Finite Volume Method

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Outline

- Finite Volume Method Overview
- Grid issues
- Discretization of the transport equation
  - Discretization of diffusive term
  - Discretization of convective term
  - TVD schemes
  - Discretization of temporal term
  - Discretization of the source term
- Interpolation and calculation of the gradient
- Boundary conditions
- SLAE formation
- Implementation issues

Applications

- The mainstream approach in CFD
  - ANSYS Fluent, CFX
  - OpenFOAM
  - Many others
- Incompressible flows
- Gas dynamics (subsonic, supersonic)
- Heat transfer

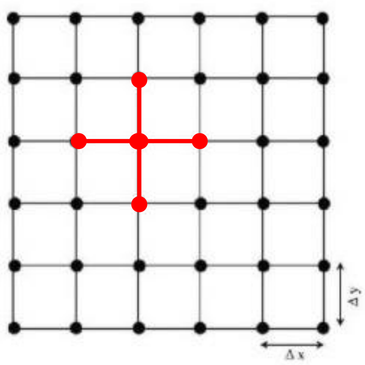
FDM vs. FVM

Finite Difference Method

- Use equation in differential form

$$\frac{\partial \varphi}{\partial t} = \Gamma\left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2}\right) + q(x,y,t)$$

- Approximate differential operators

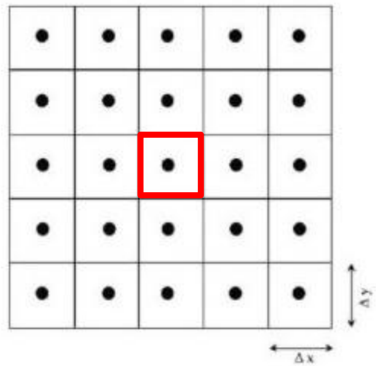


Finite Volume Method

- Use equation in integral form

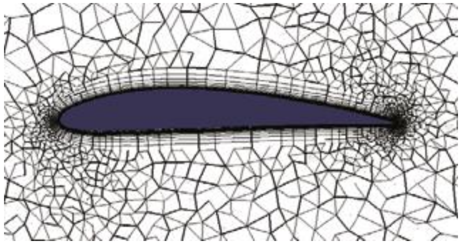
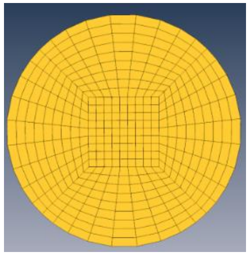
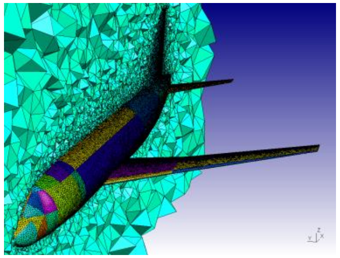
$$\frac{\partial}{\partial t}\int_{\Omega} \varphi d\omega = \int_{\partial\Omega} \Gamma \nabla \varphi \cdot \mathbf{n} ds + \int_{\Omega} q(x,y,t) d\omega$$

- Approximate integral operators



Finite volume: basic methodology

- Divide the domain into control volumes

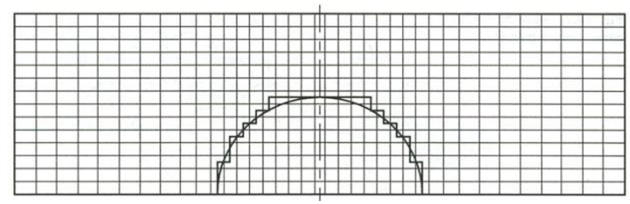
- Integrate the differential equation over the control volume and apply the divergence theorem
- To evaluate derivative terms, values at the control volume faces are needed: have to make an assumption about how the value varies
- Result is a set of linear algebraic equations: one for each control volume
- Solve iteratively or simultaneously

