Partial differential equations

Parabolic equation with constant coefficients

Let $u(x,t)$ is defined for $x \in [0,1]$ and $t \in [0,T]$.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f(x,t) \tag{1}$$

Initial condition:

$$u(x, t=0) = u_0(x)$$

Boundary conditions

$$u(0,t) = \mu_1(t) \qquad u(1,t) = \mu_2(t)$$

Numerical solutions: grids and grid functions

Consider a 2D grid $\omega_h \times \omega_\tau$:

$$\begin{aligned}\omega_\tau &= \{t_n = n\,\tau\,, \quad n = 0, \ldots, K\,; \quad K\,\tau = T\} \\ \omega_h &= \{x_j = j\,h\,, \quad j = 0, \ldots, N\,; \quad N\,h = 1\}\end{aligned}$$

Define a ***grid function*** $y_j^n \equiv y(x_j, t_n)$.

Stencils

Approximate the derivatives at (x_j, t_n) using a ***stencil***.

Explicit stencil

Using the ***explicit stencil***

Eq.(1) generates at (x_j, t_n),

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{y_{j+1}^n - 2y_j^n + y_{j-1}^n}{h^2} + \phi_j^n \tag{2}$$

This is defined at the ***internal grid points***,
$n = 0, \ldots, K-1$ and $j = 1, \ldots, N-1$.

Explicit stencil

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{y_{j+1}^n - 2y_j^n + y_{j-1}^n}{h^2} + \phi_j^n$$

At the boundary nodes, use initial and boundary conditions

$$y_0^n = \mu_1(t_n)\,, \quad y_N^n = \mu_2(t_n)\,, \qquad n = 0, \ldots, K$$

$$y_j^0 = u_0(x_j)\,, \qquad j = 0, \ldots, K$$

This is a system of linear algebraic equations for y_j^n.

Questions

1. Does this linear system have a unique solution?
2. What is the method of solving it?
3. What is the relation between the FDE, (2), and the PDE, (1), for $h, \tau \to 0$? IOW, does the FDE ***approximate*** the PDE?
4. Does the solution of the FDE ***converge*** to the solution of the PDE for $h, \tau \to 0$.

Does the FDE have a unique solution?

The number of unknowns, y_j^n, is

$$(N+1) \times (K+1)$$

The number equations is

$$\begin{array}{ll} (N-1) \times K & \text{internal nodes} \\ +(K+1) \times 2 & \text{boundary conditions: } x = 0, 1 \\ +(N+1) & \text{initial condition } t = 0 \\ -2 & \text{double-counting the corners} \end{array}$$

$$= N\,K + N + K + 1$$

Solving the FDE: proceed layer by layer

At $n = 0$ the solution is given by the initial condition.

At layer $n + 1$,

$$\frac{\color{blue}{y_j^{\mathbf{n+1}}} - y_j^n}{\tau} = \frac{y_{j+1}^n - 2y_j^n + y_{j-1}^n}{h^2} + \phi_j^n$$

At $j = 0$ and N use the boundary conditions:
$y_0^{n+1} = \mu_1(t_{n+1})$ and $y_N^{n+1} = \mu_2(t_{n+1})$.

Approximation

The FDE approximates the PDE with $O(\tau + h^2)$, provided

- $\phi_j^n - f(x_j, t_n) = O(\tau + h^2)$
- the boundary conditions are approximated with this degree.

Convergence

Define

$$z_j^n = y_j^n - u(x_j, t_n) \ .$$

Convergence means $|z_j^n| \to 0$ as $h \to 0$ and $\tau \to 0$.

The full programme: Substitute $y_j^n = z_j^n + u(x_j, t_n)$ into the FDE, derive the finite-difference equation for z_j^n, thus derive the bounds for $|z_j^n|$.

