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PDE exercises - 3 [Finite differences]

(2) $u_t + a u_x = 0$, $x \in (0,1)$, $t \geq 0$, $a > 0$ (1)
with initial condition $u(x,0) = \sin(2\pi x)$
periodic boundary condition, that is
$$u(0,t) = u(1,t)$$

(a) Propose an implicit finite difference scheme with 1st order in time and space, for the discretization of 3. Justify the selection of the approximation for the spatial derivative.

Solution: The time derivative is discretized using backward Euler method:
$$\left.\frac{\partial u}{\partial t}\right|_i^{n+1} = \frac{u_i^{n+1} - u_i^n}{\Delta t} + O(\Delta t)$$
For the spatial derivative, a backward (upwind) difference should be used:
$$\left.\frac{\partial u}{\partial x}\right|_i^{n+1} = \frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} + O(\Delta x)$$
substituting in the equation (1)
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} + O(\Delta t, \Delta x) = 0$$
and neglecting the truncation errors, the following numerical problem is obtained:
$$\frac{V_i^{n+1} - V_i^n}{\Delta t} + a \cdot \frac{V_i^{n+1} - V_{i-1}^{n+1}}{\Delta x} = 0$$
Rearranging terms, this problem can be rewritten as:
$$-c V_{i-1}^{n+1} + (1+c) V_i^{n+1} = V_i^n$$
where $c = \frac{a \Delta t}{\Delta x}$ is the Courant number

(b) How are periodic boundary conditions treated? Write in detail the system of equations to solve in each time step:
Consider the discretization with $M+2$ points $x_i = i\Delta x$, $i = 0, 1, \ldots, M+1$. In order to impose periodic boundary conditions, we need to impose $V_0 = V_{M+1}$. This can be done using the numerical scheme at point $i=1$:

$$-c\,U_0^{n+1} + (1+c)\,U_1^{n+1} = U_1^n$$
$$-c\,U_{M+1}^{n+1} + (1+c)\,U_1^{n+1} = U_1^n$$

For all other points, we can consider the numerical problem

$$-c\,U_{i-1}^{n+1} + (1+c)\,U_i^{n+1} = U_i^n, \quad i = 2, \dots, M+1.$$

Thus, the system that must be solved in each time step is $AU^{n+1} = U^n$ with

$$U^P = \begin{Bmatrix} U_1^P \\ U_2^P \\ \vdots \\ U_M^P \\ U_{M+1}^P \end{Bmatrix} \qquad A = \begin{bmatrix} 1+c & & & & -c \\ -c & 1+c & & & \\ & \ddots & \ddots & & \\ & & -c & 1+c & 0 \\ & & & -c & 1+c \end{bmatrix}$$

(c) The system's matrix is not symmetric, so we need to use a general method for solving it (we cannot use Cholesky or conjugate gradients methods). As a direct method, it is advisable to use a factorization method such as Crout (LU). The matrix does not change with iterations, therefore it can be decomposed once and use the factorization throughout all the computation. Regarding iterative methods the matrix is diagonally dominant, Thus, stationary method such as Jacobi or Gauss-Seidel would converge. If convergence is slow, GMRES can also be used

(d) Direct methods maintain the matrix skyline. Therefore, only the last colour of the matrix can be filled-in

Note: Periodic boundary conditions $u(0,t) = u(1,t)$ can also be imposed considering U_0 as an unknown and adding an equation $U_0 = U_{M+1}$. Then, the system that must be solved each time step is $AU^{n+1} = U^n$

with

$$U^P = \begin{Bmatrix} U_1^P \\ U_2^P \\ \vdots \\ U_M^P \\ U_{M+1}^P \end{Bmatrix} \qquad A = \begin{bmatrix} -1 & & & & -1 \\ -c & 1+c & & & \\ 0 & -c & 1+c & & \\ & & \ddots & \ddots & \\ & & -c & 1+c & 0 \\ & & & -c & 1+c \end{bmatrix}$$

The pattern of the matrix is the same than in the previous case. Therefore, the same methods should be used for solving the linear system, furthermore, the fill-in pattern will also be the same.