FVM features

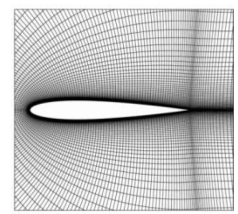
- Mass, momentum and energy are always conserved even on coarse grids
- Works well if variables may not be continuously differentiable across shocks and other discontinuities
- Applicable for unstructured grids with variable shape nodes and faces count
- The method is applicable to both steady-state and transient calculations
- Efficient, iterative solvers well developed
- The most spread and well-developed in CFD

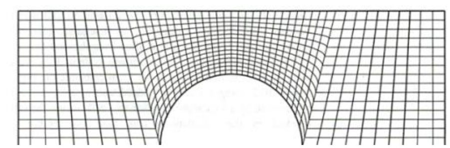
Grid issues

- Stepwise boundary approximation

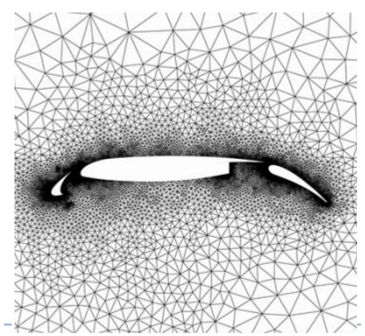


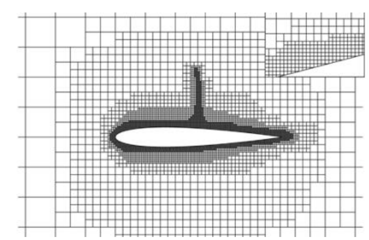
- Body fitted grids
  - Orthogonal
  - Non-orthogonal





- Block structured grids
- Unstructured grids





Discretization of transport equation

- Consider generalized transport equation for quantity φ

$$\frac{\partial \rho\varphi}{\partial t} + div\left(\rho\varphi\,\mathbf{v}\right) = div\left(\Gamma\nabla\varphi\right) + q$$

$$\begin{pmatrix} Rate\ of\ local \\ change\ of\ \varphi \end{pmatrix} + \begin{pmatrix} Net\ rate\ of\ \ advection\ of\ \varphi \\ by\ transport\ \ field\ \ \mathbf{v} = \mathbf{v}(\mathbf{x},t) \end{pmatrix} = \begin{pmatrix} Rate\ of\ change\ of \\ \varphi\ due\ to\ diffusion \end{pmatrix} + \begin{pmatrix} Rate\ of\ change\ of \\ \varphi\ due\ to\ sources \end{pmatrix}$$

$$Unsteady\ term \quad + \quad Convection\ term \quad = \quad Diffusion\ term \quad + \quad Source\ term$$

- Integrate over Control Volume Ω and apply Gauss divergence theorem

$$\int_{\Omega} \frac{\partial \rho\varphi}{\partial t} + \int_{S} \rho\varphi\,\mathbf{v}\cdot d\mathbf{S} = \int_{S} \Gamma\nabla\varphi\cdot d\mathbf{S} + \int_{\Omega} q\,d\Omega$$

$$\begin{pmatrix} Rate\ of\ \ change \\ of\ \varphi\ in\ CV \end{pmatrix} + \begin{pmatrix} Convective\ \ flux\ of\ \varphi \\ through\ CV\ \ boundary \end{pmatrix} = \begin{pmatrix} Diffusive\ \ flux\ of\ \varphi \\ through\ CV\ \ boundary \end{pmatrix} + \begin{pmatrix} Generation\ of\ \varphi \\ in\ CV\ \ by\ sources \end{pmatrix}$$

Discretization of transport equation

- Method accuracy is determined by approximation of surface and volume integrals
- If function is assumed to be constant over CV (Control Volume) and CF (CF - Cell Face) we obtain first order of accuracy

- Linear variation of function in CV and CF

$$\varphi(\mathbf{r}) = \varphi_P + \left(\mathbf{r} - \mathbf{r}_P\right) \cdot \left(\nabla \varphi\right)_P, \quad \varphi_P = \varphi(\mathbf{r}_P),$$

enables to construct the second order approximation schemes. Here P or $\mathbf{r}_P$ is a gravity center of CV/CF

$$\int_{\Omega_P} \left(\mathbf{r} - \mathbf{r}_P\right) \cdot \left(\nabla \varphi\right)_P = 0$$