Instead, use the ***von Neumann*** analysis.

von Neumann stability analysis

- Only works for linear problems.
- Does not account for boundary conditions and r.h.s.
- Only gives necessary conditions for stability and convergence.
- Is very simple.

von Neumann stability analysis

Consider the homogenous equation

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{y_{j+1}^n - 2y_j^n + y_{j-1}^n}{h^2}$$

Look for particular solutions of the form

$$y_j^n(\varphi) = q^n e^{i\varphi jh}$$

where $\varphi \in \mathbb{R}$ and $q \in \mathbb{R}$ is unknown.

von Neumann stability analysis

The corresponding initial conditions are bounded,

$$y_j^0 = e^{i\varphi jh}$$

If $|q| > 1$ for some φ, the corresponding harmonic diverges as $n \to \infty$: the FDE is ***unstable***.

von Neumann stability analysis

Substitute the harmonics into the homogenous FDE:

$$
\begin{aligned}
\frac{q-1}{\tau} &= \frac{e^{ih\varphi} - 2 + e^{-ih\varphi}}{h^2} \\
&= \frac{2(\cos h\varphi - 1)}{h^2} = -\frac{4\sin^2 h\varphi/2}{h^2}
\end{aligned}
$$

So that

$$
q(\varphi) = 1 - \frac{4\tau}{h^2}\sin^2 h\varphi/2
$$

von Neumann stability analysis

Given $q(\varphi) = 1 - \dfrac{4\tau}{h^2} \sin^2 h\varphi/2$,

$$|q| \leqslant 1 \qquad \text{for all } \varphi$$

iff

$$\frac{\tau}{h^2} \leqslant \frac{1}{2}\,.$$

$\Longrightarrow$ The explicit scheme is only ***conditionally stable***.

Implicit methods

Implicit four-point stencil

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f(x, t)$$

Using the ***implicit stencil***

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{y_{j+1}^{n+1} - 2y_j^{n+1} + y_{j-1}^{n+1}}{h^2} + \phi_j^n \tag{3}$$

NB: the r.h.s. contains y^{n+1} at the layer $(n+1)$.

Implicit four-point stencil

The boundary value problem:

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{y_{j+1}^{n+1} - 2y_j^{n+1} + y_{j-1}^{n+1}}{h^2} + \phi_j^n$$

for $j = 1, \ldots, N-1$ and $n = 0, \ldots, K-1$.

Here $\phi_j^n = f(x_j, t_{n+1}) + O(\tau + h^2)\,.$

Boundary conditions:

$$y_0^{n+1} = \mu_1(t_{n+1})\,, \qquad y_N^{n+1} = \mu_2(t_{n+1})\,, \qquad n = 0, \ldots, K-1$$

$$y_j^0 = u_0(x_j)\,, \qquad j = 0, \ldots, N$$

Solving the FDE: layer by layer

At $n = 0$ the solution is given by the initial condition.

At layer $n+1$, solve a tridiagonal system of equations

$$\gamma y_{\mathbf{j+1}}^{n+1} - (1+2\gamma) y_{\mathbf{j}}^{n+1} + \gamma y_{\mathbf{j-1}}^{n+1} = -\left(y_j^n + \tau \phi_j^n \right)$$

$$y_0^{n+1} = \mu_1(t_{n+1})\,, \quad y_N^{n+1} = \mu_2(t_{n+1}).$$

for $j = 1, \ldots N-1$.
NB: The system is diagonally dominant.

Here $\gamma \equiv \tau / h^2$.

von Neumann stability analysis

Consider the homogenous equation

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{y_{j+1}^{n+1} - 2y_j^{n+1} + y_{j-1}^{n+1}}{h^2}$$

Look for particular solutions of the form

$$y_j^n(\varphi) = q^n e^{i\varphi jh}$$

where $\varphi \in \mathbb{R}$ and $q \in \mathbb{R}$ is unknown.

von Neumann stability analysis

For the implicit scheme

$$q^{-1} = 1 + 4\gamma \sin^2 \varphi h/2$$

So that

$$|q| \leqslant 1 \qquad \text{for all } \varphi \in \mathbb{R}$$

irrespective of τ and h.

The scheme is ***absolutely stable***.

