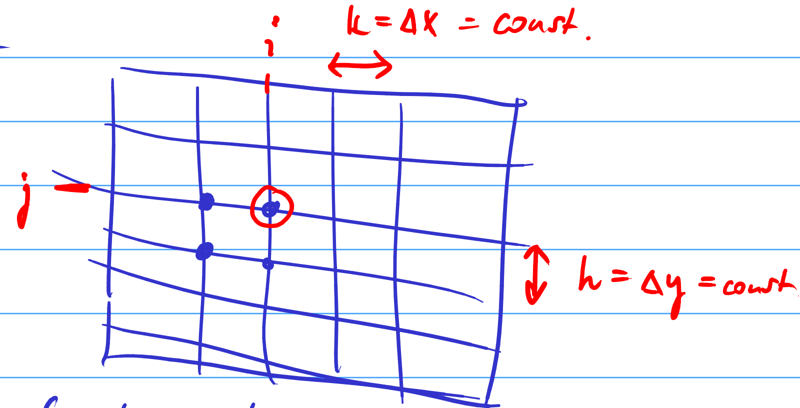
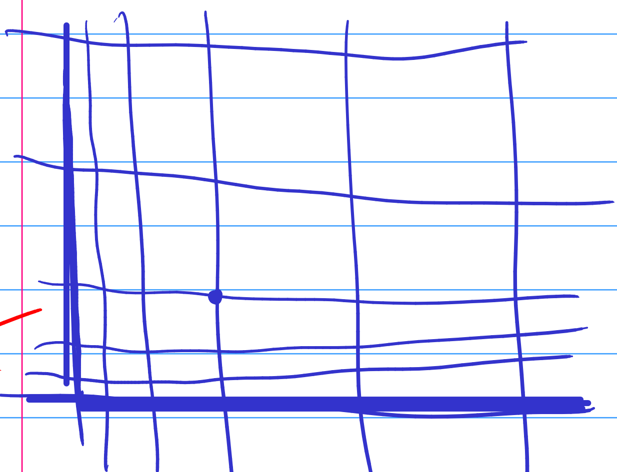
BASICS OF COMPUTATIONAL FLUID DYNAMICS

- conservation laws - the equations of fluid dynamics
- classification of PDEs, method of characteristics
- basics of the finite difference method, FDM schemes for simple problems and their properties
- finite volume method — mesh types / schemes
- advanced numerical schemes and solvers (OpenFOAM)
- other methods
- visualization

TRADITIONAL NUMERICAL METHODS

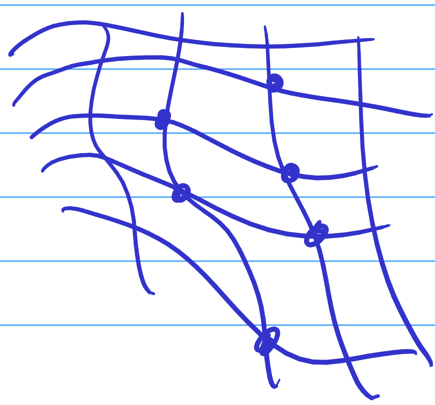


FDM – approximation of function values at grid points

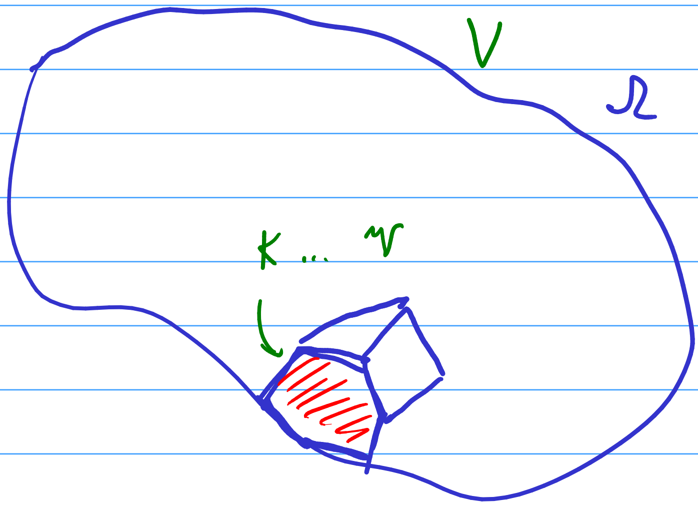


refinement close to walls

Δx, Δy may have variable size



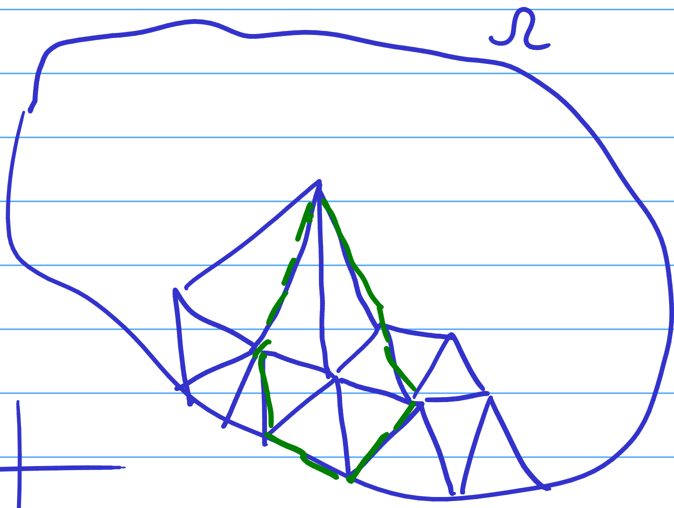
- Finite Volume Method, FVM



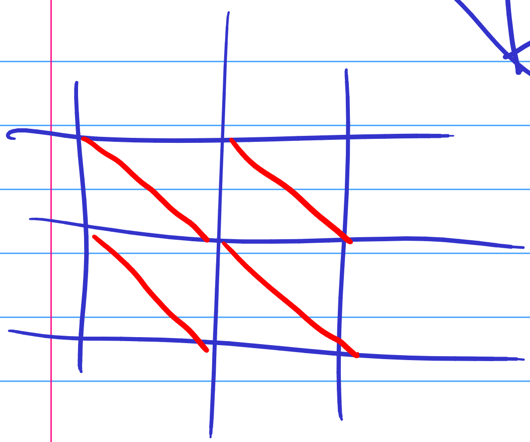
computational domain divided into polygonal (2D) or polyhedral (3D) cells (control volumes)

- approximation of integrals of the solution over the cells

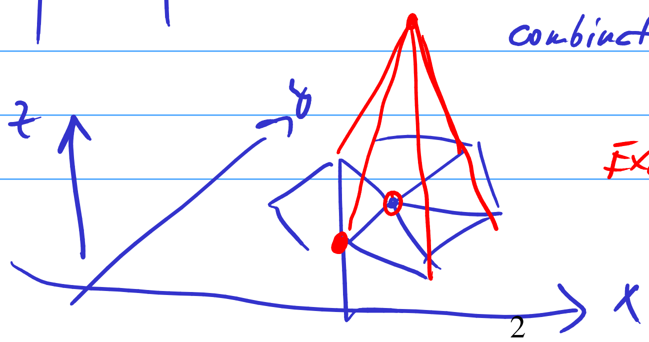
- FEM … Finite Element Method



unstructured meshes made of triangles (2D) or quadrilaterals (3D)

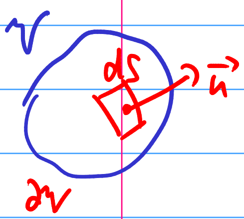


- numerical approximation of the solution as a finite linear combination of basis functions



Example: P1-elements: pyramidal basis functions

EQUATIONS OF FLUID DYNAMICS



– viscous compressible flow of a simple fluid

$$\frac{\partial \rho}{\partial t} + \partial_j(\rho V_j) = 0$$

Continuity equation

$$\frac{\partial(\rho V_i)}{\partial t} + \partial_j(\rho V_i V_j) = -\partial_i P + \partial_j \tilde{\tau}_{ij} + \rho F_i \qquad i \in \{1,2,3\}$$

Navier-Stokes eq.: conservation of linear momentum

$$\frac{\partial(\rho E)}{\partial t} + \partial_j(\rho E V_j) = -P\partial_i V_i + \underline{\tilde{\tau}_{ij}\,\partial_j V_i} + \partial_i(\lambda \partial_i T) + \rho \dot{Q}$$

conservation of internal energy

ρ .. density (of mass)

V_i ... velocity components

E .. specific internal energy

$E \to \hat{E}$

total energy $\quad \hat{E} = E + \frac{1}{2}\vec{V}^2 \qquad \vec{V}^2 = \|\vec{V}\|^2$

$$\frac{\partial(\rho \hat{E})}{\partial t} + \partial_j(\rho \hat{E} V_j) = -\partial_i(PV_i) + \underline{\partial_j(V_i \tilde{\tau}_{ij})} + \rho F_i V_i + \partial_i(\lambda \partial_i T) + \rho \dot{Q}$$

In 2D ($i \in \{1,2\}$), it is possible to write ($\vec{F} = 0$) $\dot{Q} = 0$

$\frac{\partial}{\partial t} =: \partial_t$

$$\partial_t \rho + \partial_1(\rho v_1) + \partial_2(\rho v_2) = 0$$

$$i=1: \quad \partial_t(\rho v_1) + \partial_1(\rho v_1^2 + p) + \partial_2(\rho v_1 v_2) = \partial_1 \tau_{11} + \partial_2 \tau_{12}$$

$$i=2: \quad \partial_t(\rho v_2) + \partial_1(\rho v_2 v_1) + \partial_2(\rho v_2^2 + p) = \partial_1 \tau_{21} + \partial_2 \tau_{22}$$

$$\partial_t(\rho \hat{E}) + \partial_1\big(v_1(\rho E + p)\big) + \partial_2\big(v_2(\rho E + p)\big) = \bigcirc + \square$$

$$\bigcirc = \partial_1(v_i \tilde{\tau}_{i1} + \lambda \partial_1 T)$$

$$\square = \partial_2(v_i \tilde{\tau}_{i2} + \lambda \partial_2 T)$$

$$\partial_t \vec{W} + \underbrace{\partial_1 \vec{F} + \partial_2 \vec{G}}_{\substack{\text{convective (inviscid)} \\ \text{physical fluxes} \\ = \nabla \cdot (\vec{F}, \vec{G})}} = \underbrace{\partial_1 \vec{R} + \partial_2 \vec{S}}_{\substack{\text{viscous} \\ \text{(diffusive) fluxes} \\ = \nabla \cdot (\vec{R}, \vec{S})}}$$

NOTE: Inviscid flow (Euler equations) $\rightarrow$ $\vec{R}, \vec{S} = \vec{0}$

"1D Euler equation" (for a single quantity "u")

$$\partial_t u + \partial_x (f(u)) = 0$$

linearization

$$\partial_t u + \underbrace{f'(u)}_{\approx \text{const}} \partial_x u = 0$$

$$\boxed{\partial_t u + a \partial_x u = 0}$$ transport equation (*)

on $(0,T) \times \Omega$, $\Omega = (0,1)$

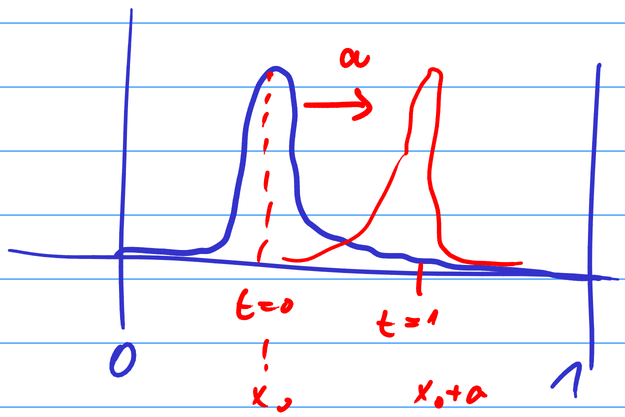
with initial cond. $u(0,x) = u_0(x)$ on Ω

with boundary cond. $u|_{\partial\Omega} = 0$ on $\partial\Omega = \{0,1\}$, i.e. $u(0) = u(1) = 0$

The exact solution reads

$$u(t,x) = \begin{cases} u(0, x-at) \\ u_0(x-at) & \text{for } x > at \\ 0 & \text{for } x < at \end{cases}$$

(plug into the equation (*) to verify)

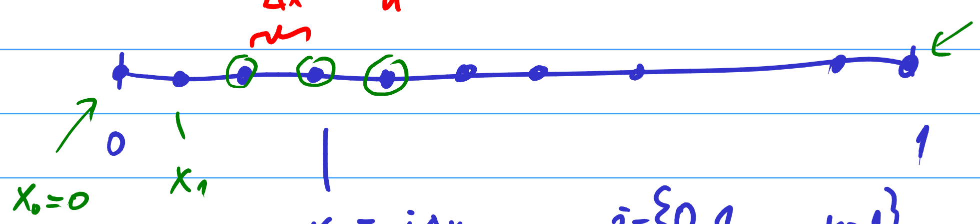


$$u(t,x_{i\pm1}) = u(t,x_i) \pm \partial_x u(t,x_i)\,\Delta x + \frac{1}{2!}\partial_{xx}u(t,x_i)\,\Delta x^2 + \mathcal{O}(\Delta x^3)$$

Attempted numerical solution

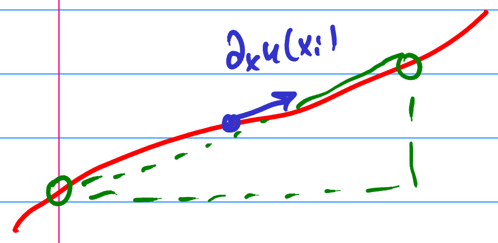
$\Delta x = \frac{1}{n}$

n grid points

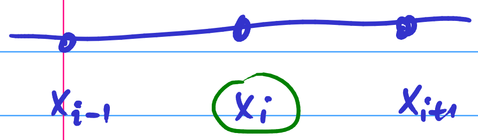


$x_i = i\Delta x \qquad i = \{0, 1, \dots, n-1\}$

$$\partial_x u(t,x_i) = \frac{u(t,x_{i+1}) - u(t,x_{i-1})}{2\Delta x} + \mathcal{O}(\Delta x^2)$$



$$\partial_t u(t_k,x) = \frac{u(t_k,x) - u(t_{k-1},x)}{\Delta t} + \mathcal{O}(\Delta t)$$



Δt … time step

$t_k = k \cdot \Delta t$

in order for the numerical scheme to "see" far enough to capture the information moving with velocity $a>0$ (from the left), we need $a\Delta t < \Delta x$, i.e. $a\frac{\Delta t}{\Delta x} < 1$ (see "CFL" later)

now replace: $u(t_k, x_i) \longrightarrow u_i^k$ { a "mesh function" = a "table" of numbers

$\Rightarrow$ we get the numerical scheme

$$\frac{u_i^k - u_i^{k-1}}{\Delta t} + a\,\frac{u_{i+1}^{k-1} - u_{i-1}^{k-1}}{2\Delta x} = 0$$

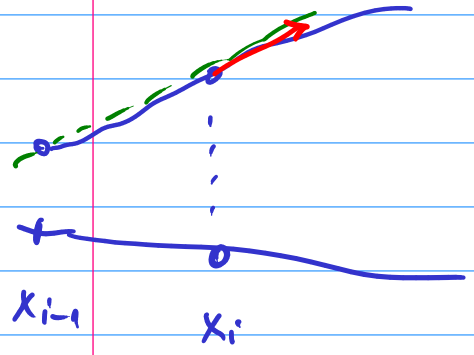
$$\Rightarrow \quad u_i^k = u_i^{k-1} - a\frac{\Delta t}{2\Delta x}\left(u_{i+1}^{k-1} - u_{i-1}^{k-1}\right)$$

for $a>0$, this value cannot have any influence on the solution in grid point x_i

… this does not work, as it propagates information in the wrong direction

Instead, let's look in the correct direction only (i.e. to the left if $a>0$)

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



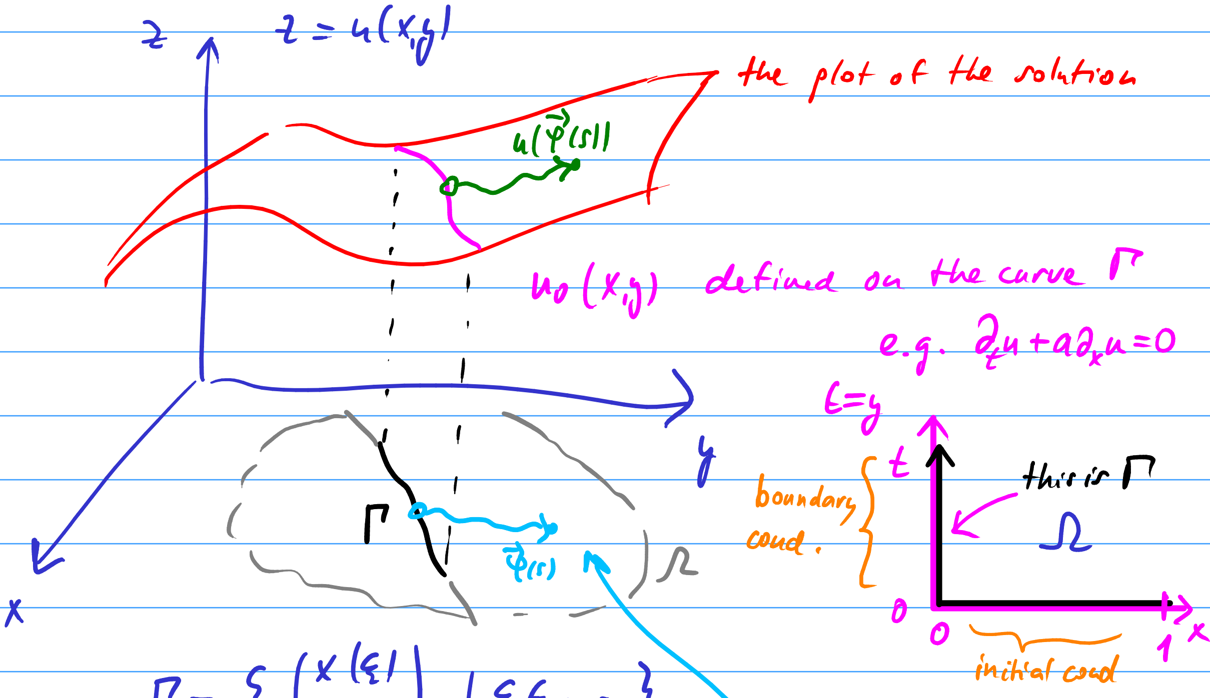
$$\uparrow \; \partial_x u(t,x_i) = \frac{u(t,x_i)-u(t,x_{i-1})}{\Delta x} + \mathcal{O}(\Delta x)$$

CLASSIFICATION OF 1. and 2. order PDE's, CHARACTERISTICS

- start with one 1. order PDE for the unknown $u=u(x,y)$ in 2D:

$$a(x,y,u)\frac{\partial u}{\partial x} + b(x,y,u)\frac{\partial u}{\partial y} = c(x,y,u) \qquad \Big| \text{ def } (*)$$

solution



$$\Gamma = \left\{ \begin{pmatrix} x(\xi) \\ y(\xi) \end{pmatrix} \;\middle|\; \xi \in \dots \right\}$$

characteristic projection from $\Gamma(\xi)$

on Γ: $\dfrac{du_0}{d\xi} = \dfrac{\partial u}{\partial x}\dfrac{dx}{d\xi} + \dfrac{\partial u}{\partial y}\dfrac{dy}{d\xi}$

$$\Rightarrow \begin{pmatrix} a & b \\ \frac{dx}{d\xi} & \frac{dy}{d\xi} \end{pmatrix} \begin{pmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial y} \end{pmatrix} = \begin{pmatrix} c \\ \frac{du_0}{d\xi} \end{pmatrix}$$

1. row = PDE

2. row =

a unique solution exists $\Leftrightarrow$ $\begin{vmatrix} a & b \\ \frac{dx}{d\xi} & \frac{dy}{d\xi} \end{vmatrix} \neq 0$

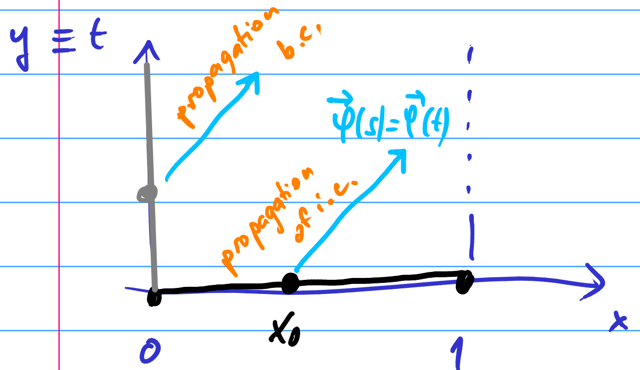
Let's solve the PDE along $\varphi = \langle \vec{\varphi} \rangle$ $\quad \vec{\varphi} = \vec{\varphi}(s)$,

starting on Γ, i.e. $\vec{\varphi}(0) = \begin{pmatrix} x(\xi) \\ y(\xi) \end{pmatrix}$ for the given ξ

The function u is a solution to $\circledast$ on φ $\Leftrightarrow$ $\vec{\varphi}(s) = \begin{pmatrix} x(s) \\ y(s) \end{pmatrix}$

$$\left.\begin{array}{c} \dfrac{du}{ds} = \dfrac{\partial u}{\partial x}\dfrac{dx}{ds} + \dfrac{\partial u}{\partial y}\dfrac{dy}{ds} \\ \| \qquad\qquad \| \qquad\qquad \| \\ \circledast: \quad c = \dfrac{\partial u}{\partial x}\cdot a + \dfrac{\partial u}{\partial y}\cdot b \end{array}\right\} \Leftrightarrow \left\{ \begin{array}{l} \dfrac{dx}{ds} = a(x,y,u(x,y)) \\ \dfrac{dy}{ds} = b(x,y,u(x,y)) \\ \dfrac{du}{ds} = c(x,y,u(x,y)) \end{array}\right.$$

Example: the transport equation $\partial_t u + a\partial_x u = 0$ $\qquad t \equiv y$, $b \equiv 1$, $c = 0$



$$\frac{dx}{ds} = a, \quad \underbrace{\frac{dt}{ds} = 1, \quad t\big|_{s=0} = 0}_{s=t}$$

$$\frac{du}{ds} = c = 0$$

$\Gamma = \left\{ \begin{pmatrix} 0 \\ t \end{pmatrix}, t > 0 \right\} \cup \left\{ \begin{pmatrix} x \\ 0 \end{pmatrix}, x \in \langle 0,1 \rangle \right\}$ $\quad \Rightarrow \dfrac{dx}{dt} = a \wedge x\big|_{t=0} = x_0 = \vec{\Gamma}(\xi) \Rightarrow x(t) = x_0 + at$

$$\Rightarrow \quad u(t,x) = u_0(0,x_0) = u_0(0,x-at)$$

For a system of quasi-linear PDE: $\quad \vec{u} = \vec{u}(x,y) \in \mathbb{R}^n$

$$\underbrace{A \frac{\partial \vec{u}}{\partial x}}_{} + B \frac{\partial \vec{u}}{\partial y} = \vec{c} \qquad A, B \in \mathbb{R}^{n\times n}, \quad A,B = A,B(x,y,\vec{u})$$

$\frac{\partial}{\partial x}\vec{f}(x,y,\vec{u}) + \frac{\partial}{\partial y}\vec{g}(\ldots)$!

: we look for so called characteristic directions

- - - -

2nd order PDE (quasilinear)

without "$+h\cdot u$"

$$a\frac{\partial^2 u}{\partial x^2} + 2b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} = g$$

$$\Rightarrow \quad v \equiv \frac{\partial u}{\partial x}, \quad w \equiv \frac{\partial u}{\partial y}$$

again, $a = a(x,y,u(x,y))$

$b = -\!\!\shortparallel\!\!-$ etc.

$$\Leftrightarrow \quad \begin{pmatrix} a & 0 \\ 0 & 1 \end{pmatrix} \frac{\partial}{\partial x}\begin{pmatrix} v \\ w \end{pmatrix} + \begin{pmatrix} 2b & c \\ -1 & 0 \end{pmatrix} \frac{\partial}{\partial y}\begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} g - dv - ew \\ 0 \end{pmatrix}$$

2nd row: $\quad \frac{\partial w}{\partial x} - \frac{\partial v}{\partial y} = 0 \Leftrightarrow$ $\boxed{\text{closedness of the differential form } du = \frac{\partial u}{\partial x}dx + \frac{\partial u}{\partial y}dy = v\,dx + w\,dy}$

1 2nd-order PDE transformed to a system of 2 1st-order PDE's

$\Rightarrow$ (Without proof), the characteristics satisfy $\quad \frac{dy}{dx} = \lambda(x,y)$

where $\quad \begin{vmatrix} 2b - a\lambda & c \\ -1 & -\lambda \end{vmatrix} = a\lambda^2 - 2b\lambda + c = 0 \qquad$ quadratic eq. for λ

a,b,c all depend on x,y (and $u(x,y)$)

$$\Rightarrow \quad \lambda_{1,2} = \frac{2b \pm \sqrt{4b^2 - 4ac}}{2a} = \frac{b \pm \sqrt{b^2 - ac}}{a}$$

with $\boxed{D = b^2 - ac}$

PDE name:

- $D > 0 \Rightarrow$ 2 roots $\Rightarrow$ 2 characteristics $\rightarrow$ HYPERBOLIC
- $D = 0 \rightarrow$ 1 root $\Rightarrow$ 1 characteristic $\Rightarrow$ PARABOLIC
- $D < 0 \Rightarrow$ imaginary roots only $\rightarrow$ ELLIPTIC

Analogy to quadratic surfaces: $\quad Q(x,y) = ax^2 - 2bxy + cy^2 + dx + ey + g = 0$

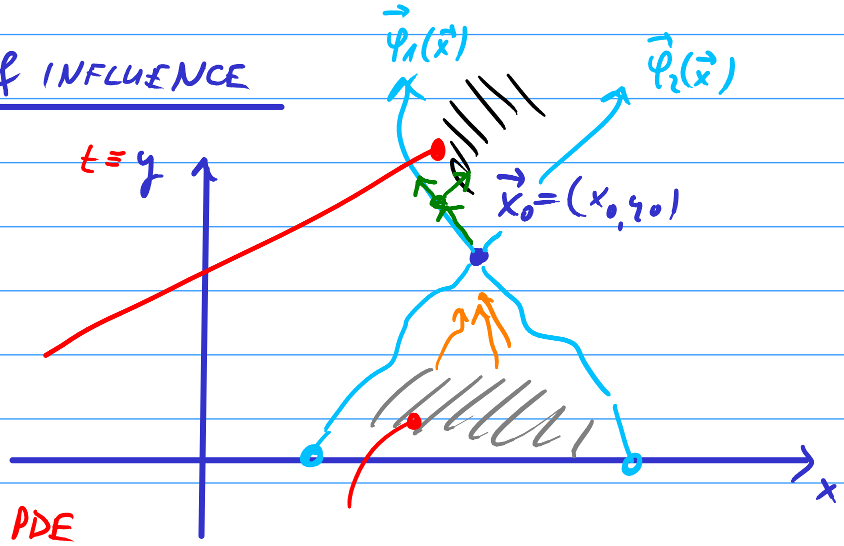
$D > 0 \Rightarrow$ $Q = 0$ is an equation of a HYPERBOLA

$D = 0$ — " — PARABOLA

$D < 0$ — " — ELLIPSE

DOMAINS OF DEPENDENCE & INFLUENCE

1) HYPERBOLIC EQUATION



DOMAIN OF INFLUENCE of the point $\vec{x}_0$

... the solution $u(\vec{x})$ of the PDE is influenced by the value of u at $\vec{x}_0$

DOMAIN OF DEPENDENCE of the point $\vec{x}_0$

... the value $u(\vec{x}_0)$ depends on the values of $u(\vec{x})$ for $\vec{x}$ in this region

2) PARABOLIC PDE

e.g. heat equation $\quad a\dfrac{\partial^2 u}{\partial x^2} \qquad\qquad - \dfrac{\partial u}{\partial t} = 0$

$a=1$ $\qquad$ $b,c,d=0$ $\qquad$ $e=-1$

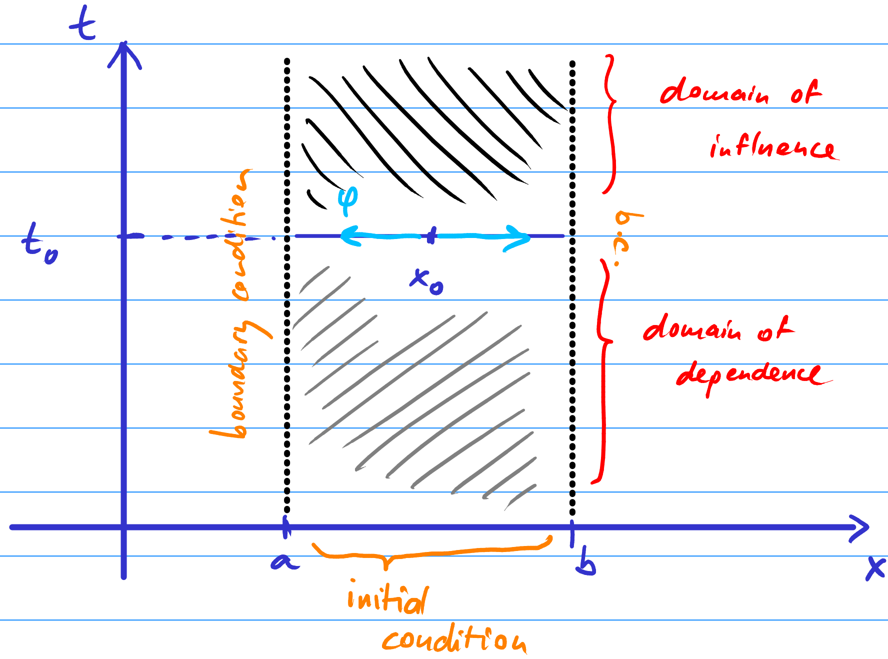
$$a\frac{\partial^2 u}{\partial x^2} + \underbrace{2b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x}}_{b,c,d=0} + e\frac{\partial u}{\partial y} = g$$

$y \equiv t$

$\Rightarrow$ we have $\lambda = \dfrac{-b \pm \sqrt{b^2 - ac}}{a} = 0$

$\Rightarrow \dfrac{dy}{dx} \equiv \dfrac{dt}{dx} = 0 \quad \Rightarrow$ characteristics are parallel with x axis

information spreads along the spatial (x) dimension at infinite speed



<u>NOTE</u>: Hyperbolic and parabolic equations can be solved as evolutionary problems, i.e. forward in time

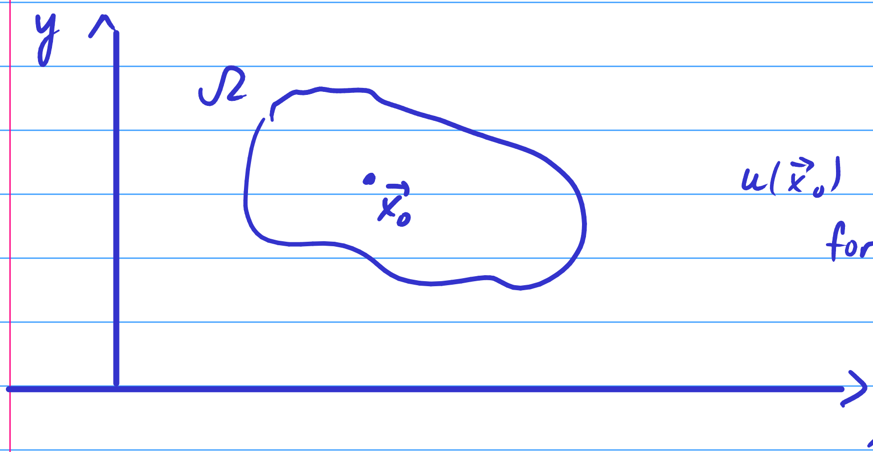
(one of the independent variables has the sense of time)

3) ELLIPTIC PDE

- characteristics do not exist
- the domain of dependence / influence is the whole domain Ω

e.g. $-\Delta u = f$

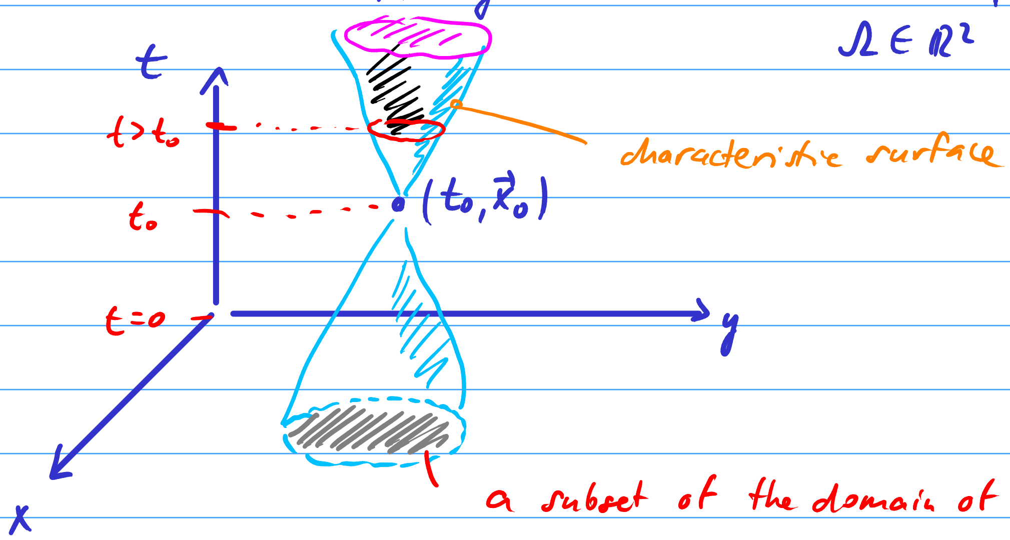
Poisson equation



$u(\vec{x}_0)$ depends on $u(\vec{x})$ for all $\vec{x} \in \Omega$

NOTE: Higher-dimensional cases, e.g.

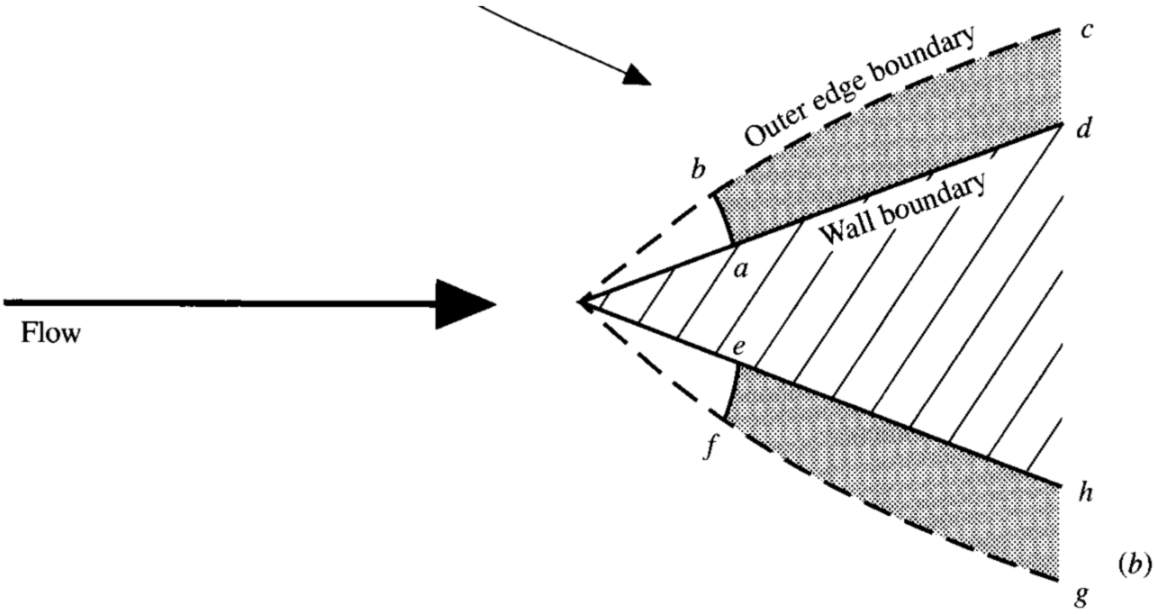
HYPERBOLIC PDE in $\mathcal{J} \times \Omega$ where $\mathcal{J} = (0, T_{max})$, $\Omega \in \mathbb{R}^2$



a subset of the domain of the initial condition which influences the value of u at $(t_0, \vec{x}_0)$

NOTE: Navier-Stokes equations are (generally) of <u>mixed type</u>

- subsonic viscous flow $\Rightarrow$ parabolic behavior
- supersonic flow $\Rightarrow$ hyperbolic behavior



- inviscid flow (Euler equations) $\Rightarrow$ hyperbolic type

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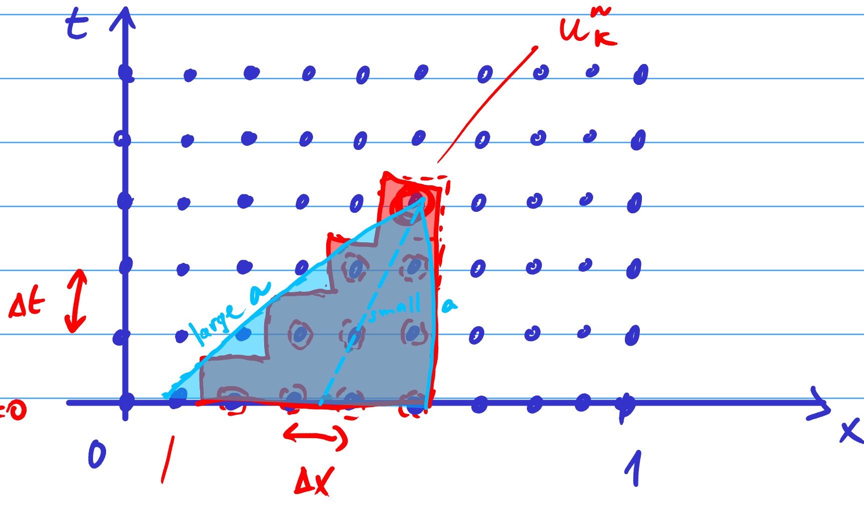
... back to the (upwind) scheme for the transport equation

$$\partial_t u + a \partial_x u = 0 \quad \rightarrow \quad u_k^{n+1} = u_k^n + a \frac{\Delta t}{\Delta x} (u_k^n - u_{k-1}^n)$$

pro $a > 0$

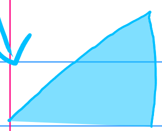
$u_k^n \approx u(n\Delta t, k\Delta x)$

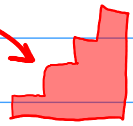


u_k^0 ... initial condition

CFL condition (Courant, Friedrichs, Lewy) (1928)

As the necessary condition for convergence of the numerical scheme, the domain of dependence of the PDE must be subset of the domain of dependence of the numerical scheme.



