Lecture 4

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Numerical Methods for PDEs

Outline of Lecture 4

- exercises of Lecture 3
- FTCS for the heat equation
- Von Neumann stability
- Lax equivalence theorem
- Conditional consistency and unconditional instability
- The heat equation in 2D
- outlook to Lecture 5

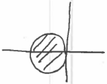
FTCS for heat equation [1]

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

κ: diffusion coefficient > 0

① Method of Lines $\underset{\text{step 1}}{\Rightarrow}$ $\frac{d\vec{u}}{dt} = \kappa D_{2c}\vec{u}$; $\lambda(D_{2c}) \in \mathbb{R}^-$ (see exercise)

step 2 (for example) EF, stability region in $\mathbb{C}$: S_{EF}



check...

$\Rightarrow$ $\kappa \cdot \lambda(D_{2c}) \in S_{EF}$ (stable num. sol.) if $\boxed{\frac{\kappa \cdot \Delta t}{(\Delta x)^2} \le \frac{1}{2}}$ conditional stability

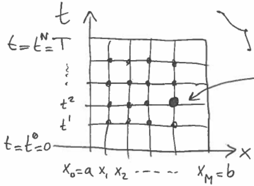
② space-time discretization ("one" step) $\Leftrightarrow$ MoL + EF (for this choice)

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

FTCS (forward in time, central in space)

with $u_i^n \approx u(x_i, t^n)$

FTCS for heat equation [2]



numerical grid in space-time domain

gridpoint (x_i, t^n)

FTCS: $u_i^{n+1} = u_i^n + \frac{\kappa \Delta t}{(\Delta x)^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)$

$i = ----$

$n = -----$

IC: $u_i^0 = ---$, $i = --$

BC's: $\begin{cases} u_0^n = --- , & n = - \\ u_M^n = --- , & n = --- \end{cases}$

Consider the general PDE: $\mathcal{L}u = 0$ and a FD-approximation: $L_\Delta u = 0$

Let $v(x,t)$ be any smooth function, then the local truncation error τ_i^n (LTE):

$$\tau_i^n = \mathcal{L}\left(v(\underbrace{i\Delta x}_{x_i}), v(\underbrace{n\Delta t}_{t^n})\right) - L_\Delta v(i\Delta x, n\Delta t)$$

FTCS for heat equation [3]

Example:

$$\begin{cases} L v = v_t - \kappa v_{xx} & \text{(heat equation)} \\ L_\Delta v = \dfrac{v_i^{n+1} - v_i^n}{\Delta t} - \kappa \cdot \dfrac{v_{i+1}^n - 2v_i^n + v_{i-1}^n}{(\Delta x)^2} & \text{(FTCS)} \end{cases}$$

$$\Rightarrow \tau_i^n = \left[(v_t)_i^n - \frac{v_i^{n+1} - v_i^n}{\Delta t} \right] - \kappa \cdot \left[(v_{xx})_i^n - \frac{v_{i+1}^n - 2v_i^n + v_{i-1}^n}{(\Delta x)^2} \right]$$

using Taylor series:

$$= -\frac{\Delta t}{2} (v_{tt})_i^n + \frac{\kappa (\Delta x)^2}{12} (v_{xxxx})_i^n + \text{H.O.T. in } \Delta t \text{ and } \Delta x$$

↖ higher order terms

Def. A FD-scheme $L_\Delta u_i^n = 0$ is consistent "with a PDE" $\mathcal{L} u = 0$ if $\tau_i^n \to 0$ as $\Delta x \to 0$ AND $\Delta t \to 0$

↳ FTCS-scheme is consistent (for the heat equation)

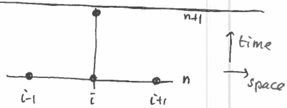
FTCS for heat equation [4]

