

Finite volume method

The *finite volume method* is based on (I) rather than (D). The integral conservation law is enforced for small control volumes defined by the computational mesh:

$$\bar{V} = \bigcup_{i=1}^N \bar{V}_i, \quad V_i \cap V_j = \emptyset, \quad \forall i \neq j$$

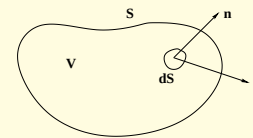
$$u_i = \frac{1}{|V_i|} \int_{V_i} u dV \quad \text{mean value}$$

To be specified

- concrete choice of control volumes
- type of approximation inside them
- numerical methods for evaluation of integrals and fluxes

Integral conservation law (I)

$$\frac{\partial}{\partial t} \int_V u dV + \int_S \mathbf{f} \cdot \mathbf{n} dS = \int_V q dV$$



$$\mathbf{f} = \mathbf{v}u - d\nabla u$$

flux function

$$\int_V \frac{\partial u}{\partial t} dV + \int_V \nabla \cdot \mathbf{f} dV = \int_V q dV$$

Partial differential equation (D)

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{f} = q \quad \text{in } V$$

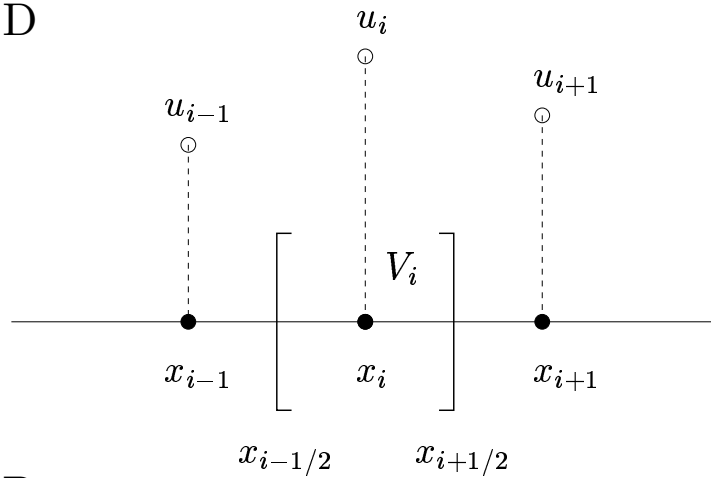
In steady state $\frac{\partial u}{\partial t} = 0$ so that

$$\nabla \cdot (u\mathbf{v}) = \nabla \cdot (d\nabla u) + q$$

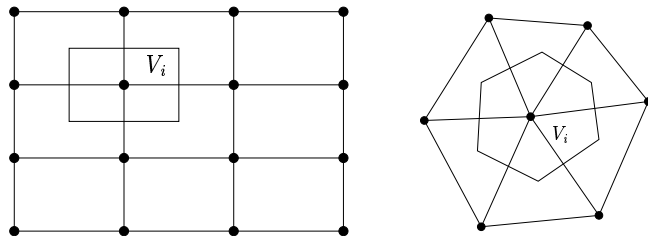
Definition of control volumes

Vertex-centered FVM

1D

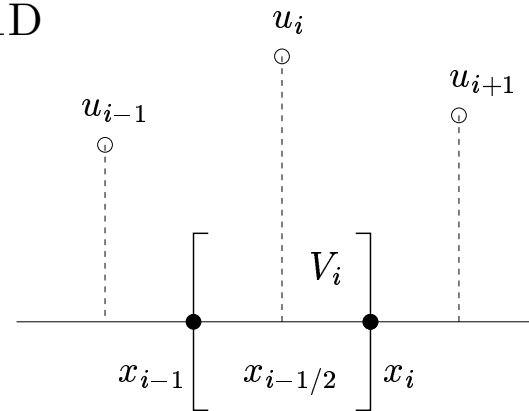


2D

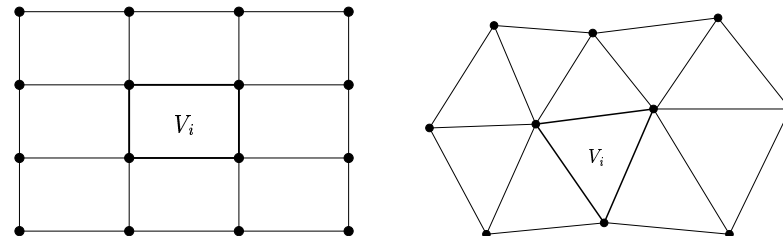


Cell-centered FVM

1D



2D



Different grids / control volumes can be used for different variables ($\mathbf{v}, p, \dots$)

