
Numerical Methods for Partial Differential Equations

Finite Differences

Starred questions (*) have to be handed in for marking.

1. Consider a bar with length 1 m and constant thermal conductivity k . The temperature at the ends of the bar is

$$T(0) = 0, \quad T(1) = 1. \quad (1)$$

In order to determine the temperature distribution on the bar, the heat equation is stated

$$k \frac{d^2 T}{dx^2} = 0, \quad x \in (0, 1) \quad (2)$$

with boundary conditions (1).

- a) Derive a numerical scheme for the solution of the boundary problem given by equations (2) and (1) using a centered approximation of order Δx^2 . Detail the linear system obtained for $\Delta x = 0.2$.
- b) Solve the linear system obtained in a) for a bar with constant thermal conductivity $k = 1$. Represent the solution. With no extra computations, justify how would the temperature distribution for a bar be with conductivity $k = 10$.
- c) Solve the linear system of equations with the Gauss-Seidel method and the Conjugate Gradient method. Compute 4 iterations with initial approximation $x_i = 1$, and comment the convergence of both methods.

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- 2.* Let us consider the differential equation

$$u_t + au_x = 0, \quad x \in (0, 1), \quad t \geq 0, \quad a > 0 \quad (3)$$

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 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.
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3. Consider the elliptic equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$$

with homogeneous Dirichlet boundary conditions (i.e $u = 0$ at the whole boundary) and source term $f(x, y) = 2(x^2 + y^2)$.

- a) Solve the problem in a square domain $[0, 4] \times [0, 4]$ with $\Delta x = \Delta y = 1$, and determine the temperature at the point $(x, y) = (1, 1)$.
- b) Solve the problem in the triangle defined by vertices $(0, 0)$, $(0, 4)$ and $(4, 0)$, with $\Delta x = \Delta y = 1$, and determine the temperature at the point $(x, y) = (1, 1)$.
- c) Using the initial approximation $\mathbf{U} = \mathbf{0}$, compute 4 iterations for the solution of the system obtained in b) with the Jacobi and Gauss-Seidel methods, and comment the results.

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

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

with boundary conditions

$$u(0, t) = 0 \quad \text{and} \quad u_x(1, t) = 0 \quad (5)$$

and the initial condition

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

In the PDE (4), $\nu > 0$ 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 (4) with boundary conditions (5) and initial condition (6). Detail the numerical treatment of boundary conditions.
- b) Which scheme is obtained for $\sigma = 0$ (diffusion equation)? And for $\nu = 0$ (reaction equation)?
- 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 .
- 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.

5. The following finite differences schemes

$$(i) \quad U_i^{n+1} = U_i^n - \frac{c}{2} (U_{i+1}^n - U_{i-1}^n) \tag{7}$$

$$(ii) \quad U_i^{n+1} = U_i^n - c (U_i^n - U_{i-1}^n)$$

with Courant number $c = a\Delta t/\Delta x$, are considered for the solution of the boundary problem

$$u_t + au_x = 0, \quad x \in (0, 4), \quad t \geq 0, \quad a > 0 \tag{8}$$

$$u(x, 0) = u_0(x), \quad u(0, t) = 0.$$

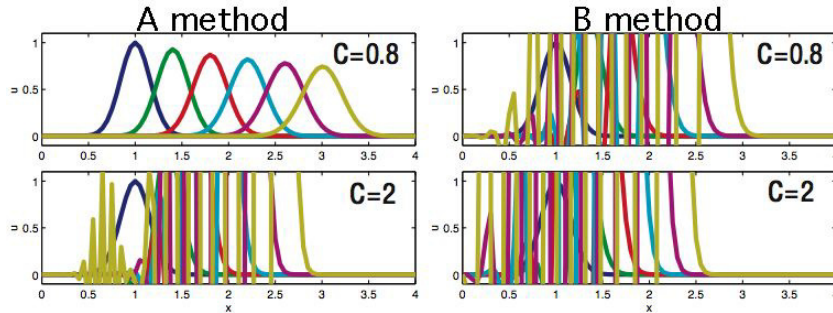


Figure 1: Numerical results with methods A and B

- Discuss for each method whether it is an explicit or implicit method and indicate the truncation order. Which linear solver would you use in each case?
- Figure 1 shows the solution with methods A and B for Courant numbers $c = 0.8$ and $c = 2$. Decide reasonably which of the schemes (i) and (ii) correspond to methods A and B.
- Comment the stability of both methods. Do the numerical results correspond to the expected behavior?

