}}\right) = \Psi(\theta_m^{st})$$

We can draw the function Ψ which is shown in the following (Fig 1)

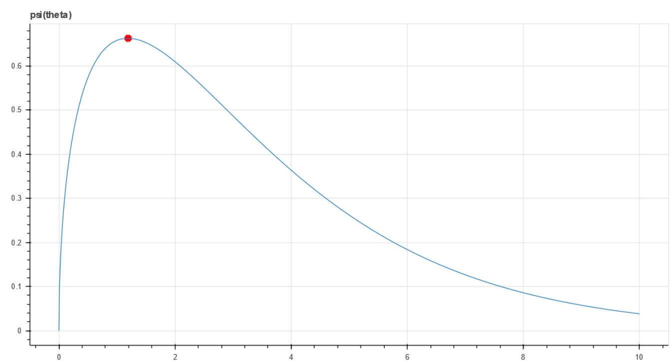


Figure 1 – Function Ψ

Numerically, we have the maximum value for $\lambda_{cr} \approx 0.878$. If λ is too large, the equation admits no solution. In this case, the diffusion of the system is not strong enough to maintain a stable temperature. Then the system explode with a $\theta_m^{st} = \infty$. **2.2.2-2.2.3**

When $\lambda > \lambda_{cr}$, there isn't a stationary point. When $\lambda < \lambda_{cr}$, there are two equilibrium but only the low temperature is stable. At λ, there is a stable equilibrium. **2.2.4**

1.3 Numerical resolution of the semi-discretized in space problem

If we use a central second order finite difference approximation, we will get for (3-4) :

$$\begin{cases} \partial_\tau \theta_k - \dfrac{1}{\lambda}\dfrac{\theta_{k-1} - 2\theta_k + \theta_{k+1}}{h^2} = \exp(\theta_k)Y_k \\ Y_k - \dfrac{1}{\lambda}\dfrac{Y_{k-1} - 2Y_k + Y_{k+1}}{h^2} = -\varepsilon\exp(Y\theta_k)Y_k \end{cases}$$

Where, h is length of spatial discretization steps. The same, if we neglect the fuel consumption, the equation (5) becomes :

$$\partial_\tau \theta_k - \frac{1}{\lambda}\frac{\theta_{k-1} - 2\theta_k + \theta_{k+1}}{h^2} = \exp(\theta_k)$$

The numerical solution is shown as below, and it converges to the analytic solution as predicted.

Yet, the diffusion of the fuel mass fraction is so fast that its initial spatial distribution has (almost) no influence on the dynamics of the problem for $\lambda < \lambda_{cr}$. In short term, the explosion happens so fast that it converges quickly to the approximate model (without fuel consumption). For the images shown below (Fig 3) we take three initial distribution into our consideration :

In long term, the dynamics of θ and Y converges to zero, which is a good response to our analysis in the first subsection (Fig 4).

This result comes from two facts (**2.3.4**) :