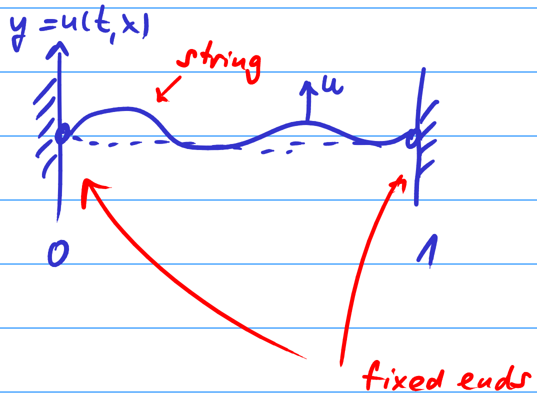


For the transport equation : $a\Delta t \leq \Delta x \iff \frac{a\Delta t}{\Delta x} \leq 1$

$$\iff \frac{\Delta t}{\Delta x} \leq \frac{1}{a}$$

Courant number

Wave equation in 1D



$$\partial_{tt} u = a^2 \partial_{xx} u$$

b.c. $u(t,0) = u(t,1) = 0 \quad \forall t$

init.c. $u(0,x) = u_0(x)$ initial position

$\partial_t u(0,x) = V_0(x)$ initial velocity

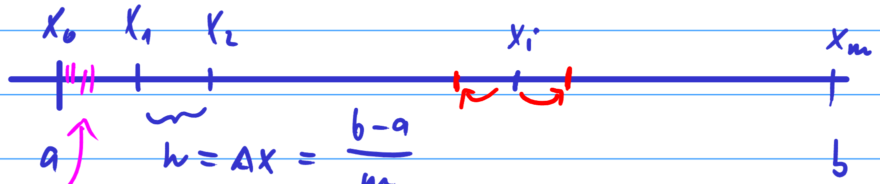
the numerical scheme for the wave eq. + convergence conditions will be shown later

Heat equation $c_p \partial_t u = k \underbrace{\partial_{xx} u}_{\Delta u}$ $u \ldots$ temperature

FINITE DIFFERENCE METHOD

difference quotients – replacements of derivatives of the function

$$\boxed{\begin{array}{l} u:(a,b)\to\mathbb{R} \\ u\in C^{(\ell)}(a,b) \end{array}}$$



(generally) refinement possible

$$h=\Delta x=\frac{b-a}{m}$$

<u>def</u> $\quad u_i := u(a+ih) \;\big(= u(x_i)\big) \qquad i\in\{0,\dots,m\}$

but generally for $i\in\mathbb{R}$

$$u_i^{(k)} := u^{(k)}(a+ih) \qquad u_i' := u_i^{(1)}$$

Let $\alpha_1,\alpha_2,\dots,\alpha_\ell\in\mathbb{R}$ are given numbers.

Then $\exists c_1,\dots,c_\ell$ such that

$$u_i' = \frac{1}{h}\sum_{j=1}^{\ell} c_j u_{i+\alpha_j} + \underbrace{\mathcal{O}(h^{\ell-1})}_{\approx K\cdot h^{\ell-1}}$$

$(\ell-1)$ = order of approximation

Proof: How to find c_j?

$$u_{i+\alpha_j} = \sum_{k=0}^{\ell-1}\frac{u_i^{(k)}}{k!}\Big(\underbrace{\underbrace{a+(i+\alpha_j)h}_{=x_{i+\alpha_j}\ \text{pro}\ \alpha_j\in\mathbb{Z}} - \underbrace{(a+ih)}_{x_i}}_{\alpha_j h}\Big)^k + \mathcal{O}(h^\ell) \qquad \forall j$$

plug this into

$$\frac{1}{h}\sum_{j=1}^{\ell} c_j u_{i+\alpha_j} = \frac{1}{h}\sum_{j=1}^{\ell} c_j\left[\sum_{k=0}^{\ell-1}\frac{u_i^{(k)}}{k!}(\alpha_j h)^k + \mathcal{O}(h^\ell)\right] =$$

$$\sum_{k=0}^{l-1} u_i^{(k)} \underbrace{\left[\sum_{j=1}^{l} \frac{\alpha_j^k h^{k-1}}{k!} c_j\right]}_{b_k} + \mathcal{O}(h^{l-1}) \overset{!}{=} u_i'$$

we need $b_1 = 1 \wedge b_k = 0$ for $k \neq 1$

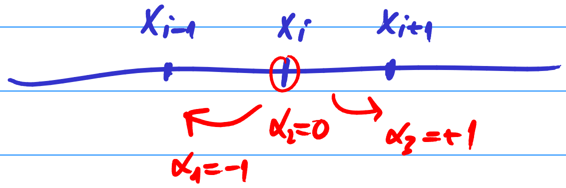
these conditions form a linear system for c_j in the form

$$A\vec{c} = \vec{b} \quad \text{where} \quad A = (a_{k,j}) = \left(\frac{\alpha_j^k h^{k-1}}{k!}\right) \in \mathbb{R}^{l \times l}$$

$$k \in \{0, \dots, l-1\}, \quad j \in \{1, \dots, l\}$$

$$\vec{b} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Example: central difference quotient: $\alpha_1 = -1$, $\alpha_2 = 0$, $\alpha_3 = 1$



$$\begin{array}{cc} & j \quad\; 1 \qquad 2 \qquad 3 \\ \begin{array}{c} k \;\; 0 \\ 1 \\ 2 \end{array} & \begin{pmatrix} \frac{1}{h} & \frac{1}{h} & \frac{1}{h} \\ -1 & 0 & 1 \\ \frac{h}{2} & 0 & \frac{h}{2} \end{pmatrix} \end{array} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\left(\begin{array}{ccc|c} \frac{1}{h} & \frac{1}{h} & \frac{1}{h} & 0 \\ -1 & 0 & 1 & 1 \\ \frac{h}{2} & 0 & \frac{h}{2} & 0 \end{array}\right) \sim \left(\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ -1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \end{array}\right) \sim \left(\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ -1 & 0 & 1 & 1 \\ 0 & 0 & 1 & \frac{1}{2} \end{array}\right)$$

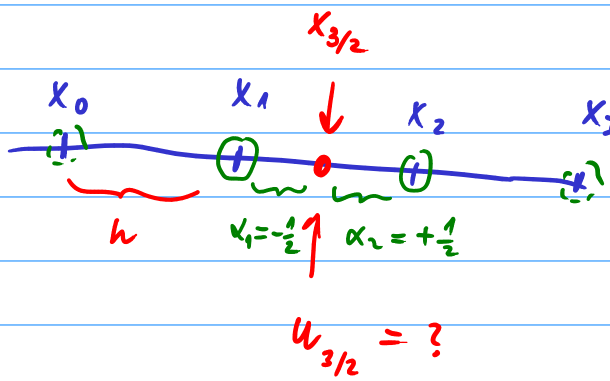
$$c_3 = \frac{1}{2}, \quad c_1 = -\frac{1}{2}, \quad c_2 = 0$$

$$u_i' = \frac{1}{h}\sum_{j=1}^{\ell} c_j u_{i+\alpha_j} \quad + \mathcal{O}(h^{\ell-1})$$

$$u_i' = \frac{1}{2h}\left(-u_{i-1} + 0\cdot u_i + u_{i+1}\right) + \mathcal{O}(h^2)$$

$$= \frac{u_{i+1} - u_{i-1}}{2h}$$

NOTE: INTERPOLATION :

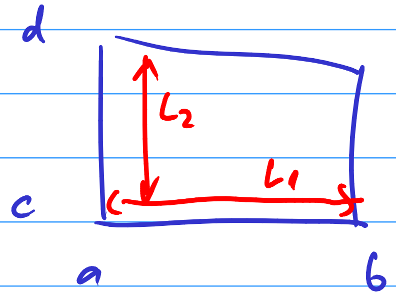


Exercise : How to find $u_{3/2}$ by means of u_1, u_2 ? / u_0, u_1, u_2, u_3

NOTATIONS OF THE FDM

on $\mathcal{J}\times\Omega$ where $\mathcal{J} = (0, t_{max})$, $\Omega = (a,b)\times(c,d) \subset \mathbb{R}^2$

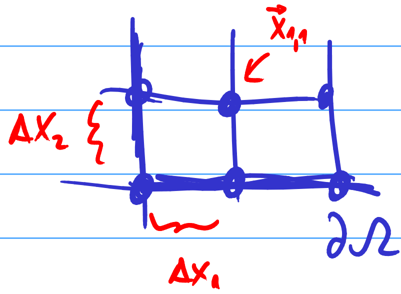
$$t \in \mathcal{J}, \quad \vec{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \in \Omega$$



- $L_1 = b - a, \quad L_2 = d - c$

on Ω, we define the grid (mesh) of $(m_1+1)\times(m_2+1)$ evenly spaced (equidistant) points

"grid nodes"



def $\quad \Delta x_1 = \frac{L_1}{m_1}, \quad \Delta x_2 = \frac{L_2}{m_2}$

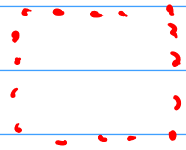
def. $\quad \vec{x}_{ij} = \begin{pmatrix} i\Delta x_1 \\ j\Delta x_2 \end{pmatrix}$

- def. $h = \max(\Delta x_1, \Delta x_2)$; $\frac{1}{h}$ $= \min\left(\frac{m_1}{L_1}, \frac{m_2}{L_2}\right)$ will be called the <u>spatial resolution of the grid</u>

- set of <u>inner grid nodes</u> $\omega_h = \{ \vec{x}_{ij} \mid i \in \{1, \dots, m_1 - 1\},\ j \in \{1, \dots, m_2 - 1\} \}$

- set of <u>all grid nodes</u> $\bar{\omega}_h = \{ \vec{x}_{ij} \mid i \in \{0, \dots, m_1\}, j \in \{0, \dots, m_2\} \}$

- set of <u>boundary nodes</u> $\gamma_h = \bar{\omega}_h \setminus \omega_h$



- def $\Delta t = \frac{t_{max}}{N}$

and $t^n = n \Delta t$ pro $n \in \{0, \dots, N\}$ is called the <u>n-th time level (layer)</u>

- set of time levels

$$\tau^{\Delta t} = \{ t^n \mid n \in \{1, \dots, N\} \}$$
$$\bar{\tau}^{\Delta t} = \{ t^n \mid n \in \{0, \dots, N\} \}$$

- space of <u>grid functions</u>

$$\mathcal{H}_h^{\Delta t} = \{ w_h^{\Delta t} \mid w_h^{\Delta t} : \bar{\tau}^{\Delta t} \times \bar{\omega}_h \to \mathbb{R} \}$$

elements of $\mathcal{H}_h^{\Delta t}$ are "grid functions"

- $w_{i,j}^n := w_h^{\Delta t}(t^n, \vec{x}_{i,j})$

- operator of projection onto the grid $\mathcal{P}_h^{\Delta t} : C(\bar{\mathcal{J}} \times \bar{\Omega}) \to \mathcal{H}_h^{\Delta t}$

def. $$\Big(\underbrace{\mathcal{P}_h^{\Delta t} u}_{\in \mathcal{H}_h^{\Delta t}}\Big)_{i,j}^n = u(t^n, \vec{x}_{i,j})$$

<u>NOTE</u>: For vector-valued functions, the same can be done component-wise.

DIFFERENCE QUOTIENTS FOR THE SPATIAL PARTIAL DERIVATIVES

$u \in C^1(I \times \Omega) \qquad w \in \mathcal{H}_h^{\Delta t}$

def. $\underbrace{\left(\overleftarrow{\delta}_{x_1} w\right)_{i,j}^n}_{\boxed{\text{grid function on } I^{\Delta t} \times \omega_h}} = \dfrac{w_{i,j}^n - w_{i-1,j}^n}{\Delta x_1}$ backward difference

if $w = \varphi_h^{\Delta t} u$: then
$$\left(\overleftarrow{\delta}_{x_1} \varphi_h^{\Delta t} u\right)_{i,j}^n = \partial_{x_1} u(t^n, \vec{x}_{ij}) + \mathcal{O}(h)$$
holds.

$$\left(\overrightarrow{\delta}_{x_1} w\right)_{i,j}^n = \frac{w_{i+1,j}^n - w_{i,j}^n}{\Delta x_1}$$ forward dif

$$\left(\overleftrightarrow{\delta}_{x_1} w\right)_{i,j}^n = \frac{w_{i+1,j}^n - w_{i-1,j}^n}{2\Delta x_1}$$ central dif.

$$\left(\overleftarrow{\delta}_{x_2} w\right)_{i,j}^n = \frac{w_{i,j}^n - w_{i,j-1}^n}{\Delta x_2}$$ etc. $\overrightarrow{\delta}_{x_2} w$, $\overleftrightarrow{\delta}_{x_2} w$

NOTE: REPLACEMENTS FOR GRADIENT & DIVERGENCE

$$\overleftarrow{\nabla}_h w = \begin{pmatrix} \overleftarrow{\delta}_{x_1} w \\ \overleftarrow{\delta}_{x_2} w \end{pmatrix}, \quad \overrightarrow{\nabla}_h = \begin{pmatrix} \dots \end{pmatrix}$$

$$\overleftrightarrow{\nabla}_h w = \begin{pmatrix} \dots \end{pmatrix}$$

$$\overleftarrow{\nabla}_h \cdot \vec{w} = \overleftarrow{\delta}_{x_1} w_1 + \overleftarrow{\delta}_{x_2} w_2$$ here $\vec{w} = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$

$w_1, w_2 \in \mathcal{H}_h^{\Delta t}$

ctd. $\overrightarrow{\nabla}_h \cdot \vec{w}$, $\overleftrightarrow{\nabla}_h \cdot \vec{w} = \dots$

DIFFERENCE QUOTIENTS FOR THE TIME DERIVATIVE

$$\left(\overleftarrow{\delta}_t w\right)^n_{i,j} = \frac{w^n_{i,j} - w^{n-1}_{i,j}}{\Delta t}, \quad \left(\overrightarrow{\delta}_t w\right)^n_{i,j} = \frac{w^{n+1}_{i,j} - w^n_{i,j}}{\Delta t}$$

backward

forward

grid functions def. on $\mathcal{I}^{\Delta t} \times \bar{\omega}_h$

CONSISTENCY, CONVERGENCE & STABILITY OF F.DIFF. SCHEMES

(Pr) upwind scheme for $\partial_t u + a\partial_x u = 0$ $\quad a > 0$

on $\mathcal{I} \times \Omega$, $\Omega = (0,1)$ $\quad \leftarrow u \in C^1(\mathcal{I} \times \Omega)$

$\downarrow$ num. solution is $u_h^{\Delta t} \in \mathcal{H}_h^{\Delta t}$ $\quad h = \Delta x$

def. $u_h^{\Delta t}(t^n, x_k) =: u_k^n$ $\leftarrow$ simplified notation

$\neq u$ ... it's the NUMERICAL solution now!

possible to be expressed explicitly

$$\frac{u_k^{n+1} - u_k^n}{\Delta t} + a\,\frac{u_k^n - u_{k-1}^n}{\Delta x} = 0 \iff \boxed{\overrightarrow{\delta}_t u_h^{\Delta t} + a\,\overleftarrow{\delta}_x u_h^{\Delta t} = 0}$$

$\forall k, \forall n$

(*) PDE: $Lu = f(t, \vec{x}, u)$ $\quad L$ ... (linear) differential operator

(**) FDS: $L_h^{\Delta t} u_h^{\Delta t} = f_h^{\Delta t}$ $\quad L_h^{\Delta t}$ ... finite difference operator

finite difference scheme

if $f = f(t, \vec{x})$ ... $f_h^{\Delta t} = P_h^{\Delta t} f$

$f_k^n := \left(f_h^{\Delta t}\right)_k^n = f(t^n, x_k)$ v 1D

if $f = f(t, \vec{x}, u)$ ... $f_k^n = f(t^n, x_k, u_k^n)$

- the norm $\|\cdot\|_h^{\Delta t}$ on $\mathcal{H}_h^{\Delta t}$ is <u>CONSISTENT</u> with the norm $\|\cdot\|_C$ on $C(\bar{\mathcal{I}} \times \bar{\Omega})$, iff

$$\lim_{\substack{h \to 0 \\ \Delta t \to 0}} \|\mathcal{P}_h^{\Delta t} u\|_h^{\Delta t} = \|u\|_C$$

<u>Example</u>: The norm $\|w\|_h^{\Delta t} = \max_{\bar{\mathcal{I}}^{\Delta t} \times \bar{\omega}_h} |w(t, \vec{x})|$ is consistent

with $\|u\|_C = \max_{\bar{\mathcal{I}} \times \bar{\Omega}} |u(t, \vec{x})|$

- the <u>APPROXIMATION ERROR</u> of the difference op. is the grid func.

$$E_h^{\Delta t}(u) = L_h^{\Delta t}(\mathcal{P}_h^{\Delta t} u) - \mathcal{P}_h^{\Delta t}(Lu) \quad : \mathcal{I}^{\Delta t} \times \omega_h \to \mathbb{R}$$

$$\underbrace{\text{where } \|\cdot\|_h^{\Delta t} \text{ is a consistent norm}}$$

- if $\|E_h^{\Delta t}(u)\|_h^{\Delta t} = \mathcal{O}(h^p + (\Delta t)^q)$, we say that $L_h^{\Delta t}$

$|\mathcal{O}(h^p)| + |\mathcal{O}(\Delta t^q)|$

<u>approximates L with order p in space and order q in time</u>

- the FD scheme (**) is <u>CONSISTENT</u> if $p > 0 \wedge q > 0$

with the "original" differential equation $Lu = f$

- the numerical scheme (**) is <u>CONVERGENT</u> $\Leftrightarrow$

$$\lim_{(\Delta t, h) \to 0} \|u_h^{\Delta t} - \mathcal{P}_h^{\Delta t} u\|_h^{\Delta t} = 0 \quad \text{where } \|\cdot\|_h^{\Delta x} \text{ is a consistent norm}$$

"$u_h^{\Delta t}$ converges to u"

num. solution

exact solution

NOTE: $e_h^{\Delta t} = u_h^{\Delta t} - P_h^{\Delta t} u$ is the <u>global approximation error</u>

NOTE: Approximation of initial & boundary conditions

initial condition

boundary condition

$$Lu = f \qquad u(0,\vec{x}) = u_{ini}(\vec{x}) \qquad Bu(t,\vec{x})\big|_{\partial\Omega} = g(t,\vec{x})$$

b.c. operator

$$u_{h,ini} = P_h u_{ini}$$

$$L_h^{\Delta t} u_h^{\Delta t} = f_h^{\Delta t} \qquad u_h^{\Delta t}\Big|_{\{0\}\times\bar{\omega}_h} = \underbrace{u_{ini}\Big|_{\bar{\omega}_h}}_{\bar{\omega}_h \to \mathbb{R}} \qquad B_h^{\Delta t} u_h^{\Delta t}\Big|_{\bar{\tau}^{\Delta t}\times\gamma_h} = g\Big|_{\bar{\tau}^{\Delta t}\times\gamma_h}$$

$$u_{h,ini} \in \mathcal{H}_h = \{w : \bar{\omega}_h \to \mathbb{R}\}$$

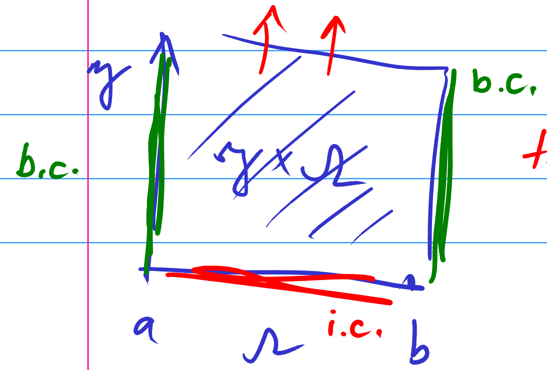
then, it is possible to extend

$$E(u) = B_h^{\Delta t}\left(P_h^{\Delta t} u\right) - P_h^{\Delta t}(Bu) \quad \text{on } \tau^{\Delta t}\times\gamma_h$$

and $$E(u) = u_h^{\Delta t}(0,\vec{x}) - u_{ini}(0,\vec{x}) = 0 \quad \text{on } \{0\}\times\bar{\omega}_h$$

- Dirichlet boundary conditions $\Rightarrow$ B, $B_h^{\Delta t}$ is an identity

$$\Rightarrow \quad E(u) = 0 \quad \text{on } \tau^{\Delta t}\times\gamma_h$$



the initial condition is just a Dirichlet b.c. in the spatio-temporal domain $\mathcal{T}\times\Omega$

u_k^n in 1D

NOTE: The consistent max. norm $\|u_h^{\Delta t}\| = \max\limits_{(t,\vec{x})\in \bar{\tau}^{\Delta t}\times\bar{\omega}_h} |u_h^{\Delta t}(t,\vec{x})| =$

$$= \max_{\bar{\tau}^{\Delta t}} \left(\max_{\bar{\omega}_h} |u_h^{\Delta t}(t,\vec{x})| \right)$$

$$= \max_{\bar{\tau}^{\Delta t}} \| u_h^n(t,\cdot) \|_h$$

max norm over spatial domain only

norm on $\mathcal{H}_h$

where $u_h^n = \underbrace{u_h^{\Delta t}(t^n,\cdot)}_{\in \mathcal{H}_h} : \bar{\omega}_h \to \mathbb{R}$

DEF: The numerical scheme $L_h^{\Delta t} u_h^{\Delta t} = f_h^{\Delta t}$ is **STABLE**

$\iff$ there exists a set $\mathcal{A} = \{(\Delta t, h) \mid \dots\} \subset \mathbb{R}^2$ such that

stability region

1) $(0,0)$ is the accumulation point of $\mathcal{A}$

2) $\forall (\Delta t, h) \in \mathcal{A}$ $\forall\, \phi \in \mathcal{H}_h^{\Delta t}$, there is a unique solution (denoted by $u_{h,\phi}^{\Delta t}$) of the problem

$$\boxed{\begin{array}{ll} L_h^{\Delta t} u_h^{\Delta t} = \phi & \\ B_h^{\Delta t} u_h^{\Delta t} = g_h^{\Delta t} & \text{b.c.} \\ u_h^0 = u_{h,ini} & \text{i.c.} \end{array}}$$

generally,

$(*)$ $\phi : \bar{\tau}^{\Delta t} \times \bar{\omega}_h \times \mathcal{H}_h^{\Delta t} \to \mathbb{R}$

(ϕ depends on the solution $u_h^{\Delta t}$ too)

3) There exists $K > 0$ such that $\forall\, (\Delta t, h) \in \mathcal{A}$, $\forall \phi_1, \phi_2 \in \mathcal{H}_h^{\Delta t}$

$$\| u_{h,\phi_1}^{\Delta t} - u_{h,\phi_2}^{\Delta t} \|_h^{\Delta t} \le K \, \| \phi_1 - \phi_2 \|_h^{\Delta t}$$

where $\| \; \|_h^{\Delta t}$ is a consistent norm

(Lax-Richtmyer equivalence theorem)

THEOREM (LAX) Let $L_h^{\Delta t}$ in (**) be a LINEAR difference operator and let ϕ not depend on $u_h^{\Delta t}$.
Let (**) have a unique solution and let $L_h^{\Delta t}$ approximate L with the order p in space and q in time where $p, q > 0$.

Then the scheme (**) is stable $\Longleftrightarrow$ it is convergent.
The order of convergence is also $\mathcal{O}(h^p + \Delta t^q)$.

we will only prove "$\Longrightarrow$"

Pf! for Dirichlet boundary conditions

orig. PDE: $\underbrace{L}_{\text{lin.}} u = \underbrace{f}_{\text{independent of } u}$ projection onto the grid

- $P_h^{\Delta t}(Lu) = P_h^{\Delta t} f$

(**) : - $L_h^{\Delta t} u_h^{\Delta t} = \phi = P_h^{\Delta t} f$ ... again, this is just projection onto the grid

subtract the two eqs.

$$P_h^{\Delta t}(Lu) - L_h^{\Delta t} u_h^{\Delta t} = 0$$

$$\underbrace{P_h^{\Delta t}(Lu) - L_h^{\Delta t}(P_h^{\Delta t} u)}_{-E(u)} + \underbrace{L_h^{\Delta t}(P_h^{\Delta t} u) - L_h^{\Delta t} u_h^{\Delta t}}_{\downarrow\ L_h^{\Delta t} \text{ is linear}} = 0$$

$-E(u)$ difference operator approximation error

$$L_h^{\Delta t}\big(\underbrace{P_h^{\Delta t} u - u_h^{\Delta t}}_{e_h^{\Delta t}}\big) \overset{\text{def.}}{=} E(u) \quad (\#)$$

$e_h^{\Delta t}$ ... glob. approx. error

(#) is a problem for $e_h^{\Delta t}$ with homogeneous (zero) Dirichlet boundary conditions & zero initial condition.

$$\boxed{\text{stability: } \| u^{\Delta t}_{h,\phi_1} - u^{\Delta t}_{h,\phi_2} \|^{\Delta t}_h \le K \| \phi_1 - \phi_2 \|^{\Delta t}_h}$$

choose $\phi_1 = E(u)$, $\quad \phi_2 = 0$

$\Updownarrow \qquad\qquad \Updownarrow$

$u^{\Delta t}_{h,\phi_1} = e^{\Delta t}_h \qquad u^{\Delta t}_{h,\phi_2} = 0$

{ Lin. dif. op. $L^{\Delta t}_h$, zero RHS $\phi_2 = 0$ + zero b.c. + zero i.c. yield constant zero solution

then

$$\| u^{\Delta t}_{h,\phi_1} - u^{\Delta t}_{h,\phi_2} \|^{\Delta t}_h = \underline{\| e^{\Delta t}_h \|^{\Delta t}_h} \le K \| E(u) \|^{\Delta t}_h = \underline{(K)\mathcal{O}(h^p + \Delta t^q)}$$

<u>THEOREM</u>: Let the assumptions (1), (2) in the definition of stability are satisfied. Consider the scheme

$$L^{\Delta t}_h u^{\Delta t}_h = f^{\Delta t}_h \qquad (*)$$

wher $L^{\Delta t}_h$ <u>is linear.</u>

Let $\exists C, D > 0$ such that $\forall (\Delta t, h) \in \mathcal{A}$ (region of stability) $\forall f_h \in \mathcal{H}^{\Delta t}_h$

$$\boxed{\| u^n_h \|_h \le C \| u^0_h \|_h + D \underbrace{n \Delta t}_{t^n} \| f_h \|^{\Delta t}_h} \quad \forall n = 1, \dots, N$$

holds.

Then the numerical scheme $(*)$ <u>is stable</u> (and hence, by Lax thm. also convergent)

Pr: Let $\phi_1, \phi_2 \in \mathcal{H}^{\Delta t}_h$. Then denote

$$L^{\Delta t}_h u^{\Delta t}_{h,\phi_1} = \phi_1$$
$$L^{\Delta}_h u^{\Delta t}_{h,\phi_2} = \phi_2$$

} subtract

denote $\varepsilon^{\Delta t}_h = u^{\Delta t}_{h,\phi_1} - u^{\Delta t}_{h,\phi_2}$

$$\overset{\text{by linearity}}{\Longrightarrow} L^{\Delta t}_h \varepsilon^{\Delta t}_h = \phi_1 - \phi_2 \quad \text{with} \quad \varepsilon^0_h = 0$$

Then:

$$\| \varepsilon^{\Delta t}_h \|^{\Delta t}_h \le \underbrace{\tilde{K}}_{\text{equivalence of norms on } \mathcal{H}^{\Delta t}_h} \max_n \| \varepsilon^n_h \|_h \le \tilde{K} \max_n \overbrace{D n \Delta t}^{= D t_{max}} \underbrace{\| \phi_1 - \phi_2 \|^{\Delta t}_h}_{\text{independent of } t} \le \overbrace{\tilde{K} D t_{max}}^{K} \| \phi_1 - \phi_2 \|^{\Delta t}_h$$

Let us consider the eq. $\underline{Lu=0}$ with the discretization $L_h^{\Delta t} u_h^{\Delta t} = 0$,

where L is $\underline{\text{linear}}$ (WLOG only in 1D)

$u_k^{n+1} = u_k^n + \Delta t(\dots)$

DEF: $L_h^{\Delta t} u_h^{\Delta t} = 0$ is $\underline{\text{positive}}$ $\Leftrightarrow$ $u_k^{n+1} = \sum_{p \in S_k} a_{p,k} u_{k+p}^n$ (see *)

$\left(L_h^{\Delta t} u_h^{\Delta t}\right)_k^n = \frac{u_k^{n+1} - u_k^n}{\Delta t} + \dots$ spatial difference quotients $\wedge$ $a_{p,k} \geq 0$ $\forall p$ $\forall k$

THEOREM: Every positive scheme is stable (and hence convergent).
(provided that L only contains derivatives of u but not u itself.)
(reaction term)

Proof

- the sum of coefficients in front of (u_{k+p}^n) in the finite difference replacement of each derivative is $\underline{0}$.

see the first row of the matrix in derivations of difference quotients

$$\Rightarrow \sum_{p \in S_k} a_{p,k} = 1 \quad \text{for each } k \quad \text{(see *)}$$

Let's choose the $\underline{\text{maximum}}$ norm $\|\cdot\|_h^{\Delta t}$

then:
$$\|u_h^{n+1}\|_h = \max_k |u_k^{n+1}| = \max_k \Big|\sum_{p \in S_k} a_{p,k} u_{k+p}^n\Big| \leq$$

$$\leq \max_k \sum_{p \in S_k} |a_{p,k}| |u_{k+p}^n| \leq \max_k \underbrace{\sum_{p \in S_k} |a_{p,k}|}_{=1} \underbrace{\left(\max_j |u_j^n|\right)}_{\|u_h^n\|_h}$$

$$\leq \max_k \underbrace{1 \cdot \|u_h^n\|_h}_{\text{no depence on } k} = \|u_h^n\|_h$$

by the same argument
$\leq \dots \|u_h^{n-1}\|_h \leq \dots \leq \|u_h^0\|_h$

$\Rightarrow$ maximum principle $\Rightarrow$ stability $\xRightarrow{\text{LAX}}$ convergence.

*) dependence on k means that the numerical scheme need not be the same for all nodes (at the boundary, it may be adapted to maintain the order of accuracy)

UPWIND SCHEME FOR THE EQUATION $\partial_t u + a\partial_x u = 0$

for a general a: $a \in \mathbb{R}$, konst. def. $a_+ = \max(a,0)$, $a_- = \min(a,0)$

$$\Rightarrow \quad \vec{\delta}_t u_h^{\Delta t} + a_+ \overleftarrow{\delta}_x u_h^{\Delta t} + a_- \vec{\delta}_x u_h^{\Delta t} = 0$$

i.e.
$$\frac{u_k^{n+1} - u_k^n}{\Delta t} + a_+ \frac{u_k^n - u_{k-1}^n}{\Delta x} + a_- \frac{u_{k+1}^n - u_k^n}{\Delta x} = 0$$

Note:
$$\partial_t u + \underline{\partial_x f(u)} = 0 \quad \Leftrightarrow \quad \partial_t u + f'(u)\,\underline{\partial_x u} = 0$$

$a_+(u) = \max(f'(u), 0)$
$a_-(u) = \min(f'(u), 0)$

Stability (and convergence) of the upwind scheme

1) positivity: $\underline{a > 0}$

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

$$= u_k^n \underbrace{\left(1 - \frac{\Delta t}{\Delta x} a\right)}_{\overset{!}{\geq} 0} + \underbrace{\frac{\Delta t}{\Delta x} a}_{> 0 \text{ always}} u_{k-1}^n$$

iff $\underline{a\frac{\Delta t}{\Delta x} \leq 1}$

this is the same condition as CFL

for convergence: CFL .. necessary condition positivity ... sufficient cond.

2) Von Neumann spectral analysis of stability

Consider $\partial_t u + a\partial_x u = 0$ with periodic boundary conditions

$\Omega = (c,d) \subset \mathbb{R}$ $\qquad u(t, x+d-c) = u(t,x) \quad \forall x \in \mathbb{R}$

DEF: The finite difference scheme $L_h^{\Delta t} u_h^{\Delta t} = f_h^{\Delta t}$ is called a **ONE-STEP scheme** $\Leftrightarrow$ the grid function $\left(L_h^{\Delta t} u_h^{\Delta t}\right)^n$ depends only on u_h^n and u_h^{n+1}, or u_h^{n-1} and u_h^n, respectively.