Discretization of local subproblems

Integral equation for a single finite volume

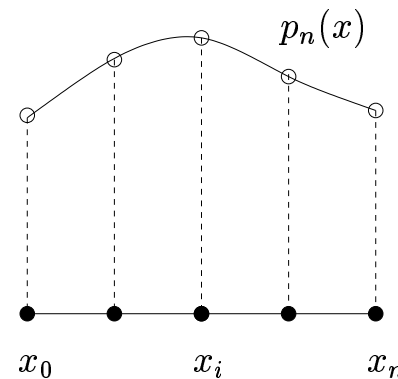
$$\frac{\partial u_i}{\partial t} + \frac{1}{|V_i|} \sum_k \int_{S_k} \mathbf{f} \cdot \mathbf{n}_k dS = q_i, \quad u_i = \frac{1}{|V_i|} \int_{V_i} u dV, \quad q_i = \frac{1}{|V_i|} \int_{V_i} q dV$$

- the integral conservation law is satisfied for each CV and for the entire domain
- to obtain a linear system, integrals must be expressed in terms of mean values

Numerical integration

$$\int_V f(\mathbf{x}) dV \approx \sum_{i=0}^n w_i f(\mathbf{x}_i)$$

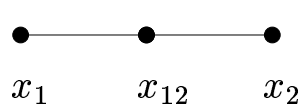
where $w_i \geq 0$ are the *weights* and $\mathbf{x}_i$ are the *nodes* of the quadrature rule



Such formulae can be derived by exact integration of an interpolation polynomial

Newton-Cotes quadrature rules for intervals

1D



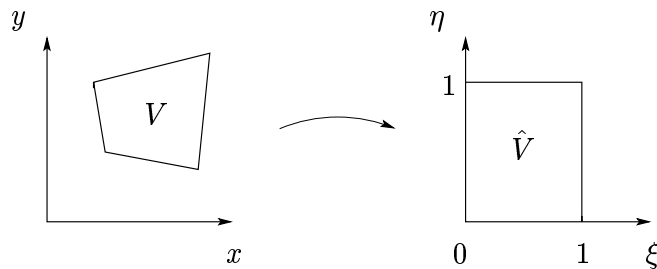
$$x_{12} = \frac{x_1 + x_2}{2}, \quad V = (x_1, x_2), \quad |V| = x_2 - x_1$$

Midpoint rule $\int_V f(x) dV \approx |V| f_{12}$ exact for $f \in P_1(V)$

Trapezoidal rule $\int_V f(x) dV \approx |V| \frac{f_1 + f_2}{2}$ exact for $f \in P_1(V)$

Simpson's rule $\int_V f(x) dV \approx |V| \frac{f_1 + 4f_{12} + f_2}{6}$ exact for $f \in P_3(V)$

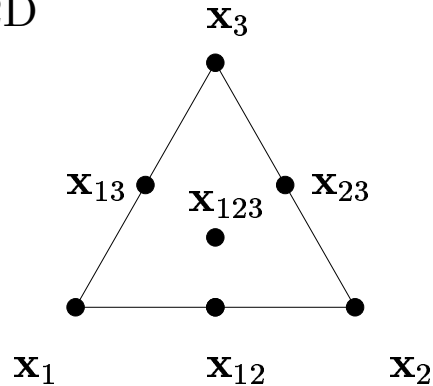
Numerical integration for quadrilaterals/hexahedra



*use a mapping onto a unit square
and apply 1D quadrature rules in
each coordinate direction*

Newton-Cotes quadrature rules for triangles

2D



Midpoints

$$\mathbf{x}_{12} = \frac{\mathbf{x}_1 + \mathbf{x}_2}{2}, \quad \mathbf{x}_{13} = \frac{\mathbf{x}_1 + \mathbf{x}_3}{2}, \quad \mathbf{x}_{23} = \frac{\mathbf{x}_2 + \mathbf{x}_3}{2}$$

