

Chap 3: Finite difference methods

for PDEs

3.1 Basic notions of discretization

while we are interested in the continuum limit of PDEs, discretization of some kind is required for most numerical approaches

$$\begin{array}{ccc} X_0 & & Y_0 \\ U & & V \\ L : X & \xrightarrow{\quad} & Y \\ (u & \mapsto & Lu = S) \\ \downarrow D_h^X & & \downarrow D_h^Y \\ L_h : X_h & \longrightarrow & Y_h \end{array}$$

continuum problem: $\boxed{Lu = S}$ continuum PDE

typically: $X_0 = C^0(\Omega), \Omega \subseteq \mathbb{R}^n$

$$X = \left\{ u \in C^2(\Omega) \mid \sup_{\Omega} |Lu| < \infty \right\} \subset X_0$$

regularity depends on differential operator L and the type of solution to be found

$$Y \subseteq Y_0 = C^0(\Omega)$$

Examples: $L = \Delta, \square, \partial_t - \partial_x f(\cdot), \dots$

discretized problem:

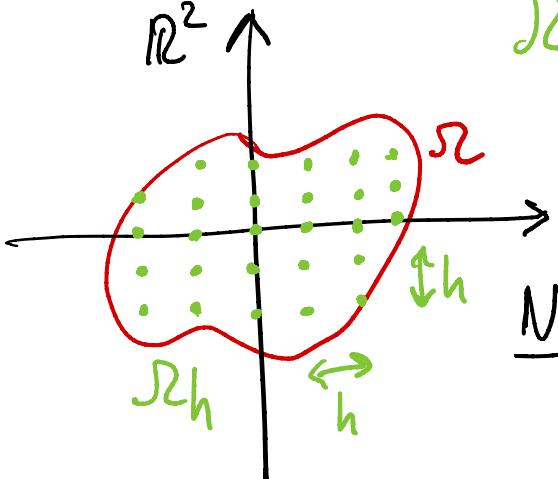
$$L_h u_h = S_h$$

discretized PDE

typically: $X_h = \{\text{grid functions}\}$

$$= \{v : \Omega_h \rightarrow \mathbb{R}^n\}$$

$$\Omega_h = \text{"grid"}, \text{e.g.: } \Omega \cap h\mathbb{Z}^n$$



$h = \text{discretization parameter}$

Notation:

