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Consider the non-dimensional linear advection-diffusion equation for the variable/unknown $u = u(x, t)$, with initial and boundary conditions:

$$u_t - a(t)u_x - \epsilon u_{xx} = 0 \quad \text{for } x \in [L_p, L] \tag{1a}$$

$$u(x, 0) = u_0(x) \tag{1b}$$

$$u(L_p, t) = u(L, t) = 0 \tag{1c}$$

(small) constant diffusion ϵ and a given function $a(t)$. The boundary conditions are classical homogeneous Dirichlet conditions. The above system arose from the research on machine learning of Choi et al. (2022). In the end, we will use $L_p = -1$ and $a(t) = 1$. [1]

QUESTION 1

Why is (1) a linear advection-diffusion equation? Explain all three terms used, i.e. "linear" (precisely), "advection" and "diffusion".

Solution:

The advection-diffusion equation describes the movement of a test particle or a substance that is being transported by a fluid (hence the "advection") but also presents a randomised spread (hence "diffusion") [2, 3]. One application for this problem is to model the spread of pollution in a river [4].

The advection term, that describes the test particle being transported by the fluid, is given by

$$a(t)u_x,$$

where $a(t)$ is the velocity of the fluid, also called "advection velocity" in [5].

The diffusion term describes random movements of the test particle. It can occur due to the internal oscillation of molecules in the substance that is being transported by the fluid, for example in "Brownian motion" [6]. This term is represented in the equation by

$$\epsilon u_{xx},$$

where ϵ is the diffusion coefficient, but it also is called the kinematic viscosity [5].

Finally, the term "linear" in Equation (1) means that it is a linear combination of derivatives of u. It only contains first-order terms and does not involve any terms of u raised to the power of 2 or higher, or any products of u. Additionally, $a(t)$ is not a function of u, which would also make the equation nonlinear.

QUESTION 2

For the θ-method, prove equations (2.80) to (2.84) in M&M. [7]

Solution:

The six-point scheme to approximate $u(x, t)$ through the Θ-method is given by Equation (2.75) from [7]

$$U_j^{n+1} - U_j^n = \mu \left[\Theta \delta_x^2 U_j^{n+1} + (1 - \Theta)\delta_x^2 U_j^n \right], \tag{2}$$

with $\mu = \Delta t/(\Delta x)^2$.

To calculate the truncation, $T_j^{n+1/2}$, error for this method we start by expanding the terms approximated by U_j^{n+1} and by U_j^n in a Taylor series around $\Delta t/2$

$$u_j^{n+1} = \left[u + \frac{1}{2}\Delta t u_t + \frac{1}{2}\left(\frac{1}{2}\Delta t\right)^2 u_{tt} + \frac{1}{3!}\left(\frac{1}{2}\Delta t\right)^3 u_{ttt} \cdots \right]_j^{n+1/2}, \tag{3a}$$

$$u_j^n = \left[u - \frac{1}{2}\Delta t u_t + \frac{1}{2}\left(\frac{1}{2}\Delta t\right)^2 u_{tt} - \frac{1}{3!}\left(\frac{1}{2}\Delta t\right)^3 u_{ttt} \cdots \right]_j^{n+1/2}. \tag{3b}$$

Next, if we replace Equations (3) on the left-hand side of Equation (2), we obtain the central difference applied on the time coordinate $delta_t u_j^{n+1/2}$

$$\delta_t u_j^{n+1/2} = u_j^{n+1} - u_j^n = \left[\Delta t u_t + \frac{1}{3!}\left(\frac{1}{2}\Delta t\right)^3 u_{ttt}\cdots\right]_j^{n+1/2}. \tag{4}$$

We can see that the even terms do annulate themselves. Equation (4) is equation 2.80 in [7].

To approximate the right-hand side, we need to apply the central difference operator twice in relation to the spatial coordinate x, to obtain $\delta_x^2 u_j^n$. From the Equation (2.28) of [7], this operator is defined as

$$\delta_x^2 u_j^n \coloneqq u_{j+1}^n - 2u_j^n + u_{j-1}^n, \tag{5}$$

therefore, the next step is to expand u_{j+1}^n and u_{j-1}^n in Taylor series, around Δx

$$u_{j+1}^n = \left[u + \Delta x u_x + \frac{1}{2}(\Delta x)^2 u_{xx} + \frac{1}{3!}(\Delta x)^3 u_{xxx} + \frac{1}{4!}(\Delta x)^4 u_{xxxx}\cdots\right]_j^n, \tag{6a}$$

$$u_{j-1}^n = \left[u - \Delta x u_x + \frac{1}{2}(\Delta x)^2 u_{xx} - \frac{1}{3!}(\Delta x)^3 u_{xxx} + \frac{1}{4!}(\Delta x)^4 u_{xxxx}\cdots\right]_j^n. \tag{6b}$$

By replacing Equations (6) in Equation (5) we get

$$\delta_x^2 u_j^n = \left[(\Delta x)^2 u_{xx} + \frac{1}{12}(\Delta x)^4 u_{xxxx}\cdots\right]_j^n, \tag{7}$$

this is equation (2.81) from [7]. The term $\delta_x^2 u_j^{n+1}$ is very similar to Equation (7), but instead of being in the line n-ish of the mesh, it will be in the line $n+1$, which make then quite complicated to be added as in Equation (2). Nevertheless, one can sort it out by expanding $\delta_x^2 u_j^n$ and $\delta_x^2 u_j^{n+1}$ around $\Delta t/2$

$$\begin{aligned}\delta_x^2 u_j^{n+1} = \Big[&\left[(\Delta x)^2 u_{xx} + \tfrac{1}{12}(\Delta x)^4 u_{xxxx} + \cdots\right] \\ &+ \tfrac{1}{2}\Delta t\left[(\Delta x)^2 u_{xxt} + \tfrac{1}{12}(\Delta x)^4 u_{xxxxt} + \cdots\right] \\ &+ \tfrac{1}{2}\left(\tfrac{1}{2}\Delta t\right)^2\left[(\Delta x)^2 u_{xxtt} + \tfrac{1}{12}(\Delta x)^4 u_{xxxxtt} + \cdots\right] + \cdots\Big]_j^{n+1/2}.\end{aligned} \tag{8}$$

$$\begin{aligned}\delta_x^2 u_j^{n} = \Big[&\left[(\Delta x)^2 u_{xx} + \tfrac{1}{12}(\Delta x)^4 u_{xxxx} + \cdots\right] \\ &- \tfrac{1}{2}\Delta t\left[(\Delta x)^2 u_{xxt} + \tfrac{1}{12}(\Delta x)^4 u_{xxxxt} + \cdots\right] \\ &+ \tfrac{1}{2}\left(\tfrac{1}{2}\Delta t\right)^2\left[(\Delta x)^2 u_{xxtt} + \tfrac{1}{12}(\Delta x)^4 u_{xxxxtt} + \cdots\right] + \cdots\Big]_j^{n+1/2}.\end{aligned} \tag{9}$$

By adding up Equations (8) and (9) as in the right-hand side of Equation (2), we get

$$\begin{aligned}\Theta\delta_x^2 u_j^{n+1} + (1-\Theta)\delta_x^2 u_j^n = \Big[&\left[(\Delta x)^2 u_{xx} + \tfrac{1}{12}(\Delta x)^4 u_{xxxx} + \cdots\right] \\ &+ \left(\Theta - \tfrac{1}{2}\right)\Delta t\left[(\Delta x)^2 u_{xxt} + \tfrac{1}{12}(\Delta x)^4 u_{xxxxt} + \cdots\right] \\ &+ \tfrac{1}{2}\left(\tfrac{1}{2}\Delta t\right)^2\left[(\Delta x)^2 u_{xxtt} + \tfrac{1}{12}(\Delta x)^4 u_{xxxxtt} + \cdots\right] + \cdots\Big]_j^{n+1/2}.\end{aligned} \tag{10}$$

Finally, with the operators calculated, we can calculate the truncation error. This quantity is what rest when we approximate $u(x_j, t_n)$, by U_j^n (section 2.5 of [7]). For the case of the Θ-method, this is given by

$$T_j^{n+1/2} = \delta_t u_j^{n+1/2} - \mu(\Theta\delta_x^2 u_j^{n+1} + (1-\Theta)\delta_x^2 u_j^n). \tag{11}$$

Then, by replacing Equations (4) and (10) in Equation (11), one ultimately obtain

$$\begin{aligned}T_j^{n+1/2} = \Big[&[u_t - u_{xx}] + \left[\left(\tfrac{1}{2} - \Theta\right)(\Delta t)u_{xxt} - \tfrac{1}{12}(\Delta x)^2 u_{xxxx}\right] \\ &+ \left[\tfrac{1}{3!}\left(\tfrac{1}{2}\Delta t\right)^2 u_{ttt} - \tfrac{1}{2}\left(\tfrac{1}{2}\Delta t\right)^2 u_{xxtt}\right] \\ &+ \left(\tfrac{1}{2} - \Theta\right)\tfrac{1}{12}\Delta t\,(\Delta x)^2 u_{xxxxt}\Big]_j^{n+1/2}.\end{aligned} \tag{12}$$

At least, this is the Equation (2.84) from [7], that can be used to calculate the truncation error of the Θ-method.

