NUMERICAL METHODS FOR PDE

List of Exercises N°3

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1. Let us consider the differential equation

$$u_t + au_x = 0, \quad x \in (0,1), \quad t \geq 0, \quad a > 0 \tag{1}$$

with initial condition

$$u(x,0) = \sin(2\pi x),$$

and periodic boundary conditions, that is

$$u(0,t) = u(1,t)$$

a) Propose an implicit finite difference scheme, with first order in time and space, for the discretization of (1). Justify the selection of the approximation for the spatial derivative.

Since we are proposing an implicit scheme of first order, we use a backward difference approximation of the derivatives:

$$f_{i\pm1} = f_i \pm \Delta\xi \left.\frac{df}{d\xi}\right|_i + \frac{\Delta\xi^2}{2!}\left.\frac{d^2f}{d\xi^2}\right|_i \pm \frac{\Delta\xi^3}{3!}\left.\frac{d^3f}{d\xi^3}\right|_i + \cdots$$

$$\left.\frac{du}{dt}\right|_i^{n+1} = \frac{u_i^{n+1} - u_i^n}{\Delta t} - \frac{\Delta t}{2!}\left.\frac{d^2u}{dt^2}\right|_i^{n+1} - \cdots = \frac{u_i^{n+1} - u_i^n}{\Delta t} + \mathcal{O}(\Delta t)$$

$$\left.\frac{du}{dx}\right|_i^{n+1} = \frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} - \frac{\Delta x}{2!}\left.\frac{d^2u}{dx^2}\right|_i^{n+1} - \cdots = \frac{u_i^n - u_{i-1}^n}{\Delta x} + \mathcal{O}(\Delta x)$$

Combining both approximations in (1):

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\left(\frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x}\right) + \tau_i^n = 0$$

$$(1+r)u_i^{n+1} - ru_{i-1}^{n+1} = u_i^n - \Delta t\tau_i^n$$

$$(1+r)U_i^{n+1} - rU_{i-1}^{n+1} = U_i^n$$

with $r = \frac{a\Delta t}{\Delta x}$. This method is implicit because we can't compute the value of u_i^{n+1} without solving a system of equations or iteration as we don't know also the value of u_{i-1}^{n+1}. Since we are required to find a method of first order in the spatial domain we use the Euler Backward difference, as opposed to the BTCS method, where we use a central difference approach. In this case, we chose i and $i-1$ because a is a velocity travelling in the positive direction, so it makes more sense to use a point in space before the actual one, where the information has already "passed".

b) How are periodic boundary conditions treated? Write in detail the system of equations to solve in each time step.

Periodic boundary conditions are treated numerically as two different boundary conditions for the beginning and the end of the row i being solved in every step. They are considered as nodes with a known value that help to compute first and last points, and that's the reason why they don't appear in the matrix formulation.

The system of equations for any time step then is:

$$\begin{cases} (1+r)U_i^{n+1} - rU_{i-1}^{n+1} = U_i^n & i = 1,\ldots,M; \quad n \geq 0 \\ U_0^{n+1} = U_{M+1}^{n+1} = u^{n+1}(0,t) & n \geq 0 \\ U_i^0 = \sin(2\pi x_i) & i = 0,\ldots,M+1 \end{cases}$$

c) Suggest a direct method and an iterative method for the solution of the linear systems of equations.

Since we are solving a system of equations with $M-2$ unknowns in every time step, dependent from the previous step, we have a system of equations of the form:

$$\boldsymbol{A}\boldsymbol{U}^{n+1} = \boldsymbol{F}$$

where we fill the matrix $\boldsymbol{A}$ with the coefficients seen in the equation. That is

$$\boldsymbol{A} = \begin{bmatrix} (1+r) & & & & & \\ -r & (1+r) & & & & \\ & \ddots & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & -r & (1+r) & \\ & & & & -r & (1+r) \end{bmatrix}$$

and $\boldsymbol{F} = \boldsymbol{U}^n + \boldsymbol{F}_\Gamma$ representing the Dirichlet boundary conditions

$$\boldsymbol{F} = (U_1^n + rU_0^{n+1}, U_2^n, \dots, U_{M-1}^n, U_M^n + rU_{M+1}^{n+1})^T$$