$$x \rightarrow x_i \in \{x_1, \dots, x_{N_x}\}$$

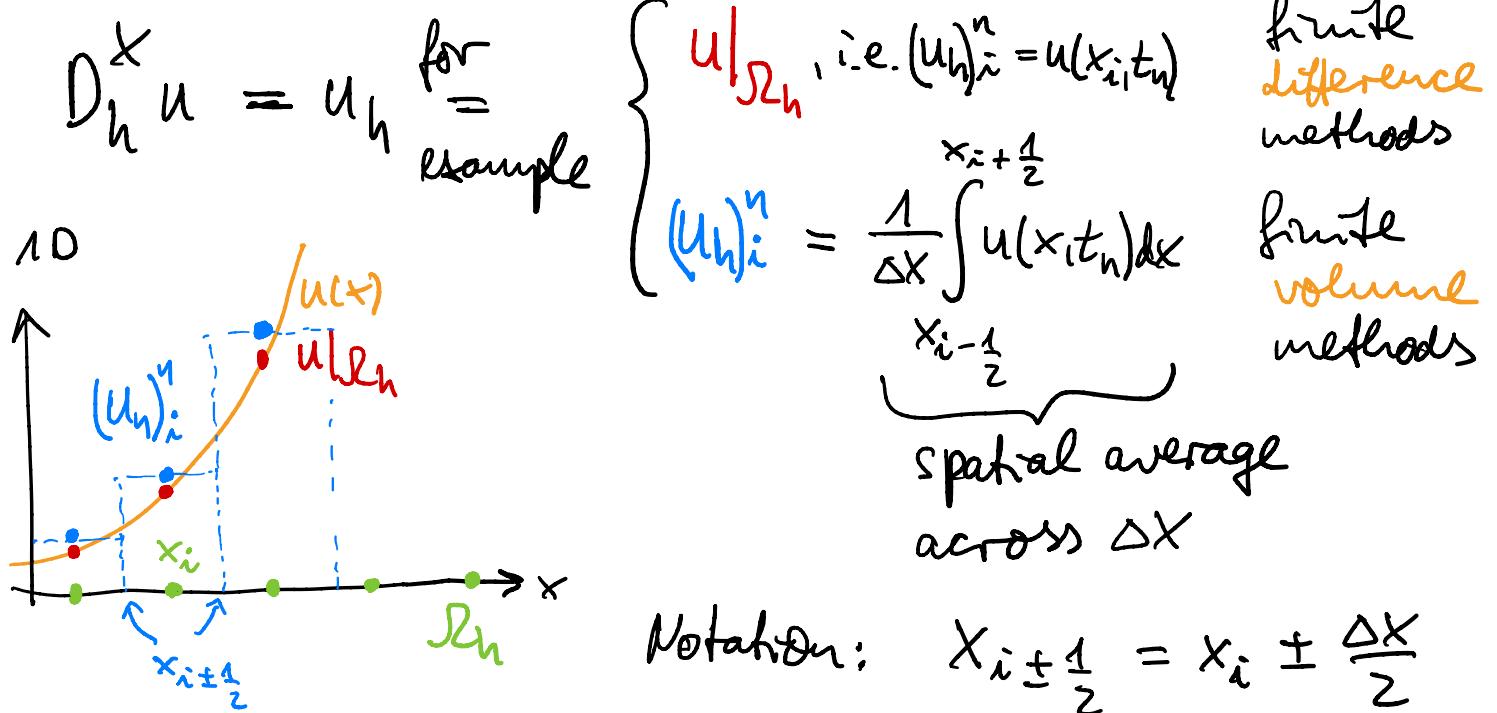
$$t \rightarrow t_n \in \{t_1, \dots, t_{N_t}\}$$

$$v \in X_h : v_i^n = v(x_i, t_n)$$

D_h^X : discretization operator

$$D_h^X : X \rightarrow X_h$$

$$u \mapsto D_h^X u \equiv u_h$$



Example: $\Omega = \mathbb{R} \times (0, \infty)$, $h = \Delta x = \Delta t$

$$\mathcal{S}_h = \{(h_i, h_n) \mid i \in \mathbb{Z}, n \in \mathbb{N}\}$$

Notation: $(x_i, t_n) \equiv (h_i, h_n)$

$$v_i^n \equiv v(x_i, t_n), \quad v \in X_h$$

3.2 Finite difference approximations

Discretize continuum PDE by discrete grid:

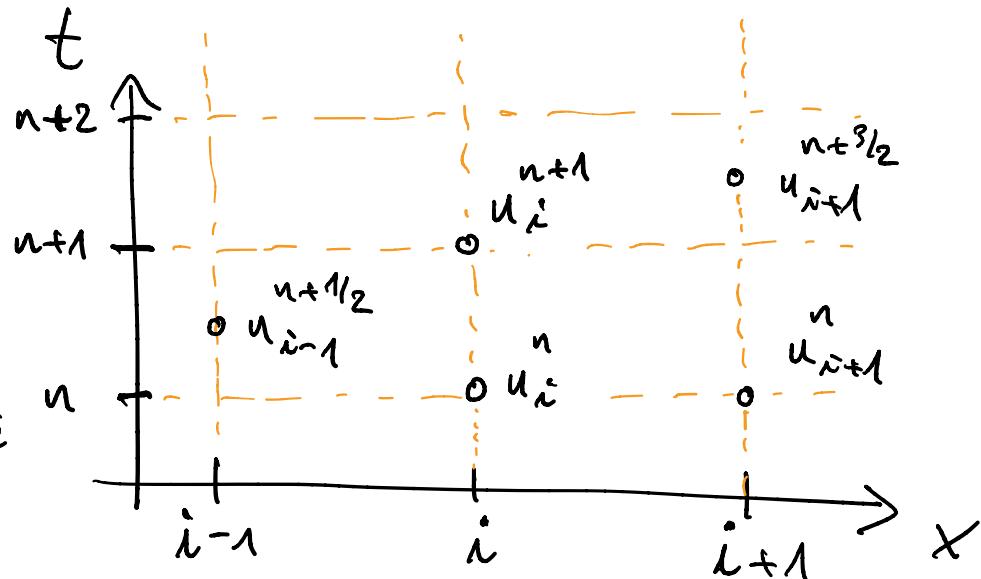
- **finite differences**: point values at grid points (or staggered)
- **finite volume**: discrete values $\hat{=}$ averages over finite volumes
(and later)