FTCS for the heat equation can be re-written as:

$$\boxed{\vec{U}^{n+1} = L_\Delta \vec{U}^n}$$

where $\vec{U}^n \stackrel{\text{def}}{=} \begin{pmatrix} \vdots \\ u_i^n \\ \vdots \end{pmatrix}$ and $L_\Delta = \begin{pmatrix} 1-2r & r & & \emptyset \\ r & 1-2r & r & \\ & & \ddots & \\ \emptyset & & r & 1-2r \end{pmatrix}$, $\boxed{r \stackrel{\text{def}}{=} K \cdot \frac{\Delta t}{(\Delta x)^2}}$

computational stencil of FTCS (heat eq.):



Note: $\|L_\Delta\|_\infty = |1-2r| + 2r$

matrix norm

if $r \leq \frac{1}{2}$, then $1-2r \geq 0$ and $\|L_\Delta\|_\infty = 1$

FTCS for heat equation [5]

Def.: $\vec{u}^n = \begin{pmatrix} \vdots \\ u(x_i,t^n) \\ \vdots \end{pmatrix}$ "exact" values at grid points

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Def.: A FD-approximation converges to the solution of a PDE on the interval $0 \le t^n \le T$, at $t = t^n$, if $\|\vec{u}^n - \vec{U}^n\| \to 0$

for $\begin{cases} n \to \infty \\ \Delta x \downarrow 0 \\ \Delta t \downarrow 0 \\ \underbrace{n \cdot \Delta t}_{=t^n} \le T \end{cases}$

Def.: A FD-scheme is stable, if there exists a positive constant C (independent of the gridspacing and initial data)

such that $\|\vec{U}^n\| \le C \cdot \|\vec{U}^0\|$, $n \to \infty$, $\Delta x \downarrow 0$, $\Delta t \downarrow 0$ at $t^n = n\Delta t \le T$

(a bound on the growth of the numerical solution)

$\sim$ well-posedness of the underlying PDE

FTCS for heat equation [6]

Thm: FTCS for the heat equation converges in the maximum norm, if $r \le \frac{1}{2}$. (*)

Proof: we have $U_i^{n+1} = r U_{i-1}^n + (1-2r) U_i^n + r U_{i+1}^n \quad \forall i$ (numerical solution)

and $u_i^{n+1} = r u_{i-1}^n + (1-2r) u_i^n + r u_{i+1}^n + \Delta t\, \tau_i^n \quad \forall i$ (exact solution)

let $e_i^n = u_i^n - U_i^n$ ("the error at (x_i, t^n)")

Because of the linearity of the problem $\Longrightarrow$

$$e_i^{n+1} = r e_{i-1}^n + (1-2r) e_i^n + r e_{i+1}^n + \Delta t\, \tau_i^n \quad \forall i$$

Taking absolute values and using the triangle inequality ($|a+b| \le |a| + |b|$)

$$\Rightarrow |e_i^{n+1}| \le |r| \cdot |e_{i-1}^n| + |1-2r| \cdot |e_i^n| + |r| \cdot |e_{i+1}^n| + \Delta t \cdot |\tau_i^n|$$

$$|\tau_i^n| \le \|\vec{\tau}^n\|_\infty$$

$$\le (|r| + |1-2r| + |r|) \cdot \|\vec{e}^n\|_\infty + \Delta t \cdot \|\vec{\tau}^n\|_\infty$$

we know that $r > 0$ and we assume (*) $r \le \frac{1}{2} \Longrightarrow |1-2r| \ge 0$

and the absolute value signs can be removed: $|r| + |1-2r| + |r| = r + 1 - 2r + r = 1$

(stability condition)

FTCS for heat equation [7]

$$\Rightarrow \quad |e_i^{n+1}| \le \|\vec{e}^{\,n}\|_\infty + \Delta t . \|\vec{\tau}^{\,n}\|_\infty \qquad \forall i$$

$$\text{and } \|\vec{e}^{\,n+1}\|_\infty \le \|\vec{e}^{\,n}\|_\infty + \Delta t . \|\vec{\tau}^{\,n}\|_\infty$$

$$\le \|\vec{e}^{\,n-1}\|_\infty + \Delta t . \|\vec{\tau}^{\,n-1}\|_\infty + \Delta t . \|\vec{\tau}^{\,n}\|_\infty$$