Discretization of transport equation

- Approximation of volume and surface integrals yields

$$\int_{\Omega} \frac{\partial \rho\varphi}{\partial t} + \int_{S} \rho\varphi \, \mathbf{v} \cdot d\mathbf{S} = \int_{S} \Gamma \nabla \varphi \cdot d\mathbf{S} + \int_{\Omega} q d\Omega$$

$$\Downarrow$$

$$\frac{\partial}{\partial t}\left(\rho_P \varphi_P \Omega_P\right) + \sum_f \varphi_f \left(\rho_f \mathbf{v}_f \cdot \mathbf{S}_f\right) = \sum_f \Gamma_f \left(\nabla \varphi_f \cdot \mathbf{S}_f\right) + q_P \Omega_P$$

- Required approximation of convective and diffusive fluxes through CF
- We know values of φ at CV centers. How to calculate values at center of CF?

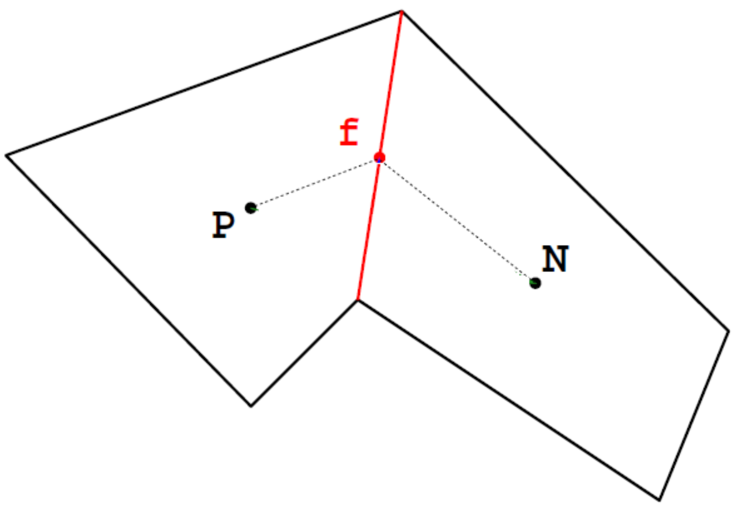
Values at CF interpolation

- Simple linear interpolation:

$$\varphi_f = \lambda_{Pf}\varphi_P + \left(1-\lambda_{Pf}\right)\varphi_N$$

$$\lambda = \frac{\left|\mathbf{r}_f - \mathbf{r}_N\right|}{\left|\mathbf{r}_f - \mathbf{r}_P\right| + \left|\mathbf{r}_f - \mathbf{r}_N\right|}$$

  - 1-st order in general case



- Linear interpolation with gradient:

$$\varphi_f = \lambda\left[\varphi_P + \left(\mathbf{r}_f - \mathbf{r}_P\right)\cdot\left(\nabla\varphi\right)_P\right] + \left(1-\lambda\right)\left[\varphi_F + \left(\mathbf{r}_f - \mathbf{r}_F\right)\cdot\left(\nabla\varphi\right)_F\right]$$

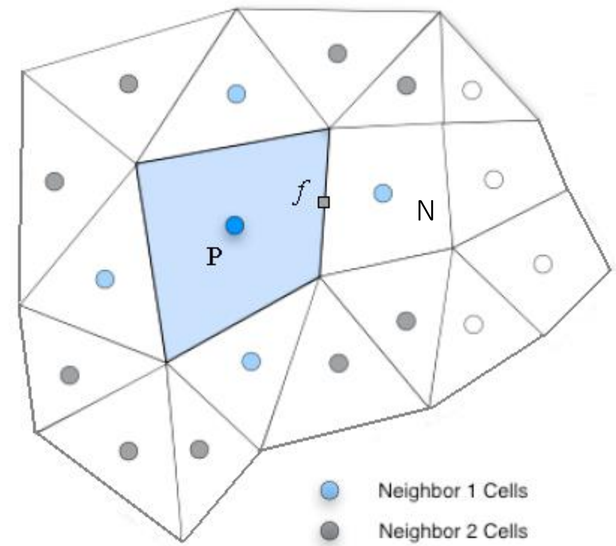
  - 2-nd order
  - Requires grad(φ) to be known

