Numerical Methods for Partial Differential Equations - Finite Differences

2. Let us consider the differential equation

$$u_t + a u_x = 0, \quad x \in (0,1), \quad t \geq 0, \quad a > 0 \tag{3}$$

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

and periodic boundary condition, 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 (3). Justify the selection of the approximation for the spatial derivative.

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

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

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

solution

Propose that the finite difference equation is obtained by replacing u_t by the first-order backward-time approximation and replacing u_x by the first-order backward-space approximation evaluated at time level $n+1$.

To get the first-order backward-time approximation, writing the Taylor series for u_i^n using grid point $(i, n+1)$ as the base point

$$u_i^n = u_i^{n+1} + u_t|_i^{n+1}(-\Delta t) + \frac{1}{2} u_{tt}|_i^{n+1}(\Delta t^2) + \dots$$

$$u_t|_i^{n+1} = \frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{1}{2} u_{tt}|_i^{n+1} \Delta t$$

Truncating the remainder term yields the first-order backward-time approximation

$$u_t|_i^{n+1} = \frac{u_i^{n+1} - u_i^n}{\Delta t} \quad \text{—— (2.1)}$$

Solution (cont.)

To get the first-order backward-space approximation, writing the Taylor series for u_{i-1}^{n+1} using grid point $(i, n+1)$ as the base point

$$u_{i-1}^{n+1} = u_i^{n+1} + u_x|_i^{n+1}(-\Delta x) + \frac{1}{2} u_{xx}|_i^{n+1}(\Delta x^2) + \ldots$$

$$u_x|_i^{n+1} = \frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} + \frac{1}{2} u_{xx}|_i^{n+1} \Delta x$$

Truncating the remainder term yields the first-order backward-space approximation

$$u_x|_i^{n+1} = \frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} \quad \text{—— (2.2)}$$

Substituting equation (2.1) and (2.2) into $u_t + a u_x = 0$ gives

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a \frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} = 0 \quad \text{—— (2.3)}$$

Rearranging equation (2.3) yields

$$-c u_{i-1}^{n+1} + (1+c) u_i^{n+1} = u_i^n \quad \text{where } c = \frac{a \Delta t}{\Delta x} \quad \text{—— (2.4)}$$ ... Answer a)

Equation (2.4) applies directly at points 2 to imax. The following system of equations is obtained

—— (2.5)