$$\le \; -- \qquad --- \qquad --$$

$$\le \|\vec{e}^{\,0}\|_\infty + n . \Delta t . \underbrace{\max_{0 \le k \le n} \|\vec{\tau}^{\,k}\|_\infty}_{\overset{\text{def}}{=} \tau}$$

neglecting round-off errors at $t=0$: $\|\vec{e}^{\,0}\|_\infty = 0$

note that $t^n = n . \Delta t \le T$ $\forall$ combinations of n and Δt

$\Rightarrow \|\vec{e}^{\,n}\|_\infty \le T . \tau$ (oo) (T: constant)

Remember: $\tau_i^n = -\frac{\Delta t}{2} (u_{tt})_i^n + \frac{\kappa (\Delta x)^2}{12} (u_{xxxx})_i^n + \text{H.O.T.}$

$$\Rightarrow |\tau| \le \underbrace{\frac{\Delta t}{2} \max_{\forall t, \forall x} |u_{tt}| + \frac{\kappa (\Delta x)^2}{12} \max_{\forall t, \forall x} |u_{xxxx}|}_{\to 0 \text{ for } \Delta t \to 0 \text{ and } \Delta x \to 0 \text{ (consistency)}} + \text{H.O.T.} \quad \Rightarrow \tau \to 0$$

(oo) $\Rightarrow \|\vec{e}^{\,n}\|_\infty \to 0$ for Δx and $\Delta t \to 0$ (convergence)

FTCS for heat equation [8]

Special case ("supra-convergence"):

FTCS heat eq. } $\tau_i^n = \left[-\frac{1}{2}\Delta t\,\kappa^2 + \frac{\kappa}{12}(\Delta x)^2\right] u_{xxxx} + O((\Delta t)^2) + O((\Delta x)^4)$

$u_t = \kappa u_{xx}$

$u_{tt} = \kappa (u_{xx})_t = \kappa(\kappa u_t)_{xx} = \kappa (u_{xx})_{xx} = \kappa^2 u_{xxxx}$

if we choose $\frac{\Delta t}{(\Delta x)^2} = \frac{1}{6\kappa}$, then $\tau_i^n = O((\Delta t)^2) + O((\Delta x)^4)$

$= O((\Delta x)^4)$

$\left(\Rightarrow \frac{\kappa\,\Delta t}{(\Delta x)^2} = \frac{1}{6} < \frac{1}{2}\right)$

fourth-order accurate!

Von Neumann stability [1]

Define: A = analytical solution of the PDE
D = exact solution of the FD equation
N = numerical solution using a computer with finite accuracy

$\Rightarrow$ discretization error $= A - D$
round-off error $\stackrel{\text{def}}{=} \varepsilon = N - D$ and $N = D + \varepsilon$

---

for FTCS applied to the heat equation with $K=1$:

$$\frac{D_i^{n+1} + \varepsilon_i^{n+1} - D_i^n - \varepsilon_i^n}{\Delta t} = \frac{D_{i+1}^n + \varepsilon_{i+1}^n - 2D_i^n - 2\varepsilon_i^n + D_{i-1}^n + \varepsilon_{i-1}^n}{(\Delta x)^2}$$

(we have added a round-off error to each term in the exact FD equation)

D "must" solve the FTCS equation exactly $\Rightarrow$ $\dfrac{\varepsilon_i^{n+1} - \varepsilon_i^n}{\Delta t} = \dfrac{\varepsilon_{i+1}^n - 2\varepsilon_i^n + \varepsilon_{i-1}^n}{(\Delta x)^2}$ $\boxed{\bullet\bullet}$

so, ε satisfies the same FD equation!
(this is, because we consider a linear PDE)

Von Neumann stability [2]

Stability: the ε_i's do not grow from step n to step $n+1$ (in the time direction)

$$\Leftrightarrow \quad |\varepsilon_i^{n+1}| \le |\varepsilon_i^n| \quad \Leftrightarrow \quad \left|\frac{\varepsilon_i^{n+1}}{\varepsilon_i^n}\right| \le 1$$

Assume: the distribution of the errors "along the x-axis" can be given by a Fourier series in x, such that the time-wise variation is exponential in time, i.e.

$$\varepsilon(x,t) = e^{at} \sum_{m=1}^{\infty} e^{i k_m x}$$

with $a \in \mathbb{C}$, k_m = wave number, $i = \sqrt{-1}$.