Center of gravity

$$\mathbf{x}_{123} = \frac{\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3}{3}$$

$$\int_V f(\mathbf{x}) dV \approx |V| f_{123}$$

exact for $f \in P_1(V)$

$$\int_V f(\mathbf{x}) dV \approx |V| \frac{f_1 + f_2 + f_3}{3}$$

exact for $f \in P_1(V)$

$$\int_V f(\mathbf{x}) dV \approx |V| \frac{f_{12} + f_{23} + f_{13}}{3}$$

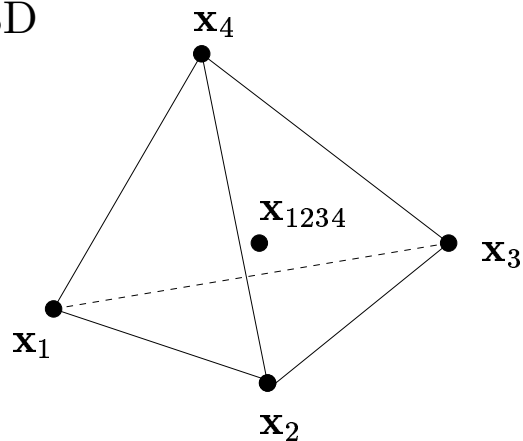
exact for $f \in P_2(V)$

$$\int_V f(\mathbf{x}) dV \approx |V| \frac{3(f_1 + f_2 + f_3) + 8(f_{12} + f_{23} + f_{13}) + 27f_{123}}{60}$$

exact for $f \in P_3(V)$

Newton-Cotes quadrature rules for tetrahedra

3D



Center of gravity

$$\mathbf{x}_{1234} = \frac{\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3 + \mathbf{x}_4}{4}$$

$$\int_V f(\mathbf{x}) dV \approx |V| f_{1234}$$

exact for $f \in P_1(V)$

$$\int_V f(\mathbf{x}) dV \approx |V| \frac{f_1 + f_2 + f_3 + f_4}{4}$$

exact for $f \in P_1(V)$

$$\int_V f(\mathbf{x}) dV \approx |V| \frac{f_1 + f_2 + f_3 + f_4 + 16f_{1234}}{20}$$

exact for $f \in P_2(V)$

Interpolation techniques

Problem: the solution is available only at computational nodes (CV centers)

Interpolation is needed to obtain the function values at quadrature points

Volume integrals $u_i = \frac{1}{|V_i|} \int_{V_i} u \, dV \approx u(\bar{\mathbf{x}}_i)$ midpoint rule

Surface integrals $\mathbf{f} = \mathbf{v}u - d\nabla u \Rightarrow \frac{1}{|V_i|} \sum_k \int_{S_k} \mathbf{f} \cdot \mathbf{n}_k \, dS = I_c + I_d$

$$I_c = \frac{1}{|V_i|} \sum_k \int_{S_k} (\mathbf{v} \cdot \mathbf{n}_k) u \, dS, \quad I_d = \frac{1}{|V_i|} \sum_k \int_{S_k} d(\mathbf{n}_k \cdot \nabla u) \, dS$$