Consider $u = u(x, t)$ find $\mathcal{S}_h = \{(i\Delta x, n\Delta t)\}_{i, n \in \mathbb{Z}\}}$

Notation:

$$u(x_i, t^n) = u_j^n$$

$$u(x_i + \frac{\Delta x}{2}, t^n) = u_{i+\frac{1}{2}}^n$$



Note: in a finite difference approximation (FDA) of a PDE, different functions can be defined at different grid locations in which case the grid is called "staggered".

and "staggered grid function"

e.g. u defined at $i + \frac{\Delta x}{2}$ is $u_{i+\frac{1}{2}}^n$

3.2.1 Partial derivatives / differential operators

Consider Taylor expansion:

$$u_{i+1}^n = u_i^n + \left. \frac{\partial u}{\partial x} \right|_i \Delta x + \frac{1}{2} \left. \frac{\partial^2 u}{\partial x^2} \right|_i (\Delta x)^2 + O((\Delta x)^3)$$

$$\left[u(x_i + \Delta x) = u(x_i) + \sum_{k=1}^n \frac{(\Delta x)^k}{k!} u^{(k)}(x_i) + O((\Delta x)^{n+1}) \right]$$

Solve for $\frac{\partial u}{\partial x}$:

$$\left. \frac{\partial u}{\partial x} \right|_j = \frac{u_{i+1}^n - u_i^n}{\Delta x} - \frac{1}{2} \left. \frac{\partial^2 u}{\partial x^2} \right|_i \Delta x + O((\Delta x)^2)$$

(*)

1D

$$D_1^+ u = \frac{u_{i+1} - u_i^n}{\Delta x}$$

"forward difference approximation"

"stencil size": max distance to neighboring grid points involved

accuracy / truncation error:

$$D_1^+ u - \frac{\partial u}{\partial x} \stackrel{(*)}{=} \frac{1}{2} \frac{\partial u^2}{\partial x^2} \Big|_i \Delta x + O((\Delta x)^2) = O(\Delta x)$$

→ first-order accurate

Similarly:

$$D_1^- u = \frac{u_i^n - u_{i-1}^n}{\Delta x}$$

"backward difference approximation"

improve accuracy:

$$\Delta x_{i+\frac{1}{2}} \equiv x_{i+1} - x_i, \quad \Delta x_{i-\frac{1}{2}} \equiv x_i - x_{i-1}$$

(can differ in general)

$$\Rightarrow \Delta x_i = \frac{1}{2} (\Delta x_{i+\frac{1}{2}} + \Delta x_{i-\frac{1}{2}})$$

$$\text{forward: } u_i^n = u_i^n + \frac{\partial u}{\partial x} \Big|_i \Delta x_{i+\frac{1}{2}} + \frac{1}{2} \frac{\partial^2 u}{\partial x^2} \Big|_i (\Delta x_{i+\frac{1}{2}})^2 + \dots$$

$$\text{backward: } u_i^n = u_i^n + \frac{\partial u}{\partial x} \Big|_i (-\Delta x_{i-\frac{1}{2}}) + \frac{1}{2} \frac{\partial^2 u}{\partial x^2} \Big|_i (\Delta x_{i-\frac{1}{2}})^2 + \dots$$