(4) Solve the diffusion-reaction PDE

$$u_t = \nu u_{xx} + 6u \quad \text{in } x \in (0,1),\ t > 0 \quad (2)$$

with boundary conditions

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

and the initial condition

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

(a) In order to obtain an explicit finite differences scheme, we need to approximate the derivatives at time step n:

$$u_t\Big|_i^n \approx \frac{U_i^{n+1} - U_i^n}{\Delta t}; \quad u_{xx}\Big|_i^n \approx \frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{\Delta x^2}$$

and substituting in the PDE we obtain the following finite differences scheme:

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \nu\,\frac{U_{i+1}^n - 2U_i^n + U_{i-1}^n}{\Delta x^2} + 6\,U_i^n$$

Rearranging terms, the equation can be rewritten as

$$U_i^{n+1} = r\,U_{i-1}^n + (1 - 2r + 6\Delta t)\,U_i^n + r\,U_{i+1}^n \quad \text{where} \quad (5)$$

$$r = \frac{\nu \Delta t}{\Delta x^2},$$

Using the discretization with $M+2$ equispaced points, $x_i = i\Delta x$, $i = 0, \dots, M+1$, we need to note that

1) Solution at first node ($i=0$) is not unknown because at $x=0$ Dirichlet boundary conditions are imposed. Therefore, we dont need to impose any equation for this point. Furthermore, the equation obtained at point x_1 must be modified in order to take into account the boundary condition:

$$U_1^{n+1} = r\,U_0^n + (1 - 2r + 6\Delta t)\,U_1^n + r\,U_2^n$$
$$\Downarrow$$
$$U_1^{n+1} = (1 - 2r + 6\Delta t)\,U_1^n + r\,U_2^n$$

2)

2) The equation corresponding to the last point in the discretisation $(i = M+1)$ is

$$U_{M+1}^{n+1} = r U_M^n + (1 - 2r + \sigma \Delta t) U_{M+1}^n + r U_{M+2}^n$$

The value of the solution at point x_{M+2} (fictitious node) can be obtained in terms of the solution at interior points using Neumann's boundary conditions. In this case, an homogeneous Neumann's boundary condition is imposed, so $U_{M+2}^n = U_M^n$ and equation at point ~~the~~ x_{M+1} can be rewritten as

$$U_{M+1}^{n+1} = 2r\, U_M^n + (1 - 2r + \sigma \Delta t) U_{M+1}^n$$

For the rest of the points, equation (5) can directly be used.

The problem can be written in matrix form as $U^{n+1} = AU^n$ with

$$U = \begin{Bmatrix} U_1 \\ U_2 \\ \vdots \\ \vdots \\ U_M \\ U_{M+1} \end{Bmatrix}, \quad A = \begin{bmatrix} \alpha & r & & & \\ r & \alpha & r & & \\ & \ddots & \ddots & \ddots & \\ & & r & \alpha & r \\ & & & 2r & \alpha \end{bmatrix}, \quad \alpha = 1 - 2r + \sigma \Delta t$$

(b) Taking $\sigma = 0$, equation (2) is reduced to $u_t = u_{xx}$ and the numerical scheme is the FTCS method for solving a diffusion problem

$$U^{n+1} = AU^n \text{ with } A = \begin{bmatrix} (1-2r) & r & & & \\ r & (1-2r) & r & & \\ & \ddots & \ddots & \ddots & \\ & & r & (1-2r) & r \\ & & & 2r & 1-2r \end{bmatrix}$$

If $\nu = 0$, the PDE (2) is reduced to an ODE $u_t = \sigma u$ and the numerical scheme obtained in the previous point is simply Euler's method:

$$U^{n+1} = (1 + \sigma \Delta t) U^n = U^n + \Delta t \cdot \underbrace{\sigma U^n}_{f(t^n, U^n)}$$