NOTE: A one-step linear scheme is in the form

$$u_h^{n+1} = A u_h^n + \Delta t f_h^n \qquad \text{explicit}$$

or
$$B u_h^{n+1} = A u_h^n + \Delta t \left(C f_h^n + D f_h^{n+1} \right) \qquad \text{implicit}$$

WLOG, let us consider an explicit one-step scheme of the above problem with zero RHS:

$$\# \qquad u_k^{n+1} = \sum_{p \in S} a_p u_{k+p}^n \quad \text{in 1D}$$

Assume $\quad \Omega = (c,d) \subset \mathbb{R}$, $\quad x_k = c + k\Delta x$, $\quad t^n = n\Delta t$

$L = d - c$

$k = 0, \dots, m \; ; \; n = 0, \dots, N$

Let $\quad u_{ini}(x) \in C(\Omega)$

$$\Rightarrow \tilde{u}_{ini}(x) = \frac{1}{2} \sum_{l=-\infty}^{+\infty} c_l \exp\left(\frac{2\pi i l x}{L}\right) \qquad c_l = \frac{2}{L}\int_c^d u_{ini}(x) \exp\left(\frac{2\pi i l x}{L}\right) dx$$

Fourier-series

$\Downarrow$ (... periodic extension of u is $\tilde{u}$)

$\Downarrow$

in the numerical scheme, the initial condition is given by $u_k^0 = u_{ini}(x_k)$

$$\Rightarrow u_k^0 = \frac{1}{2}\sum_{l=-\infty}^{+\infty} c_l \exp\left(\frac{2\pi i l(c+\overbrace{k\Delta x}^{x=x_k})}{L}\right) =$$

$$= \frac{1}{2}\sum_{l=-\infty}^{+\infty} \underbrace{c_l \exp\left(\frac{2\pi i l c}{L}\right)}_{\tilde{c}_l} \underbrace{\exp\left(i l k \frac{2\pi\Delta x}{L}\right)}_{\exp(\alpha i l k)} \qquad \alpha = \frac{2\pi\Delta x}{L}$$

$$= \frac{1}{2}\sum_{l=-\infty}^{+\infty} \tilde{c}_l \exp(\alpha i l k)$$

If the periodic b.c. are satisfied, then $u(c) = u(d)$

i.e. $u_0^n = u_m^n$

$\Rightarrow$ 1) the Fourier series expansion also holds at $x=c, x=d$

in the next time step $\Rightarrow$ 2) the scheme (#) holds $\forall k = 0, \dots, m$

then $$u_k^1 = \sum_p a_p u_{k+p}^0 = \sum_p a_p \frac{1}{2}\sum_{l=-\infty}^{+\infty} \tilde{c}_l \exp(\alpha i l(k+p)) =$$

$$= \frac{1}{2}\sum_{l=-\infty}^{+\infty} \tilde{c}_l \underbrace{\sum_p a_p \exp(\alpha i l p)}_{\lambda(\alpha l)\ \dots\ \text{amplification factor}} \exp(\alpha i l k)$$

$$\Rightarrow u_k^n = \frac{1}{2}\sum_{l=-\infty}^{+\infty} \tilde{c}_l \lambda^n(\alpha l) \exp(\alpha i l k)$$

grid refinement $\alpha \to 0$ as $\Delta x \to 0$

$\theta := \alpha l \in \mathbb{R}$ depending on $\Delta x, l$

THEN IF $|\lambda(\theta)|^2 \le 1 \quad \forall \theta \in \mathbb{R}$ $\Rightarrow u_k^n$ is bounded $\forall k, \forall n$

$\Rightarrow \|u_h^n\|_h \le C \|u_h^0\|_h$

$\Rightarrow$ stability $\Rightarrow$ convergence

IF $\exists \theta$ s.t. $|\lambda(\theta)|^2 > 1 \Rightarrow u_k^n$ grows beyond any limits for $\Delta t \to 0 \Rightarrow$ no convergence

Back to the upwind scheme:

consider the scheme $u_k^{n+1} = u_k^n - \frac{a\Delta t}{\Delta x}\left(u_k^n - u_{k-1}^n\right)$ pro $a>0$

and plug in $u_k^n = (c^1) \exp(ik\theta)$ where $\theta \in \mathbb{R}$

$$\Rightarrow u_k^{n+1} = \exp(ik\theta) - \frac{a\Delta t}{\Delta x}\left(\exp(ik\theta) - \exp(i(k-1)\theta)\right)$$
$$= \exp(ik\theta) \underbrace{\left[\left(1 - \frac{a\Delta t}{\Delta x}\right) + \frac{a\Delta t}{\Delta x}\exp(-i\theta)\right]}_{\lambda(\theta)}$$

denote $\sigma := \frac{a\Delta t}{\Delta x}$

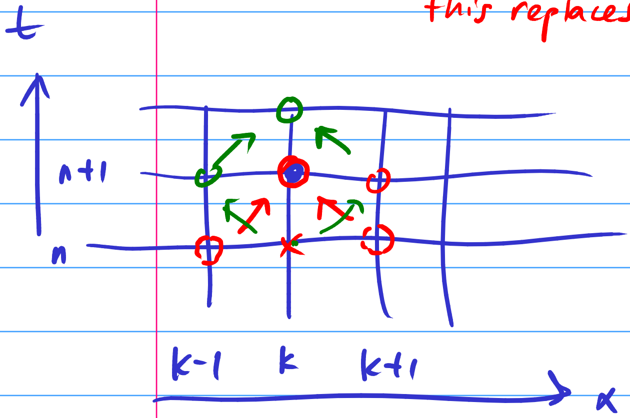
$$\Rightarrow \lambda(\theta) = 1 - \sigma\left(1 - e^{-i\theta}\right) = 1 - \sigma(1-\cos\theta) - i\sigma\sin\theta$$

$$|\lambda(\theta)|^2 = \left(1 - \sigma(1-\cos\theta)\right)^2 + \sigma^2\sin^2\theta$$
$$= \left((1-\sigma) + \sigma\cos\theta\right)^2 + \sigma^2\sin^2\theta$$
$$= (1-\sigma)^2 + 2(1-\sigma)\sigma\cos\theta + \sigma^2$$
$$= 1 - 2\sigma + 2\sigma^2 + 2(1-\sigma)\sigma\cos\theta$$
$$= 1 - \underbrace{2\sigma}_{>0}\underbrace{(1-\sigma)}_{\overset{!}{\geq} 0}\underbrace{(1-\cos\theta)}_{\geq 0} \overset{!}{\leq} 1$$

$$\Rightarrow \sigma \leq 1 \Rightarrow \frac{a\Delta t}{\Delta x} \leq 1$$

LAX-FRIEDRICHS SCHEME for $\partial_t u + a\partial_x u = 0$

$$u_k^{n+1} = \underbrace{\frac{1}{2}\left(u_{k-1}^n + u_{k+1}^n\right)}_{\text{this replaces } u_k^n} - \underbrace{\frac{a\Delta t}{2\Delta x}\left(u_{k+1}^n - u_{k-1}^n\right)}_{\frac{1}{2\Delta x}\left(u_{k+1}^n - u_{k-1}^n\right) = \left[\overleftrightarrow{\delta}_x u\right]_k^n}$$



rewrite

$$u_k^{n+1} = u_k^n - \frac{a\Delta t}{2\Delta x}\left(u_{k+1}^n - u_{k-1}^n\right) + \frac{\Delta x^2}{2\Delta t}\underbrace{\frac{\Delta t}{\Delta x^2}\left(u_{k-1}^n - 2u_k^n + u_{k+1}^n\right)}_{}$$

$$\vec{\delta}_t u_h^{\Delta t} = -a\underbrace{\overleftrightarrow{\delta}_x}_{\text{2nd order approx. of } \partial_x u} u_h^{\Delta t} + \mu_{num}\underbrace{\vec{\delta}_x \overleftarrow{\delta}_x}_{\overleftrightarrow{\delta}_{xx}} u_h^{\Delta t}$$

approximation of $\partial_{xx} u$ at the point (t^n, x_k) by a central difference

$\Rightarrow$ this scheme approximates the equation

$$\boxed{\partial_t u + a\partial_x u = \mu_{num}\partial_{xx} u}$$

"modified equation"

with the order $\mathcal{O}(\Delta t + \Delta x^2)$

Homework:
for $u \in C^3((a,b))$, prove that

$$\underbrace{\left(\overleftrightarrow{\delta}_{xx} P_h u\right)(x_k)}_{\frac{1}{\Delta x^2}\left(u(x_{k-1}) - 2u(x_k) + u(x_{k+1})\right)} = u''(x_k) + \mathcal{O}(\Delta x^2)$$

$$\mu_{num} = \frac{\Delta x^2}{2\Delta t} \quad \text{numerical viscosity}$$

MODIFIED LF SCHEME

$$\Rightarrow \mu_{num} = \varepsilon \frac{\Delta x^2}{2\Delta t}$$

$$\frac{\varepsilon}{2} \quad \text{where } \varepsilon \in [0,1]$$

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

$$\frac{\Delta x^2}{2\Delta t}\,\frac{\Delta t}{\Delta x^2} = \frac{1}{2}$$

$\varepsilon = 1 \;\ldots\; \Rightarrow$ LF scheme

$\varepsilon = 0 \;\; \Rightarrow$ explicit central scheme

Stability by the Von Neumann analysis: $\quad u_k^n = \exp(ik\theta)$

$$\lambda(\theta) = 1 - \frac{a\Delta t}{2\Delta x}\left(e^{i\theta} - e^{-i\theta}\right) + \frac{\varepsilon}{2}\left(e^{-i\theta} - 2 + e^{i\theta}\right)$$

$$= 1 - i\frac{a\Delta t}{\Delta x}\sin\theta - \varepsilon(1-\cos\theta)$$

$$|\lambda(\theta)|^2 = \left[1 - \varepsilon(1-\cos\theta)\right]^2 + \left(\frac{a\Delta t}{\Delta x}\right)^2 \sin^2\theta$$

$$= 1 - 2\varepsilon(1-\cos\theta) + \varepsilon^2(1-\cos\theta)^2 + \left(\frac{a\Delta t}{\Delta x}\right)^2\sin^2\theta$$

we solve: $1 \geq |\lambda(\theta)|^2$ $\qquad \sin^2\theta = 1-\cos^2\theta = (1-\cos\theta)(1+\cos\theta)$

$$2\varepsilon(1-\cos\theta) \geq \varepsilon^2(1-\cos\theta)^2 + \left(\frac{a\Delta t}{\Delta x}\right)^2\sin^2\theta \quad \Big| \cdot \frac{1}{1-\cos\theta}$$

$$2\varepsilon \geq \varepsilon^2(1-\cos\theta) + \left(\frac{a\Delta t}{\Delta x}\right)^2(1+\cos\theta) \qquad \theta \neq 2k\pi$$

$$z = \cos\theta$$

$$\Downarrow$$

$$2\varepsilon \geq \underbrace{\varepsilon^2(1-z) + \left(\frac{a\Delta t}{\Delta x}\right)^2 (1+z)}_{\text{linear function of } z \;\Rightarrow\; \text{assumes min./max at } z=\pm 1} \qquad \forall z \in [-1,1]$$

$z=1$: $\quad 2\varepsilon \geq 2\left(\frac{a\Delta t}{\Delta x}\right)^2$

$z=-1$: $\quad 2\varepsilon \geq 2\varepsilon^2$ ... always true for
$\qquad \varepsilon \geq \varepsilon^2 \qquad$ the considered values $\varepsilon \in [0,1]$

$\Rightarrow$ the sufficient & necessary condition for convergence of the modified LF scheme reads

$$\boxed{\frac{a\Delta t}{\Delta x} \leq \sqrt{\varepsilon}} \rightarrow \mu_{num} = \varepsilon \frac{\Delta x^2}{2\Delta t}$$

for a fixed Δx $\rightarrow \approx \frac{\Delta x}{\sqrt{\varepsilon}}$ $\Downarrow$ $\mu_{num} \approx \sqrt{\varepsilon}$

Note: for $\frac{a\Delta t}{\Delta x} = \sqrt{\varepsilon}$ ("edge of stability") .. $\mu_{num} = \varepsilon \cdot \frac{\Delta x}{2} \cdot \frac{a}{\sqrt{\varepsilon}} = \sqrt{\varepsilon}\, \frac{a}{2} \Delta x$

$\Rightarrow$ reducing Δx also reduces num. viscosity

Consequences:

- $\varepsilon = 1 \qquad \frac{a\Delta t}{\Delta x} \leq 1$ ... LF scheme has the same condition for convergence as the upwind scheme
- $\varepsilon \in (0,1)$ ... by reducing numerical viscosity, the condition on Δt gets stricter
- $\varepsilon = 0$ ... condition can never be satisfied

$\Rightarrow$ the explicit central scheme is unconditionally unstable!

Homework:
express the equation system in matrix form

IMPLICIT EULER SCHEME

$$\overleftarrow{\delta}_t u_h^{\Delta t} + a \overleftrightarrow{\delta}_x u_h^{\Delta x} = 0$$

NOTE: $n+1$ n ← explicit central

$$\left(\overleftarrow{\delta}_t u_h^{\Delta t} + a \overleftrightarrow{\delta}_x u_h^{\Delta x}\right)_k^n = \frac{u_k^n - u_k^{n-1}}{\Delta t} + a \frac{u_{k+1}^n - u_{k-1}^n}{2\Delta x} = 0$$

... a system of linear equations for the unknown vector $u_h^n = \begin{pmatrix} u_1^n \\ \vdots \\ u_{M-1}^n \end{pmatrix}$

$$\left(\overleftarrow{\delta}_t u_h^{\Delta t} + a \overleftrightarrow{\delta}_x u_h^{\Delta x}\right)_k^{n+1} = \frac{u_k^{n+1} - u_k^n}{\Delta t} + a \frac{u_{k+1}^{n+1} - u_{k-1}^{n+1}}{2\Delta x} = 0$$

with a 3-diagonal matrix

"+1" is the difference with respect to explicit central scheme

$$u_k^n = e^{ik\theta} \qquad \theta = \alpha l \in \mathbb{R} \qquad u_k^{n+1} = \lambda(\theta) e^{ik\theta}$$

plug it into the scheme:

$$\frac{1}{\Delta t}\left(\lambda(\theta) - 1\right)\cancel{e^{ik\theta}} + \frac{a}{2\Delta x}\lambda(\theta)\left(e^{i\theta} - e^{-i\theta}\right)\cancel{e^{ik\theta}} = 0 \quad \Big| \cdot \Delta t$$

let $\sigma = \frac{a\Delta t}{\Delta x}$

$$\lambda(\theta) - 1 + \frac{\sigma}{2}\lambda(\theta)\left(e^{i\theta} - e^{-i\theta}\right) =$$

$$= \lambda(\theta) - 1 + \lambda(\theta)\,\sigma\, i \sin\theta = 0$$

$$\lambda(\theta) = \frac{1}{1 + i\sigma\sin\theta}$$

$$\Rightarrow \quad |\lambda(\theta)| = 1 / \left|1 + i\sigma\sin\theta\right| \le 1$$

⇒ THE IMPLICIT SCHEME IS UNCONDITIONALLY **STABLE**!

SUMMARY:

- *explicit scheme*
  - Δt must be refined with Δx
  - more time steps necessary, but each time step easy to compute
  - easy & efficient parallelization
- *implicit scheme*
  - $\Delta t, \Delta x$ independently chosen
  - less time steps, but each time step more difficult to calculate
  - parallelization of iterative solvers

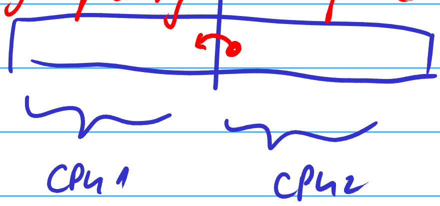
Example: upwind for $a>0$:

```
:  #pragma omp parallel for        OPENMP
for (k=1; k<m; k++)
    u_new[k] = u[k] + aΔt/Δx (u[k-1] - u[k]);
```

1 time step

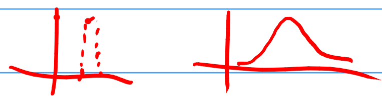
u_new[k]: u_k^{n+1} u[k]: u_k^n

message passing on 2 processes (MPI)

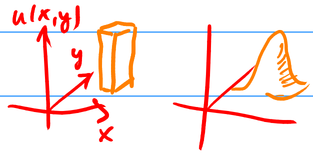


FINITE DIFFERENCE SCHEME FOR THE HEAT EQUATION

in 1D: $\partial_t u = \lambda \partial_{xx} u$ *)



in 2D, 3D: $\partial_t u = \lambda \Delta u$



with i.c. $u\big|_{t=0} = u_{ini}$

in r-D: $\partial_t u = \lambda \sum_{j=1}^{r} \partial_{jj} u$

& with b.c. $u\big|_{\partial\Omega} = 0$

*) if $\lambda = \lambda(x) \Rightarrow \partial_t = \partial_x(\lambda \partial_x u)$ — u = temperature

in 1D ... central explicit scheme

$$\left(\overleftrightarrow{\delta}_{xx} u_h^{\Delta t}\right)_k^n = \frac{u_{k+1}^n - 2u_k^n + u_{k-1}^n}{\Delta x^2}$$

$$\vec{\delta}_t u_h^{\Delta t} = \lambda \overleftrightarrow{\delta}_{xx} u_h^{\Delta t}$$

$$\frac{\partial u}{\partial x_j} = \partial_{x_j} u = \partial_j u$$

in r-D

$$\vec{\delta}_t u_h^{\Delta t} = \lambda \sum_{j=1}^{r} \overleftrightarrow{\delta}_{x_j x_j} u_h^{\Delta t}$$

$$\overleftrightarrow{\delta}_j = \overleftrightarrow{\delta}_{x_j}$$

NOTE: $\overleftrightarrow{\delta}_{xx} u_h^{\Delta t} = \underbrace{\overleftarrow{\delta}_x \vec{\delta}_x u_h^{\Delta t}}_{} = \vec{\delta}_x \overleftarrow{\delta}_x u_h^{\Delta t}$

or: $\partial_x (\lambda(x) \partial_x u(x)) =$

*) $\vec{\delta}_t u_h^{\Delta x} = \overleftarrow{\delta}_x \left[(P_h^{\Delta t} \lambda) \vec{\delta}_x u_h^{\Delta t} \right]$ $\quad = \partial_x \lambda(x) \partial_x u(x) + \lambda(x) \partial_{xx} u(x)$

Homework:
1) implement different num. schemes for this
2) analyze stability

Stability analysis in 1D: $\quad u_k^n = e^{ik\theta}, \quad u_k^{n+1} = \lambda(\theta) e^{ik\theta}$

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

$$\lambda(\theta) = 1 + \frac{\lambda \Delta t}{\Delta x^2} \left(e^{-i\theta} - 2 + e^{i\theta} \right)$$

$$= 1 + 2 \frac{\lambda \Delta t}{\Delta x^2} (\cos\theta - 1)$$

$|\lambda(\theta)| \le 1$ $\quad \Leftrightarrow \quad -1 \le 1 + 2 \frac{\lambda \Delta t}{\Delta x^2} (\cos\theta - 1) \le 1$

$\forall \theta \in \mathbb{R}$

$$\underbrace{-2 \le}_{\forall \theta} 2 \frac{\lambda \Delta t}{\Delta x^2} (\cos\theta - 1) \underbrace{\le 0}_{\text{always true}}$$

$\Leftrightarrow$

$$-2 \le -2 \cdot 2 \frac{\lambda \Delta t}{\Delta x^2}$$

$\Leftrightarrow$ $\boxed{\frac{\lambda \Delta t}{\Delta x^2} \le \frac{1}{2}}$

$\Delta t \approx \Delta x^2$

$\Rightarrow$ implicit scheme may be beneficial.

Homework: Show that the implicit scheme

$$\overleftarrow{\delta}_t u_h^{\Delta t} = \lambda \overleftrightarrow{\delta}_{xx} u_h^{\Delta t}$$

is unconditionally stable

Stability of the explicit scheme in r-D

one "mode" of the r-dimensional Fourier series has the form

$$u^n_{k_1,k_2,\dots,k_r} = e^{ik_1\theta_1} e^{ik_2\theta_2} \cdots e^{ik_r\theta_r} = \prod_{j=1}^r e^{ik_j\theta_j}$$

$\theta_1 = \frac{\Delta x_1}{2\pi}$

$$u^{n+1}_{k_1,k_2,\dots,k_r} = \lambda(\theta_1,\dots,\theta_r) \prod_{j=1}^r e^{ik_j\theta_j}$$

1D:

$$\lambda(\theta) = 1 + \frac{\lambda \Delta t}{\Delta x^2}\left(e^{-i\theta} - 2 + e^{i\theta}\right) = 1 + 2\frac{\lambda\Delta t}{\Delta x^2}\left(\cos\theta - 1\right)$$

$\downarrow$ after plugging into the r-dimensional FDM scheme

$$\lambda(\theta_1,\dots,\theta_r) = 1 + \sum_{j=1}^r 2\frac{\lambda\Delta t}{\Delta x_j^2}\left(\cos\theta_j - 1\right)$$

$$\left|\lambda(\theta_1,\dots,\theta_r)\right| \le 1 \quad \forall (\theta_1,\dots,\theta_r) \in \mathbb{R}^r$$

$$\Leftrightarrow \quad -2 \le -2\cdot\sum_{j=1}^r \frac{2\lambda\Delta t}{\Delta x_j^2} \quad \Leftrightarrow \quad \boxed{\sum_{j=1}^r \frac{\lambda\Delta t}{\Delta x_j^2} \le \frac{1}{2}}$$

... now for a uniform grid made of vertices of hypercubes with edge length h: $\Delta x_1 = \Delta x_2 = \dots = \Delta x_r = h$

$$\Rightarrow \boxed{\frac{\lambda \Delta t}{h^2} \leq \frac{1}{2r}}$$

Example: grid refinement from h to $\frac{h}{2}$ in 3D:

- $2^3 = 8$-times more grid nodes
- $2^2 = 4$-times more time steps

$\Rightarrow$ 8-times more memory
$4 \cdot 8 = 32$-times more operations ($\propto$ simulation times)

NOTE: Advection vs. diffusion-dominated problems
(N-S equations for viscous compressible flow)

- flow velocity vs. viscosity
- numerical viscosity
- turbulent viscosity

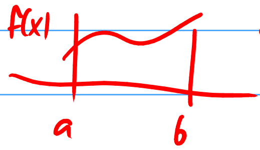
CLASSICAL SCHEMES OF THE FINITE DIFFERENCE METHOD

Crank & Nicolson scheme

$$u(t_{n+1}, x) = u(t_n, x) + \int_{t_n}^{t_{n+1}} \partial_t u(t,x)\,dt = u(t_n, x) + \frac{\Delta t}{2}\Big(\partial_t u(t_{n+1}, x) + \partial_t u(t_n, x)\Big) + \mathcal{O}(\Delta t^3)$$

which is based on the trapezoidal quadrature rule

$L = b - a$



$$\int_a^b f(x)\,dx = \underbrace{\frac{f(a)+f(b)}{2}}_{f(\xi)+O(L^2)} \cdot \underbrace{(b-a)}_{O(L)} + O(L^3)$$

$\Rightarrow$ for the equation $\partial_t u = L_x u$ — L_x is the differential operator in spatial coordinates only

$$\left(\vec{\delta}_t u_h^{\Delta t}\right)_h^n = \frac{u_h^{n+1} - u_h^n}{\Delta t} = \frac{1}{2}\Big(\underbrace{L_h u_h^n}_{\substack{\text{finite difference}\\ \text{equivalent of } L_x u\\ \text{at time } t_n}} + \underbrace{L_h u_h^{n+1}}_{\substack{-''-\\ \text{at time } t_{n+1}}}\Big)$$

L_h is the finite difference operator in spatial coordinates

E.g. for the heat equation:

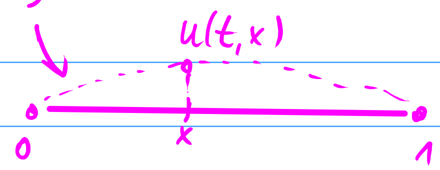
$$\frac{u_h^{n+1} - u_h^n}{\Delta t} = \lambda \cdot \frac{1}{2}\left(\overleftrightarrow{\delta}_{xx} u_h^n + \overleftrightarrow{\delta}_{xx} u_h^{n+1}\right)$$

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

$\Rightarrow$ (semi) implicit unconditionally stable scheme which is 2nd order-accurate in time

- in space, the order of approximation is given by L_h (which replaces L_x)
- in this example, it is also 2nd order

FDM SCHEME FOR THE WAVE EQ.



$$\partial_{tt} u = c^2 \partial_{xx} u \quad \dots \quad a\,\partial_{xx} u + 2b\,\partial_{xy} u + c\,\partial_{yy} u + \underbrace{\dots}_{1.\text{ord}} = 0$$

zde $t \equiv y$ $\qquad a \equiv c^2$, $\quad b \equiv 0$, $\quad c \equiv -1$

$D = b^2 - ac$

$\dfrac{dy}{dx} = \lambda$ kde $\lambda = \dfrac{-b \pm \sqrt{D}}{a}$

$\Rightarrow D = b^2 - ac \equiv c^2 > 0$

$\Rightarrow \lambda = \pm \dfrac{1}{c} = \dfrac{dt}{dx}$ $\qquad \Rightarrow$ 2nd order HYPERBOLIC PDE

FDM:
$$\overleftrightarrow{\delta}_{tt} u_h^{\Delta t} = c^2 \overleftrightarrow{\delta}_{xx} u_h^{\Delta t}$$

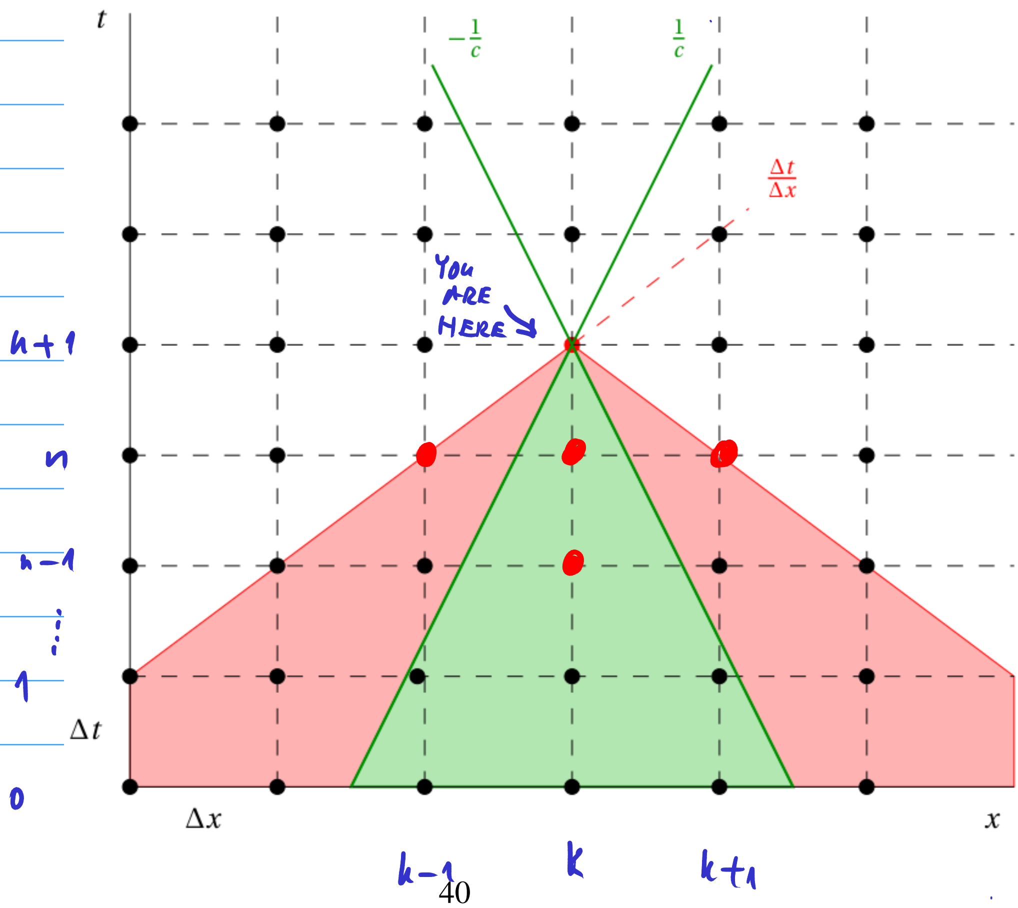
$$\frac{u_k^{n+1} - 2u_k^n + u_k^{n-1}}{\Delta t^2} = c^2 \frac{u_{k+1}^n - 2u_k^n + u_{k-1}^n}{\Delta x^2}$$

we calculate u_h^{n+1} by means of u_h^n and u_h^{n-1}

CFL:

$$\frac{\Delta t}{\Delta x} \le \frac{1}{c}$$

necessary condition for convergence



Homework:
- perform the von Neumann spectral analysis

INITIAL CONDITIONS $\quad u\big|_{t=0} = u_0 \qquad \partial_t u\big|_{t=0} = V_0 \qquad + \quad$ B.C.

init. position $\qquad$ init. velocity $\qquad u(a)=u(b)=0$ (fixed ends)

DISCRETIZATION $\downarrow \qquad \downarrow$

$$u_h^{\Delta t}\Big|_{t=0} = \left(P_h^{\Delta t} u\right)\Big|_{t=0} \qquad \vec{\delta}_t u_h^{\Delta t}\Big|_{t=0} = P_h^{\Delta t}\partial_t u\Big|_{t=0}$$

$$u_k^0 = u(0,x_k) = u_0(x_k) \qquad \underbrace{\frac{u_k^1 - u_k^0}{\Delta t}}_{} = \partial_t u(0,x_k) = V_0(x_k)$$

$\Rightarrow$ gives us the "other" time layer

$$u_k^1 = u_k^0 + \Delta t\, V_0(x_k)$$

LAX - WENDROFF FDM SCHEME FOR THE TRANSPORT EQUATION

Taylor expansion

$$u(\underbrace{t}_{t_n}+\underbrace{\Delta t}_{t_{n+1}}, x) = u(t,x) + \Delta t\, \partial_t u(t,x) + \tfrac{1}{2}\Delta t^2 \partial_{tt} u(t,x) + \mathcal{O}(\Delta t^3)$$

From the equation $\partial_t u + a\partial_x u = 0 \quad \Rightarrow \quad \partial_t u = -a\partial_x u$

$$\Rightarrow \partial_{tt} u = \partial_t \partial_t u = \partial_t(-a\partial_x u) =$$

$$= -a\partial_x \partial_t u = -a\partial_x(-a\partial_x u) = a^2\partial_{xx} u$$

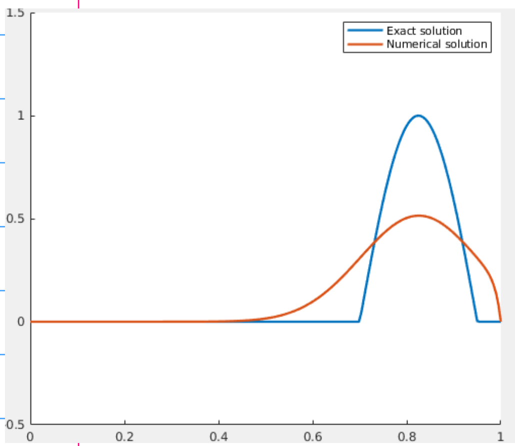
$$\Rightarrow u(t+\Delta t, x) = u(t,x) \underbrace{- a\Delta t\, \partial_x u(t,x)}_{\partial_t u} + \underbrace{\tfrac{1}{2}a^2 \Delta t^2 \partial_{xx} u(t,x)}_{\frac{1}{2}\partial_{tt} u} + \mathcal{O}(\Delta t^3)$$

$$\frac{u(t+\Delta t, x) - u(t,x)}{\Delta t} = -a\partial_x u(t,x) + \tfrac{1}{2}a^2 \Delta t\, \partial_{xx} u(t,x) + \underbrace{\mathcal{O}(\Delta t^2)}_{\text{2nd order in time}}$$

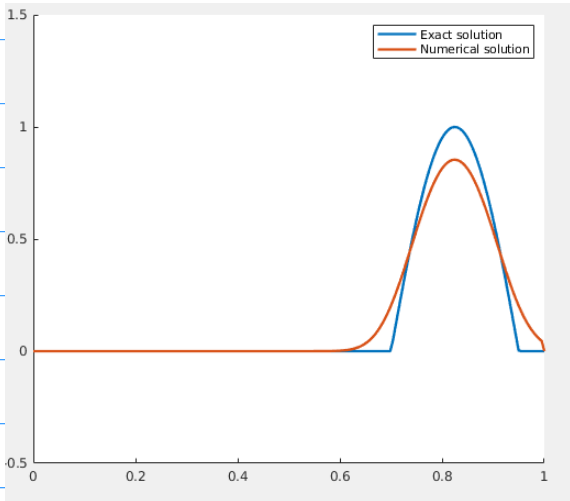
$\forall t, \forall x$

$$\boxed{\vec{\delta}_t u_h^{\Delta t}\Big|_{(t^n,x_k)} = \overbrace{-a\,\overleftrightarrow{\delta}_x u_h^{\Delta t} + \frac{1}{2}a^2\Delta t\,\overleftrightarrow{\delta}_{xx} u_h^{\Delta t}}^{\text{2nd order in space}}\Big|_{(t^n,x_k)}}$$

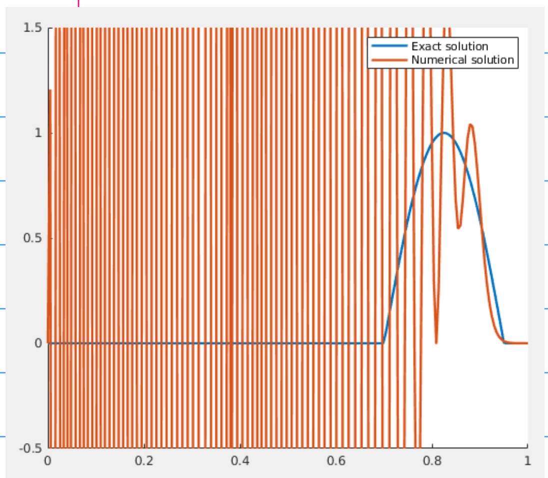
$$u_k^{n+1} = u_k^n - \frac{a\Delta t}{2\Delta x}\left(u_{k+1}^n - u_{k-1}^n\right) + \frac{1}{2}\frac{a^2\Delta t^2}{\Delta x^2}\left(u_{k+1}^n - 2u_k^n + u_{k-1}^n\right)$$



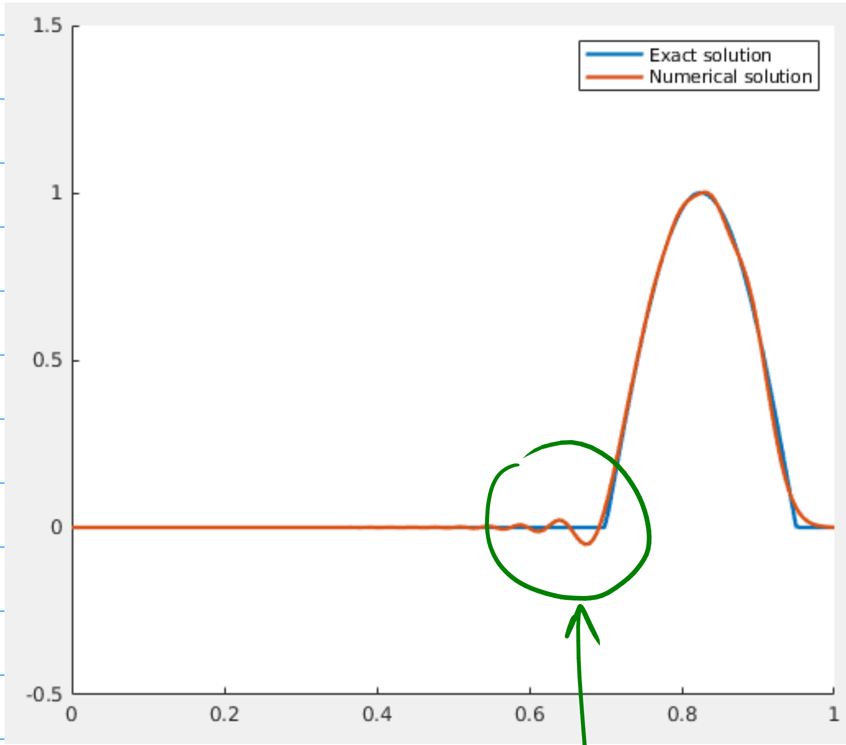
LF ... strong numerical diffusion



upwind



explicit central difference scheme (always unstable)

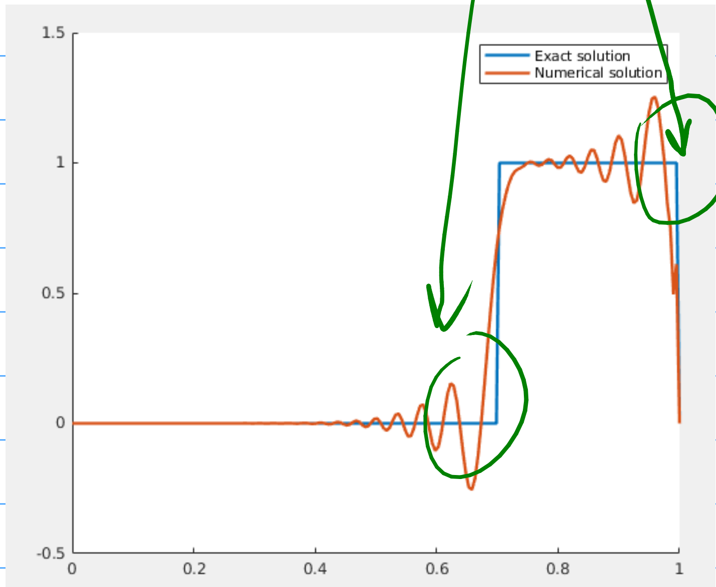


LW

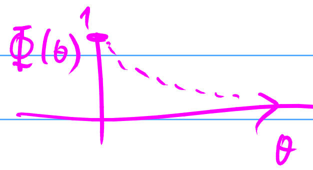
OSCILLATIONS NEAR DISCONTINUITIES

- the modified equation (see LF) contains the DISPERSION term $\partial_{xxx} u$

  ... the "source" of oscillations



SOLUTION : FOR HIGHER-ORDER SCHEMES



SLOPE LIMITER

$$\underbrace{L_h u_h^{\Delta t}}_{\text{F. difference operator in spatial coordinates}} = \underbrace{\phi\left(\left|\overleftrightarrow{\delta}_x u_h^{\Delta t}\right|\right)}_{\approx 1 \text{ for "small" arguments and } \to 0 \text{ when } \overleftrightarrow{\delta}_x u_h^{\Delta t} \to +\infty} \underbrace{L_h^{(H)} u_h^{\Delta t}}_{\text{FD (space) operator with a high order of approx.}} + \underbrace{\left(1-\phi\left(\left|\overleftrightarrow{\delta}_x u_h^{\Delta t}\right|\right)\right)}_{\text{opačné chování}} \underbrace{L_h^{(L)} u_h^{\Delta t}}_{\text{FD op. with a low (1st) order of approximation}}$$

NOTE: LW scheme for the nonlinear eq. $\partial_t u + \underbrace{\partial_x f(u)}_{f'(u)\,\partial_x u} = 0$

denote $f_k^n := f(u_k^n)$

$$\Rightarrow \quad u_k^{n+1} = u_k^n - \frac{a\Delta t}{2\Delta x}\left(f_{k+1}^n - f_{k-1}^n\right) + \frac{a^2\Delta t^2}{2\Delta x^2}\left(f_{k+1}^n - 2f_k^n + f_{k-1}^n\right)$$

PREDICTOR – CORRECTOR (2-step) form of LW schemes

Richtmyer's variant

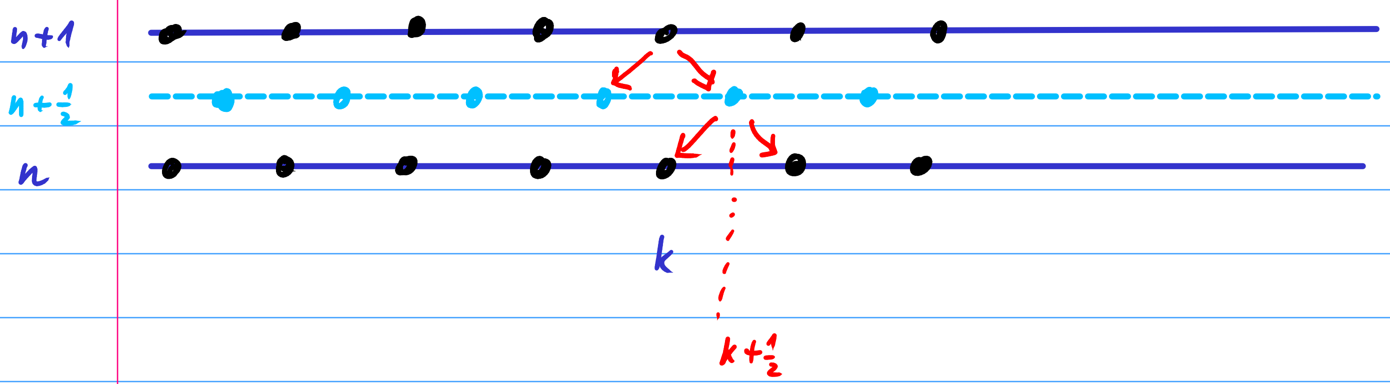
for a nonlinear transport eq.