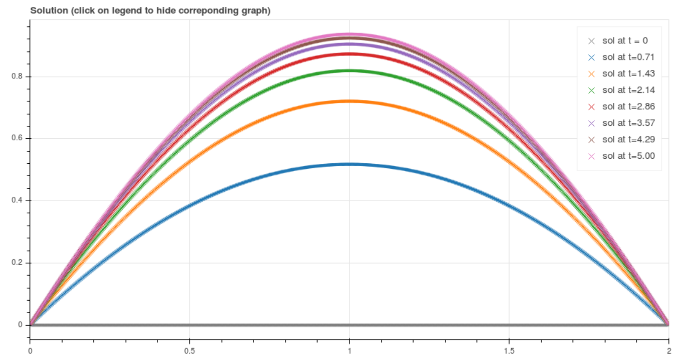
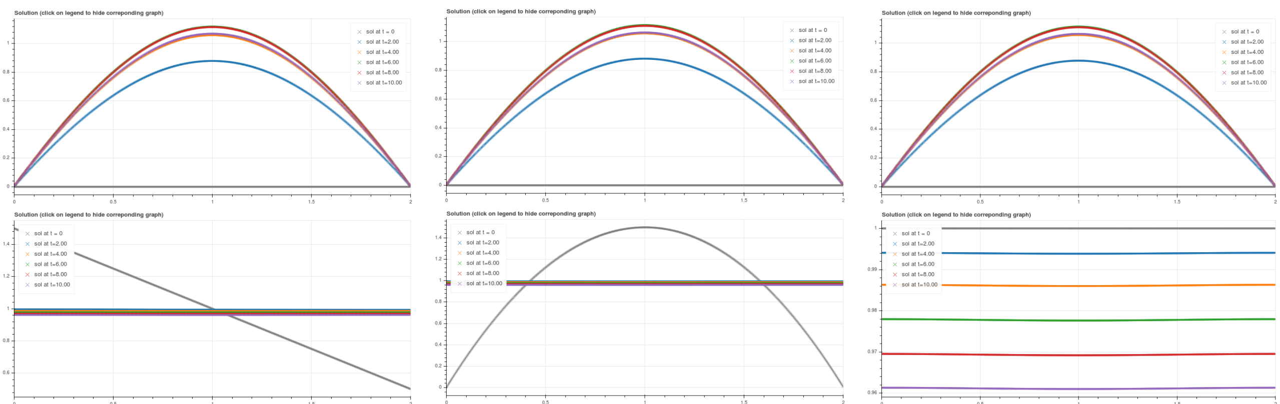
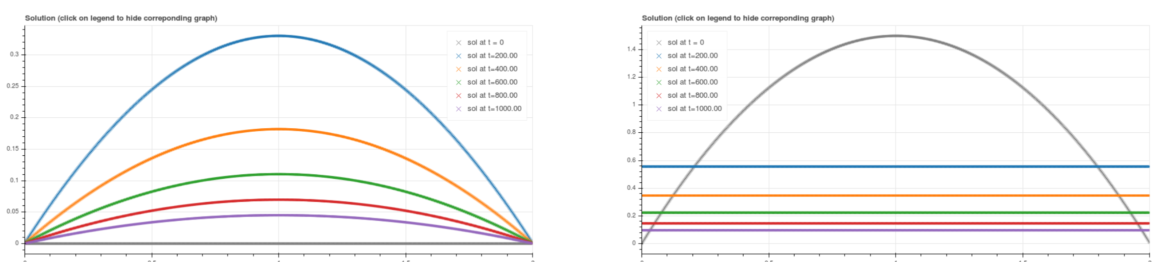


Figure 2 – Model without fuel consumption, $\lambda = 0.86$



$Y(0) = 1.5 - \xi/2, \quad \lambda = 0.9$ $\qquad$ $Y(0) = \frac{3}{4}\xi(2-\xi), \quad \lambda = 0.9$ $\qquad$ $Y(0) = 1, \quad \lambda = 0.9$

Figure 3 – Several numerical solutions during $t \in [0, 10]$ with different initial condition of the distribution of fuel



θ $\qquad$ Y

Figure 4 – Numerical solution for $t \in [0, 1000]$

1. $\varepsilon << 1$, that is $T_{FK} << (T_b - T_0)$, which is due to a large E (the activation energy). And the chemical reaction is violent and the system converges fast to the "quasi-equilibrium" thanks to the presence of heat diffusion. Instead, we have analyzed a system without thermal loss, and the temperature of the system becomes explosive.
2. $\lambda < \lambda_{cr}$, when we always have one stationary solution, then the equilibrium can be reached. Combined with the effect of violence of the reaction, the system converges easily.

2 Study of Combustion waves

2.1 Traveling waves

If we execute a substitution of the variable by $y = x - ct$, then we transform the system into **3.1.1** :

$$\begin{cases} \mathrm{cd}_y\phi(y) + D\mathrm{d}_{yy}\phi(y) = B\,\tilde{\Psi}(T_0 + (T_b - T_0)\theta(y))\phi(y), \\ \mathrm{cd}_y\theta(y) + D\mathrm{d}_{yy}\theta(y) = -B\,\tilde{\Psi}(T_0 + (T_b - T_0)\theta(y))\phi(y) \end{cases}$$

Let $\mathcal{H} = \phi + \theta$, the equation verified by $\mathcal{H}$ is written :

$$\mathrm{cd}_y\mathcal{H} + D\mathrm{d}_{yy}\mathcal{H} = 0$$

Then the analytic solution for $\mathcal{H}$ is $A\exp(-x) + B$, where A and B are two constants. From the conditions at infinity, we see that $\lim_{y\to\pm\infty}\mathcal{H} = 1$, we can have that the constant $A = 0$, therefore, $\mathcal{H} = 1, \quad \forall y \in \mathbb{R}$. Noticing that $y = x - ct$, then $\mathcal{H}$ does not depend on y, nor on $x, \quad t$. **3.1.2**

If we substitute ϕ with $1 - \phi$, we can have the equation written as :

$$c\theta' + D\theta'' + \psi(\theta) = 0$$

where $\psi(\theta) = B\tilde{\Psi}(T_0 + (T_b - T_0)\theta(y))(1 - \theta)$.