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(c) Consider $\nu = 0,1$, $\sigma = -0,1$, $\Delta x = 0,25$ and $\Delta t = 0,1$

so that $r = \nu \dfrac{\Delta t}{\Delta x^2} = 0,1 \dfrac{0,1}{0,25^2} = 0,16$

$$1 - 2r + \sigma \Delta t = 1 - 2 \cdot 0,16 + (-0,1)\,0,1 = 0,67$$

and the matrix for computing the iterations is

$$A = \begin{bmatrix} 0,67 & 0,16 & 0 & 0 \\ 0,16 & 0,67 & 0,16 & 0 \\ 0 & 0,16 & 0,67 & 0,16 \\ 0 & 0 & 0,32 & 0,67 \end{bmatrix}$$

If we use $\Delta x = 0,25$, we are considering for unknowns, namely the value of the solution at points $x_i = 0,25\, i$, $i = 1, \dots, 4$

The initial conditions is. $U^0 = (0,1,0,0)^T$ and computing 2 iterations gives:

$$U^1 = AU^0 = \begin{bmatrix} 0,16 \\ 0,67 \\ 0,16 \\ 0 \end{bmatrix} \qquad U^2 = AU^1 = \begin{bmatrix} 0,2144 \\ 0,5001 \\ 0,2144 \\ 0,0512 \end{bmatrix}$$

The solution obtained after 2 time steps is plotted in figure 1. Note that

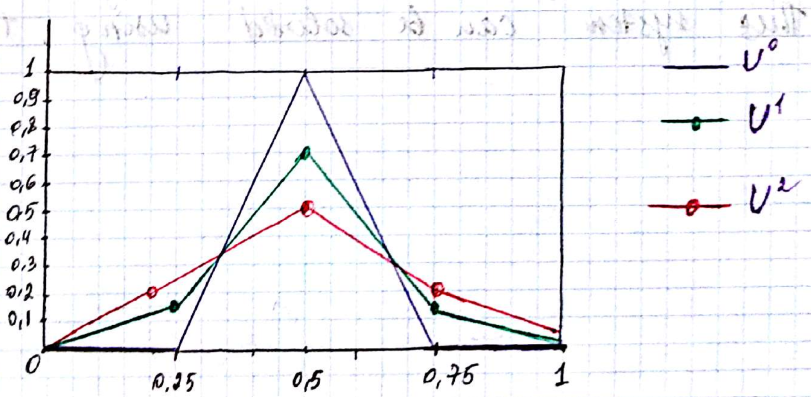

Figure 1. Initial condition and solution after 2 time steps using explicit method

- initial condition is smothed down due to diffusion and (negative) reaction term
- boundary conditions break the solution symmetry

(d) Using an implicit method, we impose the equation at time $n+1$. Derivatives are approximated as

$$u_t \Big|_i^{n+1} \approx \frac{U_i^{n+1} - U_i^n}{\Delta t} \qquad u_{xx} \Big|_i^{n+1} \approx \frac{U_{i+1}^{n+1} - 2U_i^{n+1} + U_{i-1}^{n+1}}{\Delta x^2}$$

and the finite differences scheme can be written as

$$\frac{V_i^{n+1} - V_i^{n}}{\Delta t} = \vartheta \frac{V_{i+1}^{n+1} - 2V_i^{n+1} + V_{i-1}^{n+1}}{\Delta x^2} + \sigma V_i^{n+1}$$

Rearranging terms,

$$-r V_{i-1}^{n+1} + (1 + 2r - \sigma \Delta t) V_i^{n+1} - r V_{i+1}^{n+1} = V_i^{n}, \quad \text{with } r = \vartheta \frac{\Delta t}{\Delta x^2}$$

In matrix form, the scheme can be written as

$A V^{n+1} = V^n$ where

$$V = \begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_M \\ V_{M+1} \end{bmatrix} \qquad A = \begin{bmatrix} \alpha & -r & & & \\ -r & \alpha & -r & & \\ & \ddots & \ddots & \ddots & \\ & & -r & \alpha & -r \\ & & & -2r & \alpha \end{bmatrix}, \quad \alpha = 1 + 2r - \sigma \Delta t$$

- The $2r$ term is the last equation is due to the Neumann's boundary condition (which is treated in the same way than for the explicit method)
- If the implicit method is used, at each time step we must solve a system of linear equations with tridiagonal but not symmetric matrix.

This system can be solved using thomas algorithm