6. The partial differential equation

$$\frac{\partial u}{\partial t} = b \frac{\partial^2 u}{\partial x^2}$$

is defined over the domain $0 \leq x \leq 1$, and is to be solved numerically subject to the boundary conditions $u(0, t) = 0.0$, $u(1, t) = 0.0$ and initial conditions $u(x, 0) = u_0(x)$ ($u_0(x)$ defined below), where $u(x, t)$ is the exact solution.

The explicit forward time centred space scheme is used in the form

$$U_i^{n+1} - U_i^n = r(U_{i+1}^n - 2U_i^n + U_{i-1}^n)$$

where $r = b\Delta t/\Delta x^2$, subscript i is a spatial index (x-direction) and superscript n is the time level.

- Using a Taylor series expansion, deduce the leading truncation error of the scheme and state if the scheme is consistent.

- b) A uniform grid with three interior nodes and four equally spaced intervals is used. The initial data $u_0(x)$ is defined by

$$u_1^0 = 0.0, \quad u_2^0 = 3.0, \quad u_3^0 = 6.0, \quad u_4^0 = 3.0, \quad u_5^0 = 0.0,$$

and $b = 1/4$, $\Delta t = 0.25$. Compute the solution at the 3 interior nodes after one time step. Sketch the solution. Is the scheme stable in this case? Explain.

- c) State the stability condition.
- d) State the implicit backward time centered space scheme for the above problem.
- e) Using the above data, write down the resulting system of equations (expressed in terms of general r) that must be solved in order to compute the solution at the 3 interior nodes after one time step.
- f) Determine the solution via Gaussian elimination.
- g) Will the method always be stable or is there a limitation on time step?
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7. Consider the following system of linear equations:

$$\begin{bmatrix} 10 & 4 & 0 \\ 6 & 12 & 3 \\ 0 & 5 & 9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 46 \\ 81 \\ 65 \end{bmatrix}$$

- a) Using initial data $\mathbf{x}^0 = [2, 3, 4]^T$, apply Jacobi method to the system for 3 iterations. Show your working and the results of each iteration.
- b) Using the same initial data, apply the Gauss-Seidel iterative method for the same 3×3 system for 3 iterations. Again, show your working and the results for each iteration.
- c) The exact solution of the system is $\mathbf{x}^* = [3, 4, 5]^T$. Determine which method gives the best result and explain why.
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8. Consider the following system of linear equations:

$$\begin{bmatrix} 1 & 5 \\ 5 & 100 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 17 \\ 310 \end{bmatrix}$$

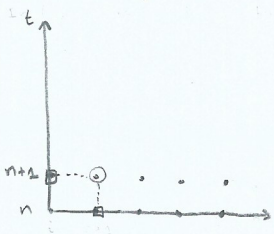
- a) As a first attempt, we have tried to solve the system using the steepest descent method, but convergence is too slow. Explain the causes of this slow convergence.
- b) Can the conjugate gradient method be used to solve the system? Will it converge? If so, how many iterations are needed?
- c) Compute two iterations of the conjugate gradient method applied to this system, using $\mathbf{x}^0 = [5, 5]^T$ as a starting vector. Which will be the results if a different starting vector is considered?
-

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0 \quad x \in (0,1) \quad t \geq 0 \quad a > 0$$

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

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

a) Implicit, 1st order in time and space.



We can't use centered differences in space because $\tau_i = O(\Delta x^2)$ (second order).
 we need to use backward differences in space (we know the previous points).
 If we use forward differences in time we get an explicit method (explicit upwind).
 we are thus going to use backward differences in time as well. (implicit upwind)

KNOWN
 0 where we apply the equation

using Taylor series:

$$\rightarrow u_i^{n+1} = u_i^n - \frac{\partial u}{\partial t} \Big|_i^{n+1} \Delta t + \frac{1}{2} \frac{\partial^2 u}{\partial t^2} \Big|_i^{n+1} \Delta t^2 + \dots \rightarrow \frac{\partial u}{\partial t} \Big|_i^{n+1} = \frac{u_i^{n+1} - u_i^n}{\Delta t} + O(\Delta t)$$