We assume D=1, then by introducing $\tilde{p} = \theta'$ we can transform the second order equation into a first order system **3.1.5** :

$$\begin{cases} \tilde{p} = \theta' \\ c\tilde{p} + \tilde{p}' + \psi(\theta) = 0 \end{cases}$$

If we reformulate the system in the phase plane by notation $p(\theta(y)) = -\tilde{p}(y)$. We have : $\mathrm{d}_y p = \mathrm{d}_\theta p\theta' = -p\mathrm{d}_\theta p$, the equation is telling :

$$-cp + p\mathrm{d}_\theta p + \psi(\theta) = 0$$

It can be easily proofed that the derivative of θ in the limit at infinity is zero (which we can proof by constructing a contradiction). Therefore $p(\theta = 0) = p(\theta = 1) = 0$. It allows us to connect two stationary states (0,0) and (1,0).

Assuming that $\mathrm{d}_\theta p(1) = \alpha$, $p = \alpha(\theta - 1)$ and $\psi(\theta) = \gamma(1 - \theta)$, from the equation above, we we have :

$$\alpha(\theta - 1)\alpha = c\alpha(\theta - 1) + \gamma(1 - \theta)$$

By solving the equation above for any θ close to one, we have :

$$\alpha = \frac{c \pm \sqrt{c^2 - 4\gamma}}{2}$$

As we can deduct that $\theta' \leq 0$, so $p \geq 0$. α is then negative, the admissible solution is $\alpha = \frac{c - \sqrt{c^2 - 4\gamma}}{2}$. **3.1.7**. We suppose the solution p is a $\mathcal{C}^2$ smooth one,

$$p\partial_\theta p = cp - \psi(\theta)$$

$$\partial_\theta p = c - \frac{\psi(\theta)}{p}$$

$$\partial_\theta(\partial_c p) = 1 + \frac{\psi(\theta)}{p^2}\partial_c p$$

If we let a certain function Y that $Y' = \frac{\psi(\theta)}{p^2}$, then we have :

$$\begin{aligned} e^{-Y}\partial_\theta(\partial_c p) - e^{-Y}Y'\partial_\theta\partial_c p &= e^{-Y} \\ \partial_\theta(e^{-Y} \times \partial_c p) &= e^{-Y} \\ 0 - e^{-Y} \times \partial_c p(\theta) &= \int_\theta^1 e^{-Y}\mathrm{d}t \\ \partial_c p(\theta) &= -e^{Y}\int_\theta^1 e^{-Y}\mathrm{d}t < 0 \end{aligned}$$

As a result, the function p decreases with c. **3.1.8** For a solution when $c = 0$, equation (9) becomes $\partial_\theta p = -\frac{\psi(\theta)}{p}$. As can be seen in the Figure 3, function $\psi(\theta) = 0, \quad \theta \in [0, \eta[$. Then $\int_0^1 \psi(\theta)\mathrm{d}\theta = \int_\eta^1 \psi(\theta)\mathrm{d}\theta$.

$$\frac{1}{2}\int_\eta^1 \mathrm{d}_\theta p^2 = -\int_0^1 \psi(\theta)\mathrm{d}\theta = -\int_\eta^1 \psi(\theta)\mathrm{d}\theta$$

As $p(1) = 0$, we have $\bar{p}(\eta) = \sqrt{2I}$ **3.1.9**

We can give directly an analytic expression for p within $[0, \eta[$ as $p = c\theta$. For $\theta \in [\eta, 1]$, $p = f(\theta, c)$ that is decreasing with c for all $\theta \in [\eta, 1]$. By comparing the value at the point $\theta = \eta$, from $c = 0$, which gives us $p(\eta^-) = 0$ and $p(\eta+) > 0$. p being continuous, we can find **an only** c who satisfies the continuous propriety.