The FD equation is linear $\Rightarrow$ each term in the series behaves in the same way as the series itself. Hence, let us deal with just one term of the series and write $\varepsilon_m(x,t) = e^{at} e^{i k_m x}$ [·]

Substitute [·] into [··] (previous page):

$t^n \leftrightarrow t$, $t^{n-1} \leftrightarrow t-\Delta t$, $t^{n+1} \leftrightarrow t+\Delta t$
$x_i \leftrightarrow x$, $x_{i-1} \leftrightarrow x-\Delta x$, $x_{i+1} \leftrightarrow x+\Delta x$ $\longrightarrow$

$$\frac{e^{a(t+\Delta t)} \cdot e^{i k_m x} - e^{at} \cdot e^{i k_m x}}{\Delta t} = \frac{e^{at} \cdot e^{i k_m (x+\Delta x)} - 2 e^{at} e^{i k_m x} + e^{at} e^{i k_m (x-\Delta x)}}{(\Delta x)^2}$$

Von Neumann stability [3]

divide by $e^{at}e^{ik_m x}$: $$\frac{e^{a\Delta t}-1}{\Delta t} = \frac{e^{ik_m\Delta x}-2+e^{-ik_m\Delta x}}{(\Delta x)^2}$$

or $$e^{a\Delta t} = 1 + \frac{\Delta t}{(\Delta x)^2}\left[e^{ik_m\Delta x}+e^{-ik_m\Delta x}-2\right]$$

remember $\cos(k_m\Delta x) = \frac{e^{ik_m\Delta x}+e^{-ik_m\Delta x}}{2}$

$$= 1 + \frac{2\Delta t}{(\Delta x)^2}\left[\cos(k_m\Delta x)-1\right]$$

remember $\sin^2\left(\frac{k_m\Delta x}{2}\right) = \frac{1-\cos(k_m\Delta x)}{2}$

$$= 1 - \frac{4\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k_m\Delta x}{2}\right)$$

from ⊡ on previous page ("dropping" the m):

$$\frac{\varepsilon_i^{n+1}}{\varepsilon_i^n} = \frac{e^{a(t+\Delta t)}\cdot e^{ik_m x}}{e^{at}\cdot e^{ik_m x}} = e^{a\Delta t}$$

$$\Rightarrow \left|\frac{\varepsilon_i^{n+1}}{\varepsilon_i^n}\right| = \left|e^{a\Delta t}\right| = \left|1-\frac{4\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k_m\Delta x}{2}\right)\right|$$

$(a \in \mathbb{C})$

Von Neumann stability [4]

$G = |e^{a\Delta t}|$ is called <u>the amplification factor</u>

stability for FTCS/heat if $G \leq 1$

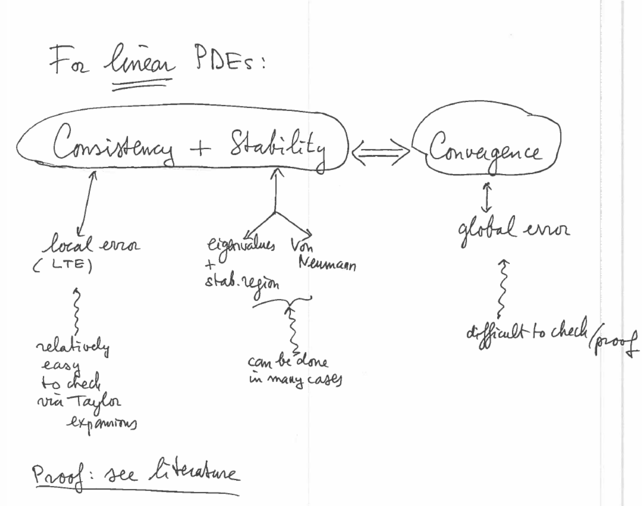
$$\Leftrightarrow \; -1 \leq 1 - \frac{4\Delta t}{(\Delta x)^2} \sin^2\left(\frac{k_m \Delta x}{2}\right) \leq 1$$