Gradients approximation

- Gauss method:

$$(\nabla\varphi)_P = \frac{1}{\Omega}\int_s \varphi \mathbf{n} dS \approx \frac{1}{\Omega}\sum_f \varphi_f \mathbf{S}_f$$

So S_f and grad(φ) are found iteratively



- Least squares method:

$$L(\nabla\varphi)_P = \sum_N w_f^2 \{\varphi_N - [\varphi_P + (\nabla\varphi)_P(\mathbf{r}_N - \mathbf{r}_P)]\}^2 \to$$

$$\left(\sum_f w_f^2 \Delta\mathbf{r}_f{}^i \cdot \Delta\mathbf{r}_f{}^j\right)(\nabla_i\phi)_P = \sum_f w_f^2 \Delta\mathbf{r}_f{}^j(\phi_S - \phi_P)$$

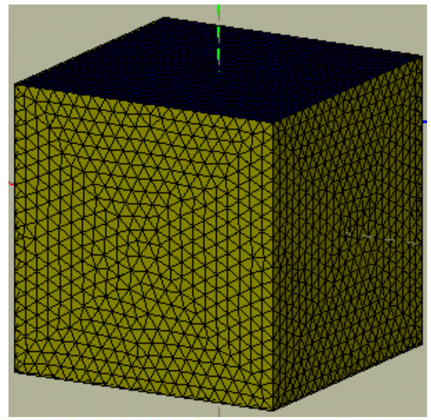
- Weight options

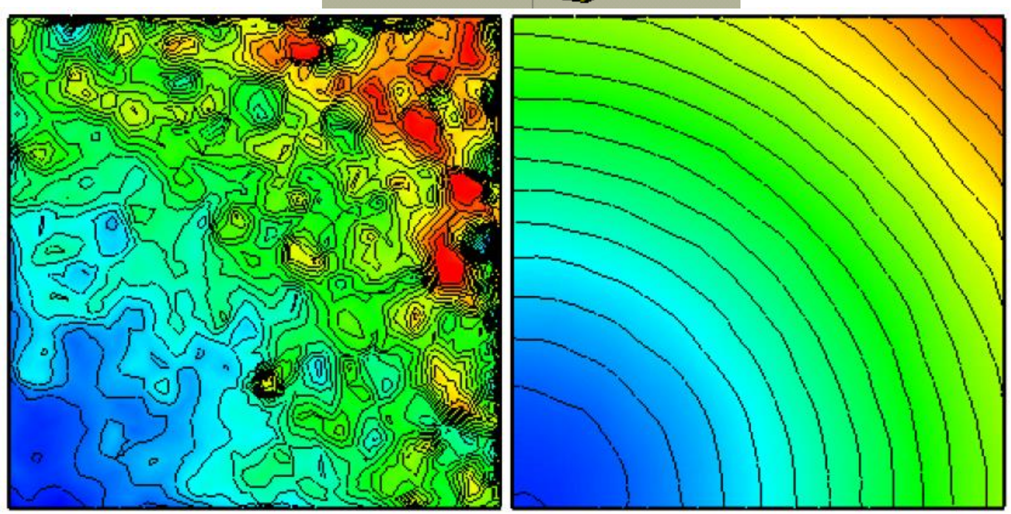
$$w_f^2 = 1;\ w_f^2 = 1/(\mathbf{r}_N - \mathbf{r}_P)^2;$$

