# Lecture 4

Paul Andries Zegeling

Department of Mathematics, Utrecht University

Numerical Methods for Time-Dependent PDEs, Spring 2024

# 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

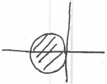
# FTCS for heat equation [1]

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

diffusion coefficient $> 0$

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

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



check ...

$\Rightarrow$ $\kappa \cdot \lambda(D_{2c}) \in S_{EF}$ if $\boxed{\dfrac{\kappa \cdot \Delta t}{(\Delta x)^2} \leq \dfrac{1}{2}}$ conditional stability

(stable num. sol.)

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

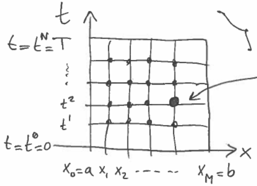
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \kappa \cdot \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2}$$

$\boxed{\text{FTCS}}$

forward in time (FT) ; central in space (CS)

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

$i = \text{----}$

$n = \text{-----}$

IC : $u_i^0 = \text{---} \quad , i = \text{--}$

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

---

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 $\tau_i^n$ (LTE):

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

# FTCS for heat equation [3]

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

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

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

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 $\Delta t \to 0$

$\Rightarrow$ FTCS-scheme is consistent (for the heat equation)

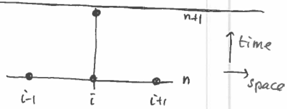
# FTCS for heat equation [4]

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 $L_\Delta = \begin{pmatrix} 1-2r & r & & \Theta \\ r & 1-2r & r & \\ & & \ddots & \\ \Theta & & r & 1-2r \end{pmatrix}$, $\boxed{r \stackrel{\text{def}}{=} K \cdot \frac{\Delta t}{(\Delta x)^2}}$

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

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

Def.: A FD-scheme is stable, if there exists a positive constant $C$ such that $\|\vec{U}^n\| \le C.\|\vec{u}^0\|$, $n \to \infty$, $\Delta x \downarrow 0$, $\Delta t \downarrow 0$ at $t^n = n\,\Delta t \le T$

independent of the gridspacing and initial data

(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 $\Rightarrow$

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

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

$$\Rightarrow |e_i^{n+1}| \le |r| . |e_{i-1}^n| + |1-2r| . |e_i^n| + |r| . |e_{i+1}^n| + \Delta t . \underbrace{|\tau_i^n|}_{\le \|\vec{\tau}^n\|_\infty}$$

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

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

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

(stability condition)

# FTCS for heat equation [7]

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

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

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

$$\leq \ldots \qquad \ldots \qquad \ldots$$

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

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

note that $t^n = n \cdot \Delta t \leq T$ $\forall$ combinations of $n$ and $\Delta t$ $\Big\} \Rightarrow \|\vec{e}^{\,n}\|_\infty \leq T \cdot \tau$ (oo)

$\uparrow$ constant

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

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

(consistency)

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

# FTCS for heat equation [8]

Special case ("supra-convergence"):

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

$u_t = \kappa u_{xx}$

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

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

$\left( \Rightarrow \dfrac{\kappa \Delta t}{(\Delta x)^2} = \dfrac{1}{6} < \dfrac{1}{2} \right)$ $= O((\Delta x)^4)$

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 $\Rightarrow \dfrac{\varepsilon_i^{n+1} - \varepsilon_i^n}{\Delta t} = \dfrac{\varepsilon_{i+1}^n - 2\varepsilon_i^n + \varepsilon_{i-1}^n}{(\Delta x)^2}$ $\boxed{\cdot\cdot}$

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

# Von Neumann stability [2]

Stability: the $\varepsilon_i$'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.

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

$a \in \mathbb{C}$, $k_m$: wave number

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

Substitute $\boxed{\cdot}$ into $\boxed{\cdot\cdot}$ (previous page):

$t^n \leftrightarrow t$, $t^{n-1} \leftrightarrow t - \Delta t$, $t^{n+1} \leftrightarrow t + \Delta t$

$x_i \leftrightarrow x$, $x_{i-1} \leftrightarrow x - \Delta x$, $x_{i+1} \leftrightarrow x + \Delta x$

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

# Von Neumann stability [3]

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

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

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

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

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

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

from $\boxed{\cdot}$ 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 $G \leq 1$

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

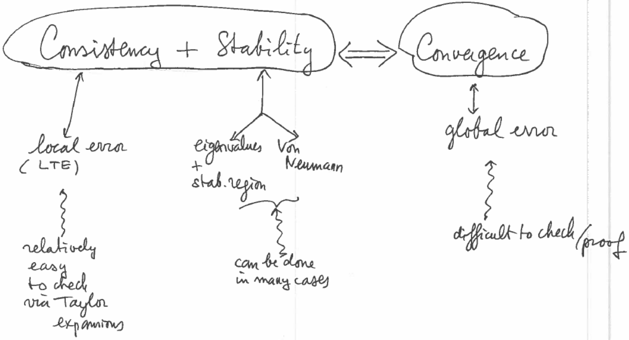
1) $\frac{4\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k_m \Delta x}{2}\right) \geq 0$ (always true) $\leftrightarrow$ gives no extra information ---

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

For linear PDEs:




Proof: see literature

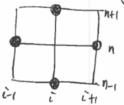
# Conditional consistency

<u>Du Fort – Frankel scheme</u> 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 : $\tau_i^n = \frac{K}{12}(u_{xxxx})_i^n (\Delta x)^2 - (u_{tt})_i^n \left(\frac{\Delta t}{\Delta x}\right)^2 - \frac{1}{6} K^2 (u_{ttt})_i^n (\Delta t)^2 + \cdots$

$\boxed{\text{IF}}$ we let $\Delta t$ and $\Delta x$ approach to zero <u>at the same rate</u> $\frac{\Delta t}{\Delta x} = \beta_{>0}$ (constant) then the method is <u>in</u>consistent. 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: <u>conditionally consistent</u>

# 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)

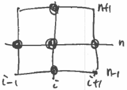
$\boxed{\text{CTCS}}$ — a three level method (n-1, n, n+1 $\Rightarrow$ requires extra numerical starting value)

central in time, central in space

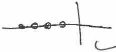
— LTE : $\tau_i^n = O((\Delta t)^2) + O((\Delta x)^2)$

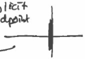
$\Rightarrow$ consistent

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)



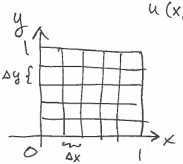


$\Rightarrow$ CTCS for heat eq. unconditionally unstable (for all $\Delta t, \Delta x$ choices)

# The heat equation in 2d [1]

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

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




approximation of $\Delta u$ in $(x_i, y_j)$:

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

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

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

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

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

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

Choice 2 Trapezoidal 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: $\mathcal{O}((\Delta x)^2) + \mathcal{O}((\Delta y)^2) + \mathcal{O}((\Delta t)^2)$

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

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

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

$\Longrightarrow$ stable, but "expensive"

Choice 3   Alternating-Direction scheme (ADI)

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

a splitting method (see also later on in the course)

# 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!? $\frac{k\cdot\Delta t/2}{(\Delta y)^2} \le \frac{1}{2}$)

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 $\Delta t$):

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

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