1) $\frac{4\Delta t}{(\Delta x)^2} \sin^2\left(\frac{k_m \Delta x}{2}\right) \geq 0$ (always true) ⟷ gives no extra information ---

2) $\frac{\Delta t}{(\Delta x)^2} \underbrace{\sin^2\left(\frac{k_m \Delta x}{2}\right)}_{\in (0,1)} \leq \frac{1}{2}$

If $\underbrace{\frac{\Delta t}{(\Delta x)^2}}_{= r \text{ (with } K=1)} \leq \frac{1}{2}$, then $G \leq 1$

Lax equivalence theorem



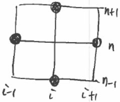
Conditional consistency

Du Fort – Frankel scheme for the heat equation

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

(not connected to the MoL approach!)

Computational stencil:



LTE : $\tau_i^n = \frac{K}{12}(u_{xxxx})_i^n(\Delta x)^2 - (u_{tt})_i^n\left(\frac{\Delta t}{\Delta x}\right)^2 - \frac{1}{6}K^2(u_{ttt})_i^m(\Delta t)^2 + \dots$

IF we let Δt and Δx approach to zero at the same rate $\frac{\Delta t}{\Delta x} = \beta$ (constant >0)
then the method is inconsistent. In fact, it approximates the PDE:

$$u_t + \beta^2 u_{tt} = K\cdot u_{xx}$$

"wave equation with damping"... large

The scheme is called: conditionally consistent

Unconditional instability

Leapfrog scheme for the heat equation ("haasje-over")

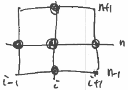
$$\frac{u_i^{n+1}-u_i^{n-1}}{2\Delta t} = \frac{k}{(\Delta x)^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)$$

(in the MoL sense it is explicit midpoint for the central in space discretization)

CTCS (central in time, central in space)

- a three level method ($n-1, n, n+1$ ⇒ requires extra numerical starting value)
- LTE: $\tau_i^n = O((\Delta t)^2) + O((\Delta x)^2)$ ⇒ consistent

computational stencil:



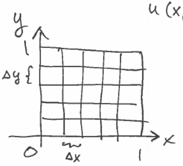
Note that $\lambda(D_{2c}) \in \mathbb{R}^-$ (see before) and $S_{\text{explicit midpoint}} \in i\mathbb{R}$ (on the imaginary axis in the complex plane)

⇒ CTCS for heat eq. unconditionally unstable (for all $\Delta t, \Delta x$ choices)

The heat equation in 2d [1]

$$u_t = \kappa \cdot (u_{xx} + u_{yy}) = \kappa \cdot \Delta u \quad , \Omega = [0,1] \times [0,1]$$

$$u(x,y,0) = u_0(x,y) \text{ + BC's on } \partial\Omega$$



approximation of Δu in (x_i, y_j):

$$u_{xx}\Big|_{(x_i,y_j)} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{(\Delta x)^2} + \dots$$

$$u_{yy}\Big|_{(x_i,y_j)} = \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{(\Delta y)^2} + \dots$$

Take, for example, $\Delta x = \Delta y = h$:

$$\Delta u\Big|_{(x_i,y_j)} = \frac{1}{h^2}\left(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}\right) - \frac{h^2}{12}\left[u_{xxxx}\Big|_{i,j} + u_{yyyy}\Big|_{i,j}\right] + \dots$$

The heat equation in 2d [2]

Time-integration:

Choice 1 (EF)

$$u_{i,j}^{n+1} = u_{i,j}^{n} + \frac{k\Delta t}{h^2}\left[u_{i-1,j}^{n} + u_{i+1,j}^{n} + u_{i,j-1}^{n} + u_{i,j+1}^{n} - 4u_{i,j}^{n}\right]$$