3 Simulation of traveling waves : Nagumo

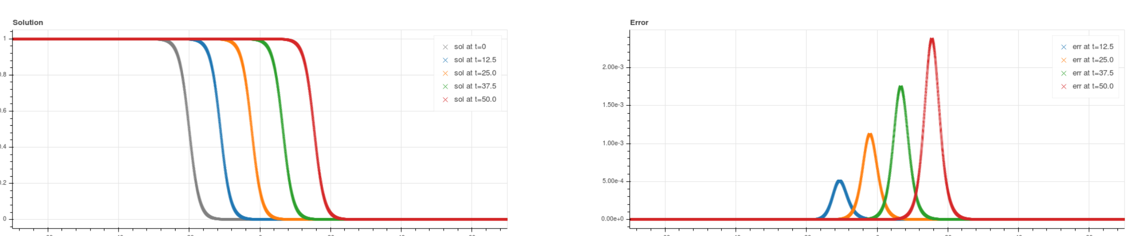
We consider the Nagumo equation :

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

3.1 Traveling waves of Nagumo type

The stiffness comes from the norm of the gradient, if the gradient becomes large in absolute value, then the system is characterized with a violent variation. Therefore, the stiffness is coming from $(k/D)^{1/2}$. **4.1.1**

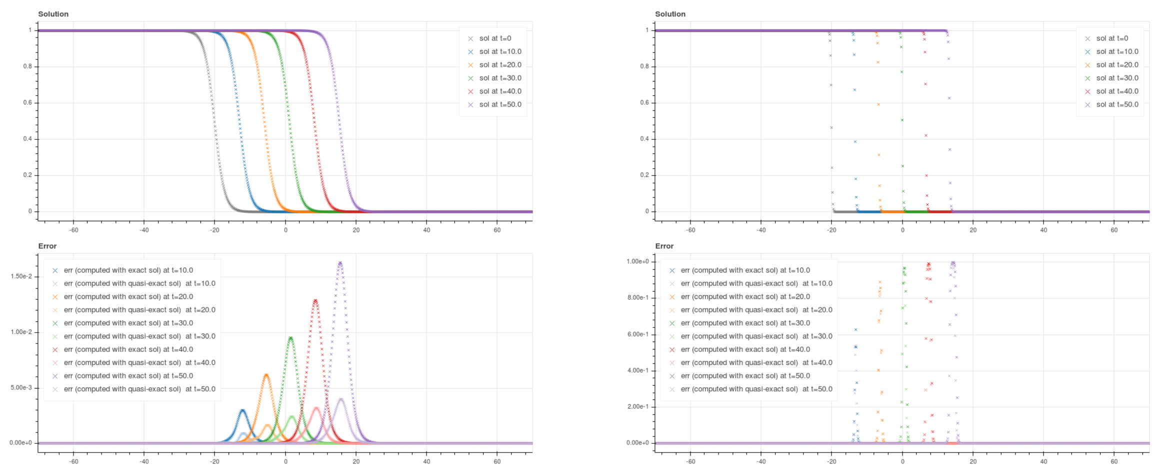
We used a RADAU5 model to solve the system. We use a "very fine" spatial-discreticized system in order to only consider the error in terms of time variation **4.1.2**.



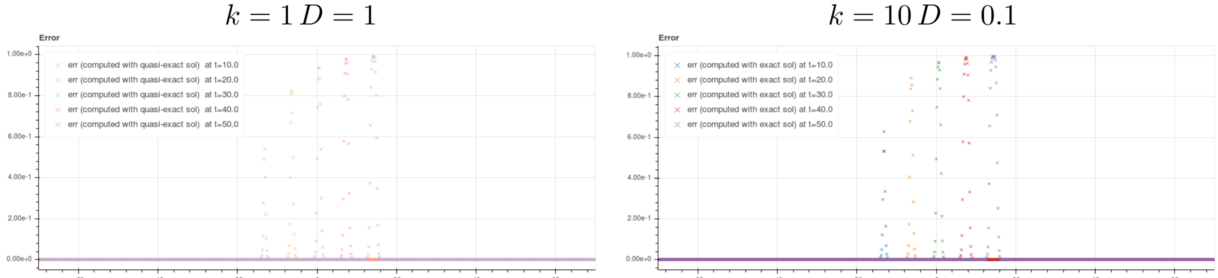
u profile — error at different moment represented by different colors

Figure 5 – Radau5 resolution with spatial discretization $N_x = 5000$

As shown in the following, we demonstrate two cases of stiffness : the right one with a moderate stiffness when $k = 1\,D = 1$. The error versus the exact one is larger than the error against the quasi-exact solution. With only 10 time steps, we reach a relatively good numerical resolution, which is close to the quasi-exact one. And when the stiffness grows, the error increases as well.