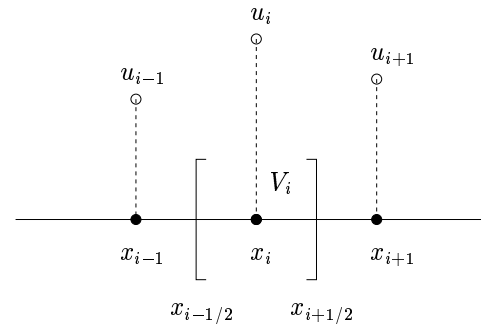
Approximation of convective fluxes

1D: $|V_i| \equiv \Delta x = \frac{1}{N}, \quad x_i = i\Delta x$

$$I_c = v \frac{u_{i+1/2} - u_{i-1/2}}{\Delta x}, \quad v = \text{const}$$

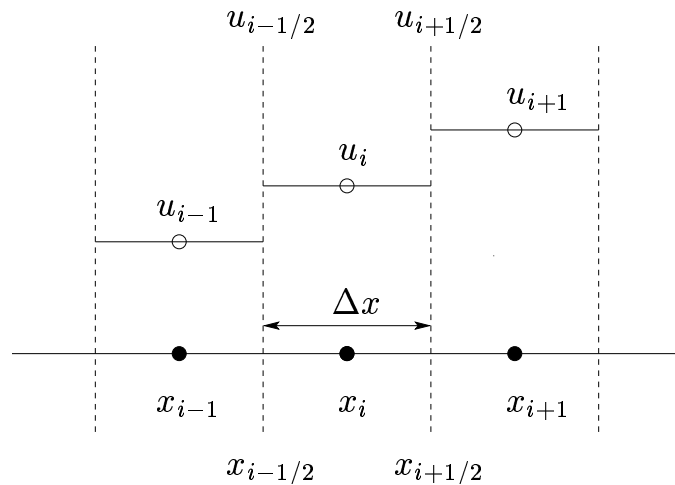
How to define the interface values $u_{i\pm 1/2}$?

vertex-centered FVM



Upwind difference approximation (UDS)

Piecewise-constant solution



Upwind-biased interface values

$$\boxed{v > 0} \quad u_{i-1/2} \approx u_{i-1}, \quad u_{i+1/2} \approx u_i$$

$$I_c \approx v \frac{u_i - u_{i-1}}{\Delta x} \quad \text{backward difference}$$

$$\boxed{v < 0} \quad u_{i-1/2} \approx u_i, \quad u_{i+1/2} \approx u_{i+1}$$

$$I_c \approx v \frac{u_{i+1} - u_i}{\Delta x} \quad \text{forward difference}$$

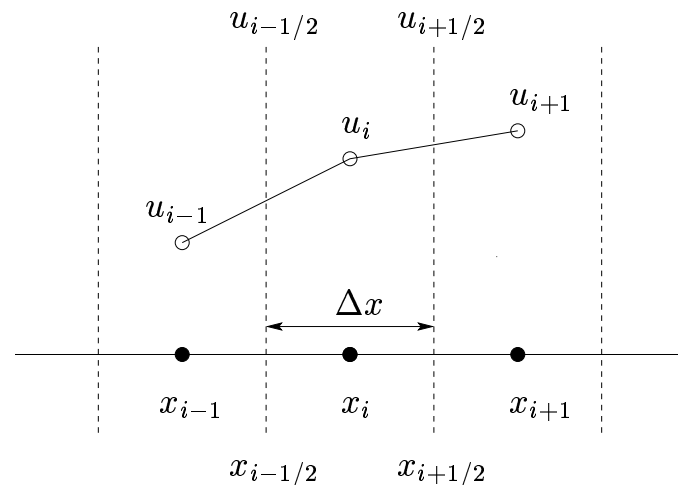
Taylor series expansion

$$vu_{i+1/2} = vu_i + \frac{v\Delta x}{2} \left(\frac{\partial u}{\partial x} \right)_i + v \frac{(\Delta x)^2}{8} \left(\frac{\partial^2 u}{\partial x^2} \right)_i + \dots$$

a first-order accurate flux approximation, the leading truncation error resembles a diffusive flux $d \frac{\partial u}{\partial x}$ with $d = \frac{v\Delta x}{2}$ being the *numerical diffusion coefficient*

Central difference approximation (CDS)

Piecewise-linear solution



Interpolation polynomial

$$p_1(x) = u_L \frac{x_R - x}{x_R - x_L} + u_R \frac{x - x_L}{x_R - x_L}$$

Averaged interface values

$$u_{i-1/2} \approx \frac{u_{i-1} + u_i}{2}, \quad u_{i+1/2} \approx \frac{u_i + u_{i+1}}{2}$$

$$I_c \approx v \frac{u_{i+1} - u_{i-1}}{2\Delta x} \quad \text{central difference}$$