First order in time and space

$$\rightarrow u_{i-1}^{n+1} = u_i^n - \frac{\partial u}{\partial x} \Big|_i^{n+1} \Delta x + \frac{1}{2} \frac{\partial^2 u}{\partial x^2} \Big|_i^{n+1} \Delta x^2 + \dots \rightarrow \frac{\partial u}{\partial x} \Big|_i^{n+1} = \frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} + O(\Delta x)$$

Substituting in the equation:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a \frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} + O(\Delta x, \Delta t) \xrightarrow{\text{we neglect the truncation error}} \frac{u_i^{n+1} - u_i^n}{\Delta t} + a \frac{u_i^{n+1} - u_{i-1}^{n+1}}{\Delta x} = 0 \rightarrow$$

$$\rightarrow \left(1 + a \frac{\Delta t}{\Delta x} \right) u_i^{n+1} - \frac{a \Delta t}{\Delta x} u_{i-1}^{n+1} = u_i^n \quad \text{for } i=1, \dots, M$$

B)

periodic boundary condition: $u(0,t) = u(1,t)$

$$\text{this way, } u_i^n = u_{M+1}^n \Rightarrow u_{i-1}^n = u_M^n$$



Imposing the scheme at the first point: $(i=0)$

$$\left(1 + a \frac{\Delta t}{\Delta x} \right) u_0^{n+1} - \frac{a \Delta t}{\Delta x} u_{-1}^{n+1} = u_0^n \quad \text{we know that } u_{-1}^{n+1} = u_M^{n+1} \rightarrow \left(1 + a \frac{\Delta t}{\Delta x} \right) u_0^{n+1} - \frac{a \Delta t}{\Delta x} u_M^{n+1} = u_0^n$$

Taking this into account, the system of equations can be written in the following way:

$$\boxed{B U^{n+1} = U^n}$$

with

$$B = \begin{pmatrix} (1 + a \frac{\Delta t}{\Delta x}) & 0 & & -\frac{a \Delta t}{\Delta x} \\ -\frac{a \Delta t}{\Delta x} & & & \\ & & & \\ 0 & & -\frac{a \Delta t}{\Delta x} & (1 + a \frac{\Delta t}{\Delta x}) \end{pmatrix} \quad U^{n+1} = \begin{pmatrix} u_0^{n+1} \\ u_1^{n+1} \\ \vdots \\ u_M^{n+1} \end{pmatrix}$$

c) Analysing the matrix B we can see that it's not symmetrical, but it is diagonally dominant. We are therefore going to suggest the Doolittle method as direct method, since it transforms our matrix $B = LU$, with L being a lower triangular matrix and U and upper triangular one. The solution is computed with 2 substitutions

*(below)

d) This would be the fill-in of the matrix for the Doolittle method proposed:

$$\begin{pmatrix} \diagdown & & \\ & \bullet & \\ & & \diagdown \end{pmatrix} = \begin{pmatrix} \diagdown & & \\ & \diagup & \\ & & \diagdown \end{pmatrix} \cdot \begin{pmatrix} \diagdown & & \\ & & \\ & & \diagdown \end{pmatrix}$$

* We would also suggest the Gauss-Seidel method as an iterative method, since it has faster convergence than the Jacobi method.

4.

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} + \sigma u \quad \text{in } x \in (0, 2), t > 0$$

$$u(0, t) = 0 \quad \text{and} \quad \frac{\partial u}{\partial x}(1, t) = 0$$

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

a) We are going to use the FTCS method: Forward in time and centered in space, which is an explicit method.