$$(1+c) u_2^{n+1} = u_2^n + c\, u(0,t) = b_2$$

$$-c u_2^{n+1} + (1+c) u_3^{n+1} = u_3^n = b_3$$

$$-c u_3^{n+1} + (1+c) u_4^{n+1} = u_4^n = b_4$$

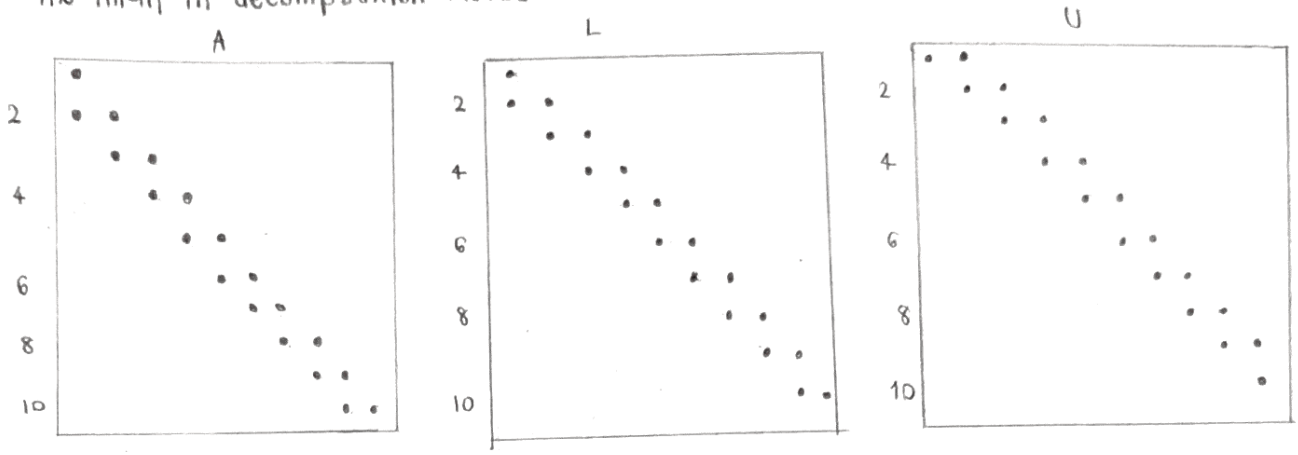
$$\vdots$$

$$-c u_{imax-1}^{n+1} = u_{imax}^n - (1+c)\, u(L,t) = b_{imax}$$ ... Answer b)

Then we may use Doolittle decomposition method or Jacobi iteration method to solve the linear system of equations above. ... Answer c)

Solution (cont.)

The fill-in in decomposition method



Numerical Methods for Partial Differential Equations - Finite Differences

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

$$u_t = \nu u_{xx} + \delta u \qquad \text{in } x \in (0,1),\ t > 0 \tag{4}$$

with boundary conditions $u(0,t) = 0$ and $u_x(1,t) = 0$ (5)

and the initial condition

$$u(x,0) = \begin{cases} 0 & \text{for } x < 1/4 \\ 4x-1 & \text{for } 1/4 \leq x < 1/2 \\ -4x+3 & \text{for } 1/2 \leq x < 3/4 \\ 0 & \text{for } 3/4 \leq x \end{cases} \tag{6}$$

In the PDE (4), $\nu > 0$ is the diffusion coefficient and $\delta < 0$ is the reaction coefficient. Both coefficients can be considered constant.

a) Propose an explicit finite difference scheme for the solution of the PDE (4) with boundary conditions (5) and initial condition (6). Detail the numerical treatment of boundary conditions.

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

c) Take $\nu = 0.1$, $\delta = -0.1$, $\Delta x = 0.25$ 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.

d) Propose an implicit finite difference scheme to solve the PDE (4) with boundary conditions (5) and initial condition (6). Detail how are boundary conditions treated, the structure of the matrix and the most suitable method to solve the linear system of equations.

solution

Propose the forward-time centered-space (FTCS) method to solve $u_t = \nu u_{xx} + \sigma u$.

Approximating u_t by the first-order forward-time approximation with grid point (i,n) as base point

$$u_t = \frac{u_i^{n+1} - u_i^n}{\Delta t}$$

Approximating u_{xx} by the second-order centered-space approximation with grid point (i,n) as the base point

$$u_{xx} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

Substituting into $u_t = \nu u_{xx} + \sigma u$ yields

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

Solving for u_i^{n+1} yields

$$u_i^{n+1} = (1+\Delta t\sigma)u_i^n + \frac{\nu \Delta t}{\Delta x^2}(u_{i+1}^n - 2u_i^n + u_{i-1}^n) \quad \text{--- (4.1)}$$

To account for the derivative boundary condition $u_x(1,t)=0$ at the right end, the first-order backward-space approximation is used to approximate the derivative boundary condition applying at grid point $(imax, n)$

$$u_x|_{imax}^n = \frac{u_{imax}^n - u_{imax-1}^n}{\Delta x} \rightarrow u_{imax}^n = u_{imax-1}^n \quad \text{since } u_x(1,t)=0$$

When $\sigma = 0$, equation (4.1) becomes

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

which is the FTCS scheme for diffusion equation.

And when $\nu = 0$, equation (4.1) becomes

$$u_i^{n+1} = (1+\Delta t\sigma)u_i^n$$

such that the solution marches linearly as the time increases.

Solution (cont.)