Taylor series expansions

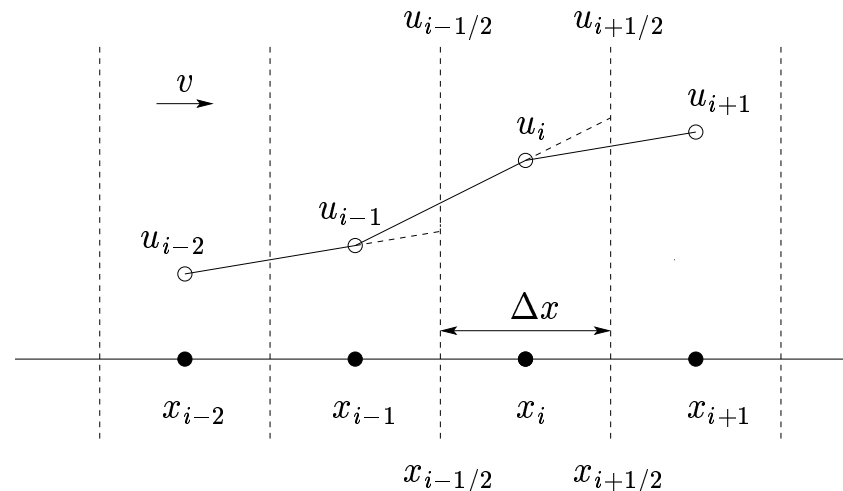
$$u_{i+1} = u_{i+1/2} + \frac{\Delta x}{2} \left(\frac{\partial u}{\partial x} \right)_{i+1/2} + \frac{(\Delta x)^2}{8} \left(\frac{\partial^2 u}{\partial x^2} \right)_{i+1/2} + \dots$$

$$u_i = u_{i+1/2} - \frac{\Delta x}{2} \left(\frac{\partial u}{\partial x} \right)_{i+1/2} + \frac{(\Delta x)^2}{8} \left(\frac{\partial^2 u}{\partial x^2} \right)_{i+1/2} - \dots$$

Hence,
$$u_{i+1/2} = \frac{u_i + u_{i+1}}{2} - \frac{(\Delta x)^2}{8} \left(\frac{\partial^2 u}{\partial x^2} \right)_{i+1/2} + \dots \quad (\text{second-order accuracy})$$

Linear upwind difference scheme (LUDS)

Piecewise-linear solution



Upwind-biased extrapolation

$$\boxed{v > 0} \quad \begin{aligned} u_{i-1/2} &\approx \frac{3u_{i-1} - u_{i-2}}{2} \\ u_{i+1/2} &\approx \frac{3u_i - u_{i-1}}{2} \end{aligned}$$

$$I_c \approx v \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x}$$

$$\boxed{v < 0} \quad \begin{aligned} u_{i-1/2} &\approx \frac{3u_i - u_{i+1}}{2} \\ u_{i+1/2} &\approx \frac{3u_{i+1} - u_{i+2}}{2} \end{aligned}$$

$$I_c \approx -v \frac{3u_i - 4u_{i+1} + u_{i+2}}{2\Delta x}$$

LUDS is second-order accurate, equivalent to the one-sided 3-point finite difference

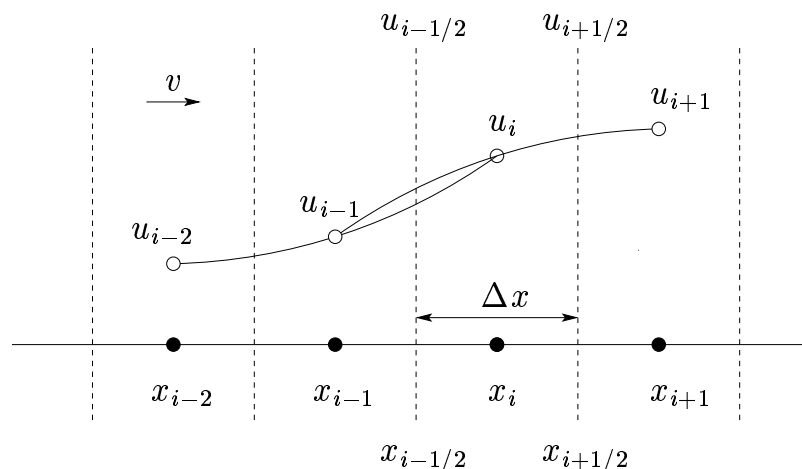
The matrix is no longer tridiagonal (shifted, upper/lower triangular if $I_d = 0$)

Defect correction: $I_{LUDS}^{(m+1)} = I_{UDS}^{(m+1)} + [I_{LUDS}^{(m)} - I_{UDS}^{(m)}], \quad m = 0, 1, 2, \dots$

Quadratic upwind difference scheme (QUICK)

Quadratic Upwind Interpolation for Convective Kinematics

$$p_2(x) = u_L \frac{x-x_M}{x_L-x_M} \frac{x_R-x}{x_R-x_L} + u_M \frac{x-x_L}{x_M-x_L} \frac{x_R-x}{x_R-x_M} + u_R \frac{x-x_L}{x_R-x_L} \frac{x-x_M}{x_R-x_M}$$