$$w_f^2 = \lambda_f S_f / \Omega_P(\mathbf{r}_N - \mathbf{r}_P)^2$$

Gradients approximation

- Comparison of Gauss and Least squares method on unstructured grids



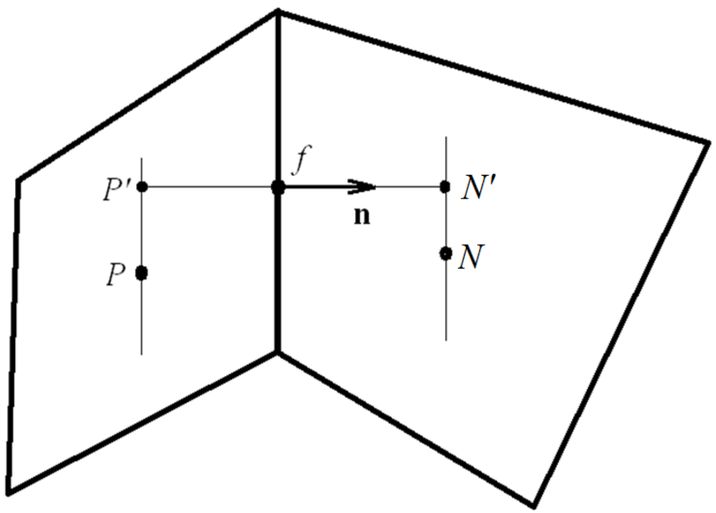


Discretization of the diffusive term

- Option 1: Using values in fictive points

$$\Gamma_f \left(\nabla \varphi_f \cdot \mathbf{S}_f \right) = \Gamma_f S_f \left(\partial \varphi / \partial \mathbf{n} \right)_f$$

$$\left(\partial \varphi / \partial \mathbf{n} \right)_f \approx \left(\varphi_{N'} - \varphi_{P'} \right) / \left| \mathbf{r}_{N'} - \mathbf{r}_{P'} \right|$$



$$\left.\begin{aligned}
\varphi_{P'} &= \varphi_P + \left(\nabla \varphi \right)_P \cdot \left(\mathbf{r}_{P'} - \mathbf{r}_P \right), \\
\varphi_{N'} &= \varphi_N + \left(\nabla \varphi \right)_N \cdot \left(\mathbf{r}_{N'} - \mathbf{r}_N \right) \\
\\
\mathbf{r}_{P'} &= \left(\mathbf{r}_f - \mathbf{r}_P \right) - \mathbf{n}\left(\left(\mathbf{r}_f - \mathbf{r}_P \right) \cdot \mathbf{n} \right), \\
\mathbf{r}_{N'} &= \left(\mathbf{r}_f - \mathbf{r}_N \right) - \mathbf{n}\left(\left(\mathbf{r}_f - \mathbf{r}_N \right) \cdot \mathbf{n} \right)
\end{aligned}\right\} \Rightarrow$$

$$\Gamma_f \left(\nabla \varphi_f \cdot \mathbf{S}_f \right) = \Gamma_f S_f \frac{\varphi_N - \varphi_P}{\left| \mathbf{r}_{N'} - \mathbf{r}_{P'} \right|} + \Gamma_f S_f \left[\frac{\left(\nabla \varphi \right)_N \cdot \left(\mathbf{r}_{N'} - \mathbf{r}_N \right) - \left(\nabla \varphi \right)_P \cdot \left(\mathbf{r}_{P'} - \mathbf{r}_P \right)}{\left| \mathbf{r}_{N'} - \mathbf{r}_{P'} \right|} \right]$$