1) Predictor ... LF scheme for time step $\frac{\Delta t}{2}$ & spatial step $\frac{\Delta x}{2}$

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

2) Corrector ... central scheme

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



McCormack's variant

1) Predictor ... Euler's explicit scheme with forward spatial difference

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

2) Corrector ... backward spatial difference

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

NOTE : FDM (Lax-Friedrichs) in 2D for Euler equations

$$\boxed{\partial_t \vec{W} + \partial_1 \vec{F} + \partial_2 \vec{G} = \vec{0}}$$

vector of unknowns (conserved quantities $\begin{pmatrix} \rho \\ \rho v_1 \\ \rho v_2 \end{pmatrix}$)

$$\vec{W}^{n+1}_{k,l} = \frac{1}{4}\left(\vec{W}^n_{k-1,l} + \vec{W}^n_{k+1,l} + \vec{W}^n_{k,l-1} + \vec{W}^n_{k,l+1}\right)$$

$$- \frac{\Delta t}{2\Delta x_1}\left(\vec{F}^n_{k+1,l} - \vec{F}^n_{k-1,l}\right) - \frac{\Delta t}{2\Delta x_2}\left(\vec{G}^n_{k,l+1} - \vec{G}^n_{k,l-1}\right)$$

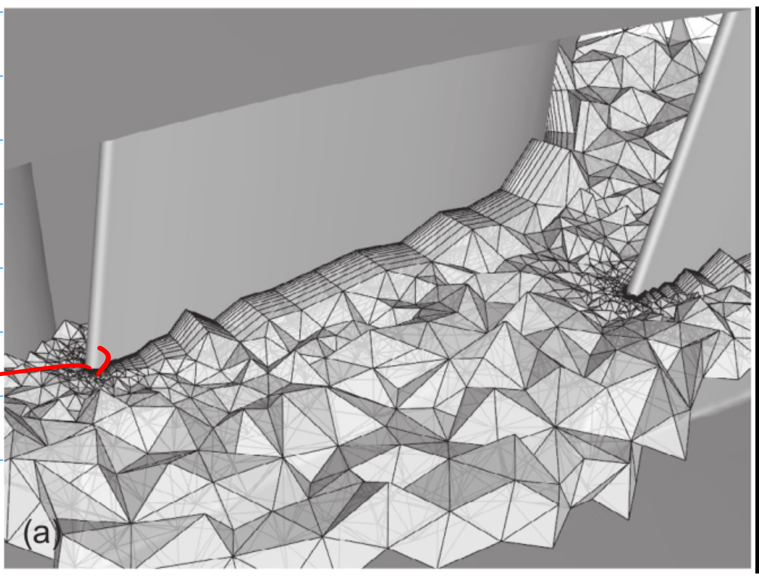
UNSTRUCTURED MESHES FOR THE FINITE VOLUME METHOD

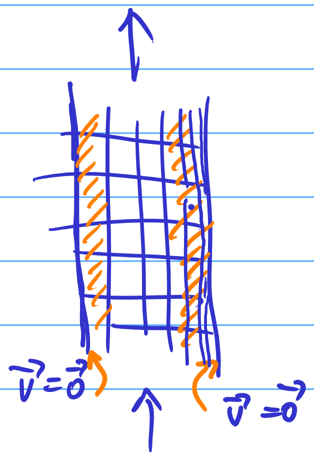
computational domain divided into polygonal (2D) or polyhedral (3D) cells

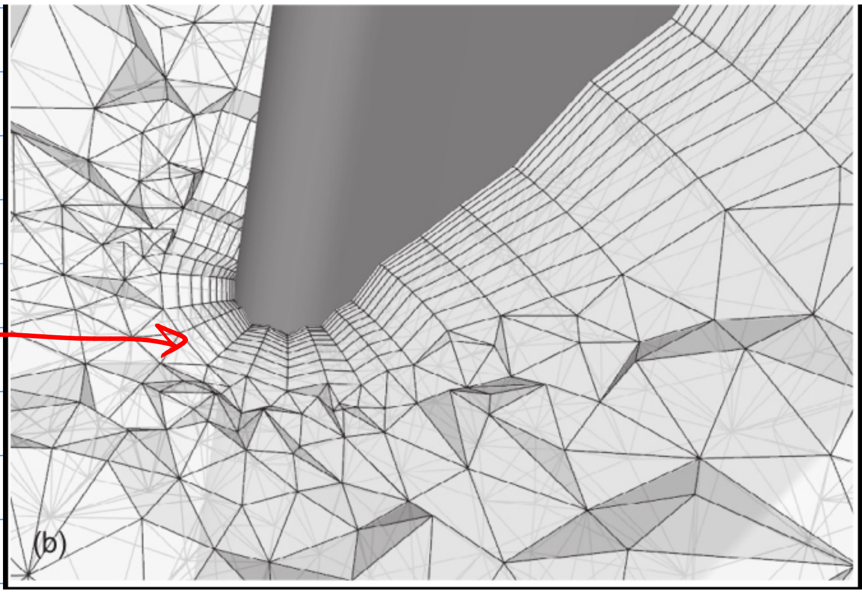
FVM - finite volume method ... approximates the integrals of unknown quantities over mesh elements (cells)

Pr

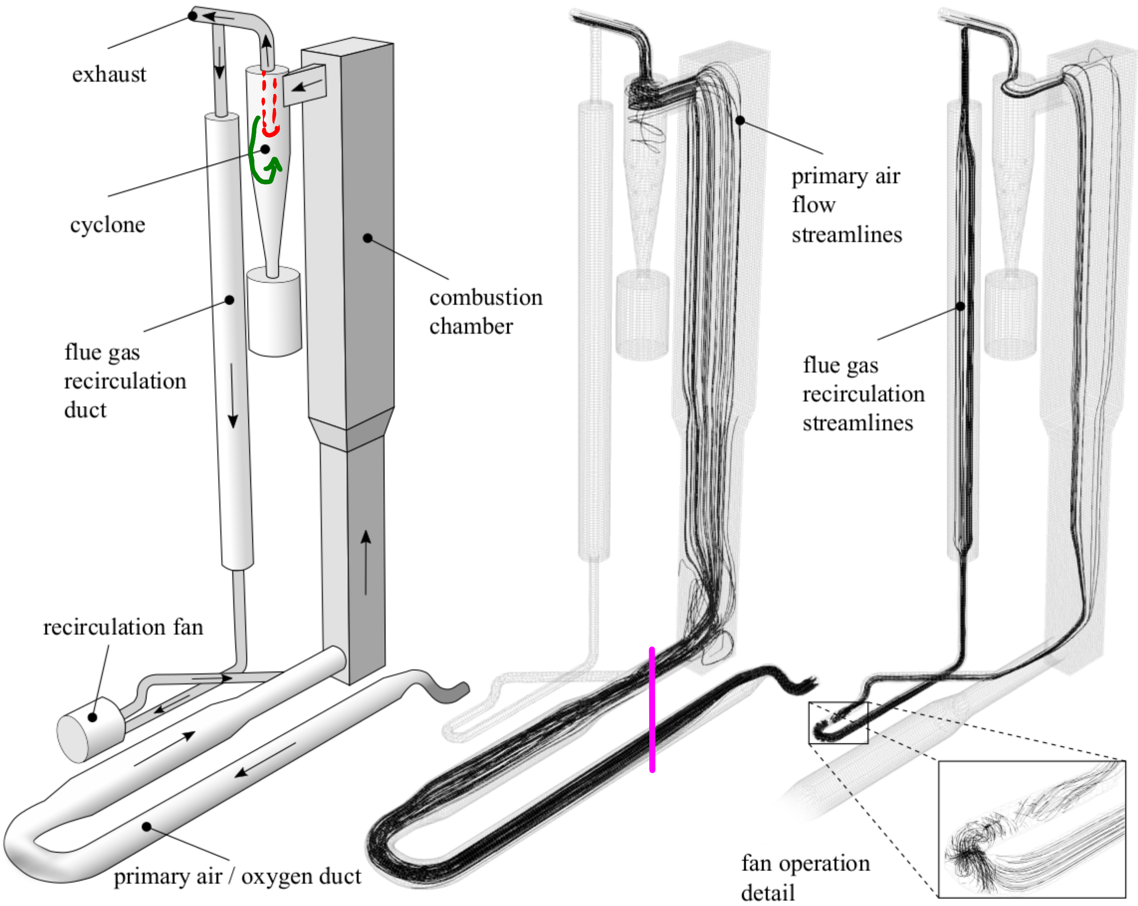
mesh refinement at the boundary



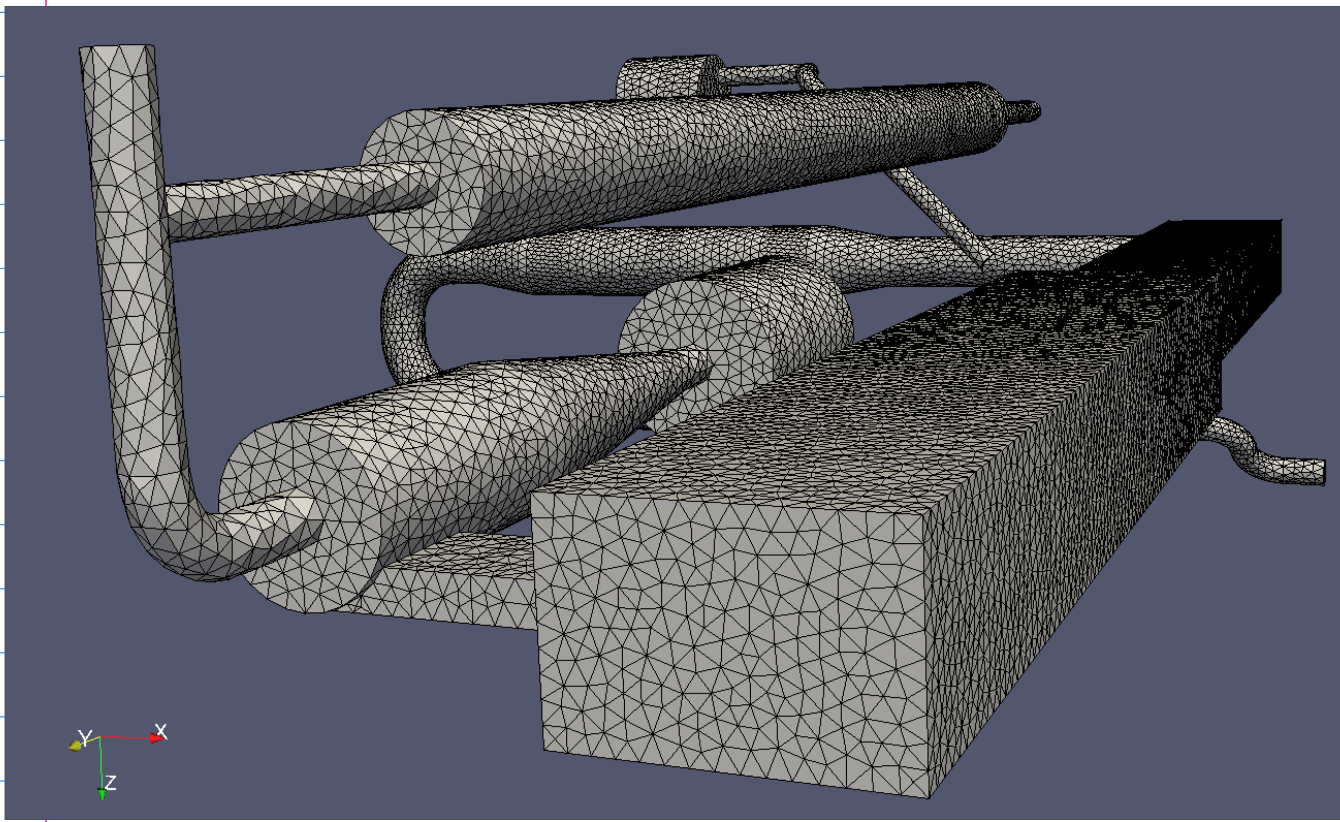




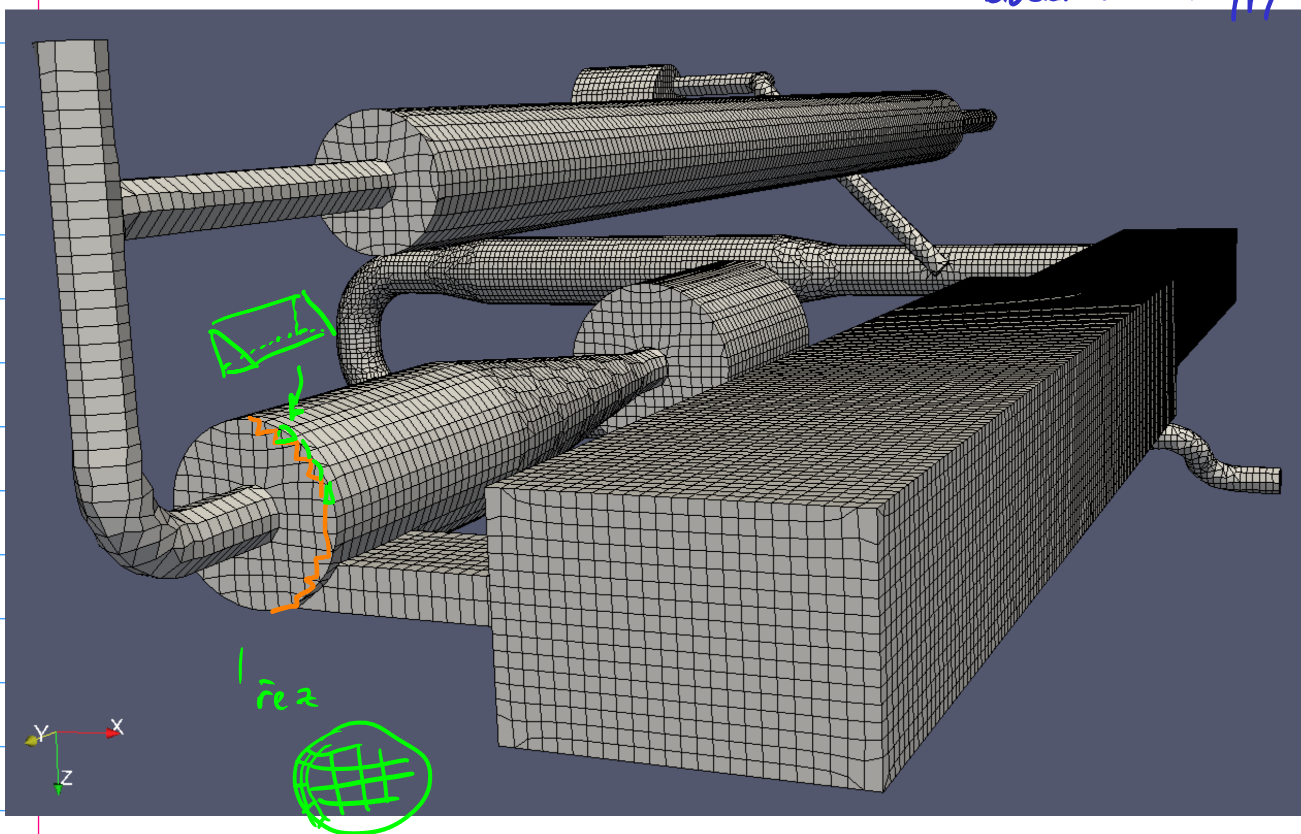
Example : a fluidized bed boiler

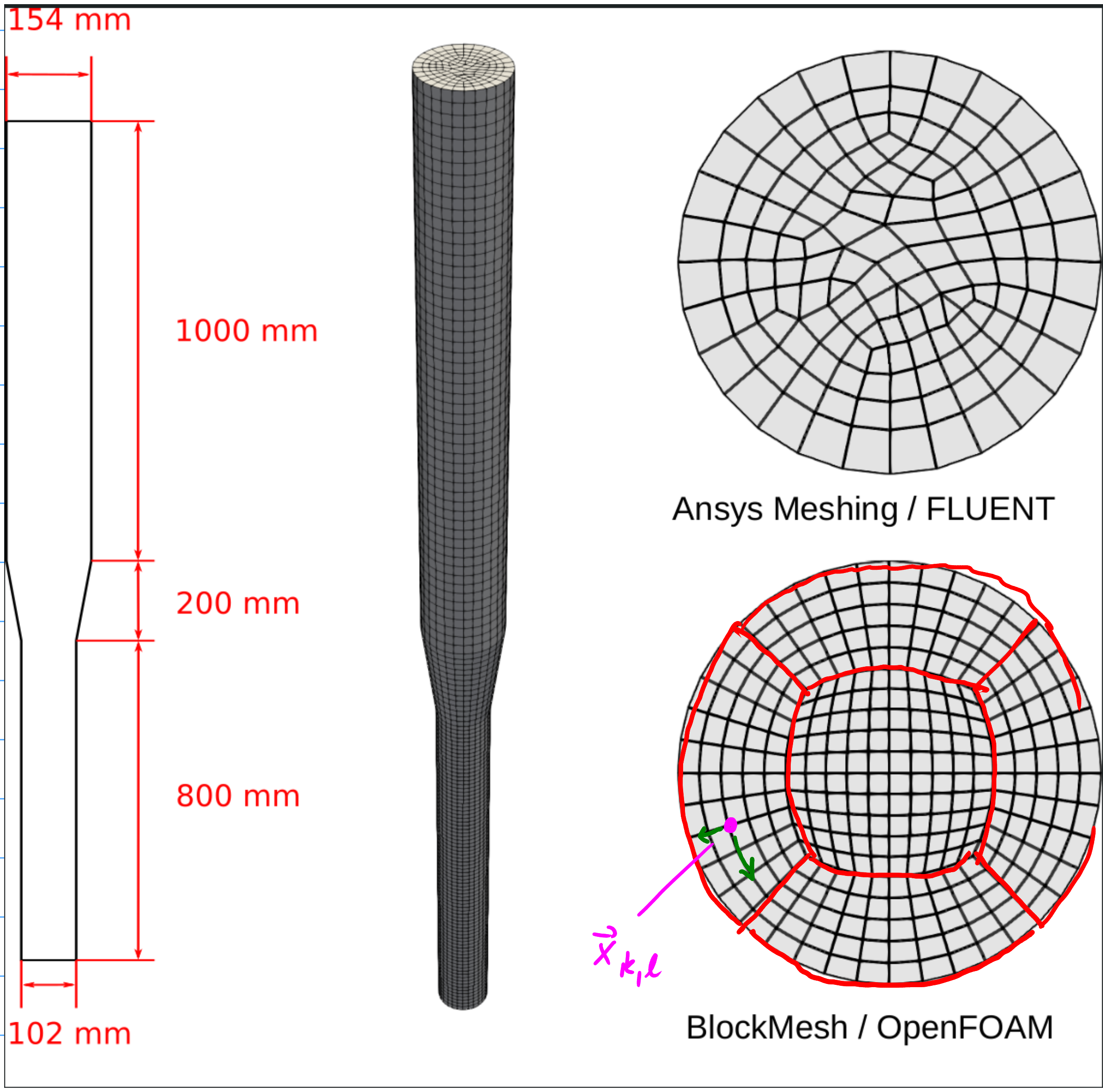


tetrahedral mesh (gmsh)

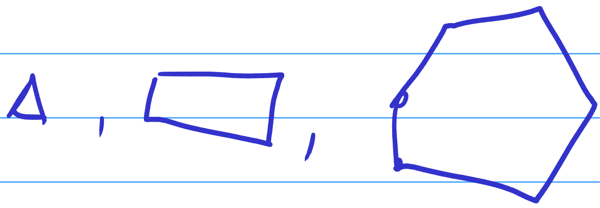


hexahedral mesh with refinement close to the walls (OpenFOAM BlockMesh + snappyHexMesh)

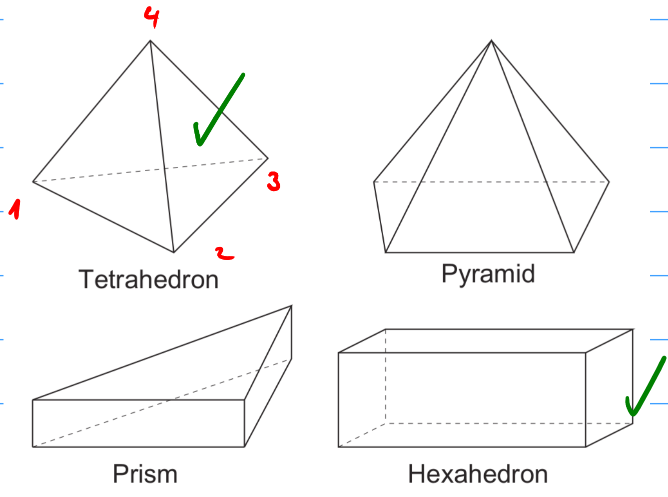




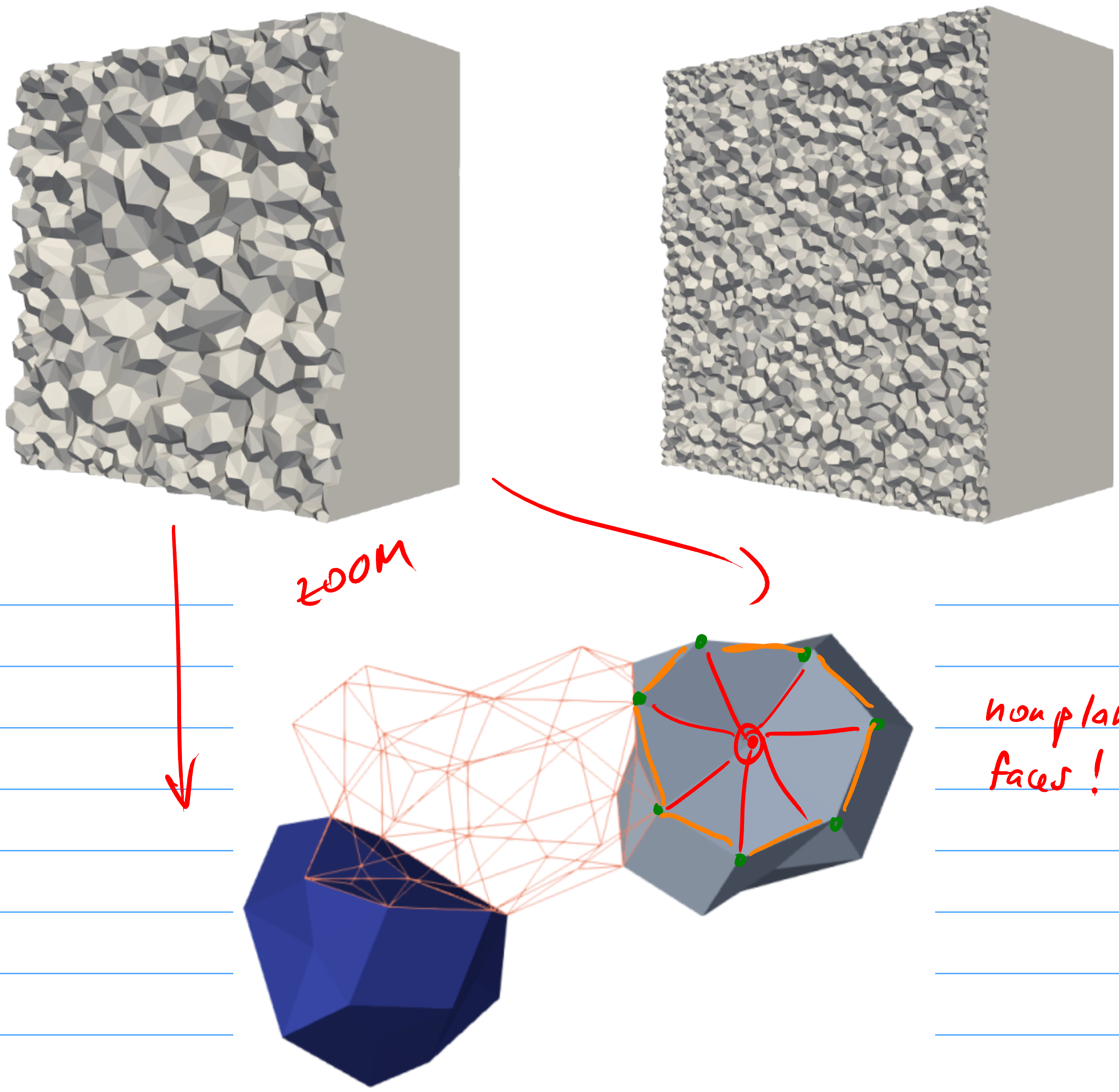
Cell types: in 2D …



in 3D



a mesh made of general polyhedra



non planar faces!

GEOMETRY & TOPOLOGY OF UNSTRUCTURED MESHES

Eymard, Gallouët

- $\mathcal{T}$ ... the mesh .. set of finite volumes (cells)

Note: $K = K^{\circ}$

- $K \in \mathcal{T}$ K ... cell $K \subset \mathbb{R}^r$ $r \in \{2,3\}$ $\overline{\Omega} = \bigcup_{K\in\mathcal{T}} \overline{K}$

- $\partial K = \bigcup_{\sigma \in \mathcal{E}_K} \sigma$ σ ... faces in 3D / edges in 2D

  $\mathcal{E}_K$ ... the set of faces forming the surface of K

\mathcal{E}

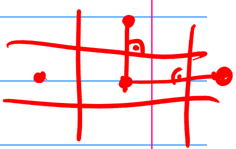
- $\mathcal{E} \ldots \bigcup_{K \in \mathcal{T}} \mathcal{E}_K$ ... set of all faces in the mesh

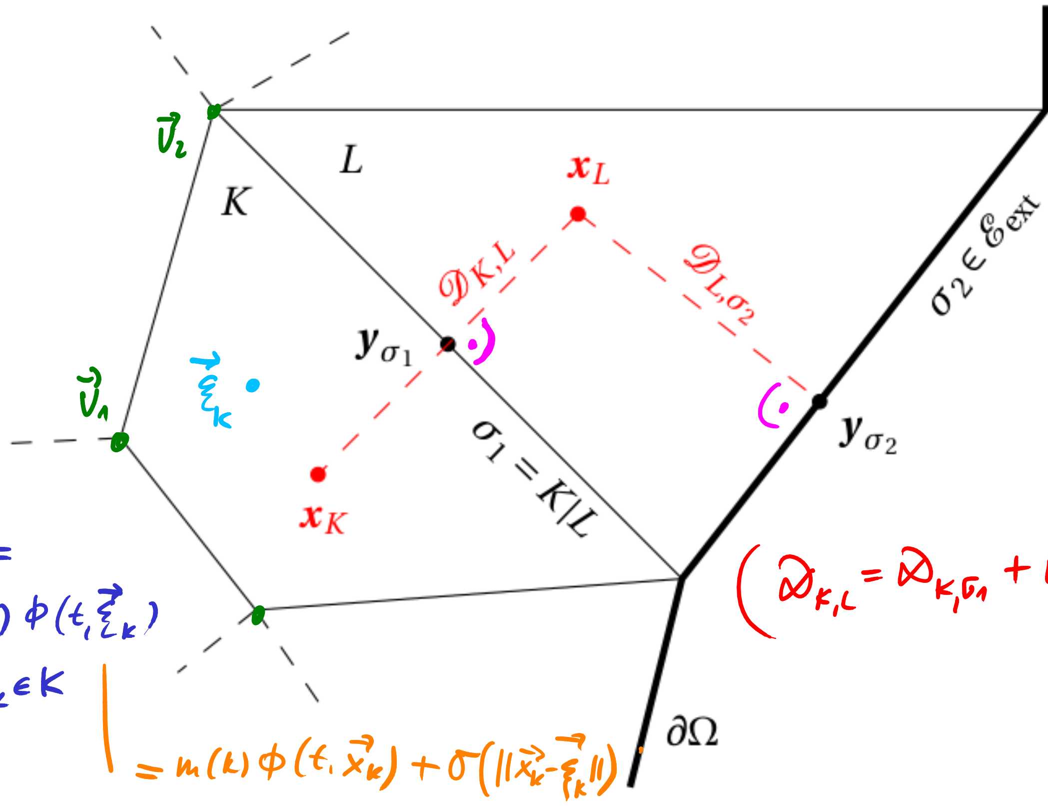
- $\mathcal{E} = \mathcal{E}_{int} \uplus \mathcal{E}_{ext}$ where $\bigcup_{\sigma \in \mathcal{E}_{ext}} \sigma = \partial\Omega$

set of interior faces   set of boundary faces

$$\sigma_1 = K|L = \partial K \cap \partial L \in \mathcal{E}_K \cap \mathcal{E}_L$$

2D example





$$\left(\mathcal{D}_{K,L} = \mathcal{D}_{K,\sigma_1} + \mathcal{D}_{L,\sigma_1} \right)$$

MEAN VALUE THEOREM:

$$\int_K \phi(t,\vec{x})\,d\vec{x} = m(K)\,\phi(t,\vec{\xi}_K)$$

where $\vec{\xi}_K \in K$

$$= m(K)\,\phi(t,\vec{x}_K) + \mathcal{O}(\|\vec{x}_K - \vec{\xi}_K\|)$$

- "cell-centered" scheme ... there is a significant point $\vec{x}_K \in K$ (a centroid) where the values of the unknown functions are approximated

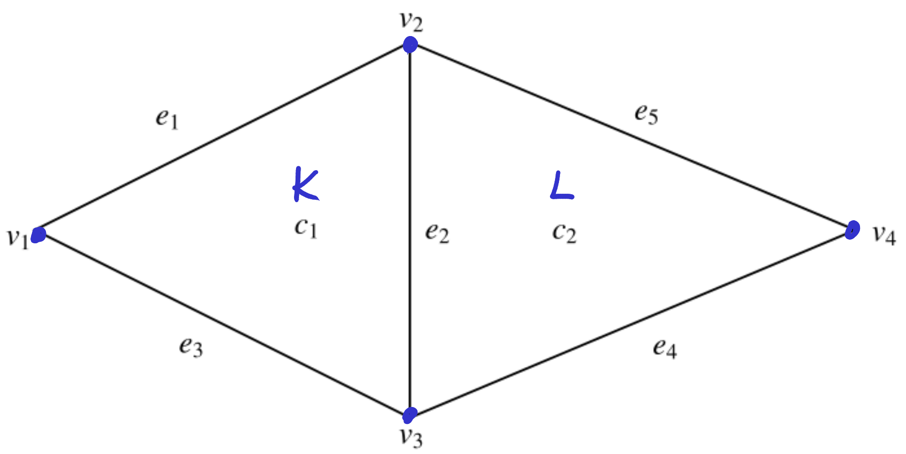
- "cell-vertex" scheme .. values are evaluated in the mesh vertices $\vec{v}_j$

- "staggered-grid" scheme ... combines both approaches

- $d_{K,L}$ .. the distance between $\vec{x}_K$ & $\vec{x}_L$ for $K|L \in \mathcal{E}_{int}$
- $D_{K,\sigma}$ .. the distance from $\vec{x}_K$ to $\vec{y}_{K,\sigma}$ ... the projection of $\vec{x}_K$ onto the boundary edge $\sigma \in \mathcal{E}_{ext}$
- $\vec{x}_K \vec{x}_L \perp \overbrace{(K|L)}^{\sigma}$ $\Rightarrow$ <u>admissible</u> mesh (admissibility / orthogonality criterion)
- $P = \{ \vec{x}_K \mid K \in \mathcal{T} \}$
- the set of functions $\mathcal{H}_{\mathcal{T}} = \{ w : P \to \mathbb{R} \}$ is referred to as <u>the set of mesh functions</u>

<u>TOPOLOGICAL INFORMATION ABOUT THE MESH – GRAPH APPROACH</u>

2D



$\{ \underbrace{v_1, v_2, v_3, v_4}_{\in \mathcal{T}^0}, \underbrace{e_1, \dots, e_5}_{\in \mathcal{T}^1}, \underbrace{c_1, c_2}_{\in \mathcal{T}^2} \} = \mathcal{T}^*$ ... all mesh "entities"

$\mathcal{T}^* = \mathcal{T}^0 \cup \mathcal{T}^1 \cup \mathcal{T}^2$

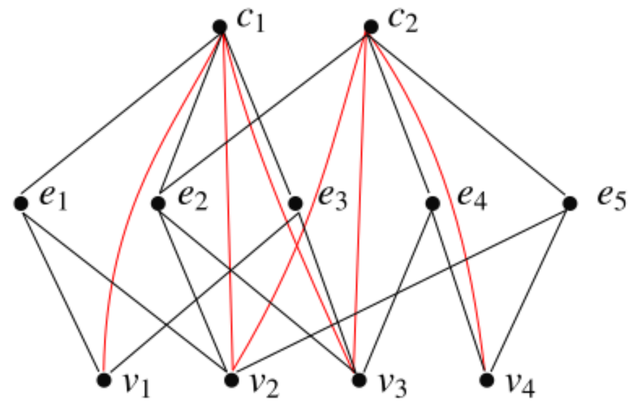
entity dimension

$e, f \in \mathcal{T}^*$ are "connected" $\iff (e \subset \partial f \vee f \subset \partial e)$

denote $E = \{ (e,f) \mid e, f \text{ are connected}, e, f \in \mathcal{T}^* \}$

... the set of edges of the graph (V, E) where $V = \mathcal{T}^*$ ... in the sense of graph theory

connection of entities



$$\mathbb{A} = (a_{ij})$$

$$a_{ij} = \begin{cases} 1 & \iff (v_i, v_j) \in E \quad (v_i, v_j \in \mathcal{T}^*) \\ 0 & \text{otherwise} \end{cases}$$

$\mathbb{A}$ can be divided into blocks according to entity dimensions:

$$\mathbb{A}^{d_1, d_2} = \left(a_{ij}^{d_1, d_2} \right)$$

$$a_{ij}^{d_1, d_2} = \begin{cases} 1 & \iff (v_i, v_j) \in E \\ 0 & \text{otherwise} \end{cases} \quad \text{where } v_i \in \mathcal{T}^{d_1}, v_j \in \mathcal{T}^{d_2}$$

$\mathbb{A}_{G_{\mathcal{T}^*}} =$ $\mathbb{A}$

	v_1	v_2	v_3	v_4	e_1	e_2	e_3	e_4	e_5	c_1	c_2
v_1	0	0	0	0	1	0	1	0	1	1	0
v_2	0	0	0	0	1	1	0	0	0	1	1
v_3	0	0	0	0	0	1	1	1	0	1	1
v_4	0	0	0	0	0	0	0	1	1	0	1
e_1	1	1	0	0	0	0	0	0	0	1	0
e_2	0	1	1	0	0	0	0	0	0	1	0
e_3	1	0	1	0	0	0	0	0	0	1	1
e_4	0	0	1	1	0	0	0	0	0	0	1
e_5	1	0	0	1	0	0	0	0	0	0	1
c_1	1	1	1	0	1	1	1	0	0	0	0
c_2	0	1	1	1	0	0	1	1	1	0	0

$\mathbb{A}_{G_{\mathcal{T}^*}} =$

	$\mathcal{T}^0$	$\mathcal{T}^1$	$\mathcal{T}^2$
$\mathcal{T}^0$	$\mathbb{A}^{0,0}_{G_{\mathcal{T}^*}}$	$\mathbb{A}^{0,1}_{G_{\mathcal{T}^*}}$	$\mathbb{A}^{0,2}_{G_{\mathcal{T}^*}}$
$\mathcal{T}^1$	$\mathbb{A}^{1,0}_{G_{\mathcal{T}^*}}$	$\mathbb{A}^{1,1}_{G_{\mathcal{T}^*}}$	$\mathbb{A}^{1,2}_{G_{\mathcal{T}^*}}$
$\mathcal{T}^2$	$\mathbb{A}^{2,0}_{G_{\mathcal{T}^*}}$	$\mathbb{A}^{2,1}_{G_{\mathcal{T}^*}}$	$\mathbb{A}^{2,2}_{G_{\mathcal{T}^*}}$

"Reconstruction" of $\mathbb{A}$ by using $\mathbb{A}^{d_i,d_j}$:

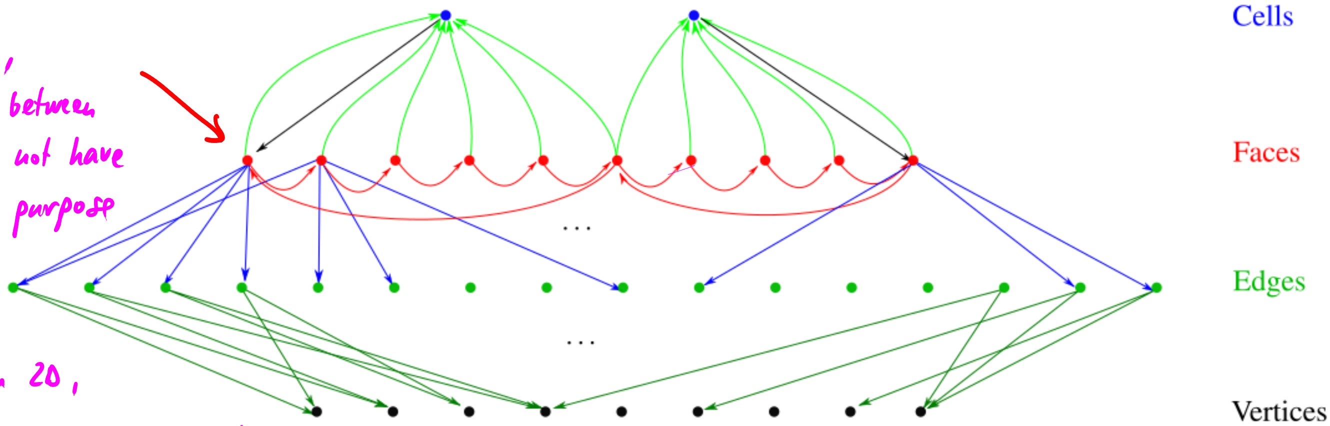
$d_1 < d_3 < d_2$

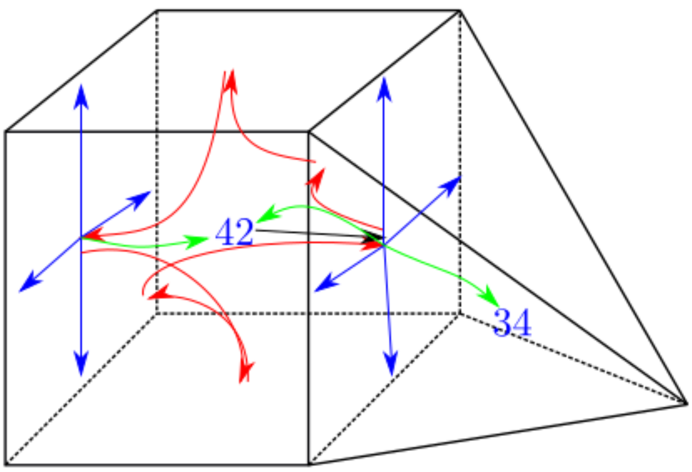
$$\left[\mathbb{A}^{d_1,d_2}_{G_{\mathcal{T}^*}}\right]_{ij} = \operatorname{connect}\left(\mathbb{A}^{d_1,d_3}_{G_{\mathcal{T}^*}}, \mathbb{A}^{d_3,d_2}_{G_{\mathcal{T}^*}}\right)$$

$$= \begin{cases} 1 & \text{if } \left(\exists k \in \left\{1,2,\ldots,N^{d_3}_{\mathcal{T}^*}\right\}\right)\left(\left[\mathbb{A}^{d_1,d_3}_{G_{\mathcal{T}^*}}\right]_{ik}\left[\mathbb{A}^{d_3,d_2}_{G_{\mathcal{T}^*}}\right]_{kj} = 1\right), \\ 0 & \text{else,} \end{cases}$$

TOPOLOGICAL INFORMATION IN 3D :

in 3D, the links between faces do not have the same purpose as links between edges in 2D, but they can be used to iterate over faces (in any order)