QUESTION 3

Write down the θ-discretisation for (1). Use a spatial (first-order) upwind discretisation for the advection term, which means that the sign of the wind $-a(t)$ determines the two-point stencil to be used. First clearly define your space-time mesh and its indexing (number according to Python-programming convention). Explicitly deal with and explain the scheme for mesh points near the boundary. That is provide complete theoretical detail. Specify a final formulation with the unknowns on the LHS and the knowns (as vector) on the RHS.

Solution:

In Equation (1), u can be approximated as

$$U_j^n \approx u(x_j, t_n). \tag{13}$$

The initial condition can be written as

$$U_j^0 = u^0(x_j), \tag{14}$$

and the boundary conditions are

$$U_0^n = 0, \tag{15}$$

and

$$U_J^n = 0. \tag{16}$$

Now, looking to equation (1a), for the first term I used a forward difference such as

$$u_t \approx \frac{U_j^{n+1} - U_j^n}{\Delta t}. \tag{17}$$

For the diffusion term (last term) I used a second order central difference

$$u_{xx} \approx \delta_x^2 U_j^n = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2}, \tag{18}$$

for the explicit term and

$$u_{xx} \approx \delta_x^2 U_j^{n+1} = \frac{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}{(\Delta x)^2}, \tag{19}$$

for the implicit term. Finally, for the advection term (second term in Equation (1a)) I am using a upwind discretisation, which I will define as

$$a(t_n)u_x \approx \frac{f_j^n}{\Delta x} = \begin{cases} a^n \frac{(U_{j+1}^n - U_j^n)}{\Delta x} & \text{for } a > 0, \\ a^n \frac{(U_j^n - U_{j-1}^n)}{\Delta x} & \text{for } a < 0, \end{cases} \tag{20}$$

for the explicity term and

$$a(t_{n+1})u_x \approx \frac{f_j^{n+1}}{\Delta x} = \begin{cases} a^{n+1} \frac{(U_{j+1}^{n+1} - U_j^{n+1})}{\Delta x} & \text{for } a > 0, \\ a^{n+1} \frac{(U_j^{n+1} - U_{j-1}^{n+1})}{\Delta x} & \text{for } a < 0. \end{cases} \tag{21}$$

Finally we can put everything together and obtain the explicit scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} - \frac{f_j^n}{\Delta x} - \epsilon \delta_x^2 U_j^n = 0, \tag{22}$$

which can be re-written as

$$U_j^{n+1} = U_j^n + \nu f_j^n + \epsilon\mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n), \tag{23}$$

where $\nu = \Delta t/\Delta x$, $\mu = \Delta t/(\Delta x)^2$ and the function f_j^n is defined in Equation (20) as the upwind scheme for the advection term. We can do the same for the implicit scheme

$$U_j^{n+1} = U_j^n + \nu f_j^{n+1} + \epsilon\mu(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}). \tag{24}$$

Ultimately we can write the Θ-method for approximating $u(x_j, t_{n+1})$ as

$$U_j^{n+1} = U_j^n + \Theta\left[\nu f_j^{n+1} + \epsilon\mu(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1})\right] + (1-\Theta)\left[(\nu f_j^n + \epsilon\mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n)\right]. \tag{25}$$

This expression is a general expression for any value of a, however, from now on I will consider only the case in which $a > 0$, and therefore use the forward difference for the advection term (first part of Equations (20) and (21)). Besides that, I will also write all the terms with $n + 1$ in the left-hand side, mas this terms will be unknown in most of the cases. By doing that Equation (25) become

$$\begin{aligned}(1 + \Theta\nu a^{n+1} + 2\Theta\epsilon\mu)U_j^{n+1} - \Theta(\nu a^{n+1} + \epsilon\mu)U_{j+1}^{n+1} - \Theta\epsilon\mu U_{j-1}^{n+1} \\ = [1 - (1 - \Theta)(\nu a^n + 2\epsilon\mu)]U_j^n + (1 - \Theta)(\nu a^n + \epsilon\mu)U_{j+1}^n + (1 - \Theta)\epsilon\mu U_{j-1}^n.\end{aligned} \tag{26}$$

To Solve this system, I defined the mesh grid shown in Figure 1. In this the space coordinate is mapped as $x_j = L_p + j\Delta x$, with $j = 0, 1, ..., J$, and the time coordinate is mapped as $t_n = n\Delta t$, with $n = 0, 1, ...$ In this Figure, the known values are represented by the blue mark, while the unknown values are represented by the purple circles. The first value of x, is defined by the boundary condition as $x_{j=0} = L_p$, and the last boundary condition is given by $x_J = L_p + J\Delta x = L$. The first unknown value is in $j = 1$. The array of unknown values are represented by z_k, such as $k = j + 1$, with $k = 0, 1, ..., m - 1$, where $m = J - 1$.

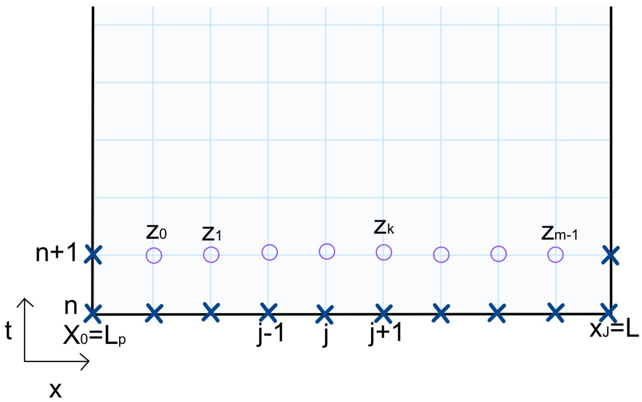

Figure 1: Space-time mesh for the Θ-method. The blue markers represents the known values (boundary condition and initial condition), while the purple circles represents the unknowns. The rows are refereed to by the index n, that is related to time as $t_n = n\Delta t$, with $n = 0, 1, ...$ The columns are labelled with the index j, that define the spatial coordinate $x_j = L_p + j\Delta x$, with $j = 0, 1, ..., J$.

With that I can define a vector of unknowns $\mathbf{z}$, a matrix A that contain the coefficients from the left side of Equation (26), and another vector $\mathbf{b}$ that contain the knowns in the right side of Equation (26). Ultimately I can use this to solve the linear systems as

$$A\mathbf{z} = \mathbf{b}. \tag{27}$$

Given that, there is three distinct cases that I came across when solving this system. The first case is represented in Figure (2a), it is for the first unknown, z_0 in $j = 1$. For this case, the term $\Theta\epsilon\mu U_0^{n+1}$ is known by the boundary condition. In the specific case of Equation (1c), this term is zero. Nevertheless, a general for of Equation (26) for this case can be written as

$$\begin{aligned}(1 + \Theta\nu a^{n+1} + 2\Theta\epsilon\mu)U_1^{n+1} - \Theta(\nu a^{n+1} + \epsilon\mu)U_2^{n+1} \\ = [1 - (1 - \Theta)(\nu a^n + 2\epsilon\mu)]U_1^n + (1 - \Theta)(\nu a^n + \epsilon\mu)U_2^n + (1 - \Theta)\epsilon\mu U_0^n - \Theta\epsilon\mu U_0^{n+1}.\end{aligned} \tag{28}$$

The second case that appears when solving this system for a middle point z_k away from the borders, this is shown in Figure (2b). In this all the terms in the left-hand side of Equation (26) are unknowns.