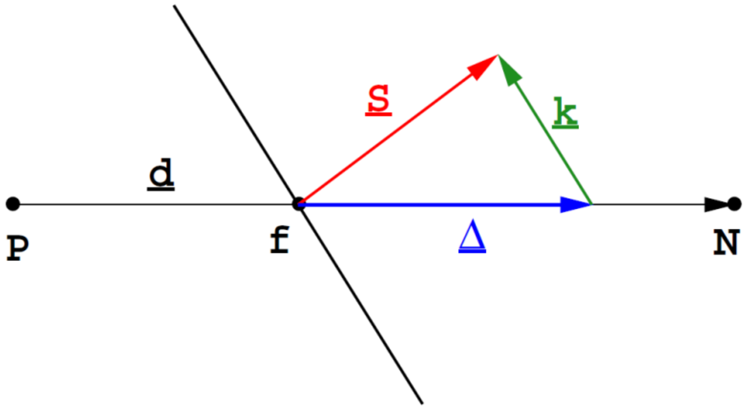
Discretization of the diffusive term

- Option 2: Interpolation of gradient

$$(\nabla\varphi)_f = \lambda(\nabla\varphi)_P + (1-\lambda)(\nabla\varphi)_N,\ \lambda = \frac{|\mathbf{r}_f - \mathbf{r}_P|}{|\mathbf{r}_f - \mathbf{r}_P| + |\mathbf{r}_f - \mathbf{r}_N|}$$

$$\nabla\varphi_f \cdot \mathbf{S}_f = \nabla\varphi_f \cdot \Delta + \nabla\varphi_f \cdot (\mathbf{S}_f - \Delta)$$

$$\nabla\varphi_f \cdot \Delta = \nabla\varphi_f \cdot k(\mathbf{r}_N - \mathbf{r}_P),\ k = \frac{\mathbf{S}_f \cdot \mathbf{S}_f}{(\mathbf{r}_N - \mathbf{r}_P)\cdot \mathbf{S}_f}$$



$$(\nabla\varphi)_f \cdot \mathbf{S}_f = k(\varphi_N - \varphi_P) + k\left[(\nabla\varphi)_N \cdot (\mathbf{r}_{Nf} - \mathbf{r}_N) - (\nabla\varphi)_P \cdot (\mathbf{r}_{Pf} - \mathbf{r}_P)\right]$$

$$\mathbf{r}_{Nf} - \mathbf{r}_N = (\mathbf{r}_f - \mathbf{r}_P) - \mathbf{n}((\mathbf{r}_f - \mathbf{r}_P)\cdot\mathbf{n}),$$
$$\mathbf{r}_{Pf} - \mathbf{r}_P = (\mathbf{r}_f - \mathbf{r}_N) - \mathbf{n}((\mathbf{r}_f - \mathbf{r}_N)\cdot\mathbf{n})$$

Convective term approximation

$$\int_S \rho\varphi\,\mathbf{v}\cdot d\mathbf{S} \approx \sum_f \varphi_f\left(\rho_f\mathbf{v}_f\cdot\mathbf{S}_f\right)$$

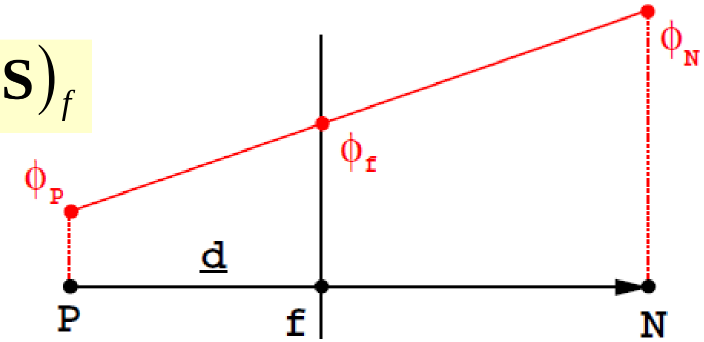
- The role of the convection differencing scheme is to determine the value of φ_f at the CF from the values in the CV centers
- The main problem is calculation of φ_f at CF’s and its convective flux across CF