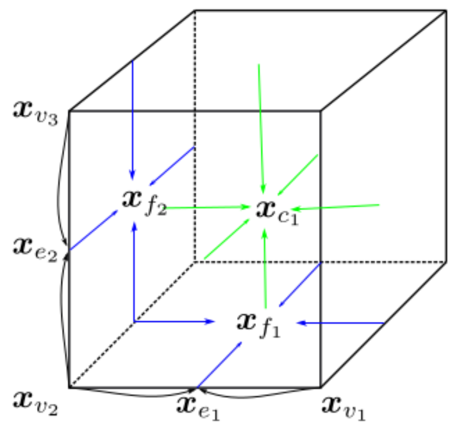




CALCULATION OF GEOMETRICAL PROPERTIES IN THE MESH

- $\vec{x}_K$ ... positions of the entity centroids

a) – hierarchically from dimension 0 up to dimension $r \in \{2,3\}$



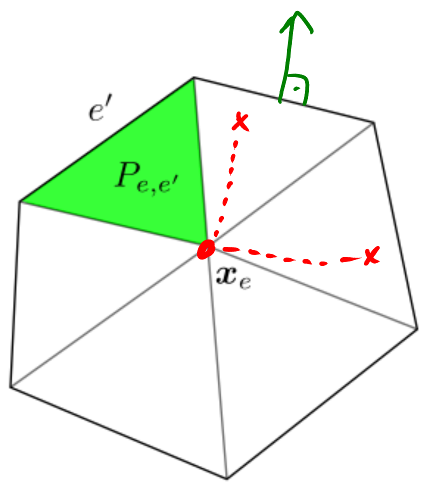
– OR –

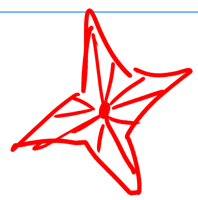
b) – centers of mass of all vertices connected to the respective entities (cells)

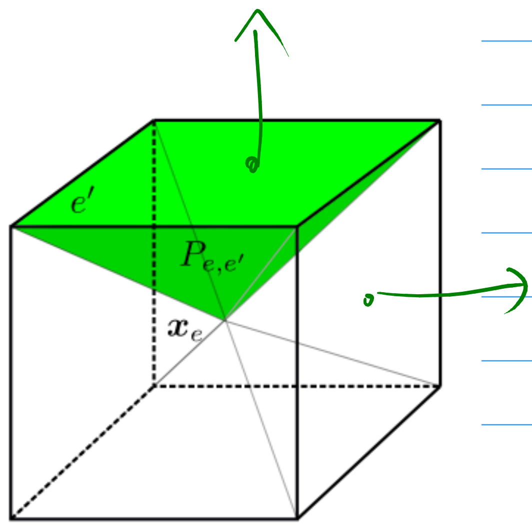
- neither of the approaches can guarantee mesh admissibility

- "size" (Hausdorff d-dimensional measure) of the entities:

– we assume the "star" property of all entities with respect to their centroids

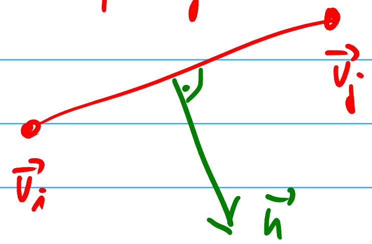


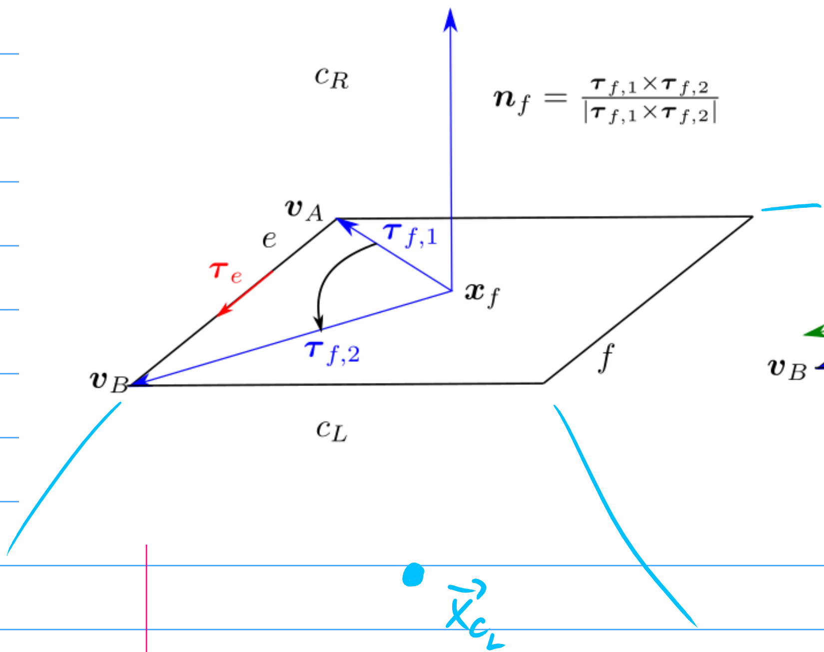


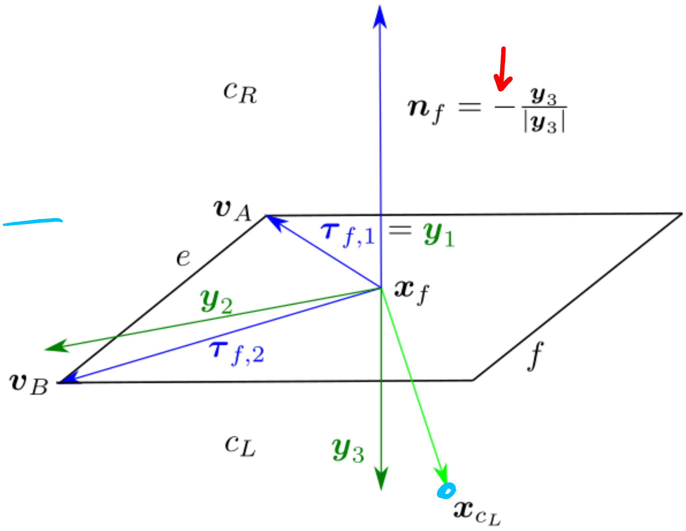


- calculation of <u>normals</u> to the faces in 3D, or edges in 2D, respectively

$\vec{v}_i - \vec{v}_j$



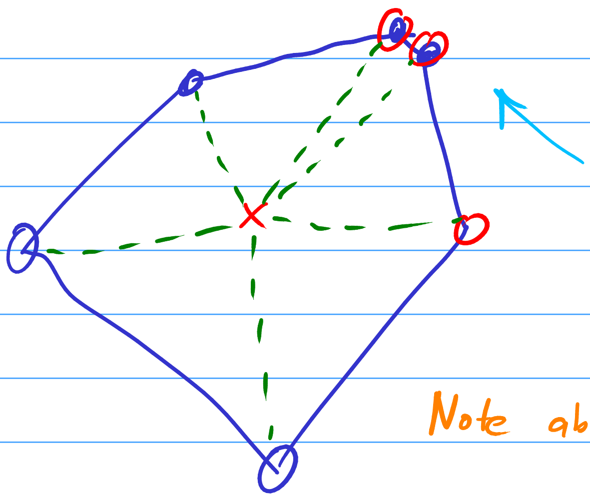




Gram-Schmidt OG process

... the orientation of $\vec{n}_f$ is unclear

$\Rightarrow$ the normal vector points outward from the cell C_L



Note about the robustness of the calculation...

Note about nonplanar faces below...

FINITE VOLUME METHOD for the NS EQUATIONS

$$\partial_t \vec{W} + \underbrace{\partial_1 \vec{F} + \partial_2 \vec{G}}_{\substack{\text{inviscid} \\ \text{(advective) physical fluxes}}} = \underbrace{\partial_1 \vec{R} + \partial_2 \vec{S}}_{\text{viscous fluxes}}$$

$\vec{R}, \vec{S}$ contain derivatives w.r.t. x_1, x_2

FVM: Integrate the NS equations over $K \in \mathcal{T}$

$$\frac{d}{dt} \int_K \vec{W} d\vec{x} + \underbrace{\int_K \partial_1 \vec{F} + \partial_2 \vec{G} \, d\vec{x}}_{\text{use the Green formula}} = \underbrace{\int_K \partial_1 \vec{R} + \partial_2 \vec{S} \, d\vec{x}}$$

$\frac{\partial \vec{W}}{\partial t}$

normal to ∂K pointing outward $\vec{n}_K = \begin{pmatrix} n_{1,K} \\ n_{2,K} \end{pmatrix}$

$$\frac{d}{dt} \int_K \vec{W} d\vec{x} + \int_{\partial K} \vec{F} n_{1,K} + \vec{G} n_{2,K} dS = \int_{\partial K} \vec{R} n_{1,K} + \vec{S} n_{2,K} dS$$

$$\frac{d}{dt} \int_K \vec{W} d\vec{x} + \sum_{\sigma \in \mathcal{E}_K} \int_\sigma \vec{F} n_{1,K,\sigma} + \vec{G} n_{2,K,\sigma} dS = \sum_{\sigma \in \mathcal{E}_K} \int_\sigma \vec{R} n_{1,K,\sigma} + \vec{S} n_{2,K,\sigma} dS$$

mind the orientation of the normal to σ

$\downarrow$ transition to <u>mesh functions</u>

physical fluxes $\quad \vec{F} n_{1,K,\sigma} \dashrightarrow \vec{F}_{K,\sigma} \ldots$ numerical fluxes

$$\vec{W} \xrightarrow[\text{in space}]{\text{discret.}} \vec{W}_K := \vec{W}_h(t, \vec{x}_K) \xrightarrow[\text{in time}]{\text{discretization}} \vec{W}_h^{\Delta t}(t^n, \vec{x}_K)$$

cell-centered scheme

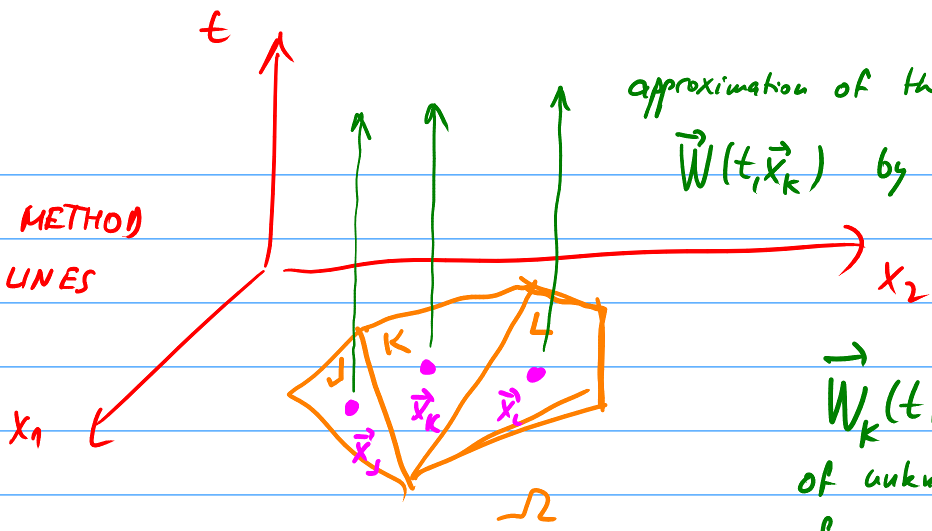
value at $\vec{x}_K$

$\vec{W}_h(t, \cdot)$ is a mesh function in space

$t^n = n \cdot \Delta t$

mesh function in space and time

NOTE: THE METHOD OF LINES



approximation of the evolution of $\vec{W}(t, \vec{x}_K)$ by $\vec{W}_K(t)$

$\vec{W}_K(t)$ is a vector of unknown functions of a single variable (t)

$\Rightarrow$ we have a system of ODE's

$\Rightarrow$ freedom in the choice of the time-integration method (explicit Euler / implicit Euler / Runge-Kutta methods etc.)

$$\frac{d}{dt}\int_K \vec{W}\,d\vec{x} + \sum_{\sigma\in\mathcal{E}_K}\int_\sigma \vec{F}\cdot n_{1,\sigma} + \vec{G}\,n_{2,\sigma}\,dS = \sum_{\sigma\in\mathcal{E}_K}\int_\sigma \vec{R}\,n_{1,\sigma} + \vec{S}\,n_{2,\sigma}\,dS$$

$$\frac{d}{dt}\underbrace{m(K)}_{\text{measure of } K\ldots}\vec{W}(t,\vec{\xi}_K) + \sum_{\sigma\in\mathcal{E}_K} m(\sigma)\left[\vec{F}(t,\vec{\xi}_\sigma)\,n_{1,\sigma} + \vec{G}(t,\vec{\xi}_\sigma)\,n_{2,\sigma}\right] =$$

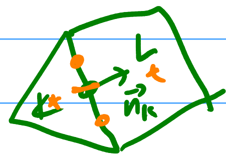
measure of K... surface area in 2D, volume in 3D

$m(\sigma)$ | the length of σ (in 3D, this would be the surface area of σ)

$\vec{\xi}_K \in K$ $\quad$ $\vec{\xi}_\sigma \in \sigma$

$$= \sum_{\sigma\in\mathcal{E}_K} m(\sigma)\left[\vec{R}(t,\vec{\xi}_\sigma)\,n_{1,\sigma} + \vec{S}(t,\vec{\xi}_\sigma)\,n_{2,\sigma}\right]$$

$\downarrow$ replacement by a mesh function



$$\frac{d}{dt}m(K)\,\vec{W}_K(t) + \sum_{\sigma\in\mathcal{E}_K} m(\sigma)\left(\vec{F}_{K,\sigma}(t) + \vec{G}_{K,\sigma}(t)\right) =$$

$$= \sum_{\sigma\in\mathcal{E}_K} m(\sigma)\left(\vec{R}_{K,\sigma}(t) + \vec{S}_{K,\sigma}(t)\right)$$

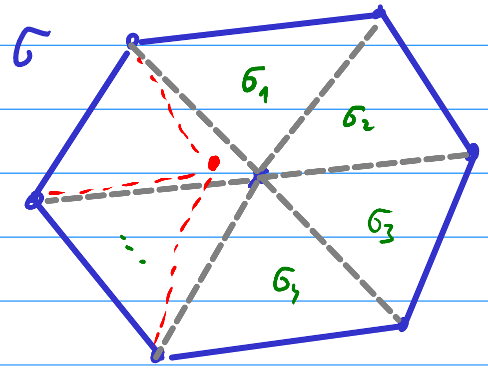
$\vec{n}_{K,\sigma} = -\vec{n}_{L,\sigma}$

$\Downarrow$

$\vec{F}_{K,\sigma} = -\vec{F}_{L,\sigma}$

$\Rightarrow$ NATURALLY CONSERVATIVE SCHEME

NONPLANAR FACES



.. triangulation of σ

$$\bar{\sigma} = \bigcup_i \bar{\sigma}_i$$

remember the replacement : $\vec{F}(t, \vec{y}_\sigma)\, n_{1,K,\sigma} \dashrightarrow \vec{F}_{K,\sigma}(t)$

denote $\underbrace{\vec{F}_{K,\sigma}}(t) = \underbrace{\vec{F}_\sigma(t)}\, n_{1,K,\sigma}$

accounts for orientation of the normal to σ w.r.t. K — does NOT account...

then, we look for an "average" normal $\vec{n}_{K,\sigma}$ such that (e.g. for $\vec{F}$)

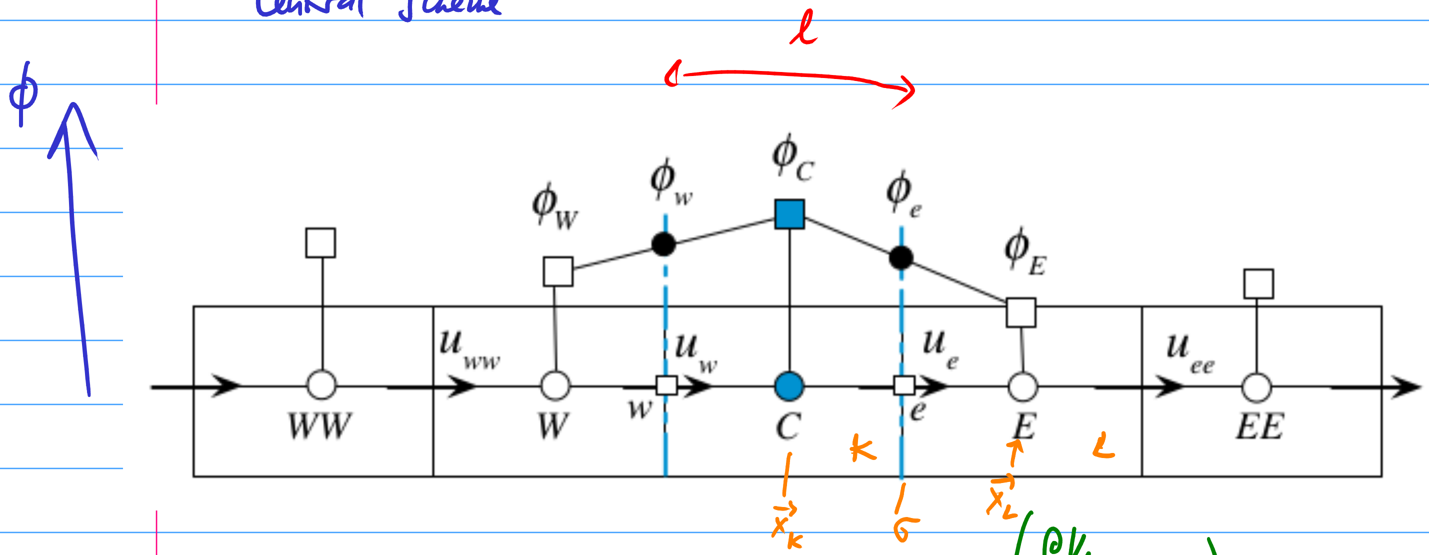
$$m(\sigma)\, \vec{F}_K(t)\, n_{1,K,\sigma} \overset{!}{=} \sum_i m(\sigma_i)\, n_{1,K,\sigma_i}\, \vec{F}_K(t)$$

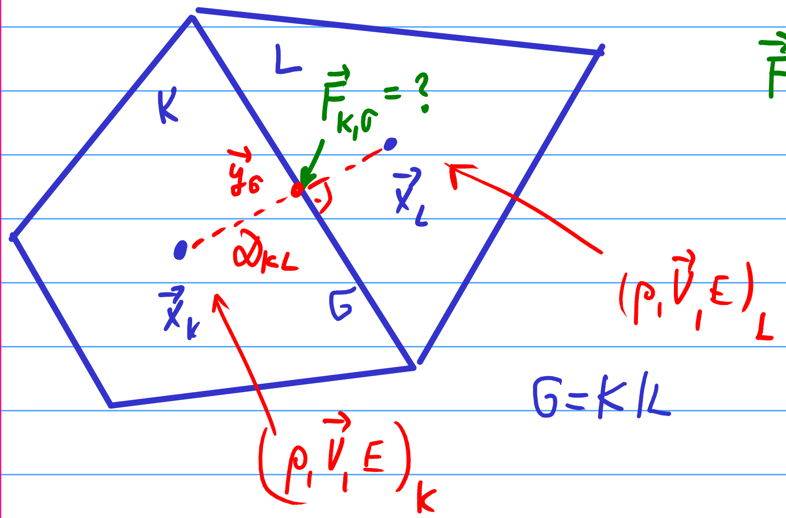
$$\Rightarrow \quad n_{1,K,\sigma} = \frac{\sum_i m(\sigma_i)\, n_{1,K,\sigma_i}}{m(\sigma)}$$

$$\Rightarrow \quad \vec{n}_{K,\sigma} = \frac{\sum_i m(\sigma_i)\, \vec{n}_{K,\sigma_i}}{m(\sigma)}$$

APPROXIMATIONS OF ADVECTIVE (INVISCID) FLUXES:

Central scheme





$$\vec{F} = \begin{pmatrix} \rho V_1 \\ \rho V_1^2 + p \\ \rho V_1 V_2 \\ (\rho E + p) V_1 \end{pmatrix}$$

ϕ ... any scalar quantity

$\sigma = K|L$

we know ϕ_K, ϕ_L, i.e., the values at the points $\vec{x}_K$, $\vec{x}_L$ (...)

... and we want to know ϕ_σ

central scheme : lin interpolation of ϕ between $\vec{x}_K$, $\vec{x}_L$

$$\phi_\sigma = \phi_K + \frac{|\vec{y}_\sigma - \vec{x}_K|}{d_{KL}} (\phi_L - \phi_K)$$

NOTE: Péclet number
$$Pe_\ell = \frac{\ell |\vec{V}|}{D}$$

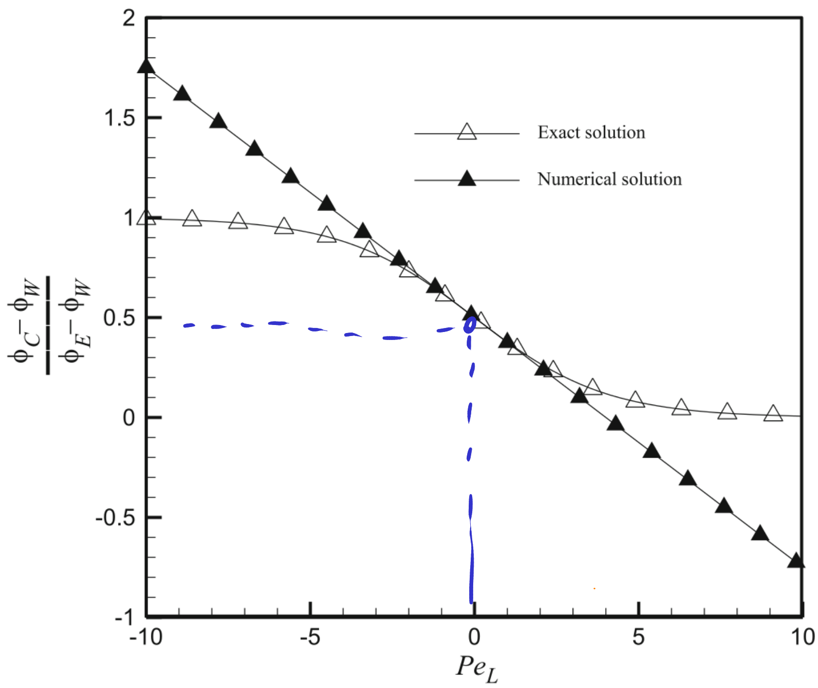
ℓ: characteristic distance

D: diffusivity of ϕ:

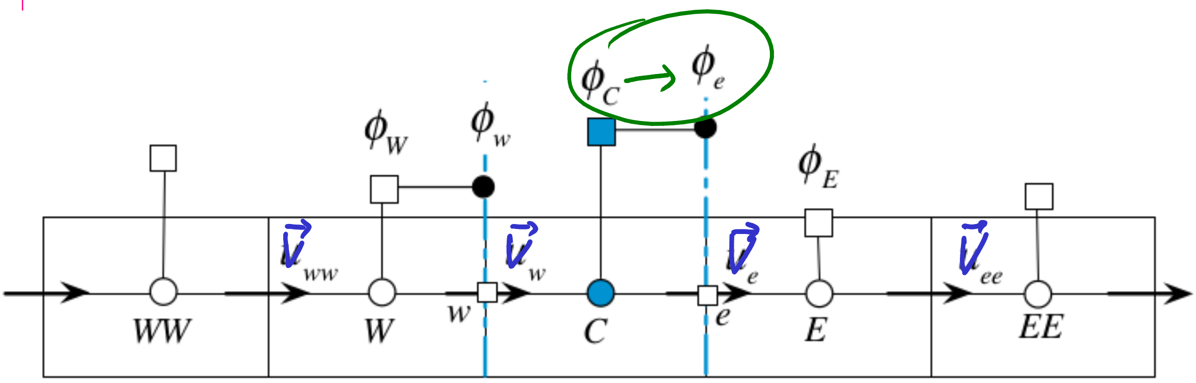
$$\frac{\partial \phi}{\partial t} = D \Delta \phi$$

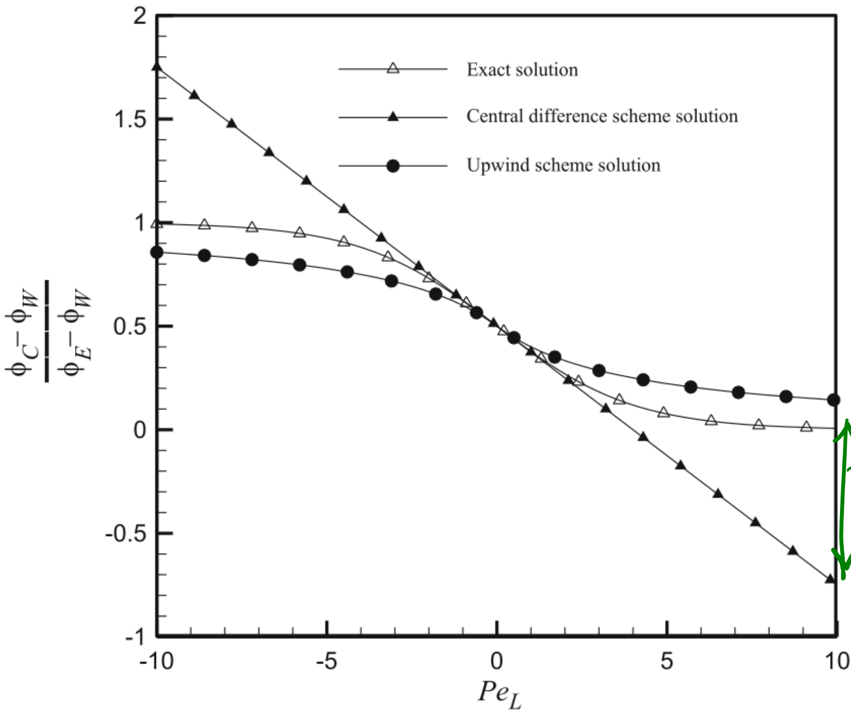
If (in 1D), ℓ is the cell size, or more accurately

$$\ell = |\vec{x}_E - \vec{x}_W|$$



1st order UPWIND scheme

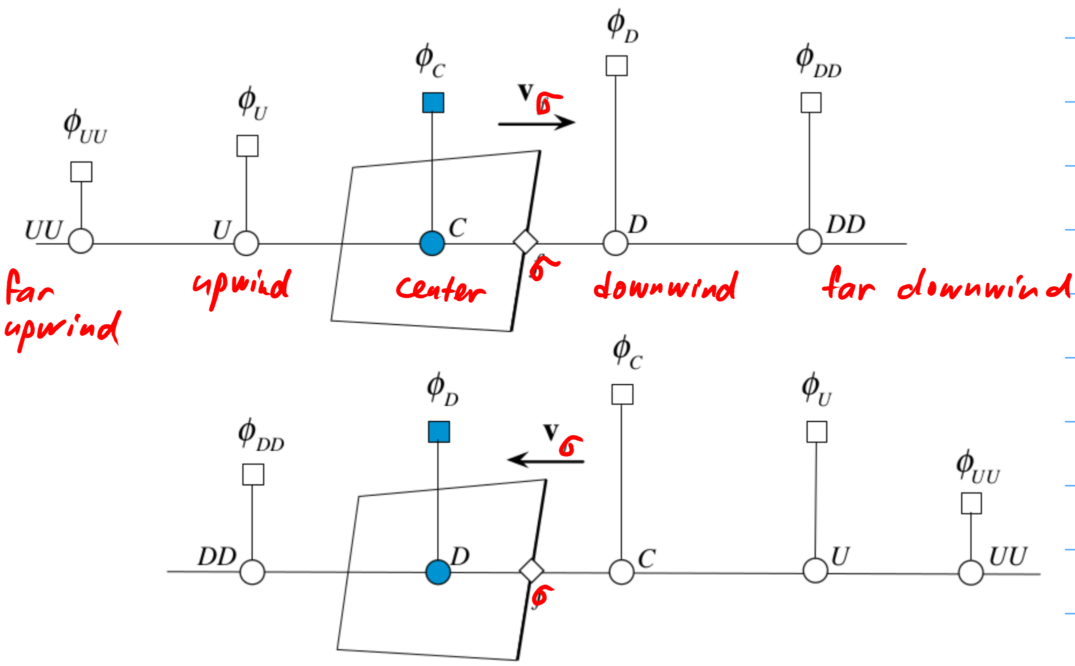




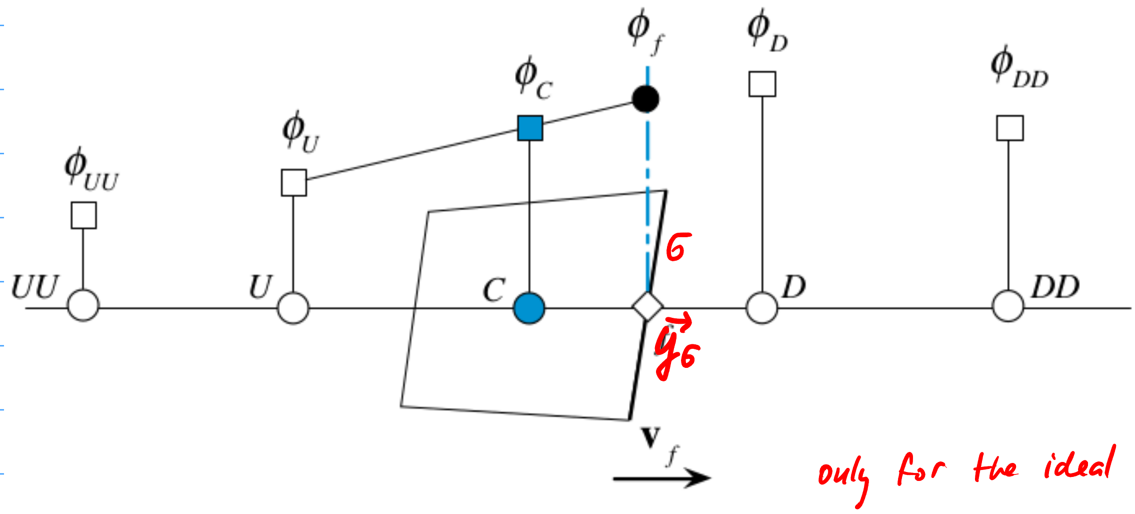
growing error of the central scheme

larger / smaller D, resp. μ

How to obtain higher (2nd) order UPWIND discretizations:

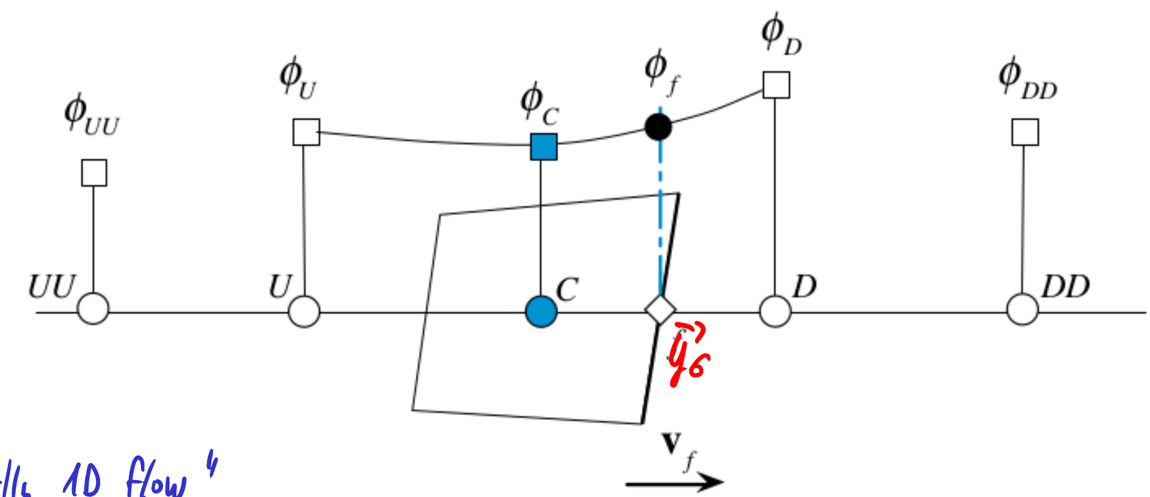


SOU scheme (Second Order Upwind)



only for the ideal case when (U, C, f), i.e. $(\vec{x}_u, \vec{x}_c, \vec{y}_\sigma)$ are on a line

QUICK scheme (Quadratic Upstream Interpolation for Convective Kinematics)

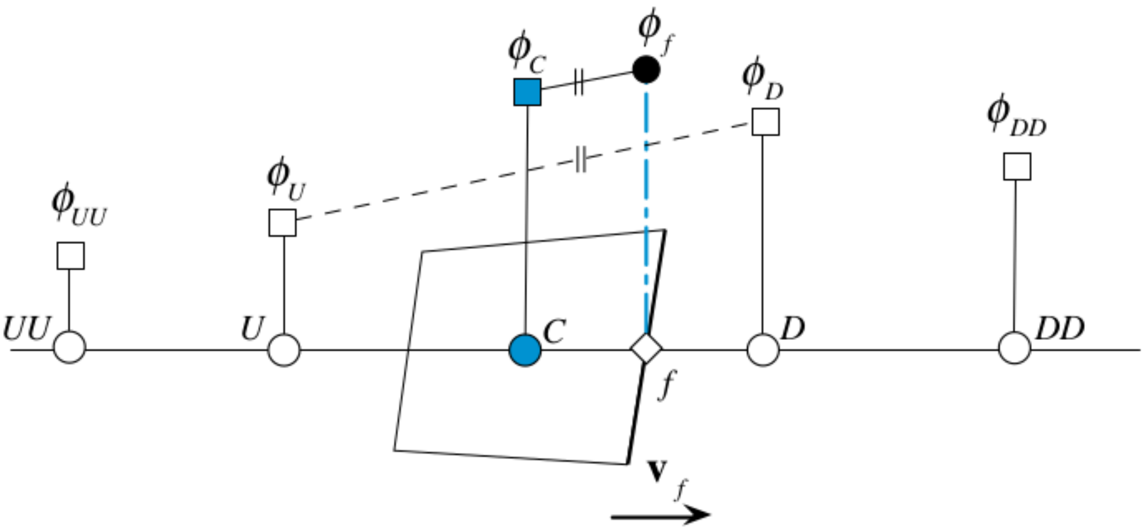


"locally 1D flow"

$$\phi = k_0 + k_1 x + k_2 x^2,$$

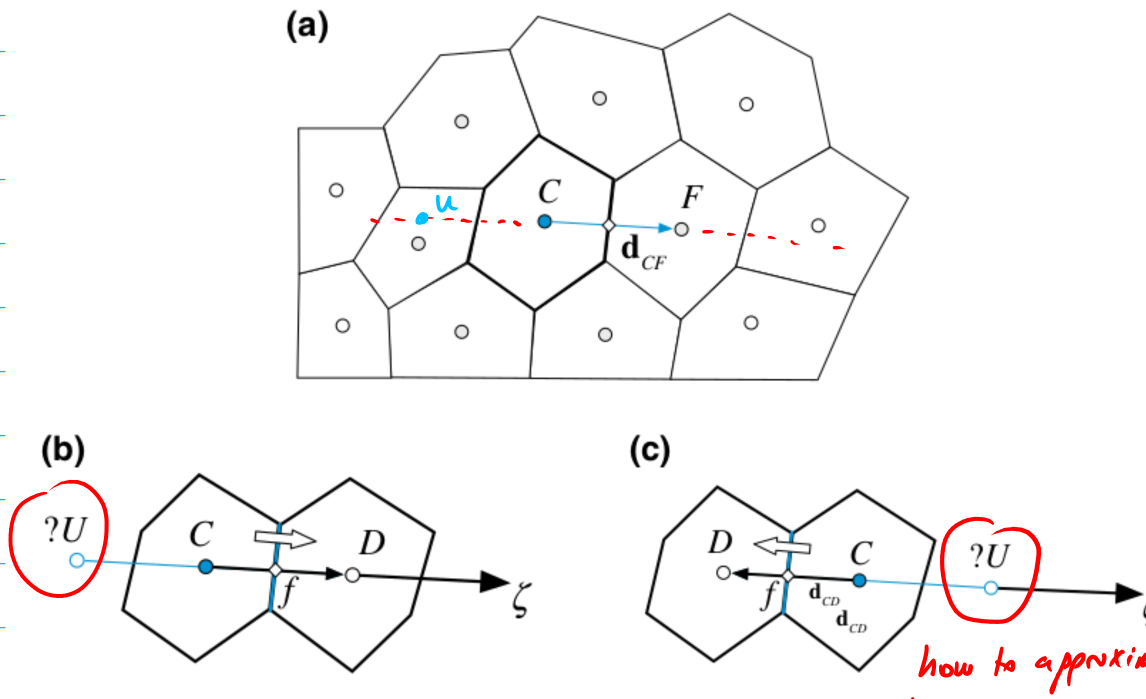
where $\phi(\vec{x}) = \begin{cases} \phi_u & \text{for } \vec{x} = \vec{x}_u \\ \phi_c & \text{for } \vec{x} = \vec{x}_c \\ \phi_D & \text{for } \vec{x} = \vec{x}_D \end{cases}$

FROMM scheme



$$\phi(x) = \phi_U + \frac{\phi_D - \phi_U}{x_D - x_U}(x - x_U)$$

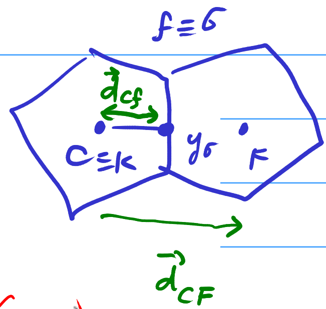
? how to do UPWIND on unstructured meshes in 2D, 3D



how to approximate ϕ in the virtual node U ?

solution : approximation of $\nabla\phi$ on the cell face $(\nabla\phi_f)$ or in the node $\vec{x}_C$ $(\nabla\phi_C)$

$\|\vec{d}_{CF}\| = \mathcal{D}_{CF}$



Upwind scheme : $\phi_f = \phi_C$

Central difference : $\phi_f = \phi_C + \nabla\phi_f \cdot \mathbf{d}_{Cf}$

SOU scheme : $\phi_f = \phi_C + (2\nabla\phi_C - \nabla\phi_f) \cdot \mathbf{d}_{Cf}$

gradient on a face

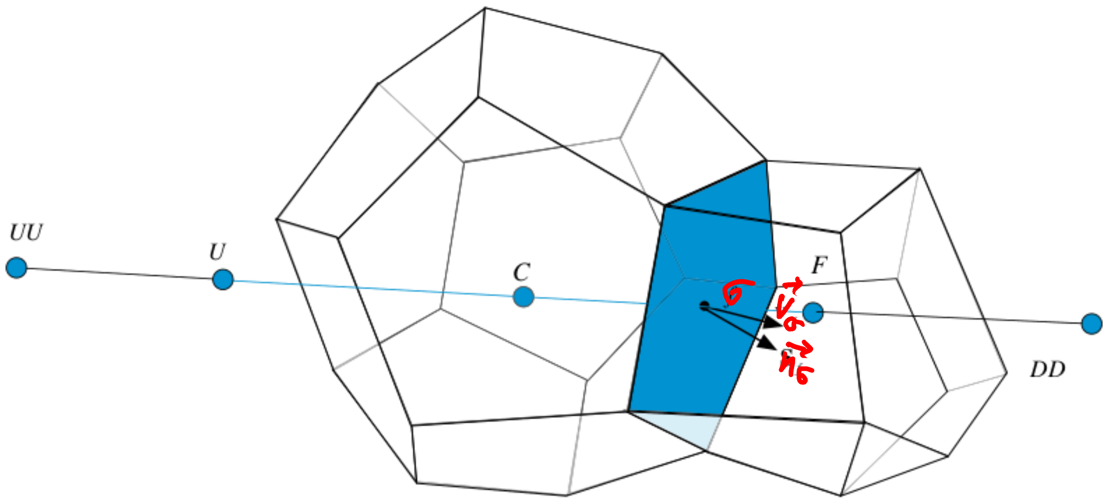
gradient in the cell center

FROMM scheme : $\phi_f = \phi_C + \nabla\phi_C \cdot \mathbf{d}_{Cf}$

QUICK scheme : $\phi_f = \phi_C + \frac{1}{2}(\nabla\phi_C + \nabla\phi_f) \cdot \mathbf{d}_{Cf}$

Downwind scheme : $\phi_f = \phi_C + 2\nabla\phi_f \cdot \mathbf{d}_{Cf}$

in 3D



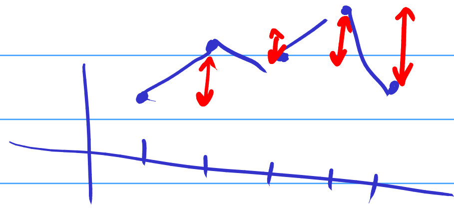
We will see later how to approximate $\nabla\phi_C$, $\nabla\phi_f$ $(f \equiv \sigma)$

SCHEME STABILITY (by the "TVD" property)

- for a finite difference scheme on a uniform grid:

$$TV(u^n) = \sum_k |u^n_{k+1} - u^n_k|$$

total variation



- "TVD" property (Total Variation Diminishing) je

$$\boxed{TV(u^{n+1}) \le TV(u^n) \quad \forall n}$$

$\Longleftrightarrow$ oscillations do NOT develop

- every TVD scheme is STABLE

- monotone scheme $\Rightarrow$ TVD scheme $\Rightarrow$ monotonicity preserving scheme

$$\boxed{\begin{array}{l} \text{if} \quad u^n_k \le v^n_k, \\ \text{then} \quad u^{n+1}_k \le v^{n+1}_k \end{array}}$$

for a linear equation: positive = monotone

$$\boxed{\begin{array}{l} \text{If } u^n \text{ is monotone in } k \\ \Rightarrow u^{n+1} \text{ is also monotone} \end{array}}$$

HARTEN'S THEOREM: A scheme in the form

$$u^{n+1}_k = u^n_k + C(u^n_{k+1} - u^n_k) - D(u^n_k - u^n_{k-1})$$

where $C, D \ge 0$ and $C + D \le 1$ is TVD. For a scalar equation, it is also convergent.