↓ subtract

$$u_{i+1}^n - u_{i-1}^n = \frac{\partial u}{\partial x} \Big|_i (\Delta x_{i+\frac{1}{2}} + \Delta x_{i-\frac{1}{2}}) + \frac{1}{2} \frac{\partial^2 u}{\partial x^2} \Big|_i \left[(\Delta x_{i+\frac{1}{2}})^2 - (\Delta x_{i-\frac{1}{2}})^2 \right]$$

$$\text{so } \frac{\partial u}{\partial x} \Big|_i = \frac{u_{i+1}^n - u_{i-1}^n}{2 \Delta x_j} - \frac{1}{2} \frac{\partial^2 u}{\partial x^2} \Big|_i \frac{(\Delta x_{i+\frac{1}{2}})^2 - (\Delta x_{i-\frac{1}{2}})^2}{2 \Delta x_j} + O((\Delta x)^2)$$

On a uniform grid:

$$D_h^0 u = \frac{u_{i+1}^n - u_{i-1}^n}{2 \Delta x} + O((\Delta x)^2)$$

"centered difference approximation"

Remark: By virtue of Taylor expansion we assume that the function u is continuously differentiable. Note that the limit

$$\lim_{\Delta x \rightarrow 0} \frac{u_{i+1}^n - u_{i-1}^n}{2 \Delta x}$$

can exist even if u is not differentiable
 (e.g. $u(x,t) = |x|$ and $\lim_{\Delta x \rightarrow 0} D_1^0 u = 0$)
 we shall explore discontinuous solutions
 later.

Higher-order derivatives:

intuitively: repeatedly apply 1st order derivatives

$$\begin{aligned}
 \text{Examples: } \frac{\partial^2 u}{\partial x^2} &\approx D_1^+ D_1^- u = \frac{1}{\Delta x} \left(D_1^+ u_i^n - D_1^- u_{i-1}^n \right) \\
 &= \frac{1}{\Delta x} \left(\frac{u_{i+1}^n - u_i^n}{\Delta x} - \frac{u_i^n - u_{i-1}^n}{\Delta x} \right) \\
 &= \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \\
 &\equiv D^2 u
 \end{aligned}$$

$$\cdot \frac{\partial^2 u}{\partial x^2} \approx D_1^- D_1^+ u = \dots = D^2 u$$

$$\cdot \frac{\partial^2 u}{\partial x^2} \approx D_{1/2}^0 D_{1/2}^0 u = \frac{1}{\Delta x} D_0^{1/2} \left(u_{i+\frac{1}{2}}^n - u_{i-\frac{1}{2}}^n \right)$$

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

$$= D^2 u$$

General approach:

goal: compute approximation to $u^{(k)} = \frac{\partial^k u}{\partial x^k}$

based on a stencil of $n \geq k+1$ points

x_1, \dots, x_n

Example: want one-sided approximation

to $\frac{\partial u}{\partial x}|_i$ based on $u_i^n, u_{i-1}^n, u_{i-2}^n$

→ Taylor expansion

$$\rightarrow u_{i-1} = u_i - u^{(1)}|_i \Delta x + \frac{1}{2} u^{(2)}|_i (\Delta x)^2 - \frac{1}{6} u^{(3)}|_i (\Delta x)^3 + O(\Delta x^4)$$

$$\rightarrow u_{i-2} = u_i - u^{(1)}|_i (2\Delta x) + \frac{1}{2} u^{(2)}|_i (2\Delta x)^2 - \frac{1}{6} u^{(3)}|_i (2\Delta x)^3 + O(\Delta x^4)$$

Ausatz:

$$D_2 u|_i = c_1 u_i + \underline{c_2 u_{i-1}} + \underline{c_3 u_{i-2}}$$

$$= c_1 u_i + \underline{c_2 u_i - c_2 u^{(1)} \Delta x + c_2 \frac{1}{2} u^{(2)} (\Delta x)^2}$$

$$\underline{- c_2 \frac{1}{6} u^{(3)} (\Delta x)^3}$$

$$+ \underline{c_3 u_i - c_3 u^{(1)} (2\Delta x) + c_3 \frac{1}{2} u^{(2)} (2\Delta x)^2}$$

$$\underline{- c_3 \frac{1}{6} u^{(3)} (\Delta x)^3} + \dots$$

$$= (c_1 + c_2 + c_3) u_i - (c_2 + 2c_3) \Delta x u^{(1)}$$

$$+ \frac{1}{2} (c_2 + 4c_3) (\Delta x)^2 u^{(2)} - \frac{1}{6} (c_2 + 8c_3) (\Delta x)^3 u^{(3)}$$