Implicit vs explicit schemes

Explicit stencil

- Simple to implement
- Requires that the time step $\tau < h^2/2$

Implicit stencil

- Requires solving a linear system at each layer
- Can choose the time step size

The choice of τ is a balance between the required accuracy and computational complexity.

Crank-Nicholson scheme

Crank-Nicholson scheme

Four-point schemes have the degree of approximation of $O(\tau + h^2)$.

Can we construct a scheme with $O(\tau^2 + h^2)$?

Crank-Nicholson scheme

a.k.a. the symmetrix six-point stencil

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \frac{1}{2}\left(\mathcal{D}_{xx} y_j^{n+1} + \mathcal{D}_{xx} y_j^n\right) + \phi_j^n$$

Where $\mathcal{D}_{xx} y_j^n \equiv \dfrac{y_{j+1}^n - 2y_j^n + y_{j-1}^n}{h^2}$

Crank-Nicholson scheme

- is $O(\tau^2 + h^2)$ provided that

$$\phi_j^n = f(x_j, t_n + \tau/2) + O(\tau^2 + h^2)$$

- is absolutely stable
- on each layer, the tridiagonal system can be solved via the Thomas algorithm
- Note the scheme is $O(\tau^2)$ even though the u_t is approximated with $O(\tau)$

Improved schemes

Consider a single-parameter family of FDEs

$$\frac{y_j^{n+1} - y_j^n}{\tau} = \sigma \mathcal{D}_{xx} y_j^{n+1} + (1-\sigma)\mathcal{D}_{xx} y_j^n + \phi_j^n$$

- $\sigma = 0$ is the explicit scheme
- $\sigma = 1$ is the fully implicit scheme
- $\sigma = 1/2$ is the Crank-Nicholson scheme

Fine-tune σ to maximize the degree of approximation.

Improved schemes

Analyze the parameterized scheme: define

$$z_j^n = y_j^n - u(x_j, t_n)\,,$$

subsitute y_j^n into the FDE, Taylor-expand the ***residual*** around $(x_j, t_n + \tau/2)$.

The scheme is $O(\tau^2 + h^4)$ and is absolutely stable if

- $\sigma = \sigma_* = \dfrac{1}{2} - \dfrac{h^2}{12\tau}$
- $\phi_j^n = f(x_j, t_{n+1/2}) + \dfrac{h^2}{12} f''(x_j, t_{n+1/2}) + O(\tau^2 + h^4)$

Three-layer schemes for parabolic equations

Two (failing) examples.

Three-layer schemes for parabolic equations

Consider the homogenous equation

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

Approximate u_t at (x_j, t_n) with a symmetric difference:

$$\frac{y_j^{n+1} - y_j^{n-1}}{2\tau} = \frac{y_{j+1}^n - 2y_j^n + y_{j-1}^n}{h^2}$$

The scheme is explicit, $O(\tau^2 + h^2)$, but ***unstable*** for all τ, h.

Three-layer schemes for parabolic equations

Try repairing the previous scheme: Replace

$$2y_j^n \quad \text{with} \quad y_j^{n+1} + y_j^{n-1}$$

$$\frac{y_j^{n+1} - y_j^{n-1}}{2\tau} = \frac{y_{j+1}^n - (y_j^{n+1} + y_j^{n-1}) + y_{j-1}^n}{h^2}$$

This scheme is absolutely stable, but approximates different equations depending on $\tau, h \to 0$.

Three-layer schemes for parabolic equations

$$\frac{y_j^{n+1} - y_j^{n-1}}{2\tau} = -\frac{\tau^2}{h^2}\mathcal{D}_{\tau\tau}y_j^n + \mathcal{D}_{xx}y_j^n$$

- for $\tau/h \to 0$ approximates

  $$u_t = u_{xx}$$

  with $O(\tau^2 + h^2 + \tau^2/h^2)$
- for $\tau = h$ approximates a hyperbolic equation

  $$u_t + u_{tt} = u_{xx}$$