TVD on an unstructured mesh: $TV = \sum_{\substack{\sigma \in \mathcal{E} \\ \sigma = K|L}} |\phi_K - \phi_L|$

u.. velocity

$$\frac{\partial(\rho\phi)}{\partial t} = -\underbrace{\frac{\partial(\rho u\phi)}{\partial x}}_{RHS}$$

and

center, upwind, downwind

$$RHS = -a(\phi_C - \phi_U) + b(\phi_D - \phi_C)$$

$$a \geq 0, \; b \geq 0, \quad \text{and} \quad 0 \leq a+b \leq 1$$

$$\Downarrow$$

TVD

$$\frac{\partial(\rho V_1)}{\partial t} + \underbrace{\nabla\cdot(\rho V_1 \vec{V})}_{\text{flux over the boundary of } \mathcal{V}} = \dots$$

Motivation: approximation of the advective flux

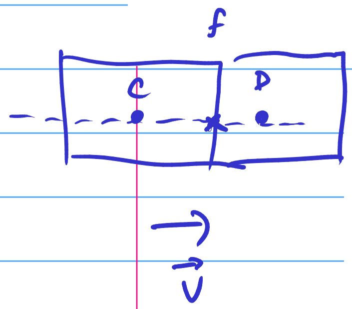
→ stable ⇐ upwind

→ more accurate (higher order) ⇐ central scheme

The central scheme artificially rewritten as:

$$\phi_f = \underbrace{\frac{1}{2}(\phi_D + \phi_C)}_{CD} = \underbrace{\phi_C}_{upwind} + \underbrace{\frac{1}{2}(\phi_D - \phi_C)}_{anti-diffusive\,flux}$$

$$\Downarrow$$



$$\phi_f = \phi_C + \frac{1}{2}\psi(r_f)(\phi_D - \phi_C)$$

flux (≈ slope) limiter

≈ 0 at discontinuities

≈ 1 if the solution is smooth

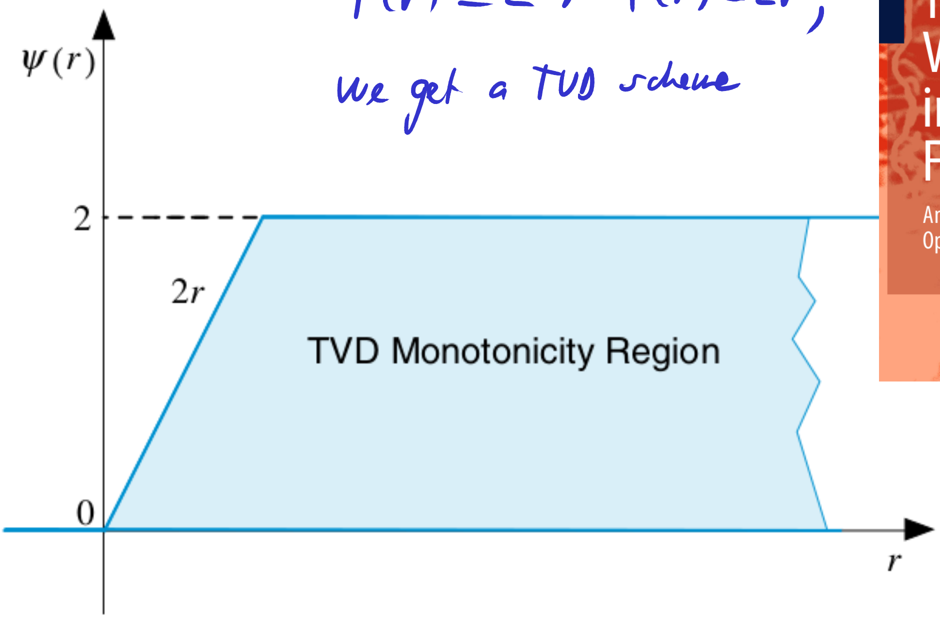
where $$r_f = \frac{\phi_C - \phi_U}{\phi_D - \phi_C}$$

ratio between the forward & backward differences a sufficient condition

one can prove that for

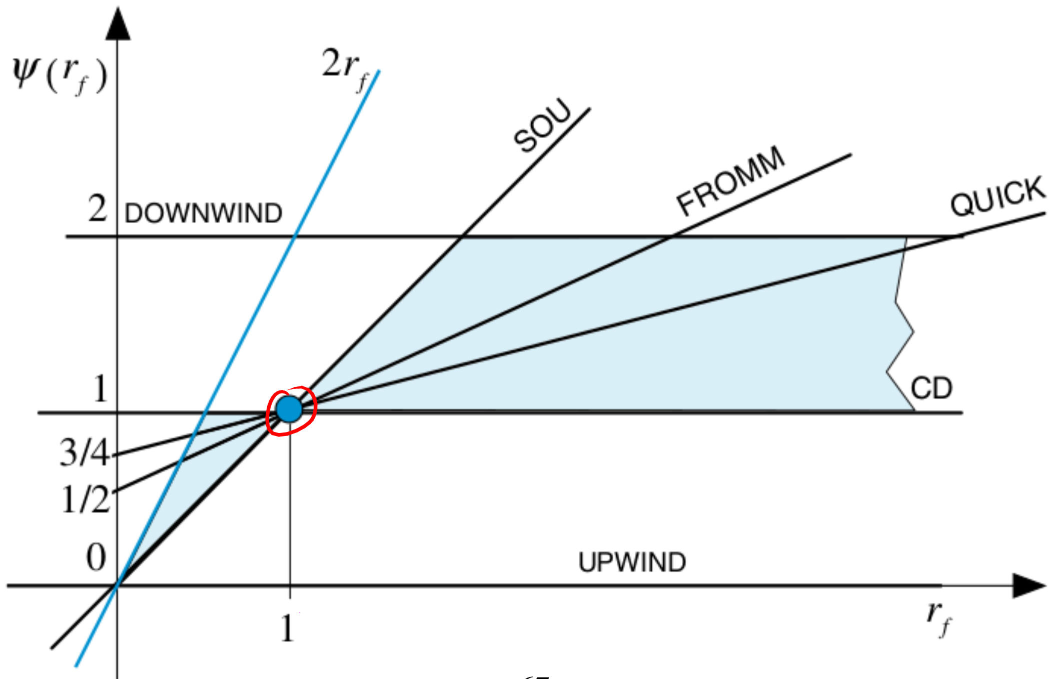
$\psi(r) \le 2 \wedge \psi(r) \le 2r$,

we get a TVD scheme



$$
\begin{cases}
Upwind & \psi(r_f) = 0 \\
Downwind & \psi(r_f) = 2 \\
FROMM & \psi(r_f) = \dfrac{1 + r_f}{2} \\
SOU & \psi(r_f) = r_f \\
CD & \psi(r_f) = 1 \\
QUICK & \psi(r_f) = \dfrac{3 + r_f}{4}
\end{cases}
$$

$\Rightarrow$

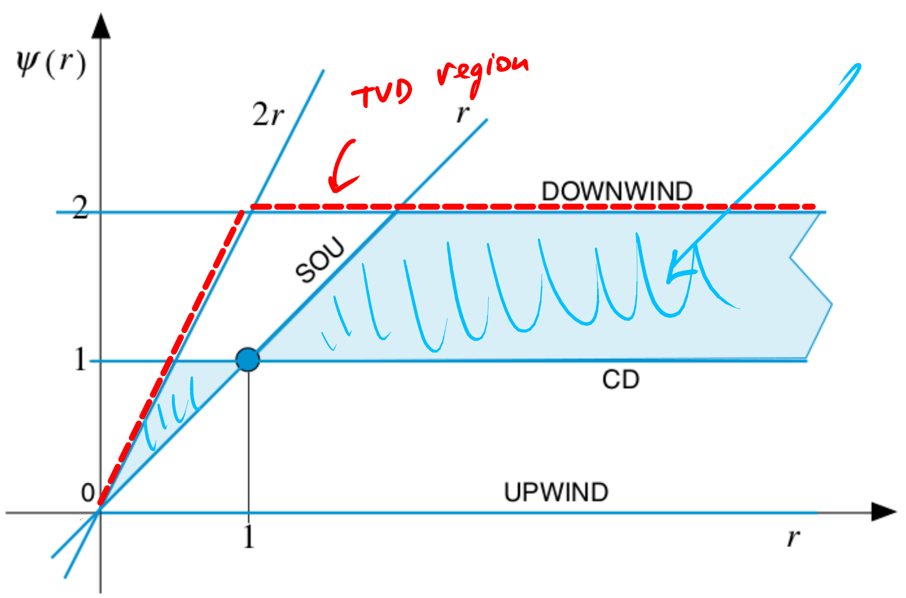


NOTE : Every 2nd-order scheme can be written as a combination of CD and SOU

$\Updownarrow$

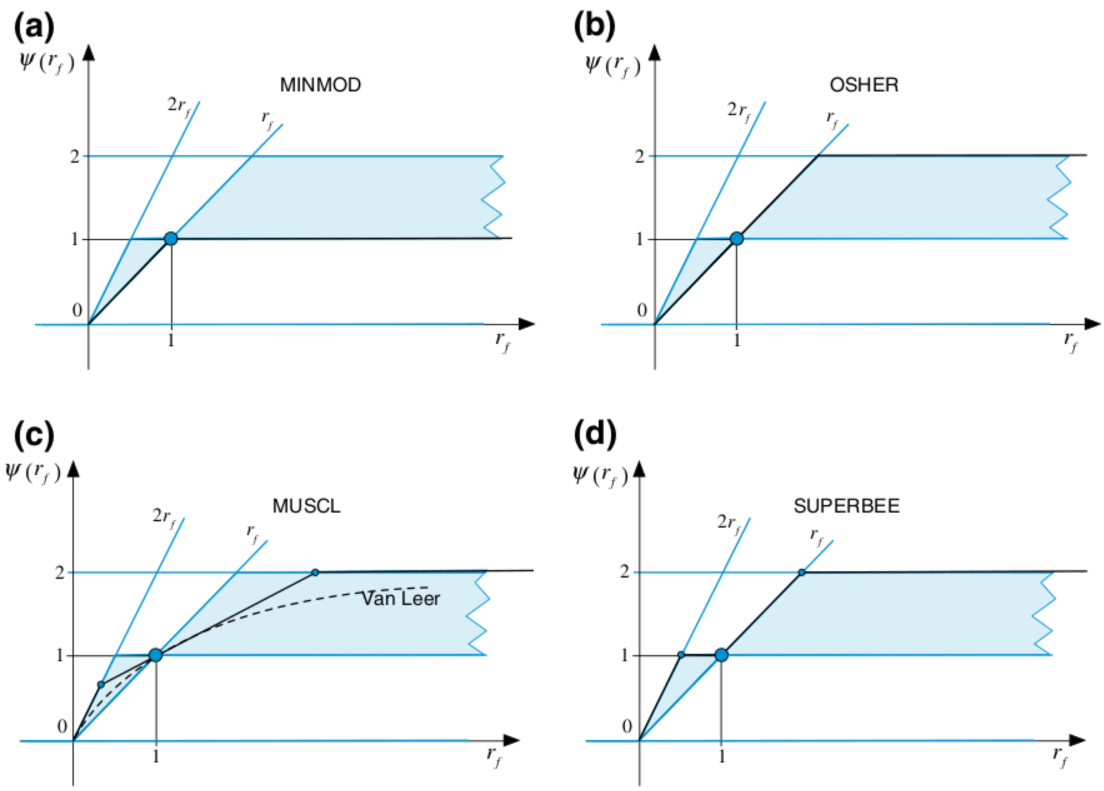
if $r=1$, the linear reconstruction of ϕ_f is exact

for the scheme to be 2nd-order, $\psi(r)$ must pass through the point $(1,1)$



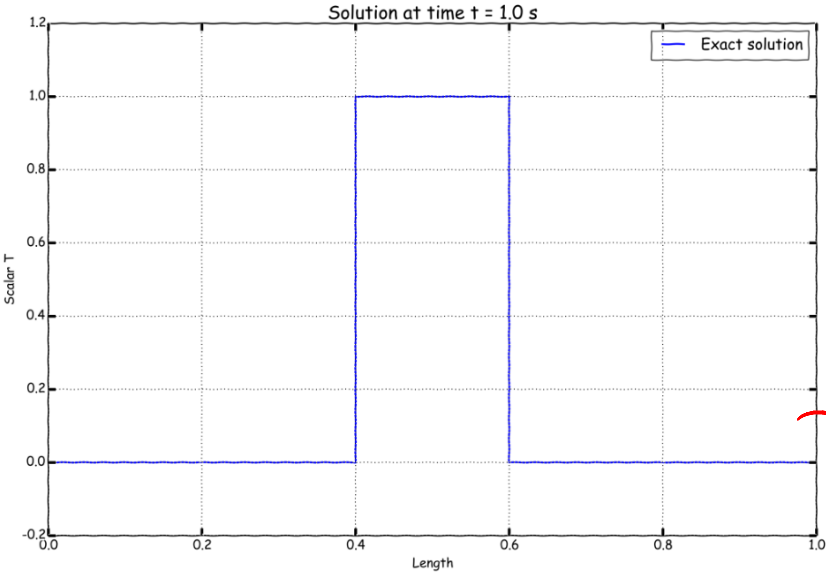
TVD + 2nd order region

LIMITERS USED IN PRACTICE

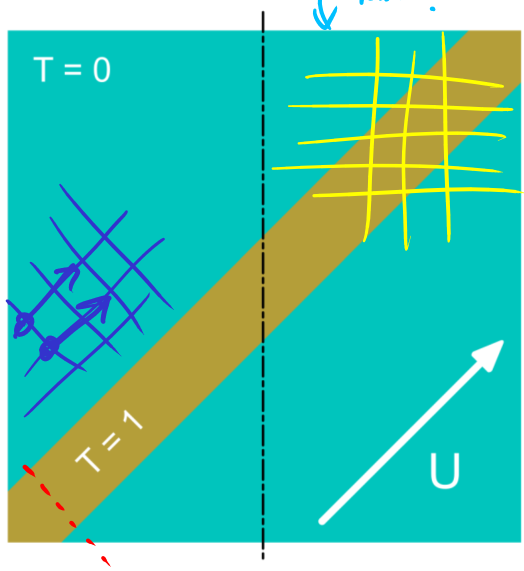


$$
\begin{array}{ll}
\textit{SUPERBEE} & \psi(r_f) = \max\left(0, \min(1, 2r_f), \min(2, r_f)\right) \\
\textit{MINMOD} & \psi(r_f) = \max\left(0, \min(1, r_f)\right) \\
\textit{OSHER} & \psi(r_f) = \max\left(0, \min(2, r_f)\right) \\
\textit{Van Leer} & \psi(r_f) = \dfrac{r_f + |r_f|}{1 + |r_f|} \\
\textit{MUSCL} & \psi(r_f) = \max\left(0, \min(2r_f, (r_f + 1)/2, 2)\right)
\end{array}
$$

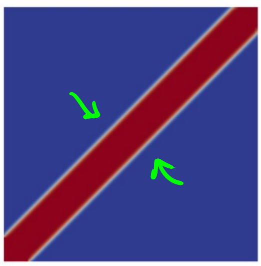
BENCHMARK



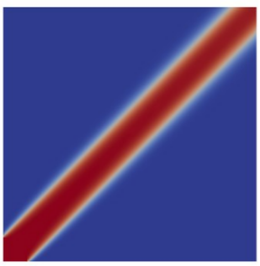
is the mesh like this?



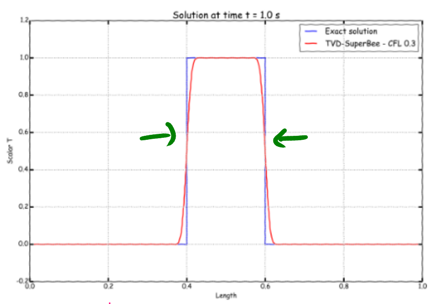
SuperBee - Compressive

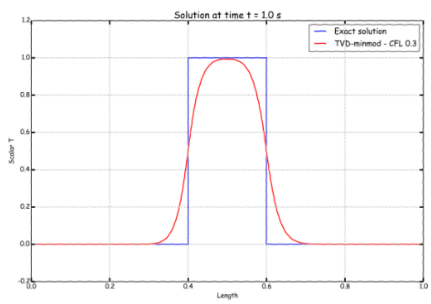


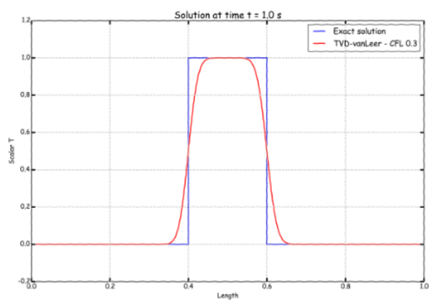
Minmod - Diffusive



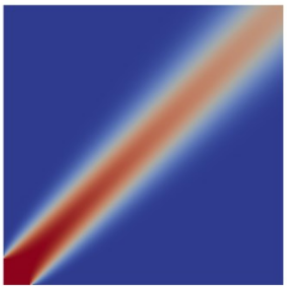
vanLeer - Smooth





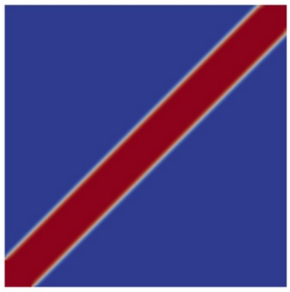


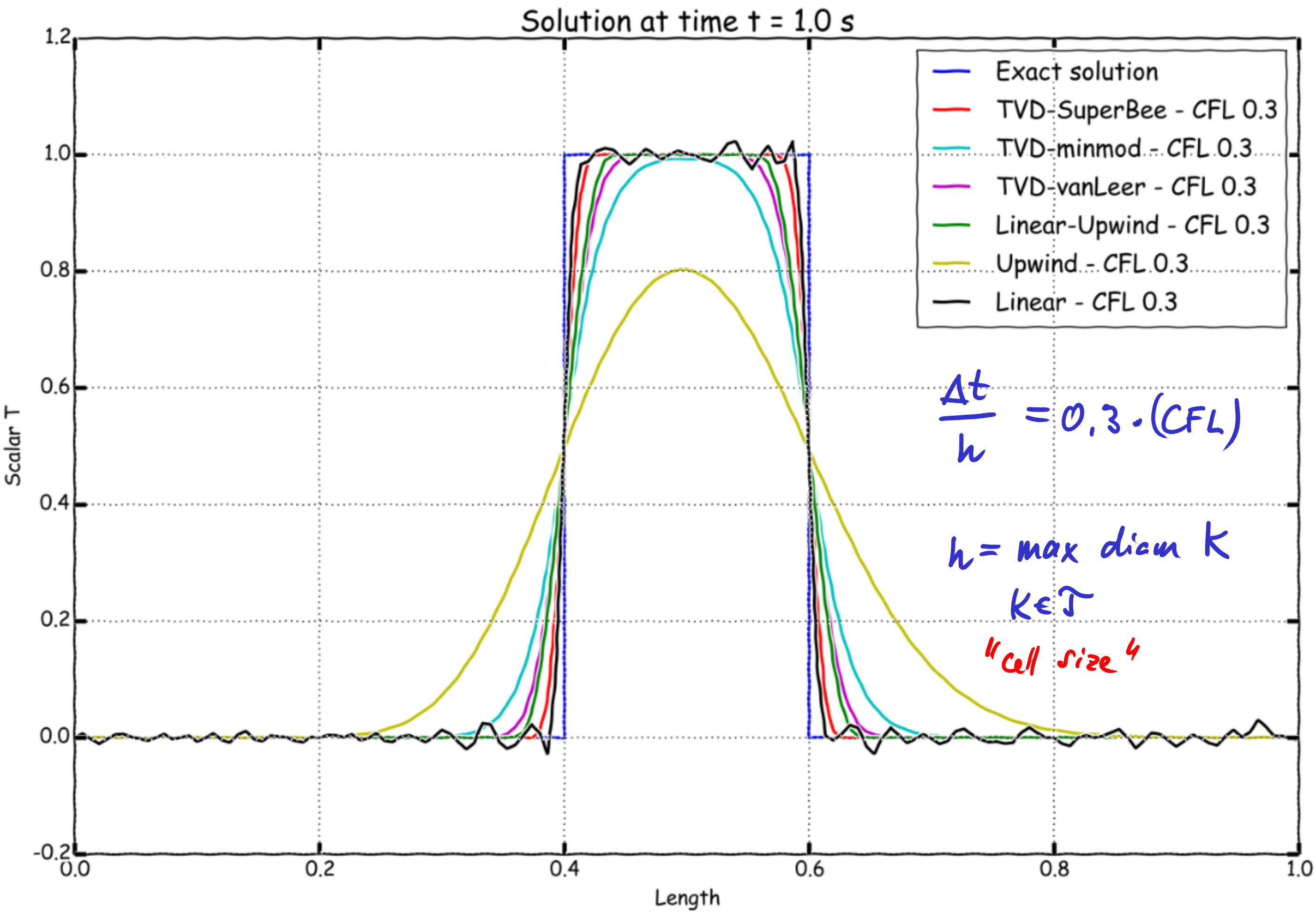
Upwind – 1st order



Linear Upwind – 2nd order

SuperBee – TVD





$$\frac{\Delta t}{h} = 0{,}3 \cdot (\mathrm{CFL})$$

$$h = \max_{K \in \mathcal{T}} \operatorname{diam} K$$

"cell size"

NOTES

- an alternative to TVD : "NVF" .. Normalized Variable Formulation

- 2nd-order schemes can be implemented as 1st order schemes + additional correction

(Deferred Correction)

Solutions to poor convergence rate of implicit solvers:

- DWF (Downwind Weighting Factor)
- NWF (Normalized WF)

OTHER APPROACHES

$$\partial_t \vec{W} + \partial_{x_1} \vec{F} + \partial_{x_2} \vec{G} = \dots$$

- **flux vector splitting**

$$\vec{F} = \begin{pmatrix} \rho V_1 \\ \rho V_1^2 + P \\ \rho V_1 V_2 \\ V_1(\rho E + P) \end{pmatrix} = $$

... AUSM

(Advective Upstream Splitting Method)

$$= \underbrace{\begin{pmatrix} \rho \\ \rho V_1 \\ \rho V_2 \\ \rho H \end{pmatrix} V_1}_{\substack{\text{advection} \\ F^{(c)}}} + \underbrace{\begin{pmatrix} 0 \\ P \\ 0 \\ 0 \end{pmatrix}}_{\substack{\text{pressure can be taken even} \\ \text{downwind (for subsonic flows)}}}$$

evaluate the Mach number locally at cell faces:

$$M = \frac{|\vec{V}|}{A}$$

$|\vec{V}|$ – (local) velocity

A – (local) speed of sound

NOTES: $\mathcal{E}$ ... total energy

$\mathcal{H}$ .. total enthalpy

$$\mathcal{H} = \mathcal{E} + \overset{\text{pressure}}{P}\,\overset{\text{volume}}{V}$$

specific enthalpy $$H = \frac{\mathcal{H}}{\underset{\text{mass}}{m}} = E + \frac{P}{\rho} \Rightarrow \rho H = \rho E + P$$

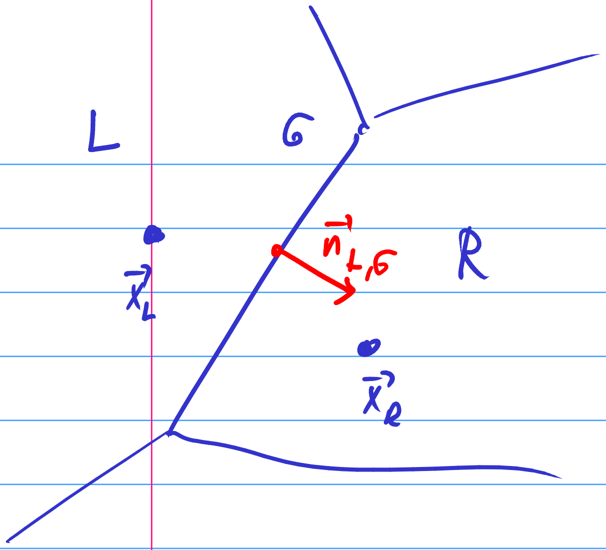
JOURNAL OF COMPUTATIONAL PHYSICS 107, 23–39 (1993)

A New Flux Splitting Scheme

MENG-SING LIOU AND CHRISTOPHER J. STEFFEN, JR.

Internal Fluid Mechanics Division, NASA Lewis Research Center, Cleveland, Ohio 44135

Received May 8, 1991



approximation of $F^{(c)}$ at the face σ

$$F_\sigma^{(c)} = \frac{V_{1,\sigma}}{A} \begin{pmatrix} A\rho \\ A\rho v_1 \\ A\rho v_2 \\ A\rho H \end{pmatrix}_\sigma = M_\sigma \begin{pmatrix} \rho A \\ \rho A v_1 \\ \rho A v_2 \\ \rho A H \end{pmatrix}_\sigma$$

where

$$(\bullet)_\sigma = \begin{cases} (\bullet)_L & \text{if } M_\sigma \geq 0 \\ (\bullet)_R & M_\sigma \leq 0 \end{cases}$$

M_σ ... characteristic velocity at the face σ $\left(\begin{array}{l} |M_\sigma| < 1 \Rightarrow \text{subsonic} \\ \qquad\;\; > 1 \Rightarrow \text{supersonic} \end{array} \right)$

$$\rightarrow M_\sigma = M_L^+ + M_R^-$$

Van Leer splitting

$$M_\bullet^\pm = \begin{cases} \pm\frac{1}{4}(M_\bullet \pm 1)^2 & \text{for } |M_\bullet| \leq 1 \quad (\text{subsonic}) \\ \frac{1}{2}(M_\bullet \pm |M_\bullet|) & \text{for } |M_\bullet| > 1 \quad (\text{supersonic}) \end{cases}$$

$M_\bullet \pm 1$ here "$\bullet$" $\in \{L, R\}$ is the characteristic velocity of a sound wave (projected into the direction $\vec{n}_{L,\sigma}$) coming from L (resp. R) to σ

Treatment of pressure: $p_\sigma = p_L^+ + p_R^-$, where

weighting by a 3rd degree polynomial in $M_\bullet$

$$p_\bullet^\pm = \begin{cases} \frac{p_\bullet}{4}(M_\bullet \pm 1)^2 (2 \mp M_\bullet) & \text{for } |M_\bullet| \leq 1 \\ \frac{p_\bullet}{2} \underbrace{(M_\bullet \pm |M_\bullet|)/M_\bullet}_{\in \{2, 0\}} & \text{for } |M_\bullet| > 1 \end{cases}$$

weighting by a 1st degree polynomial in M_0

$$p_0^{\pm} = \begin{cases} \frac{p}{2}(1 \pm M_0) & \text{for } |M_0| \le 1 \\ \frac{p}{2}(M_0 \pm |M_0|)/M_0 & \text{for } |M_0| > 1 \end{cases}$$

extensions: AUSM+, CUSP

Flux Difference Splitting – Roe's upwind scheme [Blazek, p. 104]

$$\partial_t \vec{W} + \partial_{x_1} \vec{F} + \partial_{x_2} \vec{G} \approx \partial_t \vec{W} + \underbrace{\frac{\partial \vec{F}}{\partial \vec{W}}} \partial_{x_1} \vec{W} + \underbrace{\frac{\partial \vec{G}}{\partial \vec{W}}} \partial_{x_2} \vec{W}$$

$$\vec{W} = \begin{pmatrix} \rho \\ \rho v_1 \\ \rho v_2 \\ \rho H \end{pmatrix}$$

Jacobi matrices

$\Rightarrow$ approximated by the Roe matrices $A^{(F)}_{Roe}$, $A^{(G)}_{Roe}$

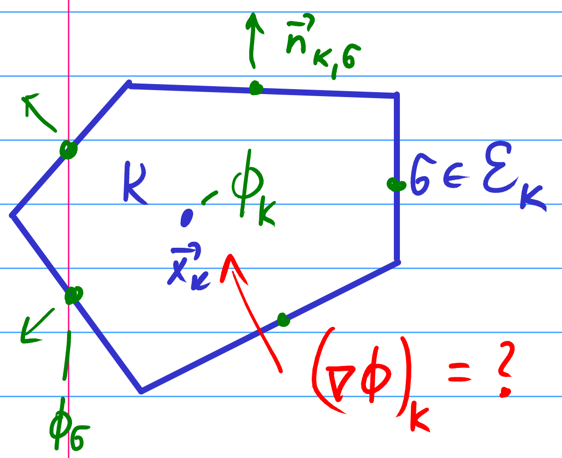
$$A^{(F)}_{Roe} = R^T \Lambda R$$

Approximation of the gradient

motivation

- viscous fluxes $\vec{R}, \vec{S}$ ... they contain $\partial_i V_k$ via σ $\Rightarrow$ values required at cell faces $\qquad \nabla \vec{V} = (\cdot)$
- solution approximations at far "virtual" nodes in 2nd-order UPWIND schemes (SOU, FROMM, QUICK, TVD ...) $\Rightarrow$ values of $\nabla\phi$ $\quad \phi \in \{\rho, \rho V_1, \ldots\}$ required at cell centers

GRADIENTS AT CELL CENTERS



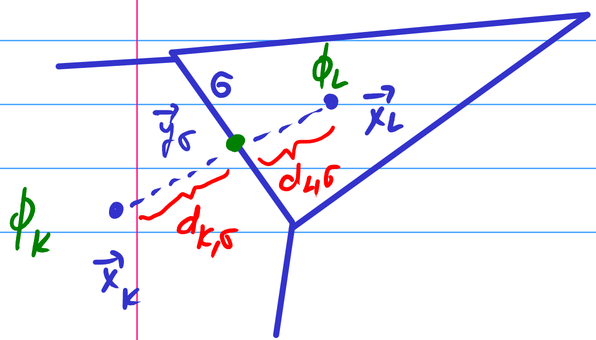
1) Gauss–Green approach

$$\int_K \partial_i \phi \, d\vec{x} = \int_{\partial K} \phi \, n_i \, dS$$

components of $\nabla\phi$ form a column vector

$$\int_K \nabla\phi \, d\vec{x} = \int_{\partial K} \phi \, \vec{n} \, dS$$

$$(\nabla\phi)_K = \frac{1}{m(K)} \sum_{\sigma\in\mathcal{E}_K} m(\sigma)\, \phi_\sigma \, \vec{n}_{K,\sigma}$$

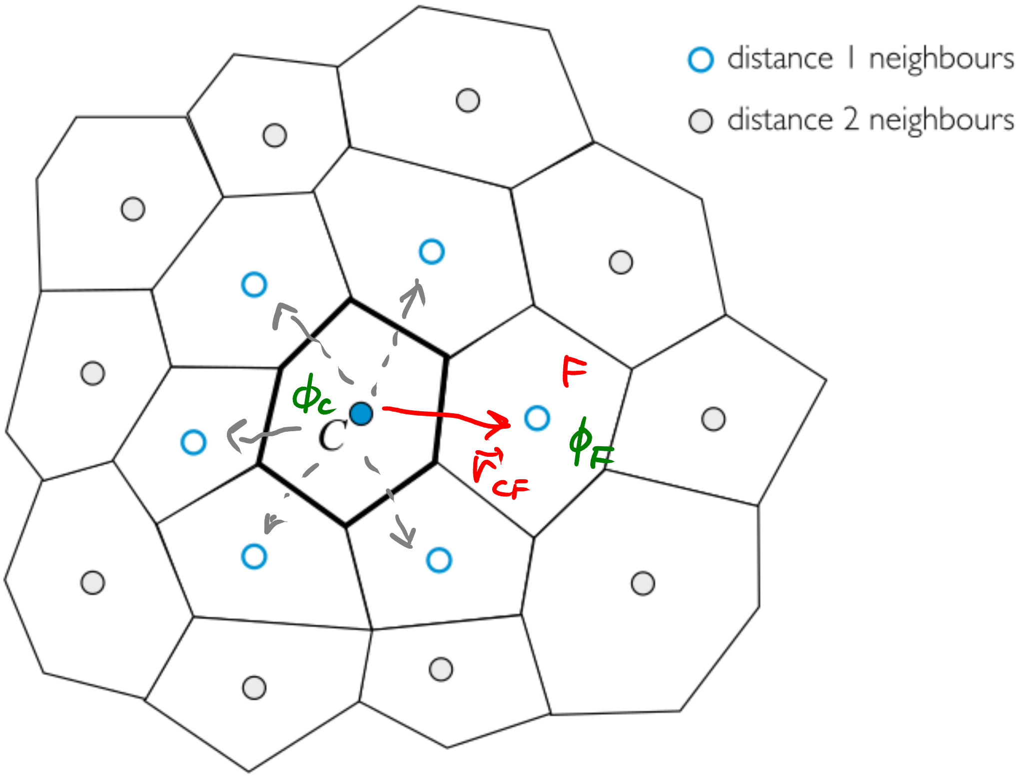


$$\phi_\sigma = \frac{1}{2}(\phi_K + \phi_L) \quad \text{(1st order)}$$

or use linear interpolation (2nd order)

$$\phi_\sigma = \frac{d_{K,\sigma}}{\mathcal{D}_{KL}} \phi_L + \frac{d_{L,\sigma}}{\mathcal{D}_{KL}} \phi_K$$

2) LEAST SQUARES GRADIENT APPROXIMATION



$$\phi_F \approx \phi_C + (\nabla\phi)_C \cdot \underbrace{(\mathbf{r}_F - \mathbf{r}_C)}_{\mathbf{r}_{CF}} + \mathcal{O}(|\vec{r}_{CF}|^2)$$

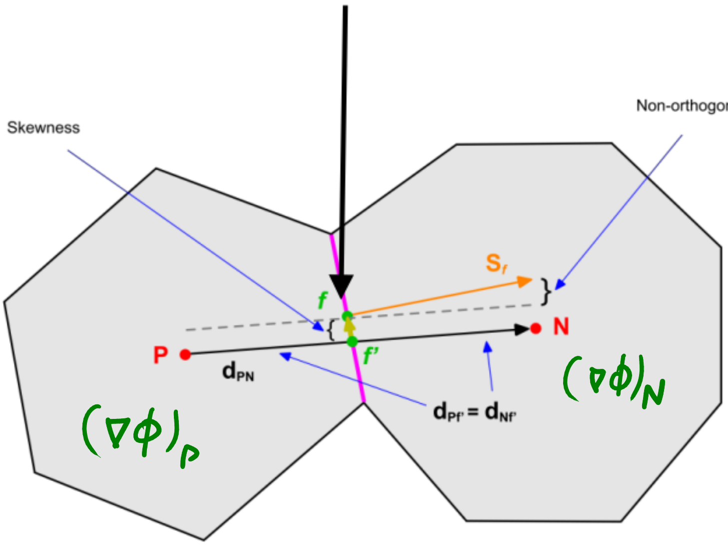
all neighbors of the cell C

minimize
$$G_C = \sum_{k=1}^{NB(C)} \left\{ \underbrace{w_k}_{\text{weights}} \Big[\underbrace{\phi_{F_k}}_{\text{the real value}} - \underbrace{(\phi_C + \nabla\phi_C \cdot \mathbf{r}_{CF_k})}_{\text{approximation}} \Big]^2 \right\}$$

APPROXIMATING GRADIENTS AT CELL FACES:

the simplest way:

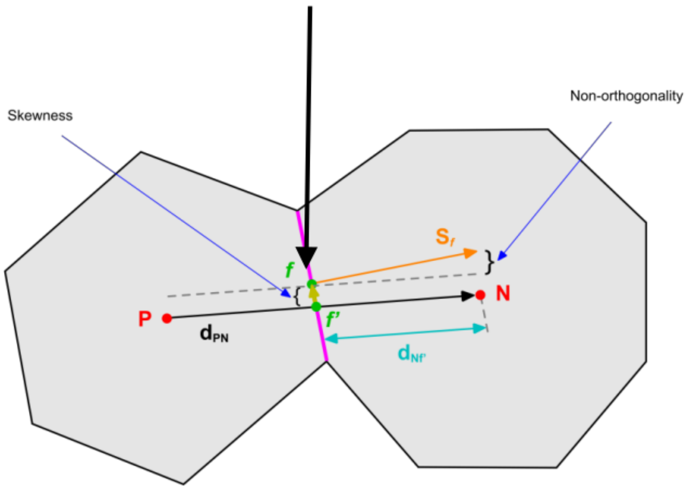
$$\nabla\phi_f = \frac{\nabla\phi_P + \nabla\phi_N}{2}$$



lin. interpolation

$$\nabla\phi_f = f_x\nabla\phi_P + (1 - f_x)\nabla\phi_N \qquad \text{where} \qquad f_x = fN/PN$$

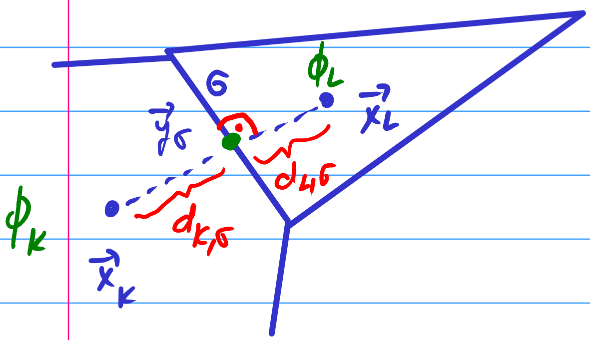
$\mathcal{D}_{PN}$



<u>NOTE:</u> Incompressible Flow: $\quad \nabla \cdot \Pi_D \longrightarrow \mu \Delta \vec{V}$

Green: $$\int_K \Delta \vec{V} \, d\vec{x} = \int_{\partial K} \underbrace{\nabla \vec{V} \cdot \vec{n}}_{\frac{\partial \vec{V}}{\partial \vec{n}}} \, dS$$

... only the derivatives in the normal direction to σ are required



$$\left(\frac{\partial \phi}{\partial \vec{n}}\right)_\sigma \approx \frac{\phi_L - \phi_K}{D_{KL}} + O(D_{KL}^2)$$

if ⊾ !!