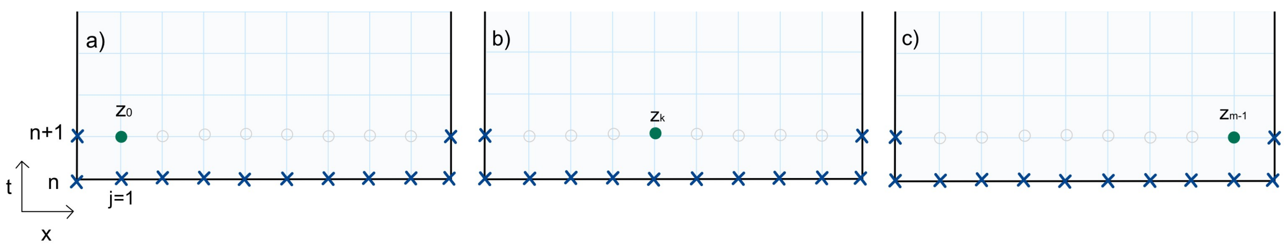

Figure 2: Grid mesh for the for the different cases considered when solving Equation(1) using the *Theta*–method.

The final case is for the last point z_{m-1}, that is in $j = J - 1$. for this case $\Theta(\nu a^{n+1} + \epsilon\mu)U_J^{n+1}$ is known from the boundary conditions, and the general for of Equation (26) can be written as

$$\begin{aligned}&(1+\Theta\nu a^{n+1}+2\Theta\epsilon\mu)U_{J-1}^{n+1}-\Theta\epsilon\mu U_{J-2}^{n+1}\\ &=[1-(1-\Theta)(\nu a^n+2\epsilon\mu)]U_{J-1}^n+(1-\Theta)(\nu a^n+\epsilon\mu)U_J^n+(1-\Theta)\epsilon\mu U_{J-2}^n+\Theta(\nu a^{n+1}+\epsilon\mu)U_J^{n+1}.\end{aligned} \tag{29}$$

QUESTION 4

Implement the explicit scheme (without matrix inversion) and reproduce Fig. 2.2 of M&M. Use the vector set-up of Python in the code. Make similar plots as in Fig. 2.2 of M&M, but display multiple time-profiles in one plot for fixed Δt. Explain the stability properties of the explicit scheme with both the results of a Fourier analysis and the maximum principle. Extend the explicit scheme to (1) above.

Solution:

The Figure 2.2 from [7] is a solution for the problem

$$u_t = u_{xx} \quad \text{for } x \in [0,1] \tag{30a}$$

$$u(x,0) = u^0(x) = \begin{cases} 2x & \text{if } 0 \le x \le 1/2 \\ 2-2x & \text{if } 1/2 \le x \le 1 \end{cases} \tag{30b}$$

$$u(0,t) = u(1,t) = 0 \tag{30c}$$

$$\tag{30d}$$

This system has exact solution, given by the Equation (2.11) from [7]

$$u(x,t) = \sum_{m=1}^{\infty} a_m sin(m\pi x), \tag{31}$$

where the coefficients a_m are given by

$$a_m = 2\int_0^1 u^0(x) sin(m\pi x)dx. \tag{32}$$

For the initial condition in Equation (30b), this is written as

$$a_m = 2\left(\int_0^{1/2} 2x\sin(m\pi x)dx + \int_{1/2}^1 (2-2x)\sin(m\pi x)dx\right) = \frac{8}{(m\pi)^2}\sin\left(\frac{m\pi}{2}\right). \tag{33}$$

Because we can not calculate the series in Equation (31) until the infinity, I define a maximum value M for the sum. And with that, the exact solution to be implemented in the code is

$$u(x,t) = \sum_{m=1}^{M} \frac{8}{(m\pi)^2}\sin\left(\frac{m\pi}{2}\right)\sin(m\pi x). \tag{34}$$

In Figure (2.2) of [7], it is stated that they used the parameters $J = 20$, and consequently $\Delta x = 0.05$, and $\Delta t = 0.0012$ and $\Delta t = 0.0013$. The explicit scheme used to solve it is given by

$$U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_j^n). \tag{35}$$

For the exact solution, they did not mentioned what is the maximum value M they used in the series, therefore I chose $M = 100$.

In Figure (3) is my solution for the reproduction of Figure (2.2) of [7]. In Figure (4) I reproduce the result in the previous Figure but for different time-steps. The code for plotting both these figures is in `Question4/step1-reproduction_fig2-2_M&M.ipynb`.

By these two figures, one ca see that the result is stable for $\Delta t = 0.0012$ and unstable for $\Delta t = 0.0013$. In section 2.6 of [7] they show, using the maximum principle, that the condition for stability of the explicit scheme is given by $\mu = \Delta t/(\Delta x)^2 \le 1/2$, in the following section, they do a Fourier analysis that endorses this result. For $\Delta x = 0.05$, when $\Delta t = 0.0012$, then $\mu = 0.48$, which fulfil the stability condition. On the other hand, when $\Delta t = 0.0013$, we get $\mu = 0.51$, which is the reson for us to obtain the instability observed on right side plots in Figures (3) and (4).

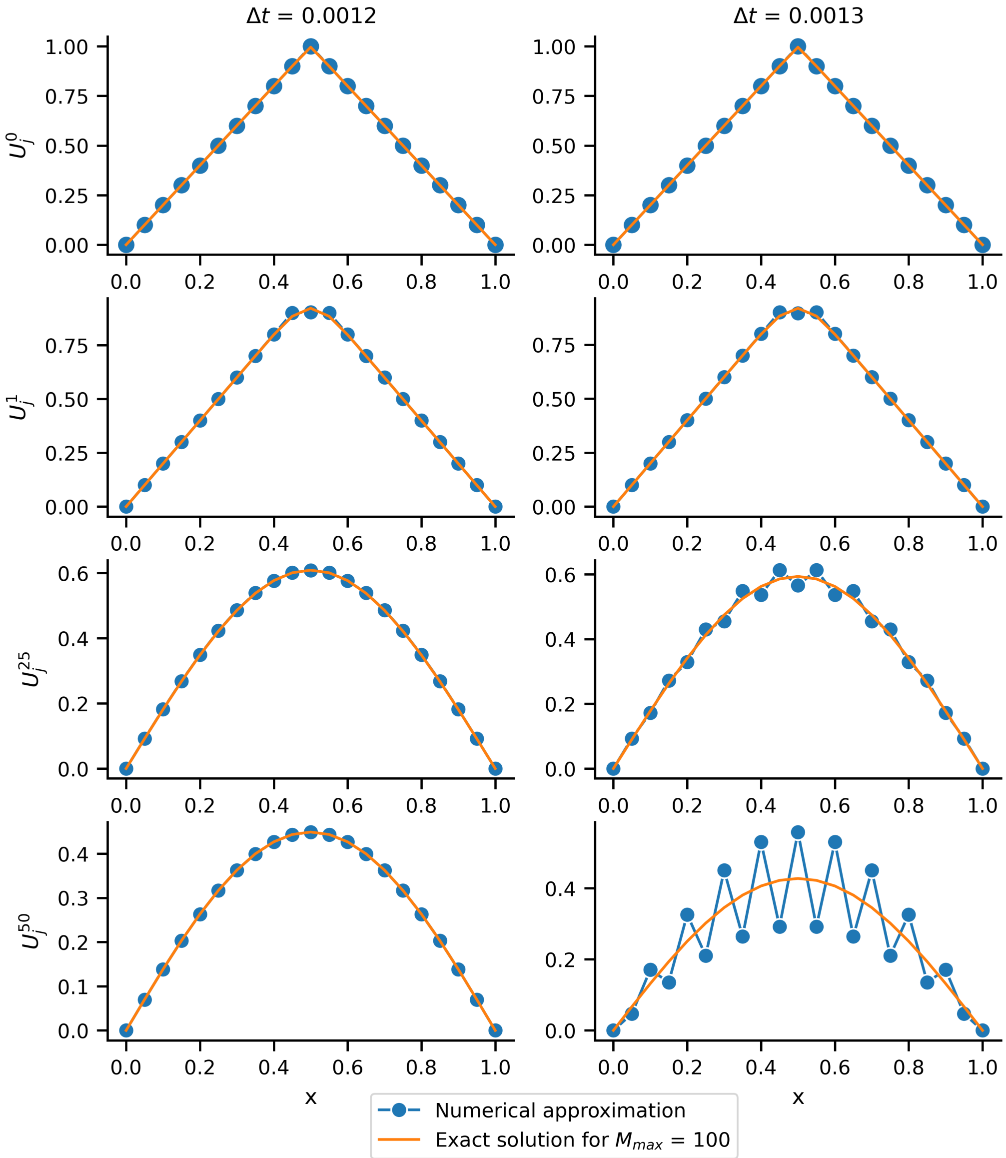

Figure 3: Reproduction of Figure 2.2 from [7].