Consider $\nu = 0.1$, $\sigma = -0.1$, $\Delta x = 0.25$, $\Delta t = 0.1$

	$u(x,t)$				
t	x = 0	x = 0.25	x = 0.5	x = 0.75	x = 1
0	0	0	1	0	0
0.1	0	0.16	0.91	0.16	0.16
0.2	0	0.2528	0.6609	0.2784	0.2784

At the first time step

$$u_{0.25}^{0.1} = (1-0.1\times0.1)\, u_{0.25}^{0} + \frac{(0.1)(0.1)}{0.25^2}\left(u_{0.5}^{0} - 2u_{0.25}^{0} + u_{0}^{0}\right) = 0.16$$

$$u_{0.5}^{0.1} = (1-0.1\times0.1)\, u_{0.5}^{0} + \frac{(0.1)(0.1)}{0.25^2}\left(u_{0.75}^{0} - 2u_{0.5}^{0} + u_{0.25}^{0}\right) = 0.91$$

$$u_{0.75}^{0.1} = (1-0.1\times0.1)\, u_{0.75}^{0} + \frac{(0.1)(0.1)}{0.25^2}\left(u_{1}^{0} - 2u_{0.75}^{0} + u_{0.5}^{0}\right) = 0.16$$

$u_{1}^{0.1} = u_{0.75}^{0.1}$ .. from derivative boundary condition.

At the second time step

$$u_{0.25}^{0.2} = (1-0.1\times0.1)\, u_{0.25}^{0.1} + \frac{(0.1)(0.1)}{0.25^2}\left(u_{0.5}^{0.1} - 2u_{0.25}^{0.1} + u_{0}^{0.1}\right) = 0.2528$$

$$u_{0.5}^{0.2} = (1-0.1\times0.1)\, u_{0.5}^{0.1} + \frac{(0.1)(0.1)}{0.25^2}\left(u_{0.75}^{0.1} - 2u_{0.5}^{0.1} + u_{0.25}^{0.1}\right) = 0.6609$$

$$u_{0.75}^{0.2} = (1-0.1\times0.1)\, u_{0.75}^{0.1} + \frac{(0.1)(0.1)}{0.25^2}\left(u_{1}^{0.1} - 2u_{0.75}^{0.1} + u_{0.5}^{0.1}\right) = 0.2784$$

$u_{1}^{0.2} = u_{0.75}^{0.2}$ .. from derivative boundary condition

From the graphic of the profile of u showing in the next page, the obtained results seem reasonable. The diffusion effect is obvious. The behavior that is different from pure diffusion is probably from the reaction term σu.

solution (cont.)

Propose Crank-Nicolson scheme to be an implicit finite difference scheme to solve the PDE $u_t = \nu u_{xx} + \sigma u$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \nu \frac{1}{2}\left(\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} + \frac{u_{i+1}^{n} - 2u_i^{n} + u_{i-1}^{n}}{\Delta x^2} \right) + \frac{1}{2}\sigma\left(u_i^{n+1} + u_i^n\right) \quad -(4.2)$$

Rearranging equation (4.2) yields

$$-d u_{i-1}^{n+1} + 2(1+d-\tfrac{1}{2}\Delta t\sigma) u_i^{n+1} - d u_{i+1}^{n+1} = d u_{i-1}^{n} + 2(1-d+\tfrac{1}{2}\Delta t\sigma) u_i^{n} + d u_{i+1}^{n} \quad -(4.3)$$

The finite difference equation (4.3) is applied at the interior points, points 2 to imax as dirichlet boundary applies at grid point 1, $u_1^{n+1} = u(0,t) = 0$ and from derivative boundary condition, we derived earlier that $u_{imax}^{n+1} = u_{imax-1}^{n+1}$.

Then we can obtain the following system of linear equations

$$2(1+d-\tfrac{1}{2}\Delta t\sigma)u_2^{n+1} - d u_3^{n+1} = d u_1^n + 2(1-d+\tfrac{1}{2}\Delta t\sigma)u_2^n + d u_3^n + d u(0,t) = b_2$$