Convective term approximation: CD and UD schemes

- Central Difference (CD) scheme

$$\varphi_f(\rho\mathbf{v}\cdot\mathbf{S})_f = \lambda\varphi_P(\rho\mathbf{v}\cdot\mathbf{S})_f + (1-\lambda)\varphi_N(\rho\mathbf{v}\cdot\mathbf{S})_f$$

$$\lambda = \frac{\left|\mathbf{r}_f - \mathbf{r}_P\right|}{\left|\mathbf{r}_f - \mathbf{r}_P\right| + \left|\mathbf{r}_f - \mathbf{r}_N\right|}$$

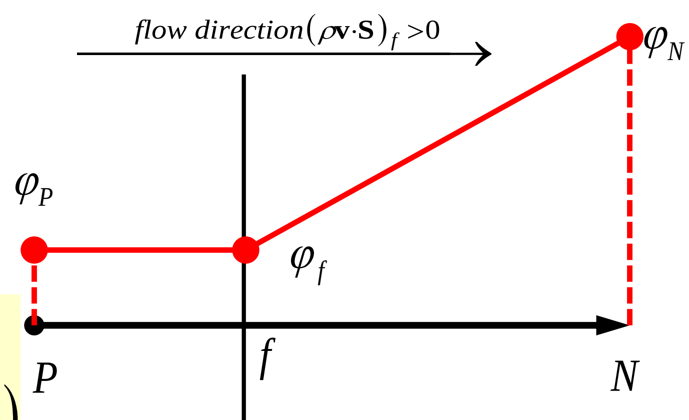


- Upwind Difference (UD) scheme

$$\varphi_f(\rho\mathbf{v}\cdot\mathbf{S})_f = \begin{cases}\varphi_P(\rho\mathbf{v}\cdot\mathbf{S})_f, & (\mathbf{v}\cdot\mathbf{S}) \geq 0\\ \varphi_N(\rho\mathbf{v}\cdot\mathbf{S})_f, & (\mathbf{v}\cdot\mathbf{S}) < 0\end{cases}$$

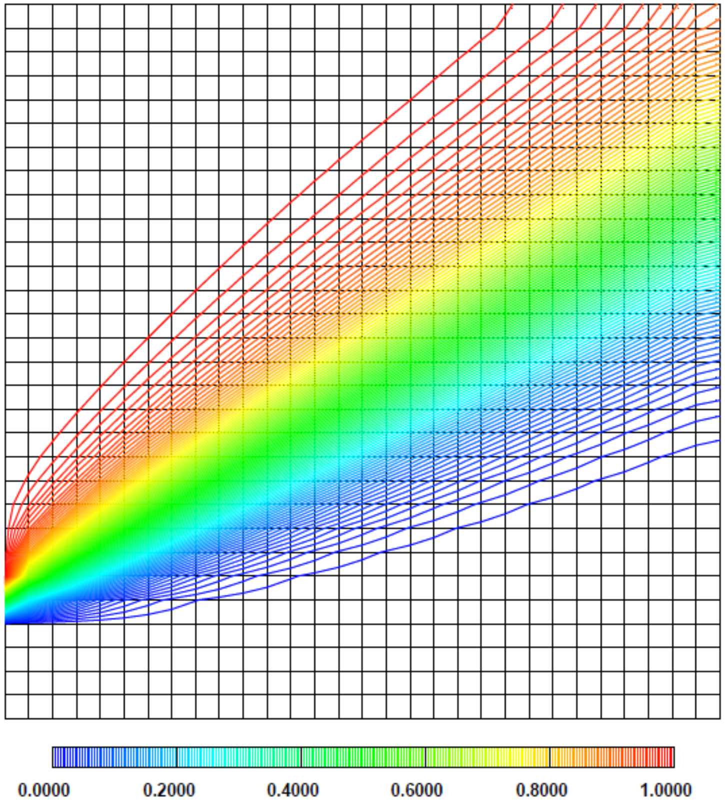
$$or \quad \varphi_f(\rho\mathbf{v}\cdot\mathbf{S})_f = \varphi_P m_f^+ + \varphi_N m_f^-$$

$$where\ m_f^+ = \max\left(0, (\rho\mathbf{v}\cdot\mathbf{S})_f\right),\ m_f^- = \min\left(0, (\rho\mathbf{v}\cdot\mathbf{S})_f\right)$$