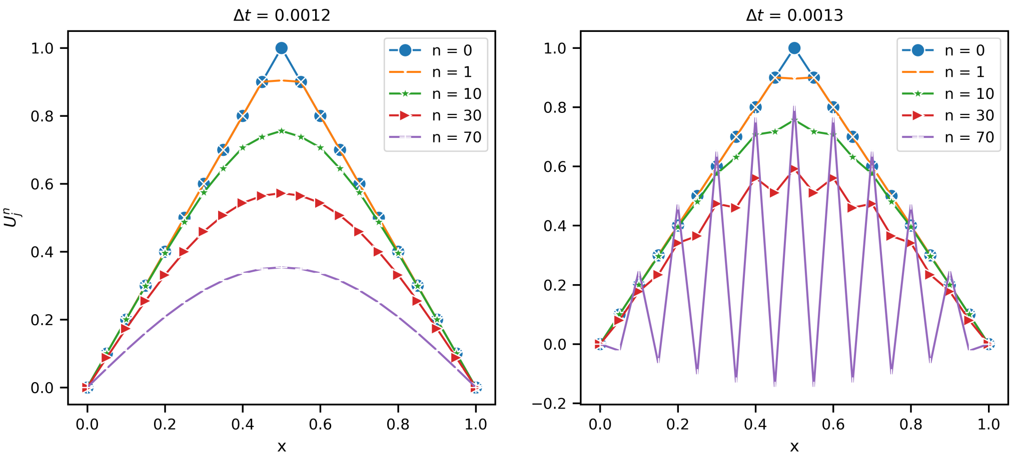

Figure 4: Reproduction of Figure 2.2 for different time-steps.

In the last step of this exercise, I will extend the explicit scheme to Equation (1). I for this case I will use the similar initial condition given in Equation (30b), but because the domain of Equation (1) is $[-1, 1]$, the

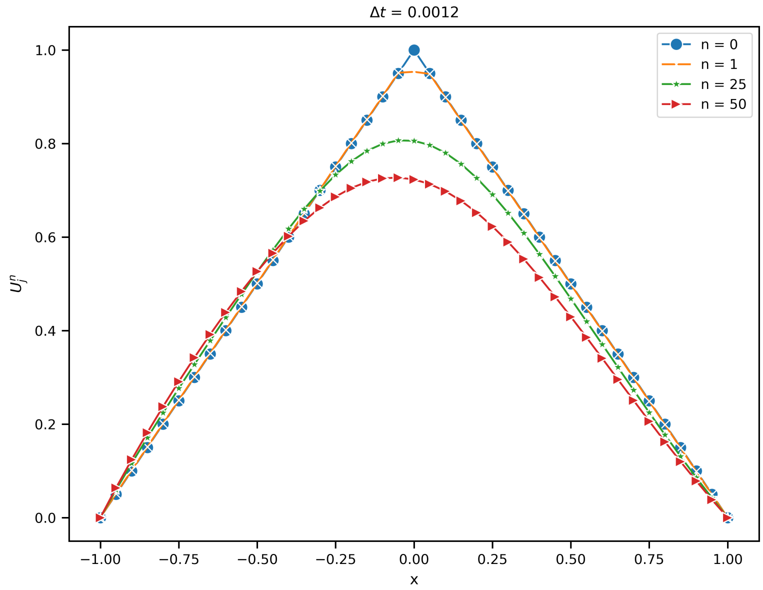

Figure 5: In this plot I extended the solution used in the previous Figures to the problem in Equation (1), I used $a = \epsilon = 1$.

initial condition will be given by

$$u(x,0) = u^0(x) = \begin{cases} 1+x & \text{if } -1 \le x \le 0 \\ 1-x & \text{if } 0 < x \le 1 \end{cases}. \tag{36}$$

Because the domain is bigger, to obtain the same $\Delta x = 0.05$, I have to set $J = 40$. The explicit scheme for this case is given in Equation (23) of the previous question. I am also assuming $a(t) = 1$ and $\epsilon = 1$. Thye results for different time steps is plotted in Figure (5). The code that solve this and plot this image is in `Question4/step2-Extend_the_explicit_sc_to Eq1.ipynb`.

QUESTION 5

Implement the θ–scheme and use the linear algebra routines in Python to solve the matrix system, for varying spatial resolutions. Explain the stability properties of the θ–scheme with both the results of a Fourier analysis and the maximum principle for the advection and diffusion parts in separation (advanced: when you can explore the full case, e.g. by numerically displaying the expressions). Oberve that the amplitude error is zero for CFL = 1 when $\epsilon = 0$.

Solution:

I implemented the Θ–method as I described in Question 3. I kept the same initial condition, boundary condition and parameters used in Question 4 for the explicit method, however I set $\Theta = 1/2$. The code that solve it is in `Question5/theta_method-diffusion_advection.ipynb`, and the first output is a plot that is a reproduce the results for the explicit scheme, shown in Figure (5), but now using the *Theta*–method, with the aforementioned parameters, this result is shown in Figure (6).

This code was made so it was possible to vary spatial and temporal resolutions, as well as vary the parameters. For the spatial resolution, specifically, the way you do it is by varying the variable J, that is the max index of the vector $\mathbf{x}$. In another words, if $\Delta x = (L - L_p)/J$, then $\Delta x/\omega = (L - L_p)/\omega J$, therefore, if one wishes to use $\Delta x/2$, it is just a matter of multiplying J by the same factor. This logic was used to produce Figure (7) for which I use $\omega = 0.5, 1, 2, 4$.

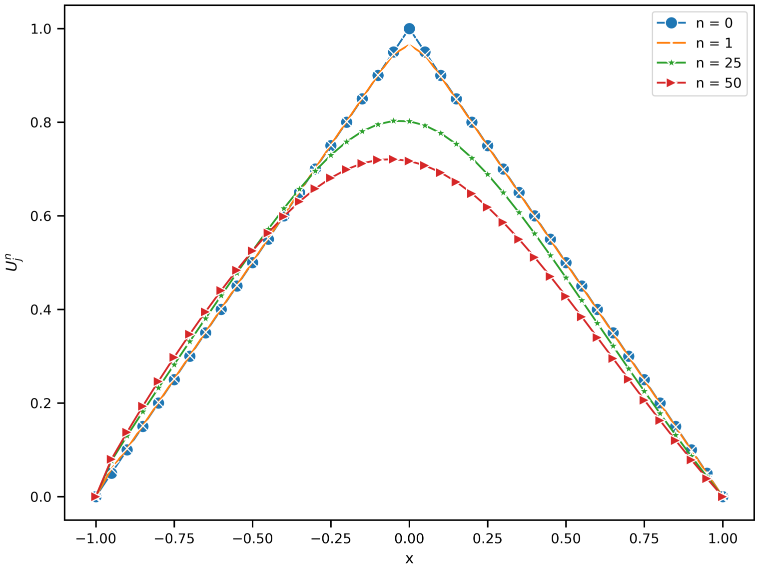

Figure 6: Reproduction of Figure (5) using Θ-method. Using $a = \epsilon = 1$, $\Delta t = 0.0012$ and $J = 40$

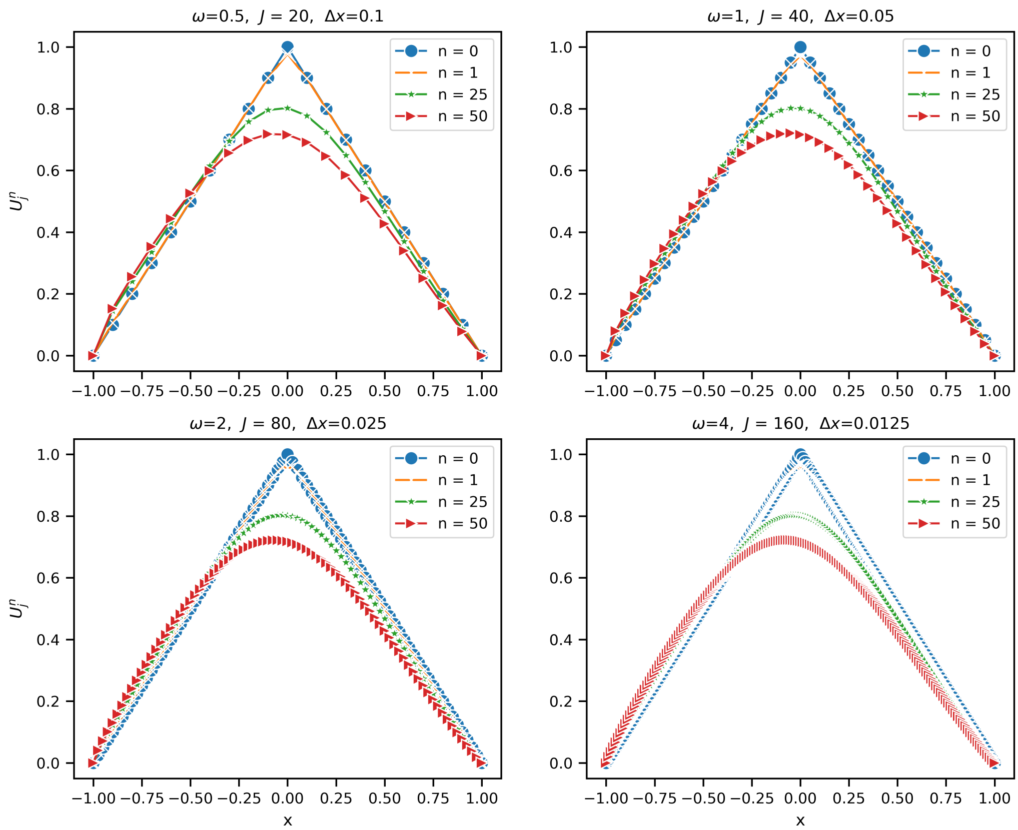

Figure 7: Solutions of Equation (1), using Θ–method with different spatial resolutions. With $a = \epsilon = 1$.