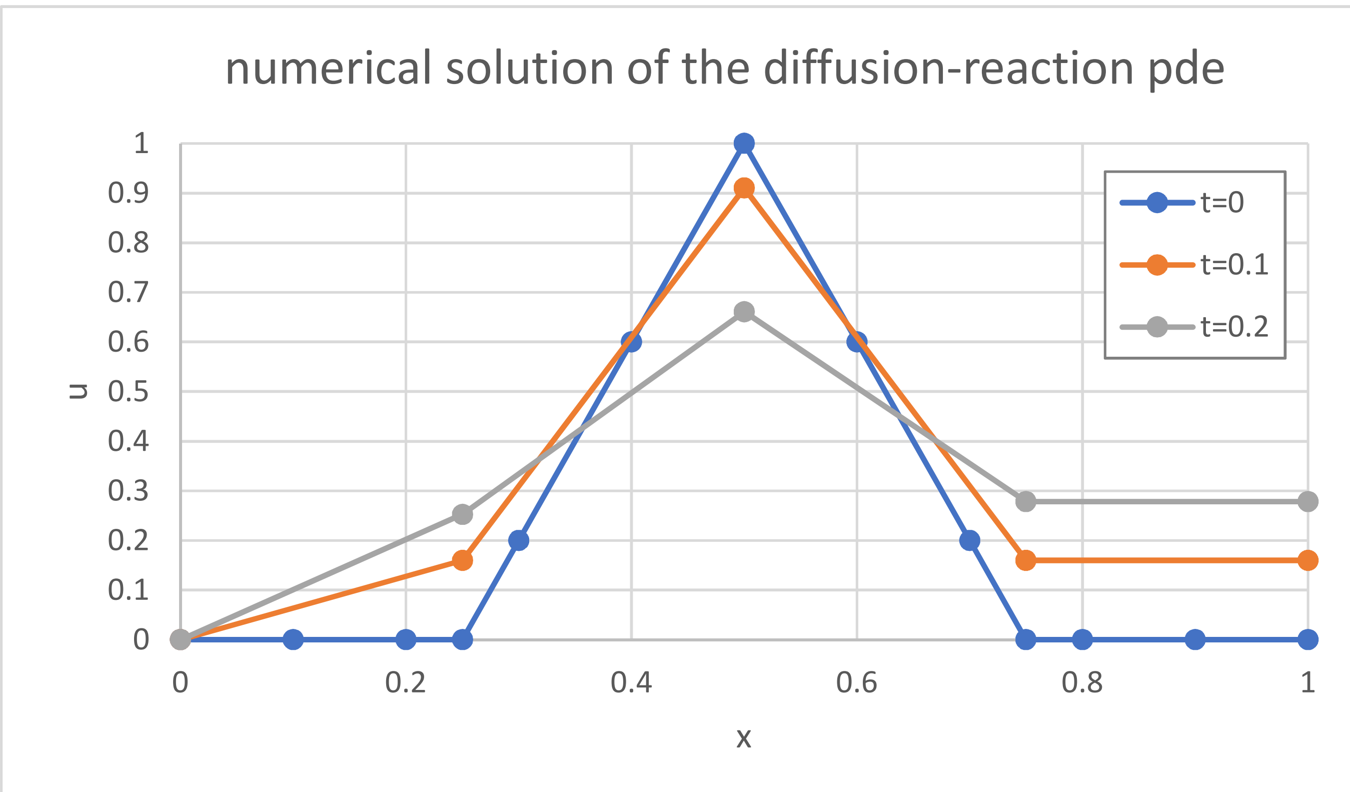
$$-d u_2^{n+1} + 2(1+d-\tfrac{1}{2}\Delta t\sigma)u_3^{n+1} - d u_4^{n+1} = d u_2^n + 2(1-d+\tfrac{1}{2}\Delta t\sigma)u_3^n + d u_4^n = b_3$$

$$-d u_3^{n+1} + 2(1+d-\tfrac{1}{2}\Delta t\sigma)u_4^{n+1} - d u_5^{n+1} = d u_3^n + 2(1-d+\tfrac{1}{2}\Delta t\sigma)u_4^n + d u_5^n = b_4$$

$$\vdots$$

$$-d u_{imax-2}^{n+1} + 2(1+d-\tfrac{1}{2}\Delta t\sigma)u_{imax-1}^{n+1} - d u_{imax-1}^{n+1} = d u_{imax-2}^n + 2(1-d+\tfrac{1}{2}\Delta t\sigma)u_{imax-1}^n + d u_{imax}^n = b_{imax}$$

which is a tridiagonal matrix and could be solved by Thomas algorithm.



numerical solution of the diffusion-reaction pde
u
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.2
0.4
0.6
0.8
1
t=0
t=0.1
t=0.2