- third-order flux approximation
- second-order overall accuracy
(because of the midpoint rule)
- marginally better than LUDS

Upwind-biased interface values

$$\boxed{v > 0} \quad \begin{aligned} u_{i-1/2} &\approx \frac{3u_i + 6u_{i-1} - u_{i-2}}{8} \\ u_{i+1/2} &\approx \frac{3u_{i+1} + 6u_i - u_{i-1}}{8} \end{aligned}$$

$$I_c \approx v \frac{3u_{i+1} + 3u_i - 7u_{i-1} + u_{i-2}}{8\Delta x}$$

$$\boxed{v < 0} \quad \begin{aligned} u_{i-1/2} &\approx \frac{3u_{i-1} + 6u_i - u_{i+1}}{8} \\ u_{i+1/2} &\approx \frac{3u_i + 6u_{i+1} - u_{i+2}}{8} \end{aligned}$$

$$I_c \approx -v \frac{3u_{i-1} + 3u_i - 7u_{i+1} + u_{i+2}}{8\Delta x}$$

Evaluation of surface integrals

Approximation of convective fluxes

- any second-order finite volume scheme is a linear combination of *CDS* and *LUDS* approximations (e.g. $I_{QUICK} = \frac{3}{4}I_{CDS} + \frac{1}{4}I_{LUDS}$)
- high-order schemes can be readily derived by polynomial fitting based on $p_m(x)$, $m > 2$ but pay off only if the quadrature rule matches their accuracy
- a high-order scheme is guaranteed to produce better results than a low-order one only *asymptotically* i.e. for sufficiently fine meshes

Approximation of diffusive fluxes

$$\left(\frac{\partial u}{\partial x}\right)_{i-1/2} \approx \frac{u_i - u_{i-1}}{\Delta x}, \quad \left(\frac{\partial u}{\partial x}\right)_{i+1/2} \approx \frac{u_{i+1} - u_i}{\Delta x} \quad \text{slopes of the straight lines}$$

Second-order accurate central difference

$$I_d = -\frac{d\left(\frac{\partial u}{\partial x}\right)_{i+1/2} - d\left(\frac{\partial u}{\partial x}\right)_{i-1/2}}{\Delta x} \approx -d\frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}$$

Discretization of transport problems

Convective transport $\rightarrow$ first derivatives $\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}$

$$\boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0} \quad \text{continuity equation (hyperbolic)}$$

Diffusive transport $\rightarrow$ second derivatives $\frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial y^2}, \frac{\partial^2}{\partial z^2}, \dots$

$$\boxed{\frac{\partial T}{\partial t} - \nabla \cdot (\kappa \nabla T) = 0} \quad \text{heat conduction (parabolic/elliptic)}$$

Dimensionless numbers: ratio of **convection** and **diffusion**

$$Pe = \frac{v_0 L_0}{d} \quad \text{Peclet number} \quad Re = \frac{v_0 L_0}{\nu} \quad \text{Reynolds number}$$

Convection-dominated transport equations (such that $Pe \gg 1$ or $Re \gg 1$) are essentially hyperbolic, which may give rise to numerical difficulties.

Example: 1D convection-diffusion equation

Boundary value problem

$$\begin{cases} v \frac{\partial u}{\partial x} - d \frac{\partial^2 u}{\partial x^2} = 0 & \text{in } (0, 1) \\ u(0) = 0, \quad u(1) = 1 \end{cases}$$

Exact solution

$$u = \frac{e^{\text{Pe} x} - 1}{e^{\text{Pe}} - 1}, \quad \text{Pe} = \frac{v}{d}$$

where Pe is the Peclet number

Vertex-centered finite volume method

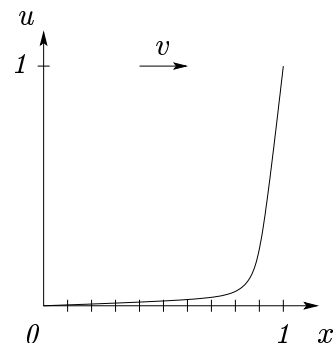
$$\text{Pe} \frac{u_{i+1/2} - u_{i-1/2}}{\Delta x} - \frac{\left(\frac{\partial u}{\partial x}\right)_{i+1/2} - \left(\frac{\partial u}{\partial x}\right)_{i-1/2}}{\Delta x} = 0$$