Regrating the convergence I will start by Equation (25) and write it by the case where $a > 0$

$$U_j^{n+1} = U_j^n + \Theta\left[\nu a^{n+1}(U_{j+1}^{n+1} - U_j^{n+1}) + \epsilon\mu(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1})\right] \\ +(1-\Theta)\left[\nu a^n(U_{j+1}^n - U_j^n) + \epsilon\mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n)\right]. \tag{37}$$

Now I will assume $U_j^n = \lambda^n e^{ikj\Delta x}$, this way, we get stability if $|\lambda| \leq 1$. Replacing this in the previous equation we have

$$\begin{aligned}\lambda^{n+1}e^{ik(j)\Delta x} &= \lambda^n e^{ikj\Delta x} \\ &+ \Theta\left[\nu a^{n+1}(\lambda^{n+1}e^{ik(j+1)\Delta x} - \lambda^{n+1}e^{ikj\Delta x}) + \epsilon\mu(\lambda^{n+1}e^{ik(j+1)\Delta x} - 2\lambda^{n+1}e^{ikj\Delta x} + \lambda^{n+1}e^{ik(j-1)\Delta x})\right] \\ &+ (1-\Theta)\left[\nu a^n(\lambda^n e^{ik(j+1)\Delta x} - \lambda^n e^{ikj\Delta x}) + \epsilon\mu(\lambda^n e^{ik(j+1)\Delta x} - 2\lambda^n e^{ikj\Delta x} + \lambda^n e^{ik(j-1)\Delta x})\right]\end{aligned}$$

after some algebra we can re-write this Equation as

$$\lambda = 1 + \lambda\Theta\left[\nu a^{n+1}(e^{ik\Delta x} - 1) + \epsilon\mu(e^{ik\Delta x} - 2 + e^{-ik\Delta x})\right] \\ + (1-\Theta)\left[\nu a^n(e^{ik\Delta x} - 1) + \epsilon\mu(e^{ik\Delta x} - 2 + e^{-ik\Delta x})\right]$$

then

$$\lambda\left\{1 - \Theta\left[\nu a^{n+1}(e^{ik\Delta x} - 1) + \epsilon\mu(e^{ik\Delta x} - 2 + e^{-ik\Delta x})\right]\right\} \\ = 1 + (1-\Theta)\left[\nu a^n(e^{ik\Delta x} - 1) + \epsilon\mu(e^{ik\Delta x} - 2 + e^{-ik\Delta x})\right]$$

and finally

$$\lambda = \frac{1 + (1-\Theta)\left[\nu a^n(e^{ik\Delta x} - 1) + \epsilon\mu(e^{ik\Delta x} - 2 + e^{-ik\Delta x})\right]}{1 - \Theta\left[\nu a^{n+1}(e^{ik\Delta x} - 1) + \epsilon\mu(e^{ik\Delta x} - 2 + e^{-ik\Delta x})\right]} \tag{38}$$

For the diffusion part, when $a = 0$, we have a case analogous to what is shown in section 2.11 of [7], we have stability when

$$\mu \leq \frac{1}{2\epsilon(1-2\Theta)}. \tag{39}$$

On the other hand, for the pure advection case, when $\epsilon = 0$, Equation (38) is given as

$$\lambda = \frac{1 + (1-\Theta)\nu a^n(e^{ik\Delta x} - 1)}{1 - \Theta\nu a^{n+1}(e^{ik\Delta x} - 1)}. \tag{40}$$

I will consider that a is constant, in a way that $a^{n+1} = a^n$, and use the Euler formula $e^{i\theta} = \cos(\theta) + i\sin(\theta)$, to write

$$\lambda = \frac{1 + (1-\Theta)\nu a[\cos(k\Delta x) + i\sin(k\Delta x) - 1]}{1 - \Theta\nu a[\cos(k\Delta x) + i\sin(k\Delta x) - 1]}. \tag{41}$$

Next I will use the identity $\cos(2\theta) - 1 = -2\sin^2(\theta)$, and "separate" the real and imaginary part

$$\lambda = \frac{[1 - 2(1-\Theta)\nu a\sin^2(k\Delta x/2)] + i(1-\Theta)\nu a\sin(k\Delta x)}{[1 + 2\Theta\nu a\sin^2(k\Delta x/2)] - i\Theta\nu a\sin(k\Delta x)}. \tag{42}$$

We have as stability condition that $|\lambda| \leq 1$, with that we cal also state that $|\lambda|^2 \leq 1$. In Equation (42), I obtained that for this case, λ is a complex number. The way to calculate the the squared magnitude of a complex number is by multiplying it for its complex conjugate λ^*, as in

$$|\lambda|^2 = \left(\frac{[1 - 2(1-\Theta)\nu a\sin^2(k\Delta x/2)] + i(1-\Theta)\nu a\sin(k\Delta x)}{[1 + 2\Theta\nu a\sin^2(k\Delta x/2)] + i\Theta\nu a\sin(k\Delta x)}\right)\left(\frac{[1 - 2(1-\Theta)\nu a\sin^2(k\Delta x/2)] - i(1-\Theta)\nu a\sin(k\Delta x)}{[1 + 2\Theta\nu a\sin^2(k\Delta x/2)] + i\Theta\nu a\sin(k\Delta x)}\right) \tag{43}$$

we can re-write this Equation as

$$|\lambda|^2 = \frac{[1 - 2(1-\Theta)\nu a\sin^2(k\Delta x/2)]^2 + (1-\Theta)^2(\nu a)^2\sin^2(k\Delta x)}{[1 + 2\Theta\nu a\sin^2(k\Delta x/2)]^2 + (\Theta\nu a)^2\sin^2(k\Delta x)} \leq 1, \tag{44}$$

next, I expand the squared term and multiply the whole inequation by the denominator

$$1 - 4(1-\Theta)\nu a\sin^2(k\Delta x/2) + 4(1-\Theta)^2(\nu a)^2\sin^4(k\Delta x/2) + (1-\Theta)^2(\nu a)^2\sin^2(k\Delta x) \\ \leq 1 + 4\Theta\nu a\sin^2(k\Delta x/2) + 4(\Theta\nu a)^2\sin^4(k\Delta x/2) + (\Theta\nu a)^2\sin^2(k\Delta x),$$

by subtracting 1 and dividing by νa in both sides we get

$$\begin{aligned}-4(1-\Theta)\sin^2(k\Delta x/2)+4(1-\Theta)^2(\nu a)\sin^4(k\Delta x/2)+(1-\Theta)^2(\nu a)\sin^2(k\Delta x)\\ \leq +4\Theta\sin^2(k\Delta x/2)+4(\Theta\nu a)\sin^4(k\Delta x/2)+(\Theta\nu a)\sin^2(k\Delta x),\end{aligned}$$

now I pass all terms to the left-hand side and expand any term $(1-\Theta)^2$

$$\begin{aligned}-4(1-\Theta)\sin^2(k\Delta x/2)-4\Theta\sin^2(k\Delta x/2)\\ +4(1-2\Theta+\Theta^2)(\nu a)\sin^4(k\Delta x/2)-4(\Theta\nu a)\sin^4(k\Delta x/2)\\ +(1-2\Theta+\Theta^2)(\nu a)\sin^2(k\Delta x)-(\Theta\nu a)\sin^2(k\Delta x)\leq 0,\end{aligned}$$

