Numerical Methods for PDEs

The θ-method

(Lecture 6, Week 2)

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Outline

1. The BTCS scheme
2. Generalisation of the FTCS and BTCS schemes: The θ-method
3. LTE analysis of the θ-method

The BTCS scheme

Goal: Schemes with better stability properties (so-called θ-schemes)

Idea: Study **BTCS schemes**, i.e., work at the forward point (x_j, t_{n+1}) and use Backward Difference Approximation in time (B_t/k) and again Central Difference Approximation in space (δ_x^2/h^2),

$$\frac{w_j^{n+1} - w_j^n}{k} =: \frac{B_t}{k} w_j^{n+1} = \frac{\delta_x^2}{h^2} w_j^{n+1} := \frac{w_{j-1}^{n+1} - 2w_j^{n+1} + w_{j+1}^{n+1}}{h^2},$$

which reads for $r := k/h^2$ as the following *implicit scheme*

$$-rw_{j-1}^{n+1} + (1+2r)w_j^{n+1} - rw_{j+1}^{n+1} = w_j^n \qquad \text{for } j = 1, 2, \ldots, J-1.$$

(Implicit means: Solve a set of simultaneous equations for each time level.)

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Matrix form of the BTCS scheme

$$S\mathbf{w}^{n+1} = \mathbf{w}^n + \mathbf{b}^{\mathbf{n+1}}$$

where

$$S = \begin{pmatrix} 1+2r & -r & 0 & \dots & \\ -r & 1+2r & -r & 0 & \dots \\ 0 & -r & 1+2r & -r & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \\ & \ddots & 0 & -r & 1+2r \end{pmatrix}, \quad \mathbf{w}^n = \begin{pmatrix} w_1^n \\ w_2^n \\ \vdots \\ \vdots \\ w_{J-1}^n \end{pmatrix},$$

$$\mathbf{b}^{n+1} = \begin{pmatrix} r\alpha(t_{n+1}) \\ 0 \\ \vdots \\ 0 \\ r\beta(t_{n+1}) \end{pmatrix}.$$

Example

Problem: For $r = 0.4$ and $J = 4$ solve

$$\begin{cases} u_t = u_{xx}\,, \\ u(0,t) = u(1,t) = 0\,, \quad t > 0 \qquad \text{(BC)} \\ u(x,0) = \sin(x\pi)\,, \qquad \text{(IC)}\,. \end{cases}$$

Solution: The I.C.s tell us that

$$\mathbf{w}^0 = \left[0, 1/\sqrt{2}, 1, 1/\sqrt{2}, 0\right].$$

At $n = 1$ the BCs tell us that $w_0^1 = w_4^1 = 0$. Setting $n = 0$ in the BTCS scheme gives ($j = 1, 2, 3$)

$$\begin{aligned} (1+0.8)w_1^1 - 0.4w_2^1 \qquad\qquad &= w_1^0 + 0.4w_0^1 \\ -0.4w_1^1 + (1+0.8)w_2^1 - 0.4w_3^1 &= w_2^0 \\ -0.4w_2^1 + (1+0.8)w_3^1 &= w_3^0 + 0.4w_4^1 \end{aligned}$$

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or

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\begin{aligned}
1.8w_1^1 - 0.4w_2^1 \qquad &= \frac{1}{\sqrt{2}} + 0.4 \times 0 \\
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\begin{pmatrix} 1.8 & -0.4 & 0 \\ -0.4 & 1.8 & -0.4 \\ 0 & -0.4 & 1.8 \end{pmatrix} \begin{pmatrix} w_1^1 \\ w_2^1 \\ w_3^1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 1 \\ \frac{1}{\sqrt{2}} \end{pmatrix}
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Solving this by Gauss elimination gives

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\mathbf{w}^1 = [0, 0.5729, 0.8102, 0.5729, 0] .
$$

We now repeat this process to get $\mathbf{w}^2, \mathbf{w}^3$, etc. The exact result is

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\mathbf{u}^1 = \exp(-\pi^2 k)\sin(\pi x_j) = [0, 0.5525, 0.7813, 0.5525, 0] .
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Natural generalisation: The θ-method

Take a weigthed average of the FTCS and BTCS scheme

$$\frac{F_t}{k} w_j^n = (1-\theta)\frac{\delta_x^2}{h^2} w_j^n + \theta\frac{\delta_x^2}{h^2} w_j^{n+1}\,, \qquad \text{with } \theta \in (0,1)\,,$$

is called the θ-method for $u_t = u_{xx}$.