using Taylor series:

$$u_i^{n+1} = u_i^n + \Delta t \frac{\partial u}{\partial t} \Big|_i^n + \frac{\Delta t^2}{2!} \frac{\partial^2 u}{\partial t^2} \Big|_i^n + \dots \rightarrow \frac{\partial u}{\partial t} \Big|_i^n = \frac{u_i^{n+1} - u_i^n}{\Delta t} + O(\Delta t)$$

$$u_{i+1}^n = u_i^n + \Delta x \frac{\partial u}{\partial x} \Big|_i^n + \frac{\Delta x^2}{2!} \frac{\partial^2 u}{\partial x^2} \Big|_i^n + \frac{\Delta x^3}{3!} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4)$$

$$u_{i-1}^n = u_i^n - \Delta x \frac{\partial u}{\partial x} \Big|_i^n + \frac{\Delta x^2}{2!} \frac{\partial^2 u}{\partial x^2} \Big|_i^n - \frac{\Delta x^3}{3!} \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4)$$

$$u_{i+1}^n + u_{i-1}^n = 2u_i^n + \frac{\Delta x^2}{2!} \frac{\partial^2 u}{\partial x^2} \Big|_i^n + O(\Delta x^4)$$

↓

$$\frac{\partial^2 u}{\partial x^2} \Big|_i^n = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} + O(\Delta x^2) \rightarrow \text{we used a second order approximation in space for higher accuracy}$$

replaces in the equation and neglects the truncation error $\tau_i^n = O(\Delta t, \Delta x^2)$:

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

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

$$\rightarrow \boxed{u_i^{n+1} = \nu \frac{\Delta t}{\Delta x^2} u_{i-1}^n + \left(1 - 2\nu \frac{\Delta t}{\Delta x^2} + \Delta t \sigma\right) u_i^n + \nu \frac{\Delta t}{\Delta x^2} u_{i+1}^n} \quad \begin{matrix} i = 0, \dots, m \\ n \geq 0 \end{matrix}$$

Applying the initial conditions:

$$u_i^0 = u(x_i, 0) \quad i=0, \dots, M+1$$

And the boundary conditions:

$$u_0^{n+1} = 0 \quad \text{for } n \geq 0 \quad (\text{Dirichlet})$$

$$\frac{\partial u}{\partial x} \Big|_1^t = 0 :$$

$$\hookrightarrow i=M+1 \rightarrow u_{M+1}^{n+1} = \frac{\Delta t}{\Delta x^2} u_M^n + (1 - 2\frac{\Delta t}{\Delta x^2} + \sigma\sigma) u_{M+1}^n + \frac{\Delta t}{\Delta x^2} u_{M+2}^n \rightarrow \text{Node } M+2 \text{ is not in our domain (fictitious)}$$

$$\hookrightarrow \frac{\partial u}{\partial x} \Big|_{M+1}^P = \frac{u_{M+2}^P - u_M^P}{2\Delta x} = 0 \Rightarrow u_{M+2}^P = u_M^P$$

↑ arbitrary

↓ centered difference

$$\hookrightarrow u_{M+1}^{n+1} = 2\frac{\Delta t}{\Delta x^2} u_M^n + (1 - 2\frac{\Delta t}{\Delta x^2} + \sigma\sigma) u_{M+1}^n$$

This way:

$$u_i^{n+1} = \frac{\Delta t}{\Delta x^2} u_{i-1}^n + (1 - 2\frac{\Delta t}{\Delta x^2} + \sigma\sigma) u_i^n + \frac{\Delta t}{\Delta x^2} u_{i+1}^n \quad i=1, \dots, M$$

$$u_{M+1}^{n+1} = 2\frac{\Delta t}{\Delta x^2} u_M^n + (1 - 2\frac{\Delta t}{\Delta x^2} + \sigma\sigma) u_{M+1}^n \quad n \geq 0$$

$$u_0^{n+1} = 0 \quad n \geq 0$$

$$u_i^0 = \begin{cases} 0 & \text{for } x < 1/4 \\ 4x-1 & \text{for } 1/4 \leq x \leq 1/2 \\ -4x+3 & \text{for } 1/2 \leq x < 3/4 \\ 0 & \text{for } 3/4 \leq x \end{cases} \quad i=1, \dots, M+1$$

13) $\sigma=0$ (diffusion equation):

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

$$u_{M+1}^{n+1} = 2\frac{\Delta t}{\Delta x^2} u_M^n + (1 - 2\frac{\Delta t}{\Delta x^2}) u_{M+1}^n \quad n \geq 0$$

$$u_0^{n+1} = 0 \quad n \geq 0$$

$$u_i^0 = \begin{cases} 0 & \text{for } x < 1/4 \\ 4x-1 & \text{for } 1/4 \leq x \leq 1/2 \\ -4x+3 & \text{for } 1/2 \leq x < 3/4 \\ 0 & \text{for } 3/4 \leq x \end{cases} \quad i=1, \dots, M+1$$