+ ... ↑ note: coefficients are of the form

$$\frac{1}{(l-1)!} \sum_{m=1}^n c_m (x_m - x_i)^{l-1}$$

Need to agree with $u^{(l)}|_i$ to highest order possible:

$$\text{and } \left. \begin{array}{l} c_1 + c_2 + c_3 = 0 \\ -(c_2 + c_3) \Delta x = 1 \\ \frac{1}{2} (c_2 + 4c_3) (\Delta x)^2 = 0 \end{array} \right\} \quad \left. \begin{array}{l} c_1 = \frac{3}{2\Delta x} \\ c_2 = -\frac{3}{\Delta x} \\ c_3 = \frac{1}{2\Delta x} \end{array} \right.$$

(Note: higher coefficients 0 would lead to over-determined system)

$$\text{and } D_2 u|_i = \frac{1}{2\Delta x} (3u_i - 4u_{i-1} + u_{i-2})$$

Truncation error:

$$\begin{aligned} D_2 u|_{\bar{x}} - u^{(4)}|_{\bar{x}} &= -\frac{1}{6} (c_2 + 8c_3) (\Delta x)^3 u^{(3)}|_{\bar{x}} + \dots \\ &= -\frac{1}{6} \left(-\frac{2}{\Delta x} + \frac{4}{\Delta x} \right) (\Delta x)^3 u^{(3)}|_{\bar{x}} + \dots \\ &= -\frac{1}{3} (\Delta x)^2 u^{(3)}|_{\bar{x}} + \dots = \Theta(\Delta x^2) \end{aligned}$$

and 2nd order accurate

General procedure: Consider stencil $\{x_e\}_{e=1,\dots,n}$ around point $\bar{x} = x_i$ (may or may not be part of stencil), $n \geq k+1$. Consider n Taylor series $e=1,\dots,n$:

$$(*) \frac{u(x_e) - \underbrace{\tilde{u}(x_i)}_{\text{known}}}{\underbrace{\Delta x}_k} = u^{(1)}|_{\bar{x}} (x_e - x_i) + \dots + \frac{1}{k!} \underbrace{(x_e - x_i)^k u^{(k)}|_{\bar{x}}}_{\text{arrow}} + \Theta(h^p)$$

and linear system of n equations in k unknowns

$$\text{Ansatz: } u^{(k)}|_{\bar{x}} = c_1 u(x_1) + \dots + c_n u(x_n) + \Theta(\Delta x^p)$$

know that we can choose (see above)

$$(***) \frac{1}{(l-1)!} \sum_{m=1}^n c_m (x_m - x_i)^{l-1} = \begin{cases} 1, & l-1=k \\ 0, & \text{otherwise} \end{cases}$$

$$l=1,\dots,n$$

If points $\{x_l\}_{l=1,\dots,n}$ are distinct, (1) is an $n \times n$ non-singular system and thus has a unique solution. Can write:

$$\left(\begin{array}{cccc|c} 1 & \cdots & \cdots & 1 \\ \vdots & & & \vdots \\ (a_{lm})_{\substack{l=2,\dots,n \\ m=1,\dots,n}} & = & \frac{1}{(l-1)!} (x_m - x_i)^{l-1} \\ \vdots & & \vdots & \vdots \\ 1 & \cdots & \cdots & 1 \end{array} \right) \left(\begin{array}{c} c_1 \\ \vdots \\ c_n \end{array} \right) = \left(\begin{array}{c} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{array} \right)$$

$\equiv A \in \text{Mat}(n \times n) \quad c$

cancellation of lower order terms
 ← $k+1$
 cancellation of higher order terms

Remarks: 1) if $n \leq k$ there are too few points in the stencil, then RHS b and solution c both zero.