$\Rightarrow$ <u>CORRECTION</u>: $(\nabla\phi)_\sigma$ is modified, so that

$$(\nabla\phi)_\sigma \cdot \vec{d}_{KL} \stackrel{!}{=} \frac{\phi_L - \phi_K}{D_{KL}}$$

$$\vec{d}_{KL} := \frac{(\vec{x}_L - \vec{x}_K)}{D_{KL}}$$

$$\Rightarrow (\nabla\phi)_\sigma^{corr} = (\nabla\phi)_\sigma + \left(\frac{\phi_L - \phi_K}{D_{KL}} - (\nabla\phi)_\sigma \cdot \vec{d}_{KL} \right) \vec{d}_{KL}$$

$\boxed{\text{check!}}$

$$\Rightarrow (\nabla\phi)_\sigma^{corr} \cdot \vec{d}_{KL} = (\nabla\phi)_\sigma \cdot \vec{d}_{KL} + \frac{\phi_L - \phi_K}{D_{KL}} \underbrace{\vec{d}_{KL} \cdot \vec{d}_{KL}}_{=1}$$

$$- \left((\nabla\phi)_\sigma \cdot \vec{d}_{KL} \right) \underbrace{\vec{d}_{KL} \cdot \vec{d}_{KL}}_{=1}$$

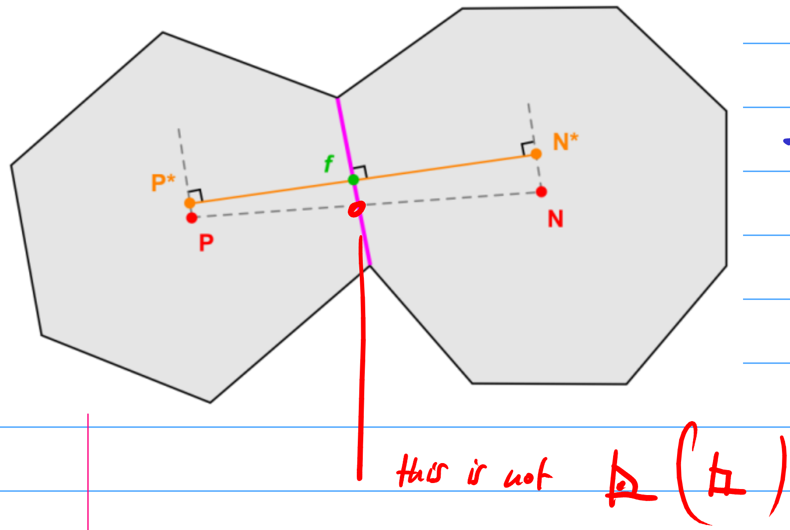
$\Rightarrow$ allows to accurately calculate

$$\frac{\partial \phi}{\partial \vec{n}} = (\nabla\phi)_\sigma^{corr} \cdot \vec{n} \quad \text{even if} \quad \vec{n} \nparallel \vec{d}_{KL}$$

NOTE: Non-admissible (non-orthogonal) meshes:

Yet another way to calculate $\frac{\partial \phi}{\partial \vec{n}}$ if the gradients at cell centers are known:

$$\phi_N^* = \phi_N + \nabla\phi_N \cdot \mathbf{d}_{N^*N} \qquad \phi_P^* = \phi_P + \nabla\phi_P \cdot \mathbf{d}_{P^*P}$$

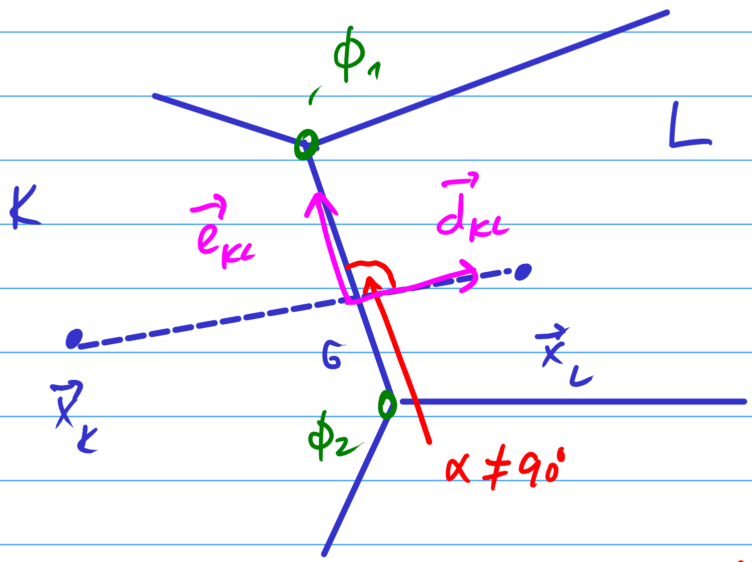


this is not ⊾ (⊥)

$$\Rightarrow \quad \nabla\phi_f = \frac{\phi_{N^*} - \phi_{P^*}}{|\mathbf{d}|_{P^*N^*}}$$

$$\frac{\partial \phi}{\partial \vec{n}}$$

In 2D, this can be used to approximate $(\nabla\phi)_G$



$$\Rightarrow \quad \frac{\partial \phi}{\partial \vec{d}_{KL}} \approx \frac{\phi_L - \phi_K}{D_{KL}}$$

$$\frac{\partial \phi}{\partial \vec{e}_{KL}} \approx \frac{\phi_1 - \phi_2}{m(G)}$$

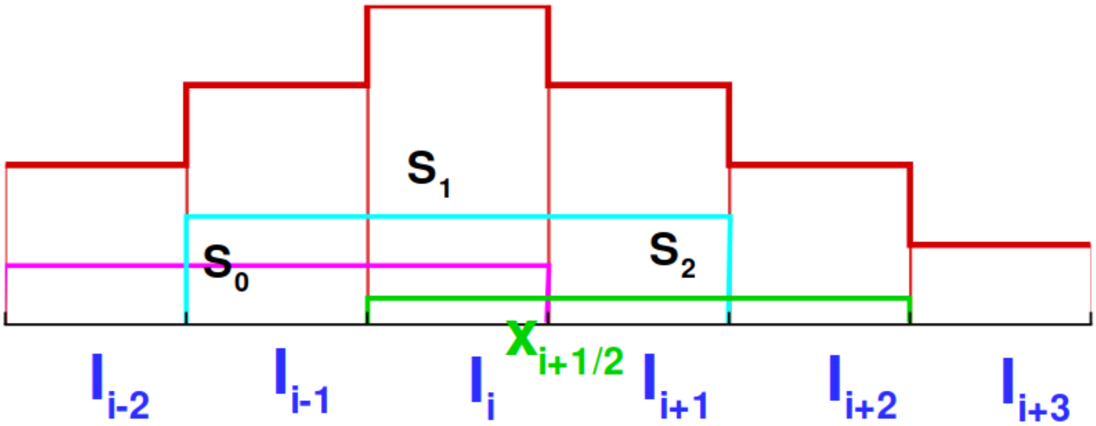
basis transformation $\Downarrow$

we calculate $(\nabla\phi)_G$, $\frac{\partial \phi}{\partial \vec{n}}$

HIGHER-ORDER METHODS (> 2nd-order)

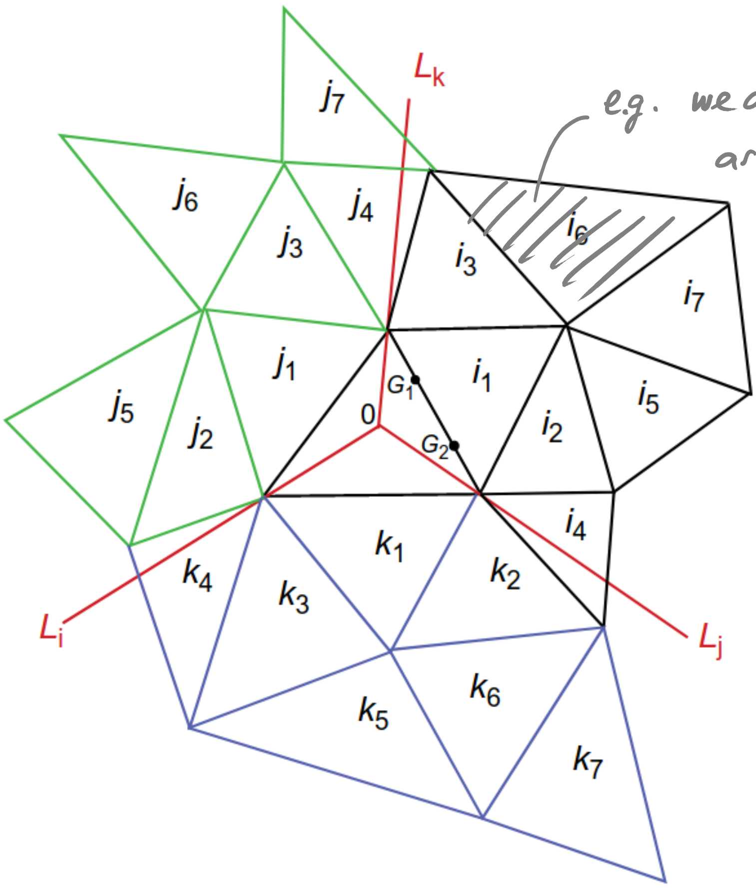
ENO – essentially non-oscillatory
WENO – weighted ENO

– an adaptive stencil that can ignore the "discontinuous" cells



– polynomial interpolation (Lagrange)

– smoothness criterion



e.g. we don't want i_6, as it does not meet the smoothness criterion

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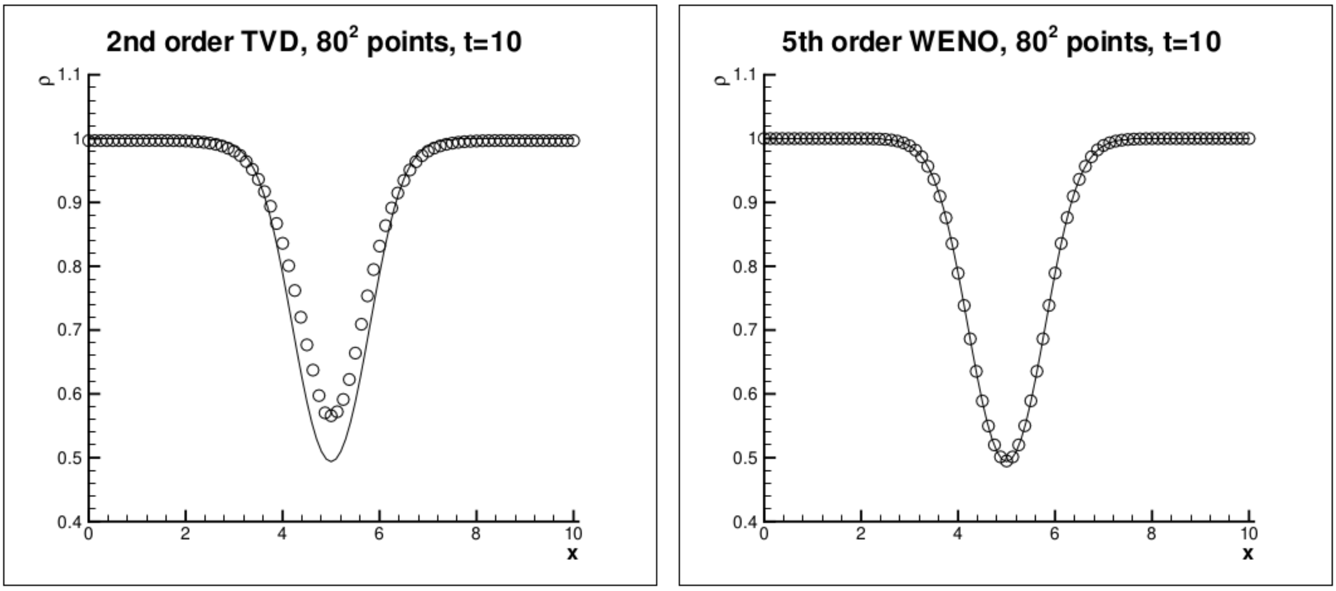


Figure 1.1: Vortex evolution. Cut at $x = 5$. Density ρ. 80^2 uniform mesh. $t = 10$ (after one time period). Solid: exact solution; circles: computed solution. Left: second order TVD scheme; right: fifth order WENO scheme.

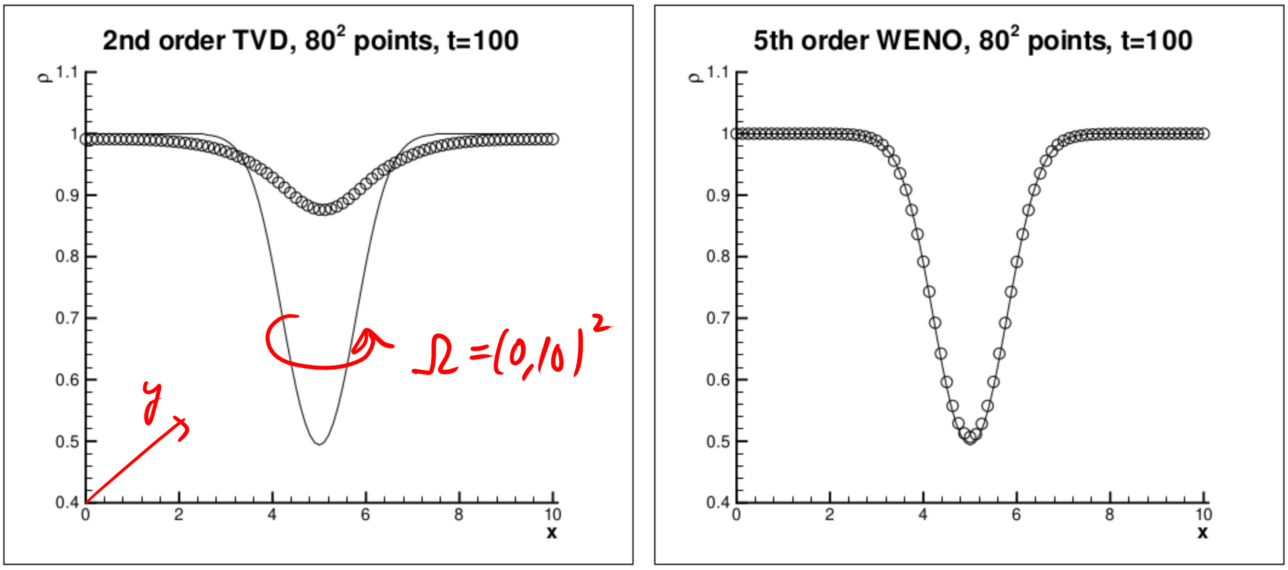


Figure 1.2: Vortex evolution. Cut at $x = 5$. Density ρ. 80^2 uniform mesh. $t = 100$ (after 10 time periods). Solid: exact solution; circles: computed solution. Left: second order TVD scheme; right: fifth order WENO scheme.

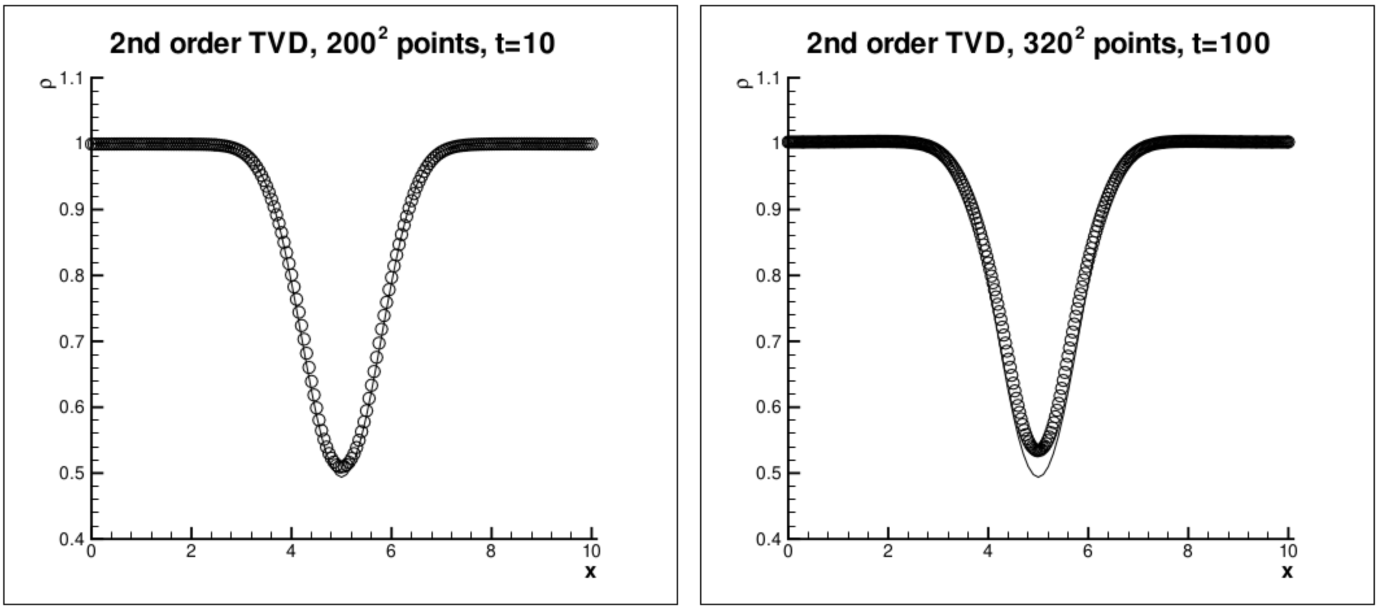


Figure 1.3: Vortex evolution. Cut at $x = 5$. Density ρ. Second order TVD scheme. Solid: exact solution; circles: computed solution. Left: 200^2 uniform mesh, $t = 10$ (after one time period); right: 320^2 uniform mesh, $t = 100$ (after 10 time periods).

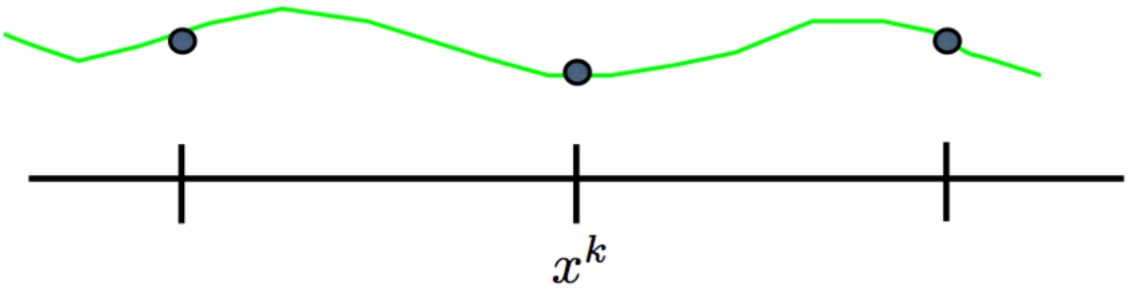
"DG"

DISCONTINUOUS GALERKIN METHOD

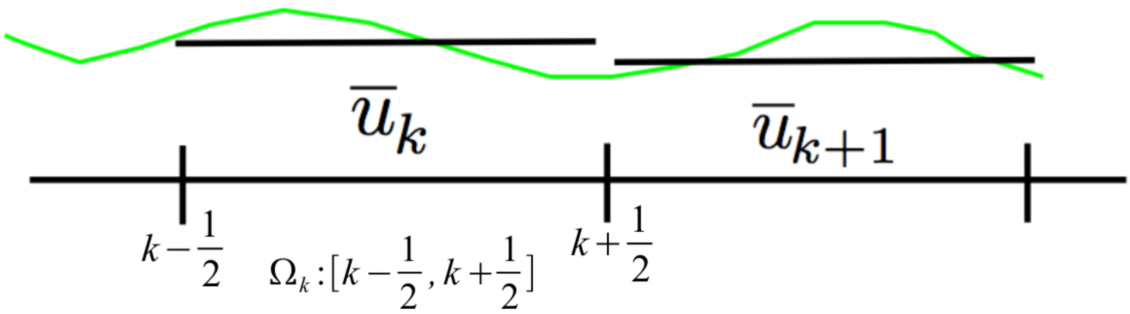
the solution is discontinuous between elements

basis functions defined only on their own elements (no overlap)

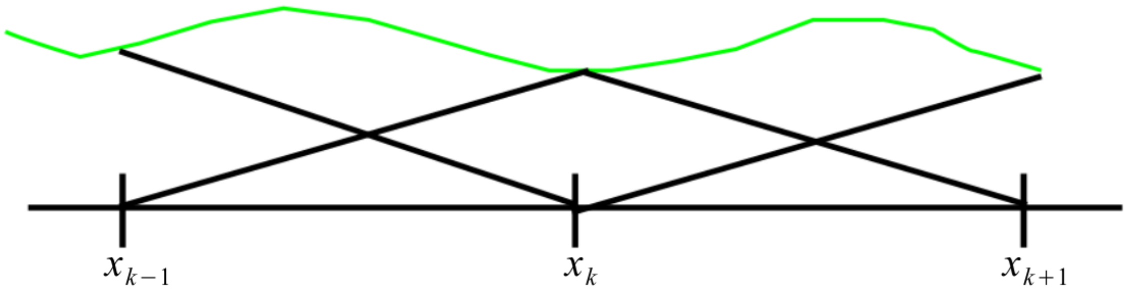
FDM



FVM

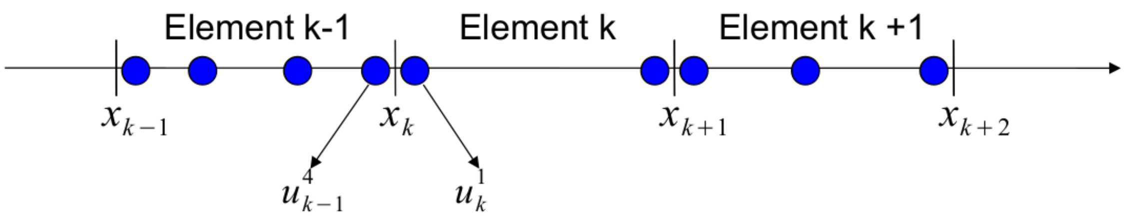


FEM



DG

"cell"



a local Galerkin method at each Ω_k

metody řešení nestlač. proudění

ZZHm $\Leftrightarrow$ $\nabla \cdot \vec{V} = 0$

ZZHyb $\Leftrightarrow$ NS ... obsahují ∇P

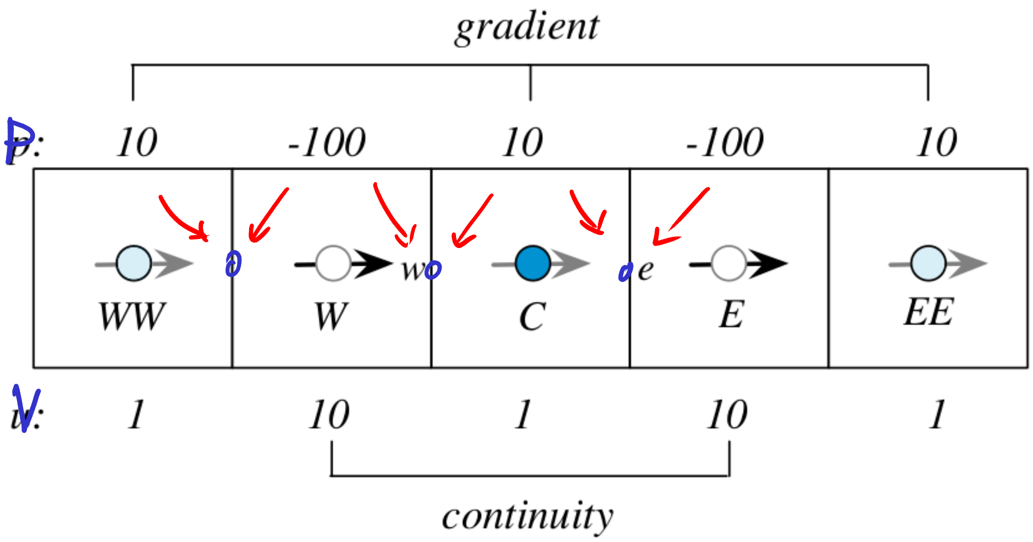
$\Downarrow$

Poissonova rovnice pro tlak

Princip num. řešičů : predikce $\leftrightarrow$ korekce

- SIMPLE .... SIMPLE C, R, ST
- PISO
- PIMPLE

PROBLÉM "ŠACHOVNICOVÝ" / "decoupling"



$$\int_C \frac{\partial P}{\partial x} dx = \left(P_e - P_w\right) m(C) = 0$$

⇒ STAGGERED GRID (střídavá síť)

- rychlosti uloženy na stěnách
- skalární veličiny ve středech buněk

- nevýhody zejména na nestrukt. sítích

<u>ALTERNATIVA</u> – speciální typ interpolace na cell-centered sítích
(Rhie–Chowova interpolace)

$$
\begin{aligned}
\overline{D^u_f \left(\frac{\partial p}{\partial x}\right)_f} - \overline{D^u_f}\,\overline{\left(\frac{\partial p}{\partial x}\right)_f} &= \frac{1}{2}\left(D^u_C\left(\frac{\partial p}{\partial x}\right)_C + D^u_F\left(\frac{\partial p}{\partial x}\right)_F\right) \\
&\quad - \frac{1}{2}\left(D^u_C + D^u_F\right) \times \frac{1}{2}\left(\left(\frac{\partial p}{\partial x}\right)_C + \left(\frac{\partial p}{\partial x}\right)_F\right) \\
&= \frac{1}{4}D^u_C\left(\left(\frac{\partial p}{\partial x}\right)_C - \left(\frac{\partial p}{\partial x}\right)_F\right) + \frac{1}{4}D^u_F\left(\left(\frac{\partial p}{\partial x}\right)_F - \left(\frac{\partial p}{\partial x}\right)_C\right) \\
&\approx O(\Delta x^2)
\end{aligned}
$$

SIMPLE :

hmot. toky přes stěny — rychlostní pole v čase $n \cdot \Delta t$ — pole hustoty / tlaku — 〃 —

set initial guess $\dot{m}^{(n)}, \mathbf{v}^{(n)}, \rho^{(n)}$, and $p^{(n)}$ at time $t+\Delta t$ to converged values at time t

assemble and solve momentum equation for $\mathbf{v}^{*}$ — NS rovnice s hodnotami $p^{(n)}$

compute $\dot{m}_f^{*}$ using the Rhie – Chow interpolation — korigované hmot. toky na stěnách

assemble and solve pressure correction equation for p' — $p^{*} = p^{(n)} + p'$

correct $\dot{m}_f^{*}, \mathbf{v}^{*}, \rho^{(n)}$, and $p^{(n)}$ to obtain $\dot{m}_f^{**}, \mathbf{v}^{**}, \rho^{*}$, and p^{*} — řešíme NS

set $\dot{m}_f^{(n)} = \dot{m}_f^{**}, \mathbf{v}^{(n)} = \mathbf{v}^{**}, \rho^{(n)} = \rho^{*}$, and $p^{(n)} = p^{*}$

converged? — no: repeat (from "assemble and solve momentum equation"); yes:

set solution at time $t+\Delta t$ to be equal to the converged solution — $\vec{v}^{(n+1)} = \vec{v}^{**}$ ...

advance in time set $t = t + \Delta t$ — $t = (n+1)\Delta t$

time exceeded? — no: repeat (from "set initial guess"); yes:

stop

variacty a vylepšení : SIMPLE $\begin{cases} C \\ R \\ ST \end{cases}$ PIMPLE

PISO

vše je v <u>OpenFOAMu</u>

<u>POZN</u> : pro <u>stlačitelné proudění</u>

"přímočaré" řešení : $\rho, \vec{V}$ ... $p = EOS(\rho, T)$

(density-based solver)

počítat korekční rovnice pro tlak : $p, \vec{V}$

(pressure-based solver)

METODY ČASOVÉ INTEGRACE

Pozn.: Metoda přímek: $\partial_t \vec{u} + \underbrace{L_{\vec{x}}}_{\text{dif. operátor v prostorových souř.}} \vec{u} = f$

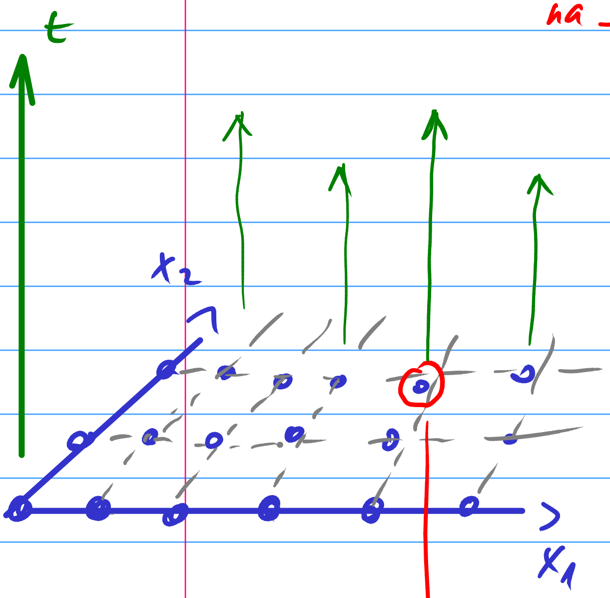
$u : (0, t_{max}) \times \Omega \to \mathbb{R}$

$u_h : (0, t_{max}) \to \underbrace{\mathcal{H}_h}_{\text{prostor síť. fcí na } \Omega}$

$$\partial_t u_h + L_{\vec{x},h} u_h = f_h \quad \Big\} \text{ konečný počet ODR}$$

$L_{\vec{x},h}$ … operátor prostorové diskretizace (MKD, MKO...)

$$\dot{\vec{u}} = \vec{F}(\vec{u})$$

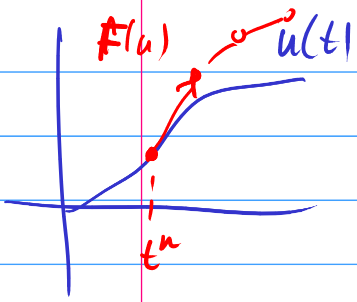


$\vec{u}$ obsahuje hodnoty u_h v jednotlivých uzlech sítě (MKD), resp. v jednotlivých buňkách (MKO)

$$[u_h(t)]_{ij} = \underbrace{(u_h(t))}_{\in \mathcal{H}_h}(\vec{x}_{ij})$$

RUNGE-KUTTOVY METODY

m-kroková RK metoda pro řešení $\dot{\vec{u}} = \vec{F}(t, \vec{u})$



$$\vec{K}_\ell = \vec{F}\left(t^n + c_\ell \Delta t,\ \vec{u}^n + \Delta t \sum_{j=1}^{m} a_{j\ell} \vec{K}_j\right)$$

$\forall \ell = 1, \dots, m$

a nakonec $$\vec{u}^{n+1} = \vec{u}^n + \Delta t \sum_{\ell=1}^{m} b_\ell \vec{K}_\ell$$

zřejmě (intuitivně) $c_\ell = \sum_{k=1}^{m} a_{\ell k}$

Butcherova tabulka

$$\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \cdots & a_{1m} \\
c_2 & a_{21} & a_{22} & \cdots & a_{2m} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
c_m & a_{m1} & a_{m2} & \cdots & a_{mm} \\
\hline
 & b_1 & b_2 & \cdots & b_m
\end{array}$$

Explicitní RK metody

pokud zde je nenulová hodnota, jde o implicitní RK metodu (alespoň v 1 kroku)

$\left(\sum_{k=1}^{m} b_k = 1\right)$

např. tzv. klasická RK metoda 4. řádu

$$\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
1/2 & 1/2 & 0 & 0 & 0 \\
1/2 & 0 & 1/2 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & 1/6 & 1/3 & 1/3 & 1/6
\end{array}$$

... pro "stiff" soustavy rovnic

6-kroková RK:

jednoduše diagonálně implicitní metoda

0	0	0	0	0	0	0
$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	0	0	0	0
$\frac{83}{250}$	$\frac{8611}{62500}$	$-\frac{1743}{31250}$	$\frac{1}{4}$	0	0	0
$\frac{31}{50}$	$\frac{5012029}{34652500}$	$-\frac{654441}{2922500}$	$\frac{174375}{388108}$	$\frac{1}{4}$	0	0
$\frac{17}{20}$	$\frac{15267082809}{155376265600}$	$-\frac{71443401}{120774400}$	$\frac{730878875}{902184768}$	$\frac{2285395}{8070912}$	$\frac{1}{4}$	0
1	$\frac{82889}{524892}$	0	$\frac{15625}{83664}$	$\frac{69875}{102672}$	$-\frac{2260}{8211}$	$\frac{1}{4}$
4. řád b_k	$\frac{82889}{524892}$	0	$\frac{15625}{83664}$	$\frac{69875}{102672}$	$-\frac{2260}{8211}$	$\frac{1}{4}$
3. řád $\hat{b}_k$	$\frac{4586570599}{29645900160}$	0	$\frac{178811875}{945068544}$	$\frac{814220225}{1159782912}$	$-\frac{3700637}{11593932}$	$\frac{61727}{225920}$

RK-Mersonova metoda s adaptivní volbou (časového) kroku 4. řádu

$\dot{\vec{x}} = \vec{f}(t, \vec{x})$

$\tau = \Delta t$

$\tau = \tau_{ini}$; $\boldsymbol{x}^\tau = \boldsymbol{x}^\tau_{ini}$;
while(1) {
  if($|T - t| < |\tau|$) {
    $\tau = T - t$; last=true;
  } else last=false;
  $\boldsymbol{K}_1 = \boldsymbol{f}(t, \boldsymbol{x}^\tau)$;
  $\boldsymbol{K}_2 = \boldsymbol{f}\left(t + \frac{\tau}{3}, \boldsymbol{x}^\tau + \frac{\tau}{3}\boldsymbol{K}_1\right)$;
  $\boldsymbol{K}_3 = \boldsymbol{f}\left(t + \frac{\tau}{3}, \boldsymbol{x}^\tau + \frac{\tau}{6}(\boldsymbol{K}_1 + \boldsymbol{K}_2)\right)$;
  $\boldsymbol{K}_4 = \boldsymbol{f}\left(t + \frac{\tau}{2}, \boldsymbol{x}^\tau + \frac{\tau}{8}(\boldsymbol{K}_1 + 3\boldsymbol{K}_3)\right)$;
  $\boldsymbol{K}_5 = \boldsymbol{f}\left(t + \tau, \boldsymbol{x}^\tau + \tau\left(\frac{1}{2}\boldsymbol{K}_1 - \frac{3}{2}\boldsymbol{K}_3 + 2\boldsymbol{K}_4\right)\right)$;
  $\varepsilon = \max_{i\in\{1,2,\dots,n\}} \frac{\tau}{3}\left|0.2K_1^i - 0.9K_3^i + 0.8K_4^i - 0.1K_5^i\right|$;
  if($\varepsilon < \delta$) {
    $\boldsymbol{x}^\tau = \boldsymbol{x}^\tau + \tau\left(\frac{1}{6}(\boldsymbol{K}_1 + \boldsymbol{K}_5) + \frac{2}{3}\boldsymbol{K}_4\right)$;
    $t = t + \tau$;
    if(last) break;
    if(ε==0) continue;
  }
  $\tau = \left(\frac{\delta}{\varepsilon}\right)^{0.2} \cdot \omega\tau$;
}

provede se vždy

$\varepsilon < \delta\omega^5 \Leftrightarrow$ τ se prodlouží

$\omega \doteq 0{,}8 \in (0,1)$

IMPLICITNÍ SCHÉMATA – ŘEŠENÍ SOUSTAV LIN. ROVNIC

$\partial_t u + a\partial_x u = 0$ transport. rovnice $\wedge$ $\underline{u(0) = u(1) = 0}$

na $\Omega = (0,1)$

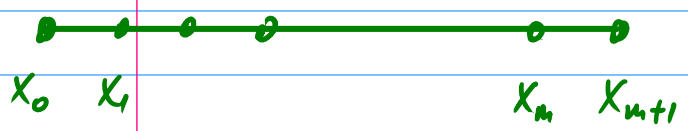
$$\overleftarrow{\delta}_t u_h^{\Delta t} + a\,\overleftrightarrow{\delta}_x u_h^{\Delta t} = 0 \iff \frac{u_k^n - u_k^{n-1}}{\Delta t} + a\,\frac{u_{k+1}^n - u_{k-1}^n}{2\Delta x} = 0$$

$$u_h^{\Delta t} \in \mathcal{H}_h^{\Delta t}$$

nebo

$$\boxed{\frac{u_k^{n+1} - u_k^n}{\Delta t} + a\,\frac{u_{k+1}^{n+1} - u_{k-1}^{n+1}}{2\Delta x} = 0}$$

PROSTOR. DISKRETIZACE



$$u_k^{n+1} + \underbrace{\frac{a\Delta t}{2\Delta x}}_{\text{ozn. } \alpha}\left(u_{k+1}^{n+1} - u_{k-1}^{n+1}\right) = u_k^n$$

soustava lin. rovnic pro u^{n+1}

$$u^{n+1} = \begin{pmatrix} u_1^{n+1} \\ \vdots \\ u_m^{n+1} \end{pmatrix}$$

$$\overbrace{\begin{pmatrix} 1 & \alpha & 0 & \cdots & & & 0 \\ -\alpha & 1 & \alpha & 0 & \cdots & & 0 \\ 0 & -\alpha & 1 & \alpha & \cdots & & \\ & & -\alpha & 1 & \alpha & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & -\alpha & 1 & \alpha \\ & & & & & -\alpha & 1 \end{pmatrix}}^{A} \begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ \vdots \\ u_m^{n+1} \end{pmatrix} = u^n$$

3-diagonální

Toeplitzova

matice

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

$\Rightarrow$ nutno najít A^{-1} ... závislé na Ω a na síti a na okraj. podm.