Since this is a trivial system of equations (given that $\boldsymbol{A}$ is lower triangular), direct solution comes from inverting $\boldsymbol{A}$ and finding the exact value for $\boldsymbol{U}^{n+1}$. An iterative solution for the system can be obtained using the Jacobi method (not Gauss-Seidel because it gives an exact solution in this case):

$$\begin{aligned} \boldsymbol{A} &= \boldsymbol{L}_A + \boldsymbol{D}_A + \boldsymbol{U}_A = \boldsymbol{L}_A + \boldsymbol{D}_A \\ \boldsymbol{D}_A\boldsymbol{U}_{k+1}^{n+1} &= \boldsymbol{F} - \boldsymbol{L}_A\boldsymbol{x}_k \\ \boldsymbol{U}_{k+1}^{n+1} &= \frac{1}{(1+r)}\left(\boldsymbol{F} - \boldsymbol{L}_A\boldsymbol{x}_k\right) \end{aligned}$$

The iterative form to obtain the exact form from the system can be written as:

$$\begin{aligned} U_i^{n+1} &= F_1/A_{11} \\ U_i^{n+1} &= \frac{1}{A_{ii}}\left(F_i - \sum_{j=1}^{i-1} A_{ij}u_j^{n+1}\right) \end{aligned}$$

which correspond to solve the system of equations one by one (i.e. to be programmed in a computer).

d) Draw schematically the fill-in of the matrix for the direct method proposed in the previous section.

An schematic of the $\boldsymbol{A}$ matrix and it's fill-in is like shown in the figure below:

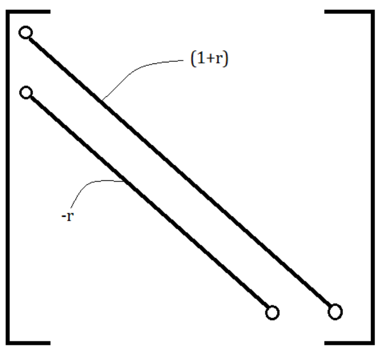

Figure 1: fill-in of $\boldsymbol{A}$.

2. For the numerical modelling of a new technique of contamination control, it is interesting to solve the diffusion-reaction PDE

$$u_t = \nu u_{xx} + \sigma u, \quad \textit{in } x \in (0,1), \quad t > 0 \tag{2}$$

with boundary conditions

$$u(0,t) = 0 \quad \textit{and} \quad u_x(1,t) = 0 \tag{3}$$

and the initial conditions

$$u(x,0) = \begin{cases} 0 & \text{for} \quad x < 1/4 \\ 4x - 1 & \text{for} \quad 1/4 \leq x < 1/2 \\ -4x + 3 & \text{for} \quad 1/2 \leq x < 3/4 \\ 0 & \text{for} \quad 3/4 \geq x \end{cases} \tag{4}$$

In the PDE (2), $\nu > 0$ is the diffusion coefficient and $\sigma < 0$ is the reaction coefficient. Both coefficients can be considered constant.

a) Propose an explicit finite difference scheme for the solution of the PDE (2) with boundary conditions (3) and initial condition (4). Detail the numerical treatment of boundary conditions.

For an explicit approach, we take a Euler Forward approximation for the first derivative and a Central Difference approximation for the second derivative. This yields:

$$\left.\frac{du}{dt}\right|_i^n = \frac{u_i^{n+1} - u_i^n}{\Delta t} - \frac{\Delta t}{2!}\left.\frac{d^2u}{dt^2}\right|_i^n - \cdots = \frac{u_i^{n+1} - u_i^n}{\Delta t} + \mathcal{O}(\Delta t)$$

$$\left.\frac{d^2u}{dx^2}\right|_i^n = \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2} - \frac{2\Delta x^2}{4!}\left.\frac{d^4u}{dx^4}\right|_i^n - \cdots = \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

Replacing everything in (2):

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \nu\left(\frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2}\right) + \sigma u_i^n + \tau_i^n$$

$$u_i^{n+1} = \frac{\nu\Delta t}{\Delta x^2}(u_{i-1}^n - 2u_i^n + u_{i+1}^n) + (1 + \Delta t\sigma)u_i^n + \Delta t\tau_i^n$$

$$U_i^{n+1} = \nu r(U_{i-1}^n - 2U_i^n + U_{i+1}^n) + (1 + \Delta t\sigma)U_i^n$$

with $r = \Delta t/\Delta x^2$. This is the explicit approximation for $u(x,t)$. The system to solve in this case is:

$$\begin{cases} U_i^{n+1} = \nu r(U_{i-1}^n - 2U_i^n + U_{i+1}^n) + (1 + \Delta t\sigma)U_i^n & i = 1, \ldots, M; \quad n \geq 0 \\ U_0^{n+1} = U_{M+1}^{n+1} = 0 & n \geq 0 \\ U_i^0 = u(x_i, 0) & i = 0, \ldots, M+1 \end{cases}$$

Boundary conditions are considered as "auxiliary nodes", in the sense that are nodes where the equation does not need to be solved, but gives data to compute the next node (i.e. U_1^{n+1} and U_{M+1}^{n+1}). The same as the initial condition, they are treated as an initiation value for the equations to be solved.

b) Which scheme is obtained for $\sigma = 0$ (diffusion equation)? And for $\nu = 0$ (reaction equation)?