LTE: $O(h^2) + O(\Delta t)$

stability: substitute (Von Neumann stability) $u_{i,j}^{n} = e^{at} e^{i\xi x} \cdot e^{i\eta y}$

$\Longrightarrow$ amplification factor $G = \left|1 - 4\frac{k\Delta t}{h^2}\sin^2\left(\frac{\xi h}{2}\right) - 4\frac{k\Delta t}{h^2}\sin^2\left(\frac{\eta h}{2}\right)\right|$

it follows that $G \le 1$, if $0 \le \frac{k\Delta t}{h^2} \le \frac{1}{4}$ ← factor two smaller than in 1D

$\Rightarrow$ conditionally stable & 1st order accuracy in time direction

Choice 2 (Trapezoïdal method in time) ← short notation for FD approx. (see also lecture 2)

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{\Delta t} = k \cdot \frac{\Delta_x^2 u_{i,j}^{n} + \Delta_x^2 u_{i,j}^{n+1}}{2(\Delta x)^2} + k \cdot \frac{\Delta_y^2 u_{i,j}^{n} + \Delta_y^2 u_{i,j}^{n+1}}{2(\Delta y)^2}$$

$$\Delta_x^2 u_i = u_{i+1} - 2u_i + u_{i-1}$$

$$\Delta_y^2 u_j = u_{j+1} - 2u_j + u_{j-1}$$

The heat equation in 2d [3]

$\Longrightarrow$ **Crank-Nicolson method** for the 2D heat equation

LTE: $O((\Delta x)^2) + O((\Delta y)^2) + O((\Delta t)^2)$

stability: $G \leq 1 \quad \forall\, \xi, \eta$ (unconditionally stable)

however, re-writing the FD equations, gives in each timestep:

$A \vec{u}^{\,n+1} = \vec{u}^{\,n}$, but no longer, as in 1d, a simple tridiagonal structure

(A: sparse matrix)

$\Rightarrow$ stable, but "explosive"

Choice 3 Alternating-Direction scheme (ADI) — a splitting method (see also later on in the course)

"in one direction (x) implicit
in the other direction (y) explicit
and also the other way round" + combine both

The heat equation in 2d [4]

i) $$\frac{u_{i,j}^{n+\frac{1}{2}} - u_{i,j}^{n}}{\frac{1}{2}\Delta t} = \frac{k}{(\Delta x)^2}\Delta_x^2 u_{i,j}^{n+\frac{1}{2}} + \frac{k}{(\Delta y)^2}\Delta_y^2 u_{i,j}^{n}$$

half time step

solve tridiagonal system (conditionally stable!! $k\cdot\frac{\Delta t/2}{(\Delta y)^2} \le \frac{1}{2}$)

ii) take another half time step:

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n+\frac{1}{2}}}{\frac{1}{2}\Delta t} = \frac{k}{(\Delta x)^2}\Delta_x^2 u_{i,j}^{n+\frac{1}{2}} + \frac{k}{(\Delta y)^2}\Delta_y^2 u_{i,j}^{n+1}$$

solve tridiagonal system (stability restriction: $k\cdot\frac{\Delta t/2}{(\Delta x)^2} \le \frac{1}{2}$)

However, the combined method of i) and ii) (full time step):

$$\frac{1}{2}(\Delta_x^2 + \Delta_y^2)(u_{i,j}^{n+1} + u_{i,j}^{n}) = \frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{\Delta t} + \frac{\Delta t}{4}\Delta_x^2\Delta_y^2(u_{i,j}^{n+1} - u_{i,j}^{n})$$

is UNconditionally stable! (see literature)

error: $O((\Delta t)^2) + O((\Delta x)^2) + O((\Delta y)^2)$

efficiency: two tridiagonal systems to be solved

Outlook to Lecture 5

- prepare exercises of Lecture 4 (see webpage!)
- the advection equation
- FTCS
- upwind, downwind
- Lax-Friedrichs
- Lax-Wendroff