I can simplify this expression as

$$-4\sin^2(k\Delta x/2)+4(1-2\Theta)(\nu a)\sin^4(k\Delta x/2)+(1-2\Theta)(\nu a)\sin^2(k\Delta x)\leq 0, \tag{45}$$

the I can write this equation as

$$-4\sin^2(k\Delta x/2)+(1-2\Theta)\nu a[4\sin^4(k\Delta x/2)+\sin^2(k\Delta x)]\leq 0. \tag{46}$$

Then I use the identity $\sin(2\theta)=2\sin(\theta)\cos(\theta)$ to write

$$-4\sin^2(k\Delta x/2)+(1-2\Theta)\nu a[4\sin^4(k\Delta x/2)+4\sin^2(k\Delta x/2)\cos^2(k\Delta x/2)]\leq 0, \tag{47}$$

I can take $4\sin^4(k\Delta x/2)$ out of the brackets to get

$$-4\sin^2(k\Delta x/2)+4(1-2\Theta)\nu a\sin^2(k\Delta x/2)[\sin^2(k\Delta x/2)+\cos^2(k\Delta x/2)]\leq 0, \tag{48}$$

and because $\sin^2(k\Delta x/2)+\cos^2(k\Delta x/2)=1$ we have

$$-4\sin^2(k\Delta x/2)+4(1-2\Theta)\nu a\sin^2(k\Delta x/2)\leq 0, \tag{49}$$

now I can divide everything by $4\sin^2(k\Delta x/2)$ and I get

$$(1-2\Theta)\nu a\leq 1, \tag{50}$$

We then finally get

$$\nu a\leq\frac{1}{(1-2\Theta)}, \tag{51}$$

which is the stability condition for when a is a constant, and >0. Just a remainder that here $\nu=\Delta t/\Delta x$. The quantity $a\nu=a\Delta t/\Delta x$ is the CFL number, and it is equal to 1 for the full explicit case, when $\Theta=0$. In Figure (8) we can observe this condition, the orange line is for $CFL=1/(1-2\Theta)$, above this line we have instability, while bellow it we have stability. The code that makes this plot is in `Question5/stability_convergence_advection.ipynb`.

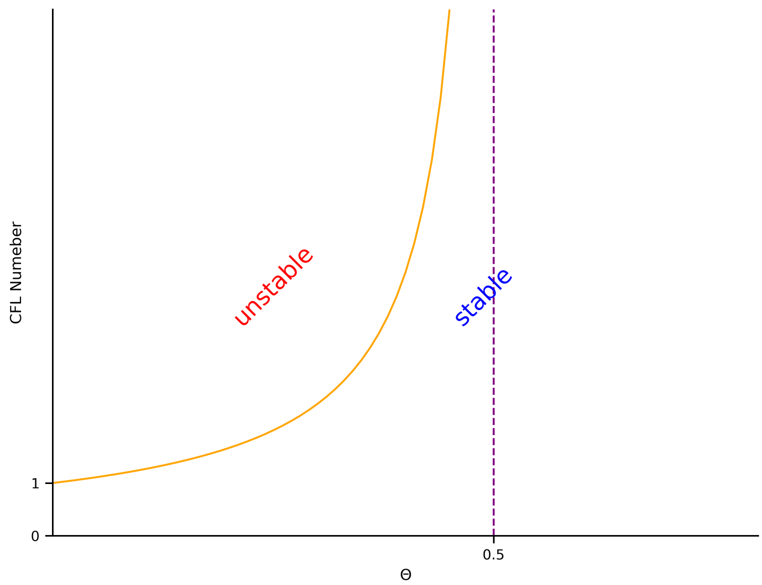

Figure 8: Stability analysis for the advection equation.

QUESTION 6

First explore the case $a(t) = 1$ with

$$u(x,0) = (1-x)^4(1+x) \quad \text{and then} \quad u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\phi_k(x) + C\right) \tag{2}$$

for $L_p = -1$, $L = 1$, $\epsilon = 10^{-3}$, $T = 1$ with $t \in [0,T]$, Legendre polynomials $\phi_k(x) = 1, x, \frac{3}{2}x^2 - \frac{1}{2}, \frac{5}{2}x^3 - \frac{3}{2}x$ and random coefficients $b_k \in [0,1)$ (uniform distribution and for $k = 0, \ldots 3$). A constant $C \geq 0$ is determined (numerically) such that $\sum_{k=0}^{3} b_k\phi_k(x) + C \geq 0$. Verify that for the appropriate θ the same numerical results are obtained as for the implementation of an explicit scheme. Display some time profiles at set times rather than set iterations for a few values of θ, μ. Use a while-time-loop with discrete time, not one using iterations. Clearly define how the stability/instability and the (violation of the) maximum principle are (numerically) determined and displayed in a μ–θ parameter plot. Find at least three μ, θ-values illustrating the three possible cases $\theta = 0, 1/2, 1$. Interpret and discuss your findings. In the end, choose $\theta = 1$, where CFL = 1 works, and argue why this choice seems necessary (Choi et al., 2024). (Report your b_k's, one of my draws was $b_k = [0.223291080, 0.523163340, 0.550701460, 0.045601950, 0.36072884]$).

Solution:

In the first part of this question I applied the theta method to Equation (1) using the first initial condition given by

$$u(x,0) = (1-x)^4(1+x). \tag{52}$$

I also actualized the diffusion term to $\epsilon = 10^{-3}$. I solved for Three values of $\Theta = [0, 1/2, 1]$ and three values of $\mu = [0.49, 0.5, 1.0]$. The results for this part is presented in Figure (9), and it was generated using the code `Question6/part-1-theta_method-diffusion_advection.ipynb`.

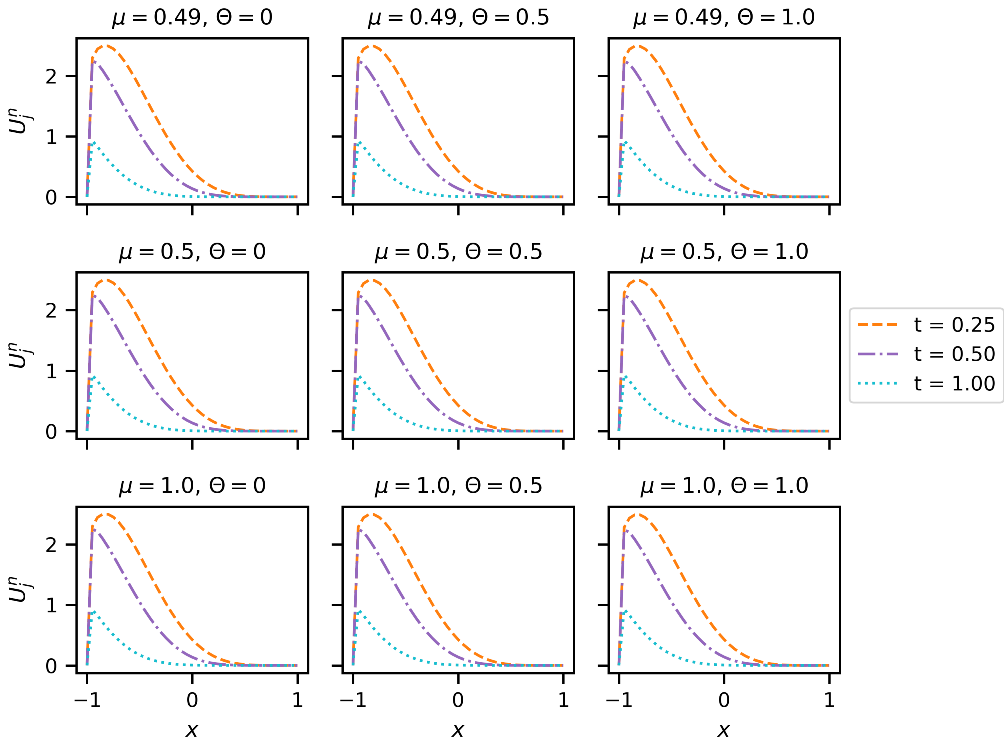

Figure 9: Solutions of Equation (1), using the initial condition given by Equation (52), $a = 1$, $\epsilon = 10^{-3}$, $\Delta x = 0.05$ and $\Delta t = \mu * (\Delta x)^2$.