$k = 1\,D = 1$ $\qquad$ $k = 10\,D = 0.1$



when $k = 10\,D = 0.1$, error terms compared with quasi exact solution and the exact one

Figure 6 – Strang solution compared with the exact one and the Radeau5 resolution

And we can see in the last row of Fig 6, neither the quasi-exact solution nor the strang method solve the system properly with a relative error close to 100%. **4.1.3**

As well, if we look at the order of Strang method, there will be a collapse of order of convergence if the system becomes too stiff. Theoretically, Strang method is of second order, which is confirmed numerically when $k = 1\,D = 1$. And if we tune to the configuration of $k = 10\,D = 0.1$. The numerical order is lower than 2 **4.1.4**.

In the meanwhile, if we look at the velocity obtained by numerical method : when the stiffness is not important, strang and quasi-exact solution give us almost the same result around 0.707 ($k = 1\,D = 1$), but when the stiffness becomes strong, Radeau5 method gives us a less satisfying result $c = 0.68$. **4.1.4**

4 Simulation of Turing pattern in 1D

The system of reaction-diffusion is the following one :

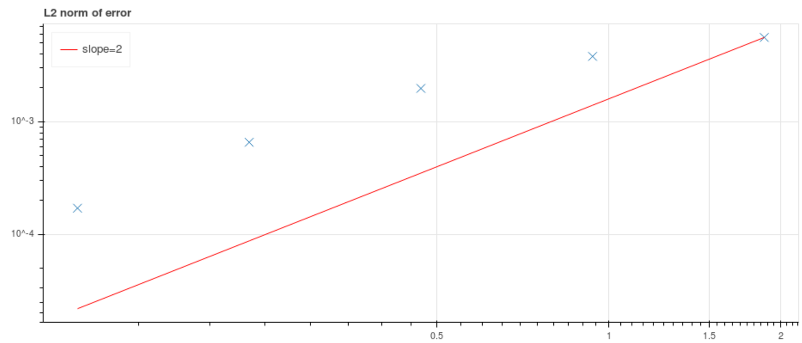


Figure 7 – $k = 10\, D = 0.1$, order of the Strang method

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

where $x \in \Omega$, $D_u = 1$, $D_v = 1.5$, $\delta = 8$.

If we neglect the presence of the diffusion term, the equilibrium can be presented as : $u = \frac{a}{5}$ and $v = 1 + \frac{a^2}{25}$. The Jacobian matrix at is described as :

$$J = \begin{bmatrix} -\frac{4v}{u^2+1} + \frac{8u^2v}{(u^2+1)^2} - 1 & -\frac{4u}{u^2+1} \\ b\delta(-\frac{v}{u^2+1} + \frac{2u^2v}{(u^2+1)^2} + 1) & -b\delta\frac{u}{u^2+1} \end{bmatrix} = \begin{bmatrix} \frac{3a^2-125}{a^2+25} & -\frac{20a}{a^2+25} \\ b\delta(\frac{10a}{25+a^2}) & -b\delta\frac{5a}{a^2+25} \end{bmatrix}$$

To obtain a Hopf bifurcation, we should have $\det(J_{eq}) = \frac{5b\delta u}{(u^2+1)} > 0$ and $trace(J) = \frac{3u^2-5-\delta bu}{u^2} = 0$. A necessary condition for b to encounter this case : $b_H = \frac{3a^2-125}{40a}$ and $b_H > 0$ **4.3.1**

1. If ab>0 (det>0) and $3a^2 - 125 - 40ab > 0$, we have two eigenvalues with positive real part, which denotes the instability of the system.
2. If ab>0 (det>0) and $3a^2 - 125 - 40ab < 0$, we have two eigenvalues with negative real part, stable.
3. If ab<0 (det<0), the solutions are always in the real plane. And there is then a positive eigenvalues, system is unstable.

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