$J=0$ (reaction equation)

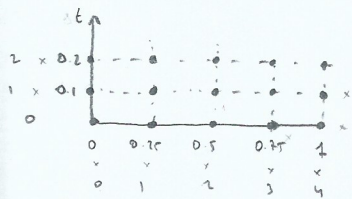
$$\begin{aligned}
 & \cdot u_i^{n+1} = (1 + \sigma \Delta t) u_i^n \quad i = 1, \dots, M \\
 & \cdot u_{M+1}^{n+1} = (1 + \sigma \Delta t) u_{M+1}^n \quad n \geq 0 \\
 & \cdot u_0^{n+1} = 0 \quad n \geq 0 \\
 & \cdot u_i^0 = \begin{cases} 0 & \text{for } x < 1/4 \\ 4x-1 & \text{for } 1/4 \leq x < 1/2 \\ -4x+3 & \text{for } 1/2 \leq x \leq 3/4 \\ 0 & \text{for } 3/4 \leq x \end{cases}
 \end{aligned}$$

c) $J=0.1 \quad \Delta x=0.25$
 $\sigma = -0.1 \quad \Delta t = 0.1$

Initial conditions:

$$u_0^0 = 0 \quad u_1^0 = 0 \quad u_2^0 = 1 \quad u_3^0 = 0 \quad u_4^0 = 0$$

$$\Rightarrow u_i^{n+1} = 0.16 u_{i-1}^n + 0.67 u_i^n + 0.16 u_{i+1}^n \quad \begin{cases} i=1, \dots, 3 \\ n=1, 2 \end{cases}$$



→ BC:

$$\Rightarrow u_0^1 = u_0^2 = 0$$

$$\Rightarrow u_4^{n+1} = 0.32 u_3^n + 0.67 u_4^n \quad \text{for } n=1, 2 \quad \begin{cases} u_4^1 = 0.32 \cdot 0 + 0.67 \cdot 0 = 0 \\ u_4^2 = 0.32 \cdot 0.16 + 0.67 \cdot 0 = 0.0512 \end{cases}$$

thus:

$$\cdot u_1^1 = 0.16 \cdot 0 + 0.67 \cdot 0 + 0.16 \cdot 1 = 0.16$$

$$\cdot u_1^2 = 0.16 \cdot 0 + 0.67 \cdot 0.16 + 0.16 \cdot 0.67 = 0.2144$$

$$\cdot u_2^1 = 0.16 \cdot 0 + 0.67 \cdot 1 + 0.16 \cdot 0 = 0.67$$

$$\cdot u_2^2 = 0.16 \cdot 0.16 + 0.67 \cdot 0.67 + 0.16 \cdot 0.16 = 0.5001$$

$$\cdot u_3^1 = 0.16 \cdot 1 + 0.67 \cdot 0 + 0.16 \cdot 0 = 0.16$$

$$\cdot u_3^2 = 0.16 \cdot 0.67 + 0.67 \cdot 0.16 + 0.16 \cdot 0 = 0.2144$$

Summarizing:

$$\begin{array}{ccccc}
 \cdot u_0^0 = 0 & \cdot u_1^0 = 0 & \cdot u_2^0 = 1 & \cdot u_3^0 = 0 & \cdot u_4^0 = 0 \\
 \cdot u_0^1 = 0 & \cdot u_1^1 = 0.16 & \cdot u_2^1 = 0.67 & \cdot u_3^1 = 0.16 & \cdot u_4^1 = 0 \\
 \cdot u_0^2 = 0 & \cdot u_1^2 = 0.2144 & \cdot u_2^2 = 0.5001 & \cdot u_3^2 = 0.2144 & \cdot u_4^2 = 0.0512
 \end{array}$$

We have plotted the profile of u in Matlab in order to check if our results are correct, the plot is attached in the .zip file that contains this homework

Looking a look at said plot it can be seen that there is a diffusion effect, since $J > 0$, and the pass of time results in it being wider. It can also be seen that there's a loss of contaminant, and that makes sense since $\sigma < 0$.