Next I change the initial conditions to

$$u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\phi_k(x) + C\right). \tag{53}$$

I determined C numeric by calculating $LP = \sum_{k=0}^{3} b_k \phi_k(x)$ for all x values, then I found the minimum value of LP, if it was less than zero then I summed the absolute value of $\min(LP)$ to the whole $LP(x)$. Besides that, I used $\epsilon = 10^{-3}$, $a = 1$, and the random generate b_k coefficients where [0.6229016948897019, 0.7417869892607294, 0.7951935655656966, 0.9424502837770503]. Ultimately, I solved Equation (1) for Three values of $\Theta = [0, 1/2, 1]$ and three values of $\mu = [0.49, 0.5, 1.0]$. The results for this is in Figure (10), and it was generated using the code `Question6/part-2-legendreIC-theta_method-diffusion_advection.ipynb`.

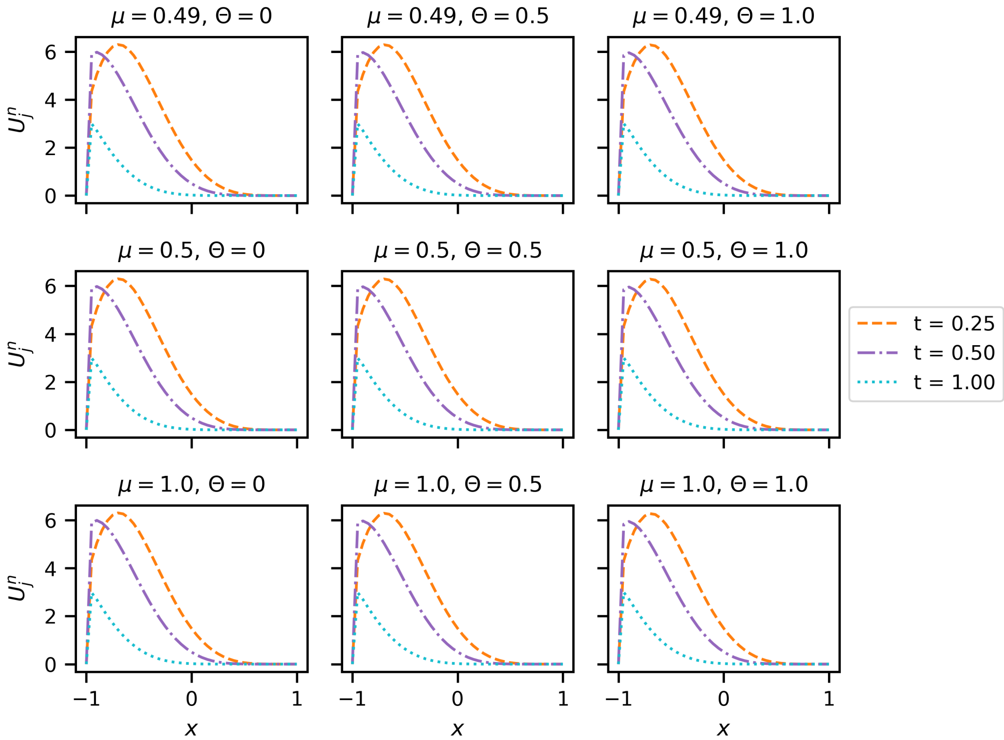

Figure 10: Solutions of Equation (1), using the initial condition given by Equation (53), with $a = 1$, $\epsilon = 10^{-3}$, $\Delta x = 0.05$ and $\Delta t = \mu * (\Delta x)^2$, and Legendre coefficients [0.6229016948897019, 0.7417869892607294, 0.7951935655656966, 0.9424502837770503].

In both Figures (9) and (10), I did not observed instabilities, even for $\mu = 1$ and $\Theta = 0$, which looks very odd. But $\mu = \Delta t/(\Delta x)^2$ is a quantity that is related to the instability of the diffusion term. However, in this example, the diffusion coefficient is very small ($\epsilon = 1^{-10}$), which means that what is dominating the stability of the problem is the advection therm, that is related to $CFL = a\nu = a\Delta t/\Delta x$, and for $\mu = 1$, $CFL = 0.05$ which is way bellow the stability condition, even for $\Theta = 0$.

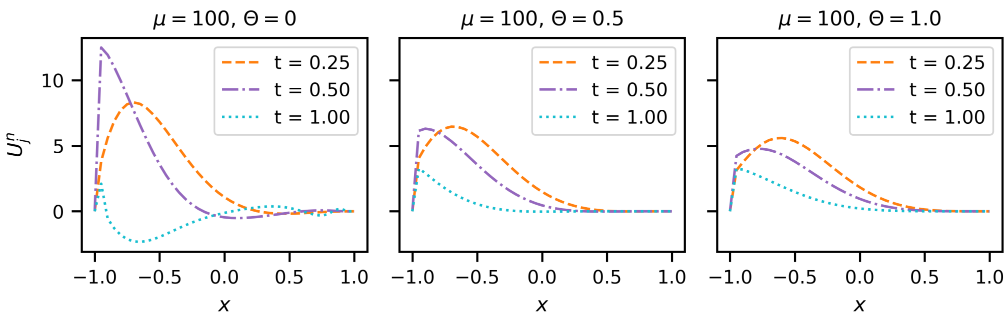

Figure 11: Solutions of Equation (1), using the initial condition given by Equation (53), with $a = 1$, $\epsilon = 10^{-3}$, $\Delta x = 0.05$ and $\Delta t = \mu * (\Delta x)^2$, and Legendre coefficients [0.6229016948897019, 0.7417869892607294, 0.7951935655656966, 0.9424502837770503].

On the other hand, if we have $CFL = 1$, we would get $\mu = 20$, with is out of the range tested in the previous figures. So I did a similar plot, but now I chose $\mu = 100$, which is well above the μ that I calculated for $CFL = 1$. The results for this is shown in Figure (11), we can see that, in this case, for $\Theta = 0$ (left most plot) we have that the curve for $t = 0.5$ is going above the curve for $t = 0.25$, and this is a sing that the convergence in unstable, once diffusion should dissipate with time. However, when we increase Θ, we see that the curves start to converge again, it is what is observed in the plot in the right for $\Theta = 1$.

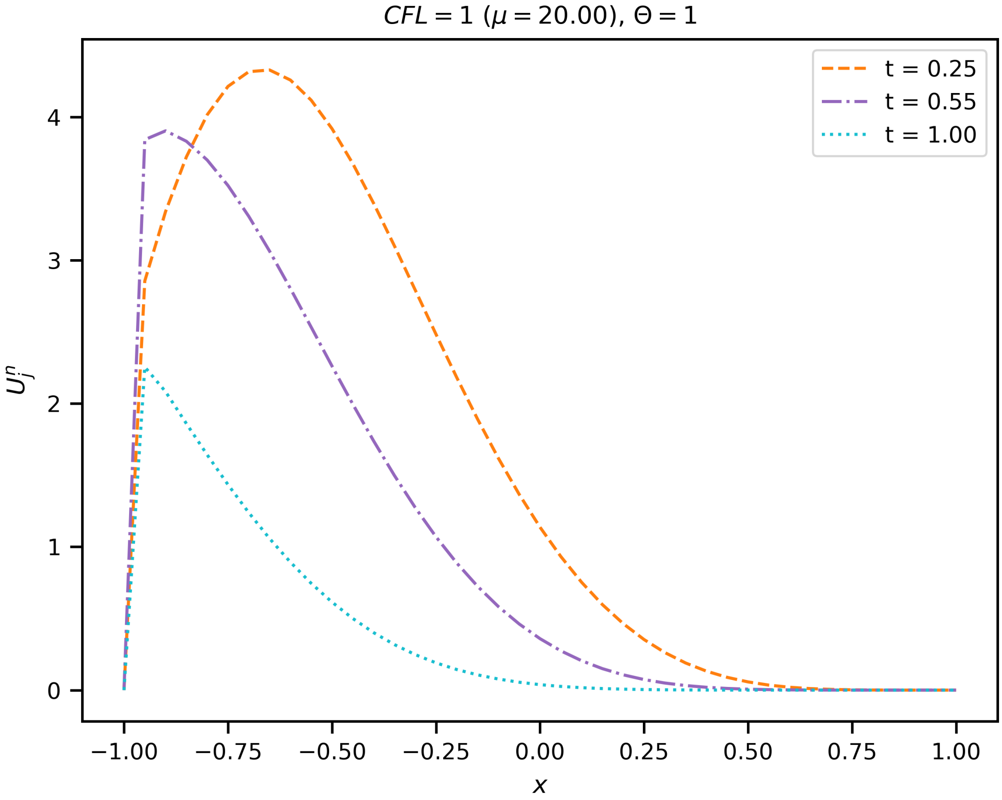

Figure 12: Solutions of Equation (1), using the initial condition given by Equation (53), with $a = 1$, $\epsilon = 10^{-3}$, $\Delta x = 0.05$ and $\Delta t = CFL * delta_x/a$, and Legendre coefficients [0.23796462709189137, 0.5442292252959519, 0.36995516654807925, 0.6039200385961945].