2) **Accuracy:** RHS and in Taylor expansions (2):

$$\left(\sum_{m=1}^n c_m (x_m - x_i)^{l-1} \right) u^{(l-1)}|_i = 0$$

$\nearrow l-1 < k$: necessary
 to cancel lower order terms
 and get $O(\Delta x)$ accuracy
 $\searrow l-1 > k$.

cancel higher
order terms and
obtain higher than
1st order accuracy

→ procedure is at least

$$O((\Delta x)^p), p = n-k \text{ accurate}$$

$p > n-k$ achievable if additional higher
order terms cancel (e.g. centered differences)

General: increasing stencil size increases
accuracy

3.2.2 Sample Discretizations

1) 1D wave equation, standard $\mathcal{O}(\Delta x^2)$

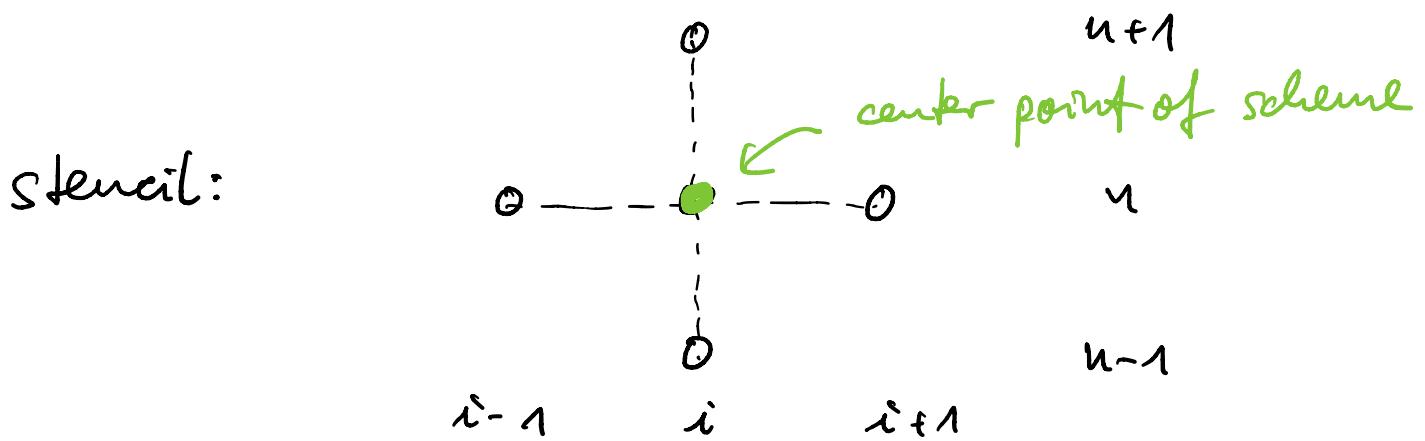
IBVP

$$\left\{ \begin{array}{l} u_{tt} - c^2 u_{xx} = 0, \quad 0 \leq x \leq 1, \quad t \geq 0 \\ u(x, 0) = u_0(x) \\ u_t(x, 0) = v_0(x) \\ u(0, t) = u(1, t) = 0 \end{array} \right. \begin{array}{l} \text{initial data} \\ \text{fixed (Dirichlet)} \\ \text{boundary conditions} \end{array}$$

Consider standard centered $\mathcal{O}(h^2)$ discretization
in space & time

$$\frac{\partial^2 u}{\partial t^2} \Big|_i^n = \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{(\Delta t)^2} + \mathcal{O}(\Delta t^2)$$

$$\frac{\partial^2 u}{\partial x^2} \Big|_i^n = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + \mathcal{O}(\Delta x^2)$$



1D FEA approximation to $O(\Delta x^2, \Delta t^2)$:

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

$$\left. \begin{array}{l} u_i^0 = u(x_i, 0) \\ u_i^1 = v(x_i, 0) \Delta t \end{array} \right\} \text{discretized initial data}$$

$$\left. \begin{array}{l} u_1^n = u_I^n = 0 \\ u_{x=0} = u_{x=1} \end{array} \right\} \text{discretized boundary condition}$$

explicitly solve for u^{n+1} :

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

\Rightarrow linear system for unknowns $\{u_i^{n+1}\}_{i=1, \dots, I}$

write:

$$A u^{n+1} = b$$

$$\begin{pmatrix} 1 & & & \\ & \ddots & & \\ & & 0 & \\ 0 & & & 1 \end{pmatrix} \begin{pmatrix} u_1^{n+1} \\ \vdots \\ u_I^{n+1} \end{pmatrix} = \begin{pmatrix} 2u_1^n - u_1^{n+1} + \lambda^2 () \\ \vdots \\ 2u_I^n - u_I^{n+1} + \lambda^2 () \end{pmatrix}$$

accuracy: $\Theta(\Delta x^2, \Delta t^2)$

A: diagonal and explicit scheme
 (will see: stable if $\lambda = \frac{c\Delta t}{\Delta x} \leq 1$ CFL condition)

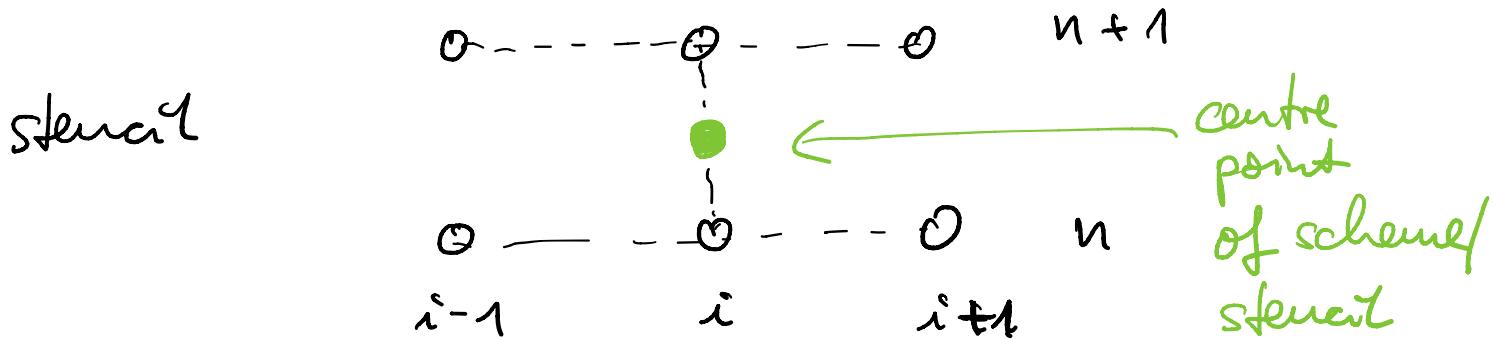
2) 1D diffusion equation, Crank-Nicholson

IBVP $\left\{ \begin{array}{l} u_t - \sigma u_{xx} = 0, \quad 0 \leq x \leq 1, \quad t \geq 0 \\ u(x, 0) = u_0(x) \\ u(0, t) = u(1, t) = 0 \end{array} \right.$

Consider: centered in time & space
 (minimizes truncation error,
 minimizes instabilities)

$$u_t \Big|_i^{n+\frac{1}{2}} = \frac{u_i^{n+1} - u_i^n}{\Delta t} + \theta(\Delta t^2)$$

$$u_{xx} \Big|_i^n = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + \theta(\Delta x^2)$$



need to apply time averaging on RHS:

$$T^{n+\frac{1}{2}}(v) = \frac{1}{2}(v^{n+1} + v^n) = v^{n+\frac{1}{2}} + O(\Delta t^2)$$

and FDA approximation to $O((\Delta x)^2, (\Delta t)^2)$:

at $t = n + \frac{1}{2}$

$$\begin{aligned} \frac{u_i^{n+1} - u_i^n}{\Delta t} &= \sigma T^{n+1}(u_{xx}|_i) \quad i = 2, \dots, I \\ &= \sigma \frac{1}{2} \left[\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{(\Delta x)^2} \right. \\ &\quad \left. - \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} \right] \end{aligned}$$

and linear system for $\{u_i^{n+1}\}_{i=2, \dots, I-1}$

write as

$$A u^{n+1} \equiv a_+ u_{i+1}^{n+1} + a_0 u_i^{n+1} + a_- u_{i-1}^{n+1} = b, \quad i = 2, \dots, I-1$$

$$\begin{pmatrix} \frac{1}{\Delta t^2} + \frac{1}{\Delta x^2} & -\frac{1}{\Delta x^2} & & & \\ -\frac{1}{\Delta x^2} & \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & -\frac{1}{\Delta x^2} \\ & & \ddots & \ddots & \\ 0 & & & -\frac{1}{\Delta x^2} & \frac{1}{\Delta t^2} + \frac{1}{\Delta x^2} \end{pmatrix} \begin{pmatrix} 0 \\ u_2^{n+1} \\ \vdots \\ u_{I-1}^{n+1} \end{pmatrix} = \begin{pmatrix} \left(\frac{1}{\Delta t^2} + \frac{1}{\Delta x^2} \right) u_i^n + \\ \frac{1}{2(\Delta x)^2} (u_{i+1}^n + u_{i-1}^n) \end{pmatrix}$$

and tridiagonal matrix and implicit scheme,

couples unknowns

u_{i+1}, u_i, u_{i-1} at
advanced time level
 $n+1$!

accuracy: $\theta(\Delta x^2, \Delta t^2)$

3) 1D advection equation

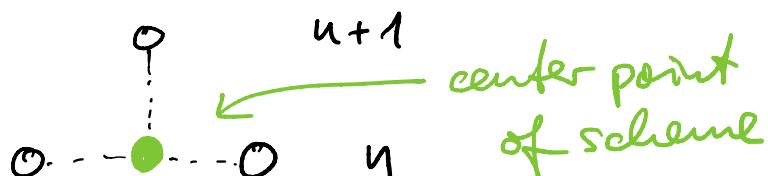
IBVP

$$\begin{cases} u_t + a u_x = 0 & 0 \leq x \leq 1, t \geq 0 \\ u(x, 0) = u_0(x) \\ u(0, t) = u(1, t) = 0 \end{cases}$$

(i) Consider simple forward in time, centered in space FDA:

$$u_x|_i^n \approx \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}, \quad u_t|_i^n = \frac{u_i^{n+1} - u_i^n}{\Delta t}$$

stencil



$i-1 \quad i \quad i+1$

and

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{a}{2\Delta x} (u_{i+1}^n - u_{i-1}^n) = 0$$

$$\Leftrightarrow u_i^{n+1} = u_i^n - \underbrace{\frac{a\Delta t}{2\Delta x}}_{=\lambda} (u_{i+1}^n - u_{i-1}^n)$$

linear system for u^{n+1} : $A u^{n+1} = b$

$$\begin{pmatrix} 1 & & & \\ & \ddots & & \\ & & \ddots & \\ & & & 1 \end{pmatrix} \begin{pmatrix} u_1^{n+1} \\ \vdots \\ u_I^{n+1} \end{pmatrix} = \begin{pmatrix} u_1^n - \lambda (u_{i+1}^n - u_{i-1}^n) \\ \vdots \\ u_I^n - \lambda (u_{i+1}^n - u_{i-1}^n) \end{pmatrix}$$

and explicit scheme $\Theta(\Delta t, \Delta x^2)$

(will see: unstable for any fixed $\frac{\Delta t}{\Delta x}$)

(ii) Lax-Friedrichs method

$$\text{replace } u_i^n \rightarrow \frac{1}{2} (u_{i-1}^n + u_{i+1}^n)$$

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

accuracy: $\Theta(\Delta t, \Delta x^2)$

(will see: stable if $\left| \frac{a\Delta t}{\Delta x} \right| \leq 1$)