From the equation

$$U_i^{n+1} = \nu r(U_{i-1}^n - 2U_i^n + U_{i+1}^n) + (1 + \Delta t\sigma)U_i^n$$

we can see that taking $\sigma = 0$ gives us the typical FTCS scheme, while taking $\nu = 0$ gives a ODE solved by the typical Euler scheme:

$$\sigma = 0 \longrightarrow \quad U_i^{n+1} = \nu r U_{i-1}^n + (1 - 2\nu r)U_i^n + \nu r U_{i+1}^n$$
$$\nu = 0 \longrightarrow \quad U_i^{n+1} = (1 + \Delta t\sigma)U_i^n$$

c) Take $\nu = 0.1$, $\sigma = -0.1$, $\Delta x = 0.25$ and $\Delta t = 0.1$, and compute two time steps with the explicit scheme proposed in section a. Are the obtained results reasonable? Discuss with the help of the graphic of the profile of u.

Using the values given, we get for every step:

$$U_i^{n+1} = 0.16U_{i-1}^n + 0.67U_i^n + 0.16U_{i+1}^n$$

Since discretization in x is 0.25, we have that $M = 3$. Boundary conditions give us that $U_0^n = U_4^n = 0$, while initial conditions give

$$U_0^0 = 0 \quad U_1^0 = 0 \quad U_2^0 = 1 \quad U_3^0 = 0 \quad U_4^0 = 0$$

With this information we can solve the system. For $n = 0$:

$$\begin{aligned} U_0^1 &= 0 \\ U_1^1 &= 0.16U_0^0 + 0.67U_1^0 + 0.16U_2^0 = 0.16 \\ U_2^1 &= 0.16U_1^0 + 0.67U_2^0 + 0.16U_3^0 = 0.67 \\ U_3^1 &= 0.16U_2^0 + 0.67U_3^0 + 0.16U_4^0 = 0.16 \\ U_4^1 &= 0 \end{aligned}$$

and for $n = 1$:

$$\begin{aligned} U_0^2 &= 0 \\ U_1^2 &= 0.16U_0^1 + 0.67U_1^1 + 0.16U_2^1 = 0.2144 \\ U_2^2 &= 0.16U_1^1 + 0.67U_2^1 + 0.16U_3^1 = 0.5001 \\ U_3^2 &= 0.16U_2^1 + 0.67U_3^1 + 0.16U_4^1 = 0.2144 \\ U_4^2 &= 0 \end{aligned}$$

The process can be seen in the following images:

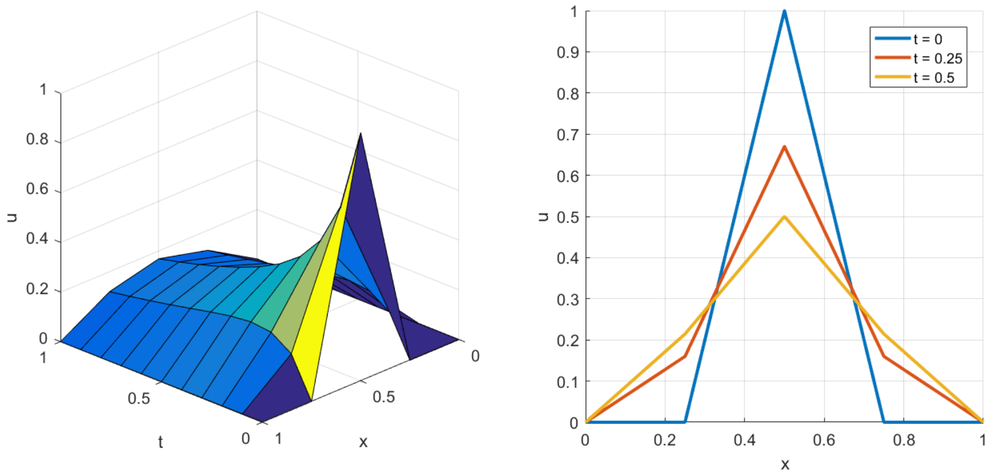

Figure 2: diffusion plots(left solved for 10 steps, right for 2)