Finally, in Figure (12) I chose $CFL = 1$ and $\Theta = 1$, and plotted the same time steps. The Legendre coefficients obtained for this Figure were [0.23796462709189137, 0.5442292252959519, 0.36995516654807925, 0.6039200385961945].

QUESTION 7

Second, consider the case $a(t) = 1$ and initial condition (see Choi et al. 2024)

$$u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k \phi_k(x) + C\right) \tag{3}$$

for $L_p = -1$, $L = 1$, $\epsilon = 10^{-3}$, $T = 1$ with $t \in [0, T]$. Graphically confirm convergence of your simulations by refining Δx. Display some time profiles at set times (e.g., $t = 0, 0.25, 0.5, 0.75, 1$ in one plot and also zoom-in near $x = -1$) rather than set iterations for $\theta = 1$. Interpret and discuss your findings. (Report your b_k's).

Solution:

In this question I explore the effect of the spatial resolution in the convergence of the solution of Equation (1). Just like in Figure (12) I fixed $CFL = 1$ and used $\Theta = 1$. To variate Δx I used the method I explained on Question 5, where I consider a factor ω such that $\Delta x/\omega = (L - L_p)/\omega J$, and I vary the spatial resolution by varying ω. I start with $J = 40$, and therefore $\Delta x = 0.05$. Then I use $\omega = [1, 2, 4]$, which lead to $\Delta x = [0.05, 0.025, 0.0125]$. The results are shown in Figure (13), the b_k's obtained for the Legendre polynomial in this case were [0.5714025946899135, 0.4288890546751146, 0.5780913011344704, 0.20609823213950174]. And all of this is made on the notebook `Question7/legendreIC-theta_method-diffusion_advection.ipynb`.

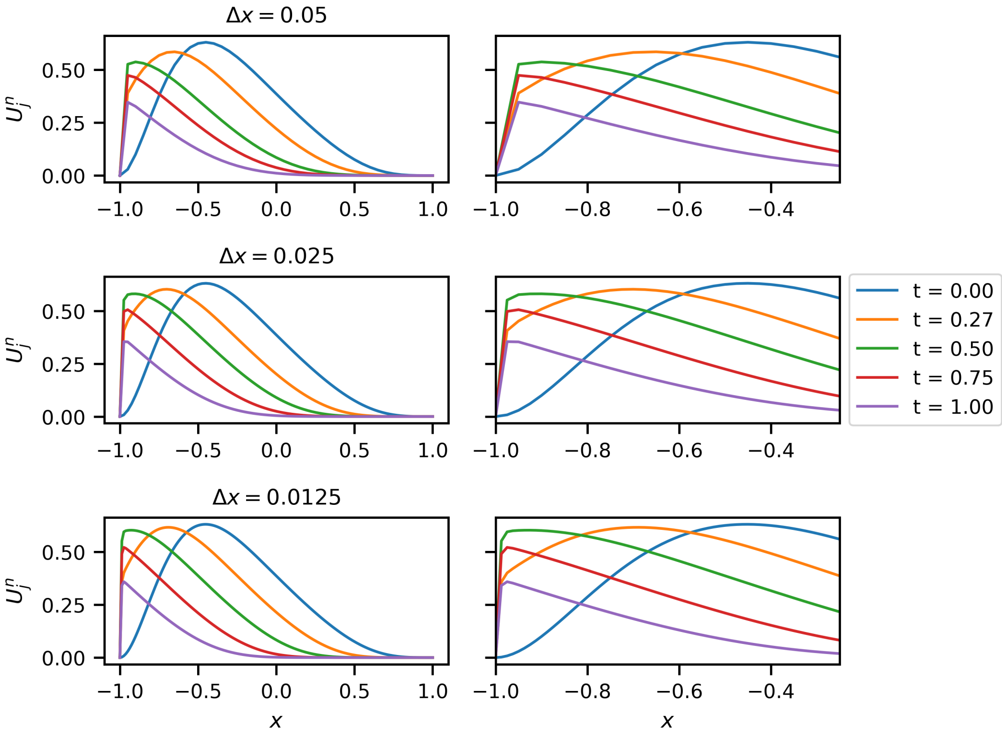

Figure 13: Solutions of Equation (1), using the initial condition given by Equation (52), $a = 1$, $\epsilon = 10^{-3}$, $CFL = 1$, $\Theta = 1$ and $\Delta t = CFL * (\Delta x)/a$. The Legendre coefficients obtained for this figure were [0.5714025946899135, 0.4288890546751146, 0.5780913011344704, 0.20609823213950174]. The left plots are the whole domain, and the right plots are the zoom close to -1.

In Figure (13), in the plots of the columns in the right we can see a zoom close to L_p of the plots of the left columns. What stand out from the refinement of the spatial resolution is the fact that, for smaller Δx, the line get closer to the border. It seems clear that the advection term is responsible for a transport in direction to L_p.

QUESTION 8

Third, explore the previous case for smaller values of ϵ, $10^{-4}, \ldots, 10^{-6}$. Report, interpret and discuss your findings (see Choi et al., 2024).

Solution:

In this question I explore different values for the diffusion coefficient. I used $a = 1$, $CFL = 1$, $\Theta = 1$, $\Delta x = 0.05$ and $\epsilon = [1, 1e-3, 1e-6, 1e-9]$, the results for this are displayed on Figure (14), and it is generated with the code in `Question7/legendreIC-theta_method-diffusion_advection.ipynb`.

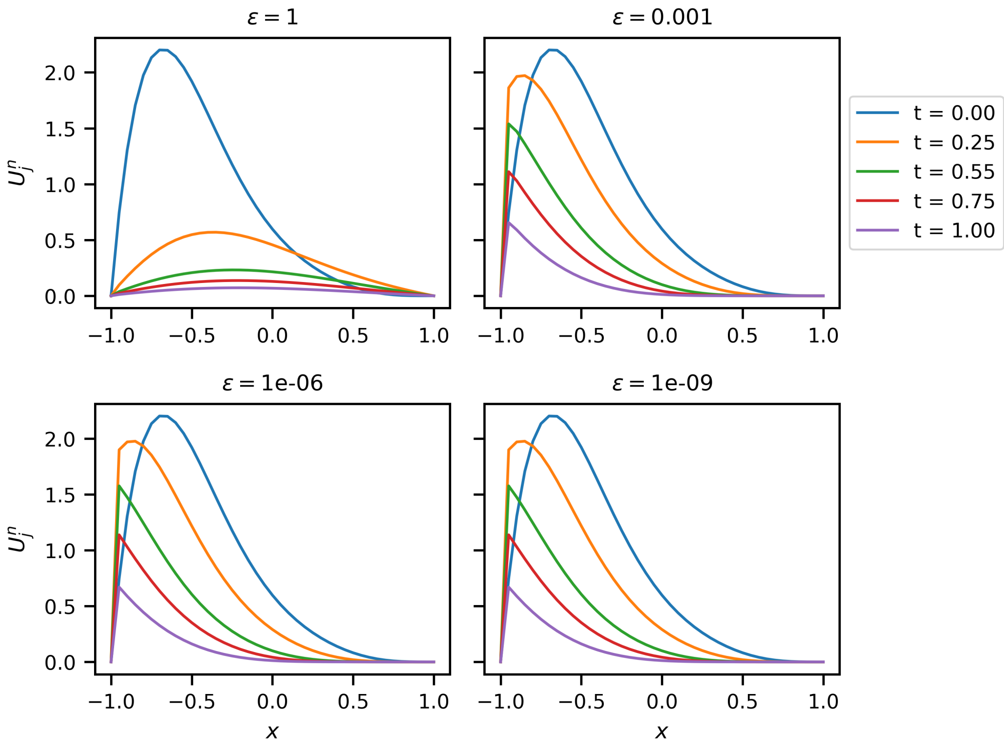

Figure 14: Solutions of Equation (1), using the initial condition given by Equation (52), $a = 1, CFL = 1, \Theta = 1, \Delta x = 0.05$ and $\Delta t = CFL * (\Delta x)/a$. The Legendre coefficients obtained for this figure were [0.965242141552123, 0.011654693792141124, 0.7359916197968754, 0.15801272476474815].

When ϵ is big, the effects of diffusion competes with the effects of advection, and U_J^n start to be spread along x as the time passes. As ϵ start to get smaller, the advection term start to take over, and U_j^n start to be transported closer to the border.

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