

Seminar 3

Implement the numerical methods using a programming language of your choice (Python, MATLAB, C++, etc.). Use the Crank–Nicolson method in time and centered finite differences in space. All variables are dimensionless. Problems 1–5 are one-dimensional; Problem 6 is an optional extension.

Problem 1. Basic Diffusion

Consider the one-dimensional heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 \leq x \leq 1, \quad (1)$$

with initial and boundary conditions

$$u(x, 0) = \sin(\pi x), \quad u(0, t) = u(1, t) = 0. \quad (2)$$

Tasks:

1. Derive the Crank–Nicolson scheme and write the resulting tridiagonal system.
2. Solve the system at each time step using the Gaussian elimination algorithm.
3. Compute the solution up to $T = 0.1$ using $N = 20, 40$, and 80 equal grid intervals, with $\Delta x = 1/N$ and $\Delta t = 0.1/N$.
4. Plot the numerical solution at $T = 0.1$ together with the analytical solution

$$u(x, t) = e^{-\pi^2 t} \sin(\pi x). \quad (3)$$

5. Calculate the maximum error

$$E_N = \max_j \left| u_j^{\text{num}}(T) - u(x_j, T) \right| \quad (4)$$

and estimate the convergence order using

$$p = \log_2 \left(\frac{E_N}{E_{2N}} \right). \quad (5)$$

Questions: Does simultaneous refinement of the spatial and temporal grids give $p \approx 2$? Does unconditional stability guarantee accuracy for arbitrarily large time steps?

Problem 2. Nonzero Boundary Values

Consider the one-dimensional heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 \leq x \leq 1, \quad (6)$$

with initial condition

$$u(x, 0) = x + \sin(\pi x) \quad (7)$$

and boundary conditions

$$u(0, t) = 0, \quad u(1, t) = 1. \quad (8)$$

Tasks:

1. Derive the Crank–Nicolson system for the interior grid points. Show explicitly how the prescribed boundary values enter the right-hand side.
2. Adapt the program from Problem 1.
3. Use $N = 20$, 40 , and 80 grid intervals, $\Delta t = 0.1/N$, and final time $T = 0.1$.
4. Compare the numerical solution with

$$u(x, t) = x + e^{-\pi^2 t} \sin(\pi x). \quad (9)$$

5. Plot the departure from the steady solution, $u(x, T) - x$, and calculate E_N and p as defined in Problem 1.

Questions: Why is the steady solution $u_s(x) = x$? How does imposing the boundary conditions change the first and last equations of the interior linear system?

Problem 3. Diffusion with a Reaction Term

Consider the equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u, \quad 0 \leq x \leq 1, \quad (10)$$

with initial and boundary conditions

$$u(x, 0) = \sin(\pi x), \quad u(0, t) = u(1, t) = 0. \quad (11)$$

Tasks:

1. Derive the Crank–Nicolson scheme, averaging both the diffusion and reaction terms between time levels n and $n + 1$.
2. Identify the change in the matrix diagonal relative to Problem 1.
3. Solve the problem up to $T = 0.1$ using $N = 20, 40$, and 80 grid intervals and $\Delta t = 0.1/N$.
4. Compare the numerical solution with

$$u(x, t) = e^{(1-\pi^2)t} \sin(\pi x). \quad (12)$$

5. Calculate E_N and p . Compare the value at $x = 0.5$ with the corresponding value in Problem 1.

Questions: Why does the solution decay even though the reaction term is positive? For the more general equation $u_t = u_{xx} + cu$, at what value of c does this initial mode change from decay to growth?

Problem 4. Advection and Diffusion

Consider the advection–diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - 2 \frac{\partial u}{\partial x}, \quad 0 \leq x \leq 1, \quad (13)$$

with initial condition

$$u(x, 0) = e^x \sin(\pi x) \quad (14)$$

and boundary conditions

$$u(0, t) = u(1, t) = 0. \quad (15)$$

Tasks:

1. Approximate the first and second spatial derivatives using centered differences.
2. Derive the Crank–Nicolson system and give the lower, main, and upper diagonal coefficients.
3. Solve the resulting tridiagonal system using the Thomas algorithm.
4. Use $N = 20, 40$, and 80 grid intervals, $\Delta t = 0.1/N$, and final time $T = 0.1$.
5. Compare the numerical solution with

$$u(x, t) = e^{x - (\pi^2 + 1)t} \sin(\pi x). \quad (16)$$

Plot the final profile and calculate E_N and p .

Questions: Why are the lower and upper diagonal coefficients unequal? How do these coefficients change if the advection term is changed from $-2u_x$ to $+2u_x$?

Problem 5. Variable Diffusion Coefficient

Consider the equation

$$\frac{\partial u}{\partial t} = a(x) \frac{\partial^2 u}{\partial x^2}, \quad a(x) = 1 - \frac{x^2}{2}, \quad 0 \leq x \leq 1, \quad (17)$$

with initial condition

$$u(x, 0) = 1 - \frac{x^2}{2} \quad (18)$$

and time-dependent boundary conditions

$$u(0, t) = e^{-t}, \quad u(1, t) = \frac{1}{2}e^{-t}. \quad (19)$$

Tasks:

1. Derive the Crank–Nicolson system using $a_j = a(x_j)$ at each interior grid point.
2. Include the boundary contributions from both time levels n and $n + 1$ in the right-hand side.
3. Fix $N = 40$ grid intervals and evolve to $T = 0.1$. Repeat with $\Delta t = 0.02, 0.01$, and 0.005 .
4. Compare the numerical solution with

$$u(x, t) = e^{-t} \left(1 - \frac{x^2}{2} \right). \quad (20)$$

5. Calculate the maximum error for each time step and estimate the temporal convergence order.

Questions: Why is the centered second derivative exact for the spatial profile in this example? Does $a(x)u_{xx}$ equal $\partial_x[a(x)u_x]$ when a varies with x ?

Problem 6. Two-Dimensional Diffusion (Optional)

Consider the two-dimensional heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}, \quad 0 \leq x, y \leq 1, \quad (21)$$

with initial condition

$$u(x, y, 0) = \sin(\pi x) \sin(\pi y) \quad (22)$$

and boundary conditions

$$u(0, y, t) = u(1, y, t) = u(x, 0, t) = u(x, 1, t) = 0. \quad (23)$$

Tasks:

1. Use centered differences with a five-point spatial stencil and derive the full Crank–Nicolson linear system.
2. Map the interior grid values to a vector and solve the system using a sparse linear solver.
3. Use $N = 10, 20$, and 40 intervals in each spatial direction, with $\Delta x = \Delta y = 1/N$, $\Delta t = 0.1/N$, and final time $T = 0.1$.
4. Compare with the analytical solution

$$u(x, y, t) = e^{-2\pi^2 t} \sin(\pi x) \sin(\pi y). \quad (24)$$

5. Plot the final solution and its cross-section at $y = 0.5$. Calculate the maximum error over all interior grid points.

Questions: Why is the matrix no longer an ordinary tridiagonal matrix? Why does this initial mode decay twice as fast as the corresponding mode in Problem 1?

Submission Requirements

For each completed problem, submit:

1. The program source code.
2. Plots comparing numerical and analytical solutions.
3. A table of errors and estimated convergence orders.
4. Brief answers to the questions.