Solution behavior for $v > 0$

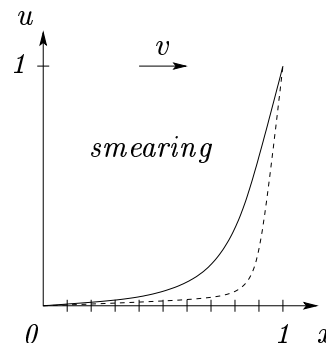
$$x_i = i\Delta x, \quad \Delta x = \frac{1}{N}, \quad i = 0, 1, \dots, N$$

$$\text{Pe} = 40$$

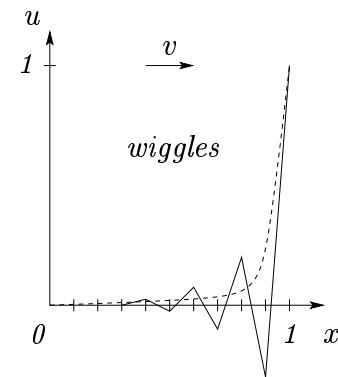
$$\Delta x = 0.1$$



exact solution



upwind difference



central difference

Discretized convection-diffusion equation

Upwind difference scheme

$$\text{Pe} \frac{u_i - u_{i-1}}{\Delta x} - \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2} = 0, \quad i = 1, \dots, N-1$$

Central difference scheme

$$\text{Pe} \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2} = 0, \quad i = 1, \dots, N-1$$

Boundary conditions $u_0 = 0, \quad u_N = 1$

Linear system

$$Au = F$$

$$A \in \mathbb{R}^{N-1 \times N-1} \quad u, F \in \mathbb{R}^{N-1}$$

$$A = \frac{1}{(\Delta x)^2} \begin{bmatrix} b & c & & \\ a & b & c & \\ & a & b & c \\ & & \ddots & \\ & & a & b \end{bmatrix}, \quad u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-1} \end{bmatrix}, \quad F = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ -\frac{c}{(\Delta x)^2} \end{bmatrix}$$

where A is a tridiagonal, nonsymmetric matrix with constant coefficients

Exact solution of the difference scheme

Linear equation for an interior node

$$au_{i-1} + bu_i + cu_{i+1} = 0 \quad a < 0, \quad b > 0, \quad a + b + c = 0$$

	a	b	c
upwind difference	$-1 - \text{Pe } \Delta x$	$2 + \text{Pe } \Delta x$	-1
central difference	$-1 - 0.5 \text{Pe } \Delta x$	2	$-1 + 0.5 \text{Pe } \Delta x$

Trial solution $u_i = \alpha + \beta r^i$, $u_0 = 0$, $u_N = 1$ (boundary conditions)

$$ar^{i-1} + br^i + cr^{i+1} = 0, \quad b = -(a + c) \quad \Rightarrow \quad cr^2 - (a + c)r + a = 0$$

$$r_{1,2} = \frac{(a + c) \pm \sqrt{(a + c)^2 - 4ac}}{2c} = \frac{(a + c) \pm (a - c)}{2c}, \quad r_1 = \frac{a}{c}, \quad r_2 = 1$$

A constant solution does not satisfy the BC $\Rightarrow r = \frac{a}{c}$ is the root we need.

Numerical behavior of the difference scheme

Trial solution $u_i = \alpha + \beta \left(\frac{a}{c}\right)^i$ subject to the boundary conditions

$$u_0 = \alpha + \beta = 0, \quad u_N = \alpha + \beta \left(\frac{a}{c}\right)^N = 1 \quad \Rightarrow \quad \alpha = -\beta = \frac{1}{1 - \left(\frac{a}{c}\right)^N}$$

Hence, $u_i = \frac{1 - \left(\frac{a}{c}\right)^i}{1 - \left(\frac{a}{c}\right)^N} = \frac{P}{Q}$ is the exact solution of the difference scheme.