As we can see, the results are reasonable, since we have a source in the center (given by the initial condition) that spreads to the sides, tending to cover the whole space, which is the basis for every Reaction-Diffusion system. The initial and last quarter of the space have no value at the beginning, but get "filled" as time passes. Since the value of σ is too small the effects are dominated by the ν part of the equation, which accounts for the diffusion of the problem.

d) Propose an implicit finite difference scheme to solve the PDE (2) with boundary conditions (3) and initial condition (4). Detail how are boundary conditions treated, the structure of the matrix and the most suitable method to solve the linear system of equations.

For an implicit approach, we take a Euler Backward approximation for the first derivative and a Central Difference approximation for the second derivative. This yields:

$$\left.\frac{du}{dt}\right|_i^{n+1} = \frac{u_i^{n+1}-u_i^n}{\Delta t} - \frac{\Delta t}{2!}\left.\frac{d^2u}{dt^2}\right|_i^{n+1} - \dots = \frac{u_i^{n+1}-u_i^n}{\Delta t} + \mathcal{O}(\Delta t)$$

$$\left.\frac{d^2u}{dx^2}\right|_i^{n+1} = \frac{u_{i-1}^{n+1}-2u_i^{n+1}+u_{i+1}^{n+1}}{\Delta x^2} - \frac{2\Delta x^2}{4!}\left.\frac{d^4u}{dx^4}\right|_i^{n+1} - \dots = \frac{u_{i-1}^{n+1}-2u_i^{n+1}+u_{i+1}^{n+1}}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

Replacing everything in (2):

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = \nu\left(\frac{u_{i-1}^{n+1}-2u_i^{n+1}+u_{i+1}^{n+1}}{\Delta x^2}\right) + \sigma u_i^{n+1} + \tau_i^{n+1}$$

$$u_i^{n+1}-u_i^n = \frac{\nu\Delta t}{\Delta x^2}(u_{i-1}^{n+1}-2u_i^{n+1}+u_{i+1}^{n+1}) + \Delta t\sigma u_i^{n+1} + \Delta t\tau_i^{n+1}$$

$$(1-\Delta t\sigma)U_i^{n+1} - \nu r(U_{i-1}^{n+1}-2U_i^{n+1}+U_{i+1}^{n+1}) = U_i^n$$

with r defined the same as the explicit case. The system to solve in this case is:

$$\begin{cases} (1-\Delta t\sigma)U_i^{n+1} - \nu r(U_{i-1}^{n+1}-2U_i^{n+1}+U_{i+1}^{n+1}) = U_i^n & i=1,\dots,M;\quad n\geq 0 \\ U_0^{n+1} = U_{M+1}^{n+1} = 0 & n \geq 0 \\ U_i^0 = u(x_i,0) & i=0,\dots,M+1 \end{cases}$$

This system can be expressed in matrix form as

$$\boldsymbol{A}\boldsymbol{U}^{n+1} = \boldsymbol{I}\boldsymbol{U}^n + \boldsymbol{F}$$

where $\boldsymbol{A}$ is of $M-1$ dimension defined as

$$\boldsymbol{A} = \begin{bmatrix} (1+2\nu r-\Delta t\sigma) & -\nu r & & & & \\ -\nu r & (1+2\nu r-\Delta t\sigma) & -\nu r & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\nu r & (1+2\nu r-\Delta t\sigma) & -\nu r \\ & & & & -\nu r & (1+2\nu r-\Delta t\sigma) \end{bmatrix}$$

and $\boldsymbol{F}$ is

$$\boldsymbol{F} = (\nu r U_0^{n+1}, 0, \dots, 0, \nu r U_{M+1}^{n+1})^T = \boldsymbol{0}$$

Boundary conditions are treated the same as the explicit method. They are removed from the computation of the matrix, since are values known, and that's the reason why they appear in the $\boldsymbol{F}$ vector.

Since in this case we have a null $\boldsymbol{F}$, the equation reduces to a simple form that can be solve by inverting $\boldsymbol{A}$. The system then can be solved as

$$\boldsymbol{U}^{n+1} = \boldsymbol{A}^{-1}\boldsymbol{U}^n$$

Approximate methods can also be used. Since we have a diagonal dominant matrix, Jacobi method can give precise solutions, same as Gauss-Seidel method (which will probably render better results also).