Remark. The θ-scheme is

1. the FTCS scheme for $\theta = 0$,
2. the BTCS scheme for $\theta = 1$,
3. implicit for any $\theta > 0$.

For $\theta \in (0,1)$ the computational molecule looks as follows

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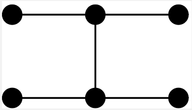

The Crank-Nicolson method: $\theta = 1/2$

For $\theta = 0.5$ we get the so-called *Crank-Nicolson* scheme

$$\frac{F_t}{k} w_j^n = \frac{1}{2}\frac{\delta_x^2}{h^2} w_j^n + \frac{1}{2}\frac{\delta_x^2}{h^2} w_j^{n+1} \,.$$

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LTE analysis of the θ-method

The θ-scheme can be written as

$$L_\Delta w_j^n := \frac{F_t}{k} w_j^n - (1-\theta)\frac{\delta_x^2}{h^2} w_j^n - \theta \frac{\delta_x^2}{h^2} w_j^{n+1} = 0.$$

LTE-procedure:

1. Plug in the exact solution $u(x_j, t_n)$ instead of w_j^n (for all j, n) into $L_\Delta w_j^n$,
2. Taylor expand about $(x, t) = (x_j, t_n)$,
3. Eliminate terms using the PDE.

Remember, do not multiply or divide $L_\Delta w_j^n$ by k or h when working out the LTE.

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We make Taylor series of smooth enough functions $u(x,t)$, i.e.,

$$
\begin{aligned}
F_t u(x_j,t_n) &= u(x_j,t_n+k) - u(x_j,t_n) \\
&= \left[k\frac{\partial}{\partial t} + \frac{k^2}{2!}\frac{\partial^2}{\partial t^2} + \frac{k^3}{3!}\frac{\partial^3}{\partial t^3} + O(k^4) \right] u(x_j,t_n) \\
&= \left[k\,u_t + \frac{k^2}{2!}u_{tt} + \frac{k^3}{3!}u_{ttt} \right]_{(x_j,t_n)} + O(k^4).
\end{aligned}
$$

Expanding the 2nd central space difference term $\delta_x^2 u(x_j,t_n)$ gives

$$
\begin{aligned}
\delta_x^2 u(x_j,t_n) &= u(x_j+h,t_n) - 2u(x_j,t_n) + u(x_j-h,t_n) \\
&= \left[h^2\frac{\partial^2}{\partial x^2} + \frac{2h^4}{4!}\frac{\partial^4}{\partial x^4} + O(h^6) \right] u(x_j,t_n) \\
&= \left[h^2\,u_{xx} + \frac{h^4}{12}u_{xxxx} \right]_{(x_j,t_n)} + O(h^6).
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The similar term $\delta_x^2 u(x_j, t_{n+1})$ (time level $n+1$) becomes

$$\begin{aligned}\delta_x^2 u(x_j, t_n+k) &= u(x_j+h, t_n+k) - 2u(x_j, t_n+k) + u(x_j-h, t_n+k) \\ &= \left[h^2 u_{xx} + \frac{h^4}{12} u_{xxxx} + O(h^6)\right]_{(x_j, t_n+k)}.\end{aligned}$$

Note that this term is evaluated at time $t = t_n + k$ and so it must also be expanded in k. That is

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We now substitute each of the three terms into $L_\Delta w_j^n$ and collect terms of the same order to get

$$\mathrm{LTE} = (u_t - u_{xx}) + k\left(\frac{1}{2}u_{tt} - \theta u_{txx}\right) - \frac{h^2}{12}u_{xxxx} + O(k^2,\, kh^2,\, h^4).$$

Since u is a solution of the PDE, this eliminates $u_t - u_{xx}$.
Also, differentiating the PDE once with respect to t gives

$$u_{tt} = u_{txx} = u_{xxxx}$$

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Therefore,

$$\text{LTE} = \begin{cases} \mathcal{O}(k, h^2) & \text{for } \theta,\ k,\ h \text{ arbitrary}\,, \\ \mathcal{O}(h^2) & \text{for } k = \mathcal{O}(h^2)\,, \\ \mathcal{O}(k^2, h^2) & \text{for } \theta = 1/2\,, \\ \mathcal{O}(h^4) & \text{for } \theta = \frac{1}{2} - \frac{1}{12r},\ r = k/h^2,\ k = \mathcal{O}(h^2)\,, \end{cases}$$

where the last property (4th order accurate) is a result of setting

$$k\left(\frac{1}{2} - \theta\right) - \frac{h^2}{12} = 0\,,$$

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