$$\boxed{c < 0} \quad a < 0, \quad \frac{a}{c} > 0 \quad \left\{ \begin{array}{ll} \frac{a}{c} > 1 & \Rightarrow P < 0, \quad Q < 0 \Rightarrow u_i > 0 \\ 0 < \frac{a}{c} < 1 & \Rightarrow P > 0, \quad Q > 0 \Rightarrow u_i > 0 \end{array} \right.$$

positivity-preserving

$$\boxed{c > 0} \quad a < 0, \quad \frac{a}{c} < 0; \quad a + c = -b < 0 \quad \Rightarrow \quad c < -a \quad \Rightarrow \quad \frac{a}{c} < -1$$

P changes its sign so that $\text{sign}(u_i) = -\text{sign}(u_{i\pm 1}) \Rightarrow$ nonphysical oscillations

$$\boxed{c = 0} \quad u_i = -\frac{a}{b}u_{i-1} = 0, \quad i = 1, \dots, N-1 \quad u_0 = 0, \quad u_N = 1$$

no spurious oscillations but the accuracy leaves a lot to be desired

Evaluation of the central difference scheme

Criterion: *the difference scheme produces no oscillations if $c \leq 0$*

Under this condition the matrix A is diagonally dominant

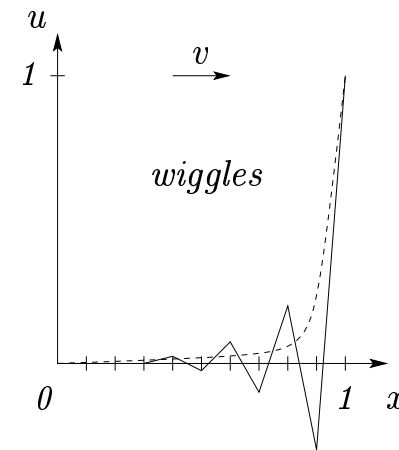
$$a < 0, \quad b = -(a + c) \quad \Rightarrow \quad \begin{aligned} |b| &= |a| + |c| && \text{for } c \leq 0 \\ |b| &< |a| + |c| && \text{for } c > 0 \end{aligned}$$

Moreover, A is an M-matrix so that all the entries of its inverse are nonnegative

Central difference scheme

$$c = -1 + \frac{\text{Pe} \Delta x}{2} \leq 0 \quad \Rightarrow \quad \text{Pe} \Delta x \leq 2$$

- this condition is very restrictive for large Pe
- wiggles occur just in the vicinity of steep gradients
- local mesh refinement is useful for moderate Pe



Evaluation of the upwind difference scheme

Upwind difference scheme $c = -1$ is negative unconditionally

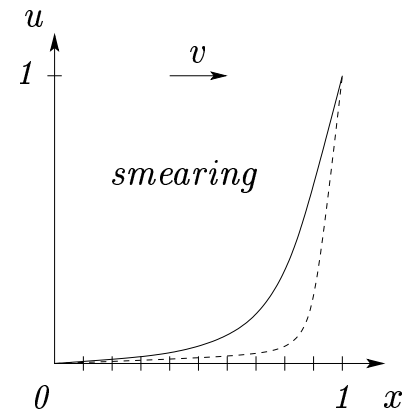
Taylor series
$$u_{i\pm 1} = u_i \pm \Delta x \left(\frac{\partial u}{\partial x} \right)_i + \frac{(\Delta x)^2}{2} \left(\frac{\partial^2 u}{\partial x^2} \right)_i \pm \frac{(\Delta x)^3}{6} \left(\frac{\partial^3 u}{\partial x^3} \right)_i + \dots$$

$$\text{Pe} \frac{u_i - u_{i-1}}{\Delta x} - \frac{u_{i-1} - 2u_i + u_{i+1}}{(\Delta x)^2} = \text{Pe} \left(\frac{\partial u}{\partial x} \right)_i - \left(\frac{\partial^2 u}{\partial x^2} \right)_i - \frac{\text{Pe} \Delta x}{2} \left(\frac{\partial^2 u}{\partial x^2} \right)_i + \mathcal{O}(\Delta x)^2$$

The truncation error is $\mathcal{O}(\Delta x)$ for the original equation but $\mathcal{O}(\Delta x)^2$ for the so-called *modified equation*

$$v \frac{\partial u}{\partial x} - \left(d + \frac{v \Delta x}{2} \right) \frac{\partial^2 u}{\partial x^2} = 0$$

where $\frac{v \Delta x}{2}$ is the numerical (artificial) diffusion coefficient



UDS is nonoscillatory but not to be recommended because of its low accuracy.