$\Rightarrow \quad u^{n+1} = \mathbb{A}^{-1} u^n$

inverze 3-diag. matice má **všechny** prvky nenulové

$\Rightarrow$ u_k^{n+1} závisí na u_ℓ^n pro všechna $\ell = 1, \dots, m$

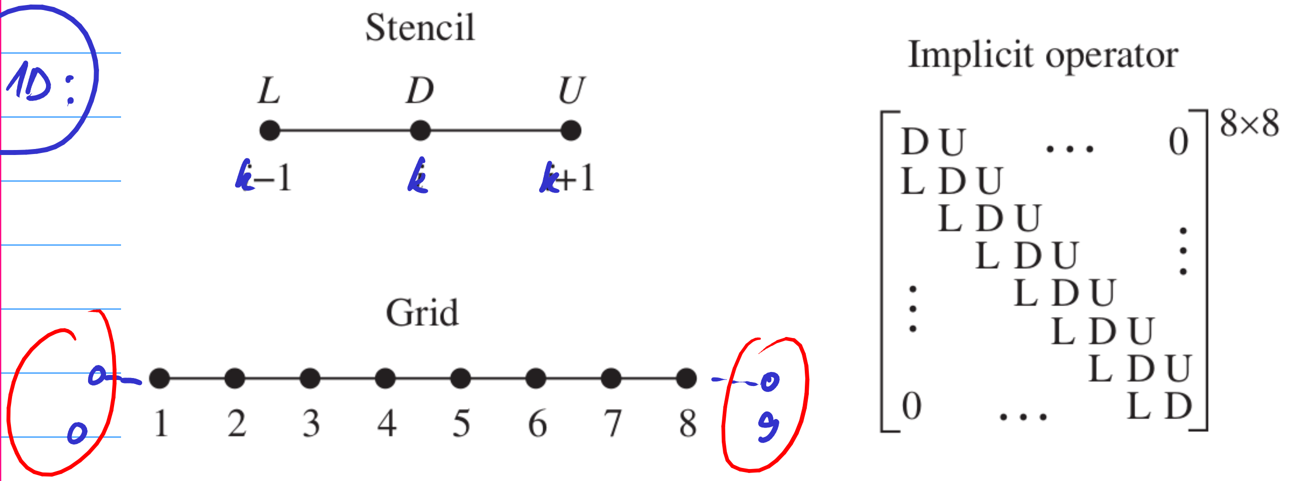
pevné

$\Rightarrow$ CFL podmínka je splněna pro lib. hodnotu rychlosti a

$\Leftarrow$ implic. schéma je nepodmíněně stabilní (víme z Von Neumannovy analýzy)

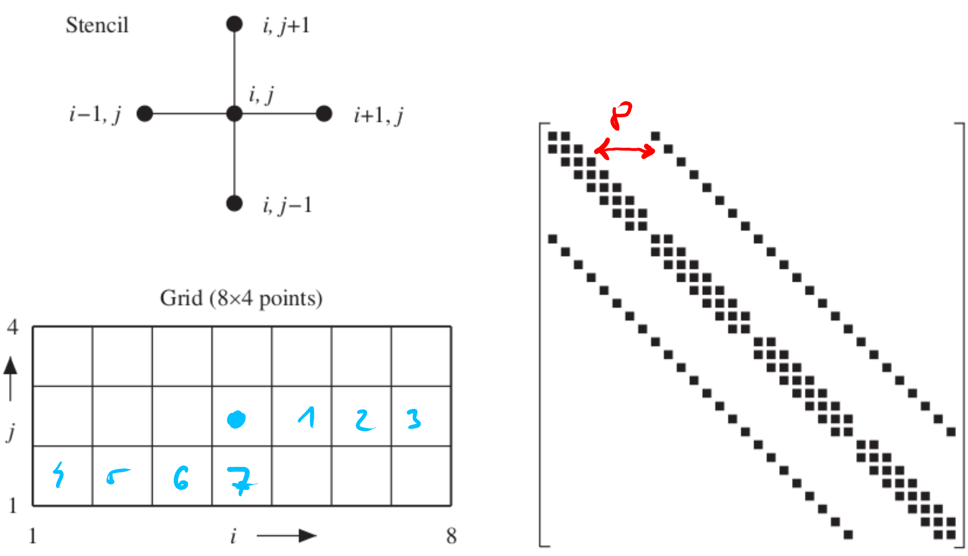
Struktury matice $\mathbb{A}$ pro úlohy v 1D, 2D:

v 1D:



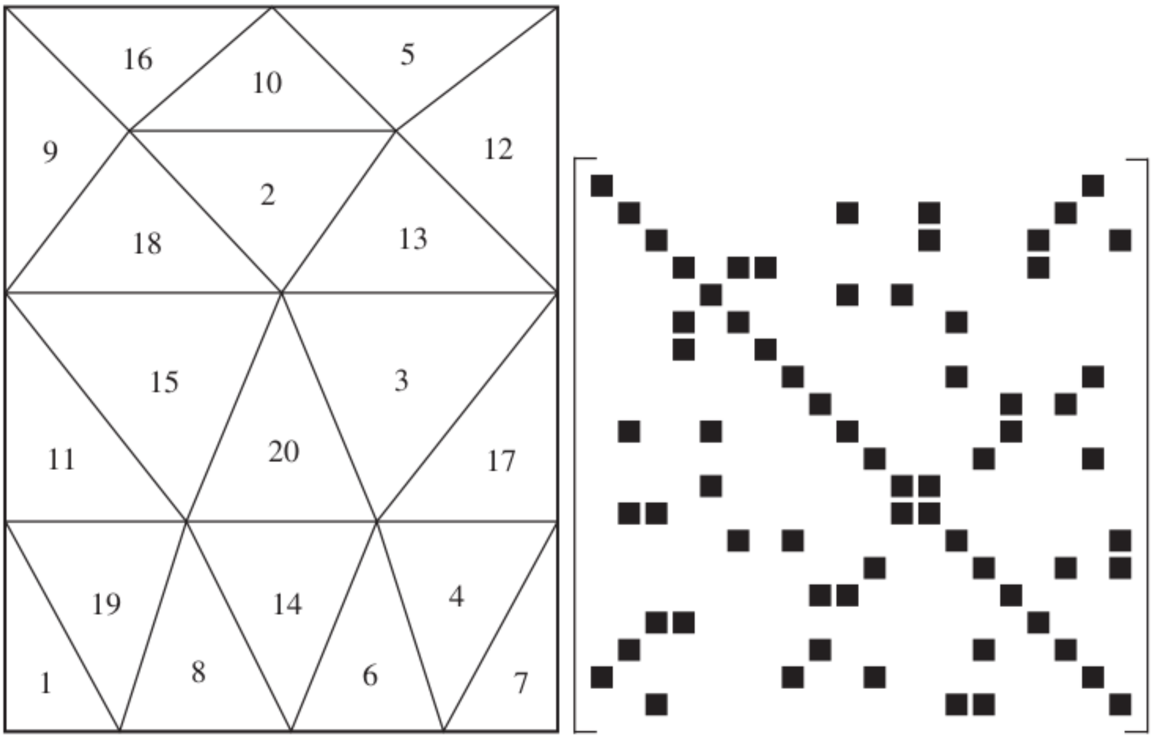
okraj. podm.

ve 2D



2D – nestrukturovaná síť:

zdroj: (Blazek – CFD – Principles & Practice 3rd ed.)



⇒ řídká matice ⇒ pro reprezentaci v počítači se hodí speciální formáty (CSR, ...)

algoritmus seřazení složek u^{n+1}

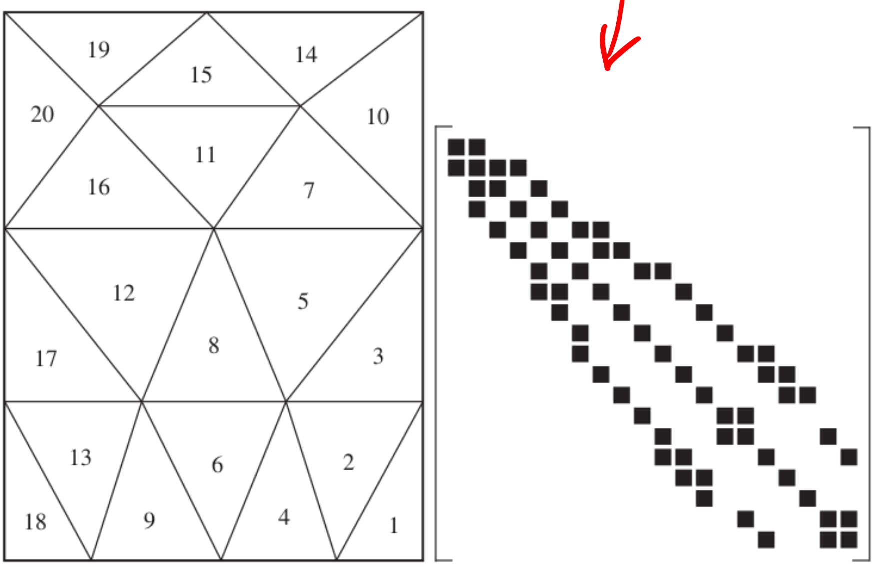


Figure 6.4 Reduced bandwidth (from 18 to 5) of the implicit operator from Fig. 6.3 with reverse-Cuthill-McKee ordering. Nonzero block matrices are displayed as filled rectangles.

$$\mathbb{A}\vec{u} = \vec{f}$$

ITERAČNÍ METODY ŘEŠENÍ $\mathbb{A}u^{n+1} = u^n$

snaha najít aproximaci $\mathbb{A}^{-1}$ $\Leftrightarrow$ předpodmínění soustavy

(číslo podmíněnosti matice $\varkappa = \|A\| \|A^{-1}\|$)

$$A\vec{u} = \vec{f}$$

$$\underbrace{M^{-1}}\mathbb{A}\vec{u} = M^{-1}\vec{f} \quad \text{kde } M \text{ je regulární}$$

"lépe podmíněné" $\Leftarrow$ pokud M^{-1} bude jistá aproximace A^{-1}

Obecná iterační metoda

$$\vec{u}^{(n+1)} = \vec{u}^{(n)} + M^{-1}(\underbrace{\vec{f} - \mathbb{A}\vec{u}^{(n)}}_{\vec{r}^{(n)}})$$

REZIDUUM

.. kdyby $M = \mathbb{A}$ tak $\vec{u}^{(n+1)} = \mathbb{A}^{-1}\vec{f}$

$$\vec{e}^{(n)} = \mathbb{A}^{-1}\vec{f} - \vec{u}^{(n)} \quad \text{CHYBA}$$

$$\text{platí} \quad \mathbb{A}\vec{e}^{(n)} = \vec{r}^{(n)}$$

$$\vec{e}^{(n+1)} = \mathbb{A}^{-1}\vec{f} - \vec{u}^{(n+1)} = \underline{\mathbb{A}^{-1}\vec{f} - \vec{u}^{(n)}} - M^{-1}(\vec{f} - \mathbb{A}\vec{u}^{(n)})$$

$$= \vec{e}^{(n)} - M^{-1}A\,\underline{(A^{-1}\vec{f} - \vec{u}^{(n)})} = \underbrace{(I - M^{-1}A)}_{\mathbb{R}}\vec{e}^{(n)}$$

relaxační matice

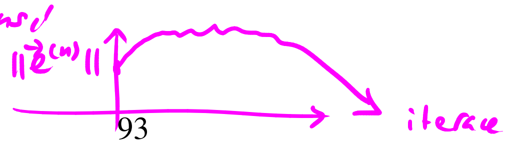
existuje norma, která je libovolně blízko $\rho(\mathbb{R})$

$\||\vec{e}^{(n+1)}\|| \leq \underbrace{\||\mathbb{R}\||}_{<1} \||\vec{e}^{(n)}\||$ vekt. norma konzistentní s danou mat. normou

Metoda konverguje $\Leftrightarrow$ $\vec{e}^{(n)} \xrightarrow{n\to\infty} 0$

$$\Leftrightarrow \quad \boxed{\rho(\mathbb{R}) < 1}$$

v této (neznámé) normě klesá chyba monotónně, ale v euklidovské zdaleka nemusí



Pozn.: Pokud $\vec{e}^{(n)} = \sum_{j=1}^{m} \alpha_j \vec{v}_j$ kde $(\vec{v}_j)_{j=1}^{m}$ jsou vl. vektory $\mathbb{R}$ příslušné (λ_j) $(|\lambda_j|<1)$

$$\vec{e}^{(n+1)} = \mathbb{R}\left(\sum_{j=1}^{m} \alpha_j \vec{v}_j\right) = \sum_j \alpha_j \mathbb{R}\vec{v}_j = \sum_j \alpha_j \lambda_j \vec{v}_j$$

Pokud $\underbrace{|\lambda_j| \ll 1}_{\rho(\mathbb{R}) \ll 1}$ $\forall j$, pak $\vec{e}^{(n)}$ konverguje k $\vec{0}$ "rychle"

Příklad: Jacobiho iterační metoda: $A = -L + D - U$

$$\vec{u}^{(n+1)} = \vec{u}^{(n)} + M^{-1}(\vec{f} - A\vec{u}^{(n)})$$

v J. metodě volíme $M = D \Rightarrow M^{-1} = D^{-1}$ což umožní

$$D\vec{u}^{(n+1)} = D\vec{u}^{(n)} + \left(f - D\vec{u}^{(n)} + (L+U)\vec{u}^{(n)}\right)$$

$$\boxed{D\vec{u}^{(n+1)} - (L+U)\vec{u}^{(n)} = \vec{f}}$$

Pozn. nejprve vl. čísla A pro úlohu ještě jednodušší než

$$\overleftarrow{\partial}_t u + a \overleftrightarrow{\partial}_x u = 0,$$

protože tam by Jacobiho metoda nekonvergovala

$\Downarrow$

POZN: Rotheho metoda

$$\partial_t u = \partial_{xx} u$$

$$\frac{u^{n+1} - u^n}{\Delta t} = \partial_{xx} u^{n+1} \quad u = u(x)$$

$$u^{n+1} = u^n + \Delta t \, \partial_{xx} u^{n+1}$$

sekvence úloh, které je nutné řešit iterační metodou

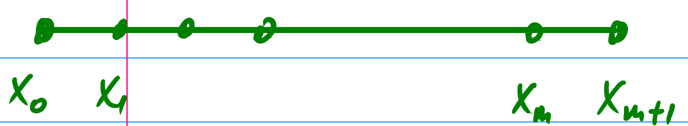
$$\Downarrow$$

Uvažujme úlohu pro Poissonovu rovnici v 1D na $\Omega = (0,1)$

$$\boxed{-u'' = f} \quad \text{s okraj. podmínkami} \quad u(0) = u(1) = 0$$

$$-\delta_{xx} u_h = f_h \quad \Longleftrightarrow \quad \boxed{\begin{gathered} -\frac{u_{k-1} - 2u_k + u_{k+1}}{\Delta x^2} = f_k \\ \forall k = 1, \dots, m \\ u_k = 0 \\ \forall k \in \{0, m+1\} \end{gathered}}$$

PROSTOR DISKRETIZACE



$\Rightarrow u_h \in \mathbb{R}^m$, pak je soustava lin. rovnic ve tvaru

$$A u_h = f_h \quad \text{kde} \quad A = \begin{array}{r} -1 \\ \\ \\ \\ \\ \end{array}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & & \ddots & \\ & & & -1 & 2 \end{pmatrix}\begin{array}{l} \\ \\ \\ \\ -1 \end{array}$$

Ukážeme, že vl. vektory A jsou $\underline{(\vec{v}_j)_k = \sin\left(\frac{jk\pi}{m+1}\right)}$ $\forall j = 1, \dots, m$

$\forall k = \underline{1}, 2, \dots, m-1, \underline{m}$

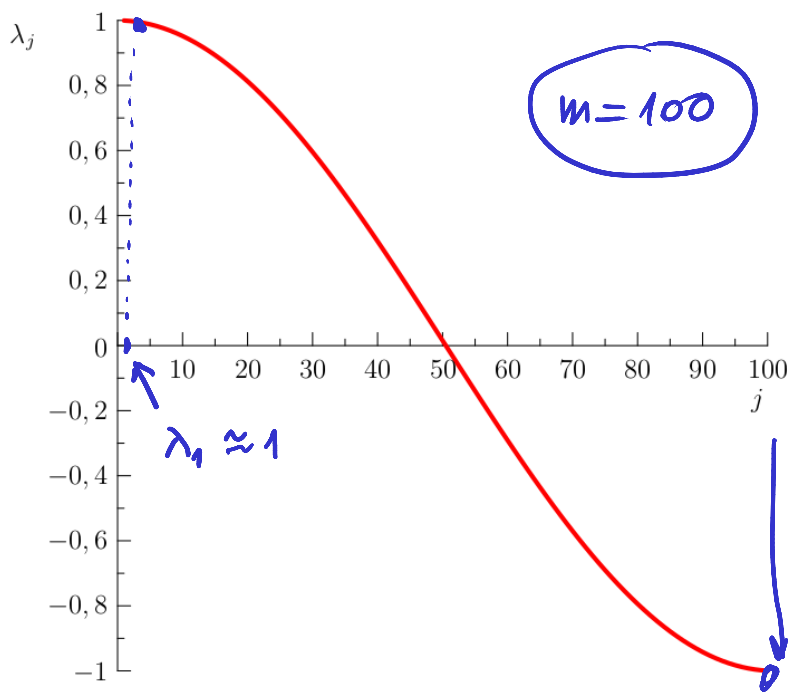
$$(A\vec{v}_j)_k = \underbrace{-\sin\left(\frac{j(k-1)\pi}{m+1}\right)}_{\sin(\alpha-\beta)} + 2\sin\left(\frac{jk\pi}{m+1}\right) \underbrace{- \sin\left(\frac{j(k+1)\pi}{m+1}\right)}_{\sin(\alpha+\beta)}$$

$$= \underbrace{2\left(1 - \cos\left(\frac{j\pi}{m+1}\right)\right)}_{\tilde{\lambda}_j} \sin\left(\frac{jk\pi}{m+1}\right)$$

$$\mathbb{D} = \begin{pmatrix} 2 & & \\ & \ddots & \\ & & 2 \end{pmatrix} \qquad \mathbb{D}^{-1} = \frac{1}{2}\mathbb{I}$$

$$R = \mathbb{I} - \mathbb{M}^{-1}\mathbb{A} = \mathbb{I} - \mathbb{D}^{-1}\mathbb{A} = \underline{\mathbb{I} - \tfrac{1}{2}\mathbb{A}}$$

$$\Rightarrow \lambda_j = 1 - \tfrac{1}{2}\tilde{\lambda}_j = 1 - \left(1 - \cos\left(\frac{j\pi}{m+1}\right)\right) = \cos\left(\frac{j\pi}{m+1}\right)$$



pro $m = 100$

$$\underbrace{\lambda_{100} \approx -1}_{\text{"Moiré efekt"}}$$

$\Rightarrow$ <u>Tzv. TLUMENÁ JACOBIHO METODA</u>

Jacobi:

$$\boxed{D\vec{u}^{(n+1)} - (L+U)\,\vec{u}^{(n)} = \vec{f}}$$

$$D\vec{u}^{*} - (L+U)\,\vec{u}^{(n)} = \vec{f}$$

$$\vec{u}^{(n+1)} = \omega\,\vec{u}^{*} + (1-\omega)\,\vec{u}^{(n)}$$

$\omega = 1 \Rightarrow$ "obyč." Jacobiho m. $\quad \omega \in (0, 1\rangle$

dosadíme: $\vec{u}^{(n+1)} = \omega\left[\vec{u}^{(n)} + \mathbb{D}^{-1}\left(\vec{f} - \mathbb{A}\vec{u}^{(n)}\right)\right] + (1-\omega)\vec{u}^{(n)}$

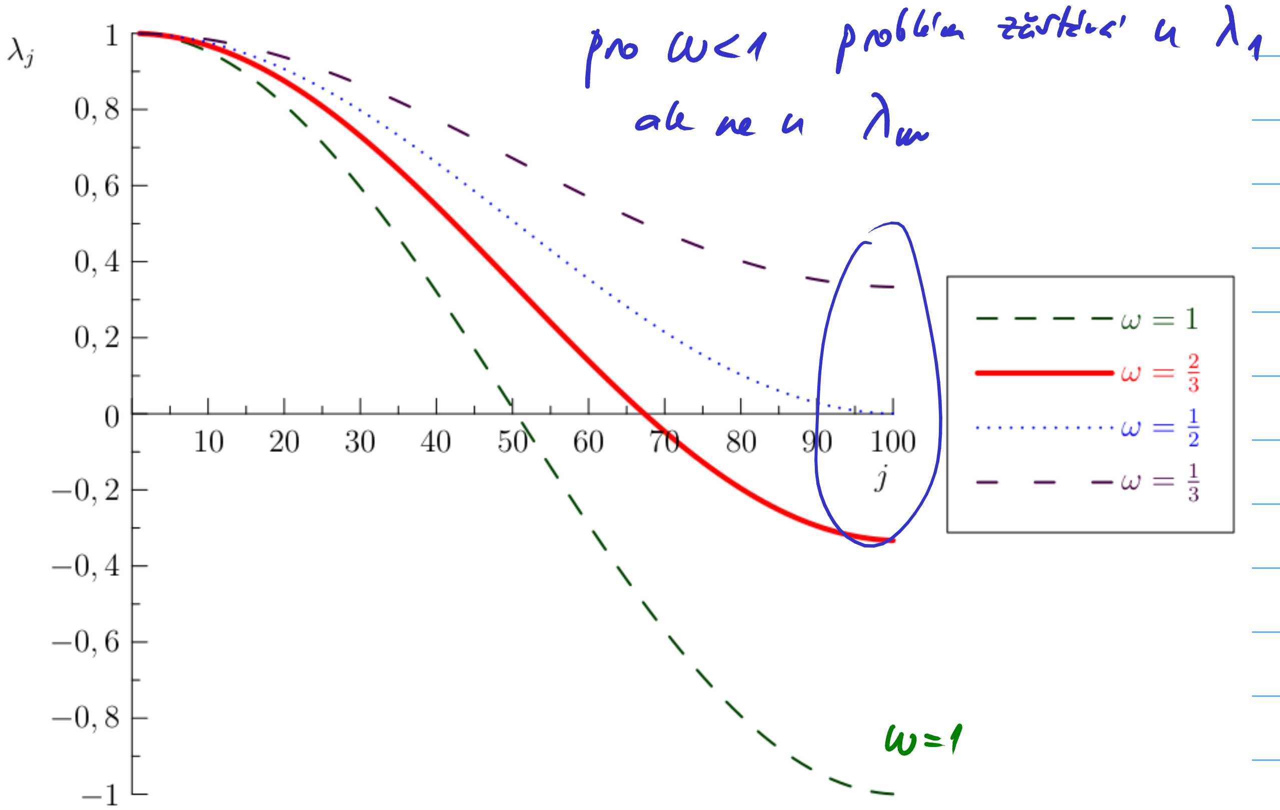
$$= \vec{u}^{(n)} + \underbrace{\omega\mathbb{D}^{-1}}_{\mathbb{M}^{-1}}\left(f - \mathbb{A}u^{(n)}\right)$$

tj.: $\mathbb{M} = \omega^{-1}\mathbb{D}$

$$\mathbb{R} = \mathbb{I} - \mathbb{M}^{-1}\mathbb{A} = \mathbb{I} - \omega\mathbb{D}^{-1}\mathbb{A} = \mathbb{I} - \frac{\omega}{2}\mathbb{A}$$

$$\Rightarrow \lambda_j = 1 - \frac{\omega}{2}\tilde{\lambda}_j = 1 - \frac{\omega}{2}\cdot 2\Big(\underbrace{1 - \cos\left(\frac{j\pi}{n+1}\right)}_{2\sin^2\left(\frac{j\pi}{2(n+1)}\right)}\Big)$$

$$= 1 - 2\omega\sin^2\left(\frac{j\pi}{2(n+1)}\right)$$



Pozn: Gaussova-Seidelova metoda: $M = -L + D$

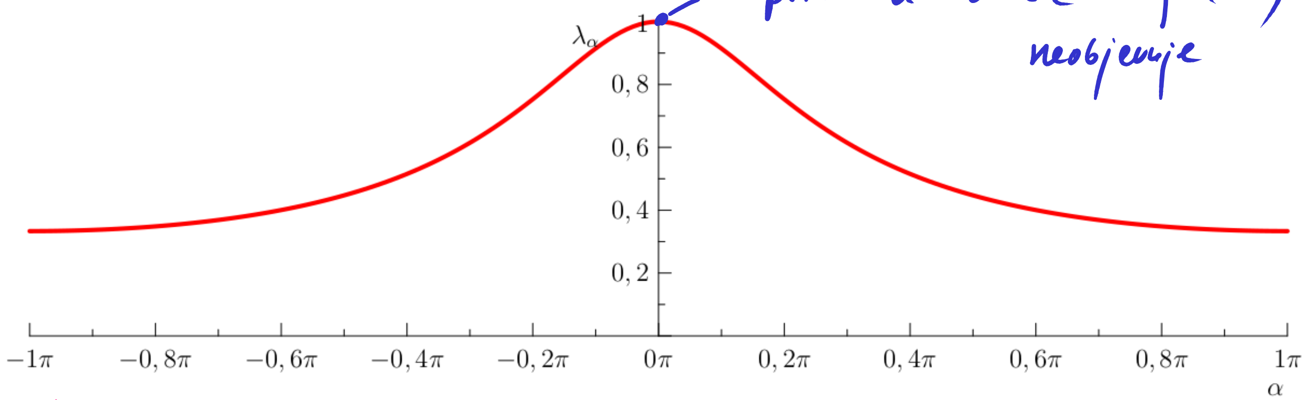
$$\Longleftrightarrow \quad (-L+D)\,\vec{u}^{(n+1)} - U\vec{u}^{(n)} = \vec{f}$$

ale $\vec{v}_j$, λ_j neumíme přesně spočítat

$\Rightarrow$ Von Neumannova spektrální analýza

$\Rightarrow$ obdobný výsledek

přímo $\alpha = 0$ se v $\rho(R)$ neobjevuje



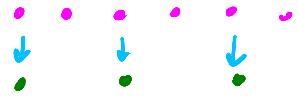
ŘEŠENÍ – URYCHLENÍ KONVERGENCE
je METODA ŘEŠENÍ NA VÍCE SÍTÍCH
tzv. MULTIGRID metoda

Uvažujme dvě sítě

1) o $(m+2)$ prvcích (jemná) s krokem $h = \Delta x$ (m sudé)

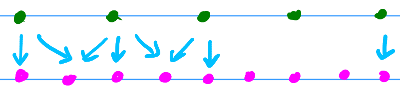
2) o $\frac{m+2}{2}$ prvcích (hrubá) s krokem $2h$

Def. operátorů přechodu mezi sítěmi



$\vec{v}_{2h} = I_{h}^{2h}\uparrow \vec{v}_h$ kde $v_{2h,k} = v_{h,2k}$ (restrikce)

funguje jen pro nulovou okraj. podm.



$$\vec{v}_h = I_{2h}^{h}\uparrow \vec{v}_{2h} = \frac{1}{2} \underbrace{\begin{pmatrix} 1 & & & & \\ 2 & & & & \\ 1 & 1 & & & \\ & 2 & & & \\ & 1 & 1 & & \\ & & \vdots & & \\ & & & 1 & 1 \\ & & & & 2 \\ & & & & 1 \end{pmatrix}}_{J \in \mathbb{R}^{(m+2)\times\left(\frac{m}{2}+1\right)}} \vec{v}_{2h}$$ (interpolace)

POZN: Restrikce lze i: $\vec{v}_{2h} = I_h^{2h}\, \vec{v}_h = J^T \vec{v}_h$

Korekční schéma na 2 sítích

řešíme $A\vec{u} = \vec{f}$ na 2 sítích:

$$A_h \vec{u}_h = \vec{f}_h \;, \quad A_{2h}\vec{u}_{2h} = \vec{f}_{2h}$$

jemná   hrubá

1) provedeme několik (ν_1) iterací řešení $A_h \vec{u}_h = \vec{f}_h$ na jemné síti

$\Rightarrow$ spočítáme $\vec{r}_h$

2) omezíme r ze sítě "h" na "$2h$": $\vec{r}_{2h} = I_h^{2h}\vec{r}_h$

(příslušná chyba $\vec{e}_h$, a tedy ani $\vec{r}_h$ už neobsahuje vysokofrekvenční složky)

$$\boxed{A_{2h}\vec{e}_{2h} = \vec{r}_{2h}}$$

3) provedeme ν_2 iterací řešení $A_{2h}\vec{e}_{2h} = \vec{r}_{2h}$ na hrubé síti "2h" $\Rightarrow$ utlumí se rychleji i nižší frekvence chyby

4) interpolujeme $\vec{e}_{2h}$ na jemnější síť $\vec{e}_h = I^h_{2h}\,\vec{e}_{2h}$

a provedeme opravu $\vec{u}_h := \vec{u}_h + \vec{e}_h$

5) provedeme ν_3 iterací řešení $A_h\vec{u}_h = \vec{f}_h$ opět na jemnější síti s krokem "h"

Zobecnění – přechody mezi více úrovněmi sítí

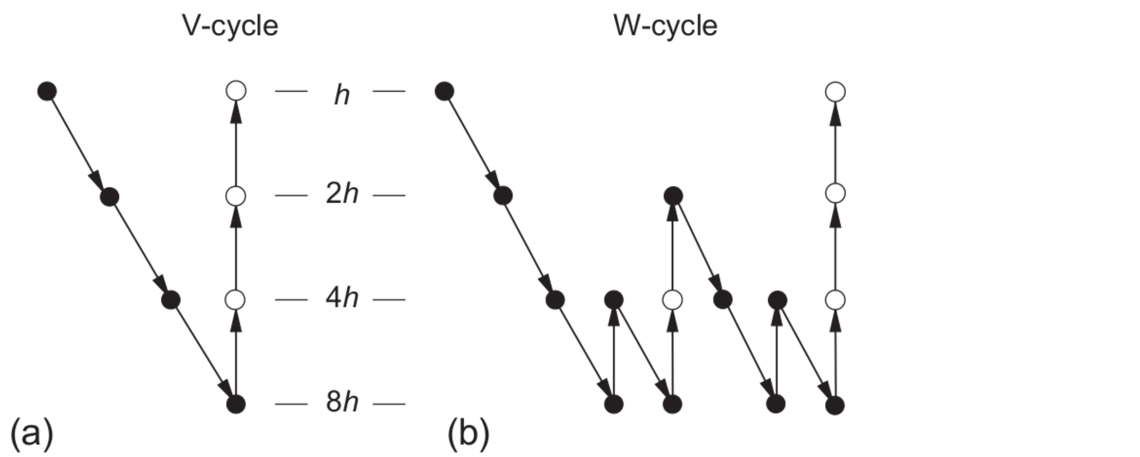
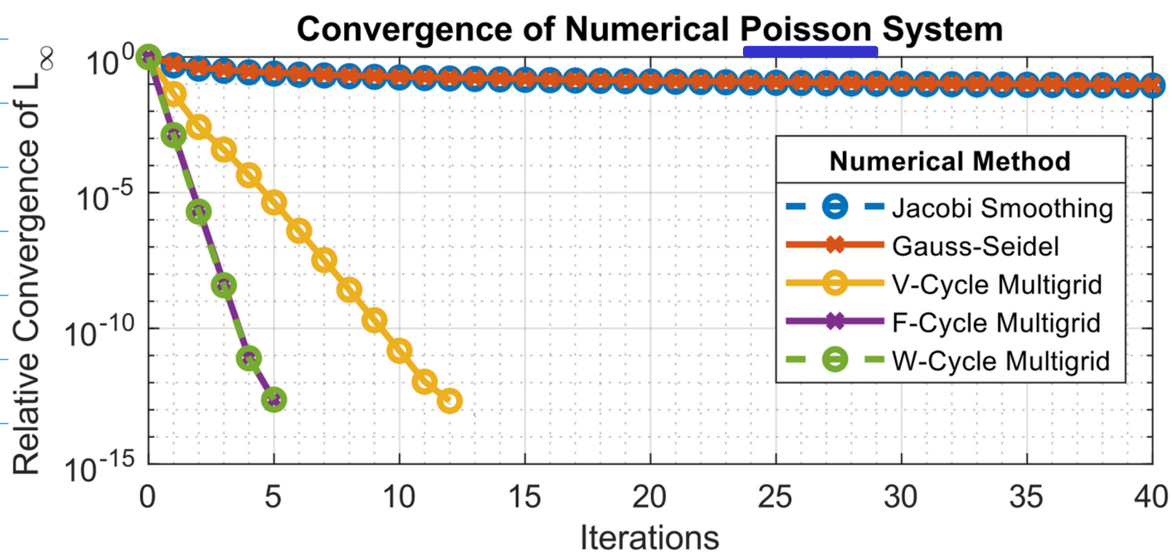
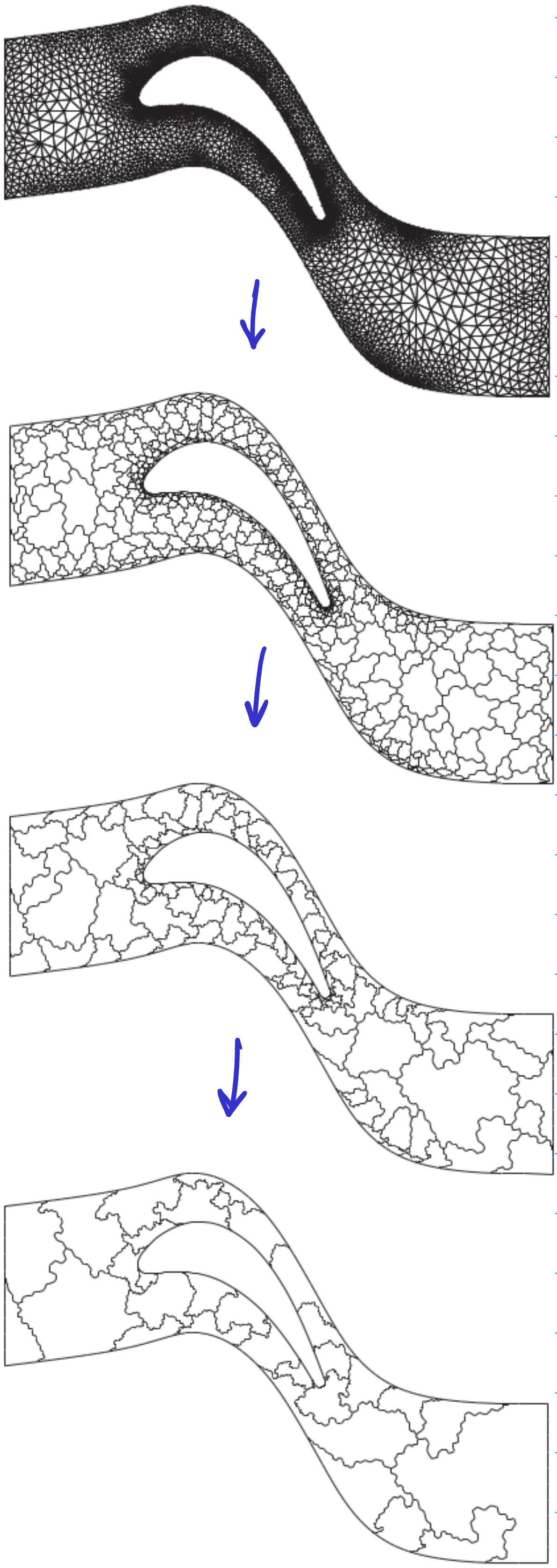


Figure 9.5 Types of multigrid cycles. • denotes time steps before restriction; ∘ represents time steps after prolongation.



MULTIGRID VE 2D NA NESTRUKT. SÍTI



[Blazek - CFD Principles & Practice]

ZAJÍMAVOST – DALŠÍ METODY V CFD

- ALE – Arbitrary Lagrangian Eulerian – MKP + pohyblivá síť

- částicové / bezsíťové metody
  - DEM … Discrete Element Method (interakce mezi částicemi – kolize)
  - MP-PIC (Multiphase Particle-in-Cell)

    MKO (proudění) ↔ pohyb částic

- Viscous Vortex Particle Method
  - virtuální částice reprezentují víry v turbulentním proudění