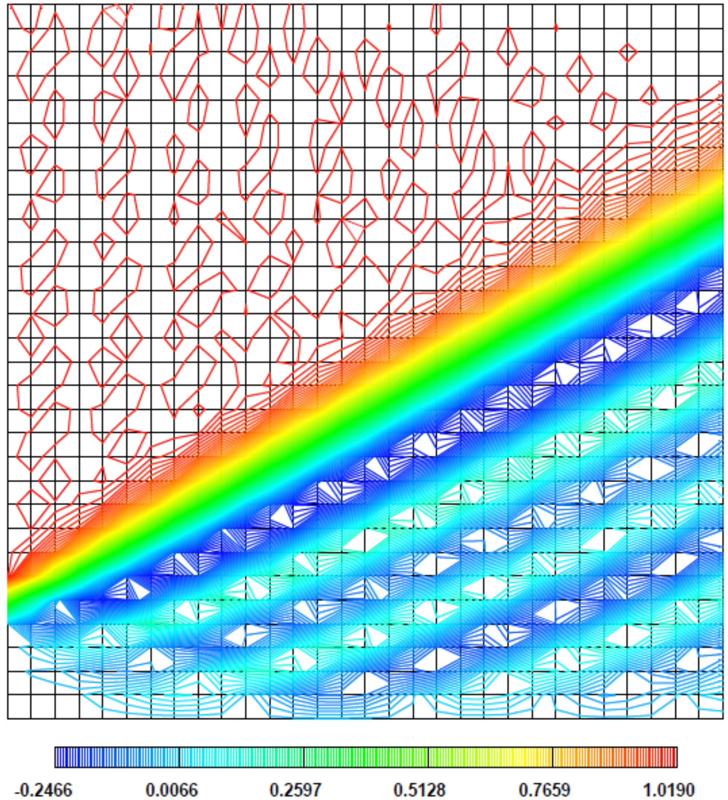


Convective term approximation: UD and CD scheme features

- Advection of stepwise profile



UD



CD

Properties of discretization scheme

- Conservativeness
  - To ensure conservation of φ for the whole solution domain the flux of φ leaving a CV across a certain face must be equal to the flux of φ entering the adjacent CV through the same face adjacent CV through the same face.
  - To achieve this the flux through a common face must be represented in a consistent manner (by one and the same expression) in adjacent CV's.
- Boundedness
  - In the absence of sources the internal nodal values of φ should be bounded by its boundary values.
- Transportiveness
  - No influence of downstream nodal values of φ in absence of diffusion

Convective term approximation: Comparison of CD and UD schemes

- CD scheme
  - Conservative
  - Conditionally bounded
  - Not transportive
  - Has 2-nd order of accuracy
  - May generate oscillations
- UD scheme has 1-nd order of accuracy
  - Conservative
  - Bounded
  - Transportive
  - Has 1-nd order of accuracy
  - Smooths the solution
- How to combine best properties of these scheme?

Convective term approximation: Blended Differencing Scheme

- Linear combination of CD and UD yields

$$\varphi_f(\rho\mathbf{v}\cdot\mathbf{S})_f = (\varphi_f)_{UD}(\rho\mathbf{v}\cdot\mathbf{S})_f + \tilde{\gamma}\left[(\varphi_f)_{CD} - (\varphi_f)_{UD}\right](\rho\mathbf{v}\cdot\mathbf{S})_f =$$

- $\tilde{\gamma}$ – is switcher between UD and CD.
- $\tilde{\gamma}$ = 0 => UD,
  $\tilde{\gamma}$ = 1 => CD
- $\tilde{\gamma}$ determines how much numerical diffusion will be introduced
- Different functions $\tilde{\gamma}$ corresponds to different schemes
- Rewrite in more common form

$$\varphi_f(\rho\mathbf{v}\cdot\mathbf{S})_f = \left[\varphi_P + \frac{\psi}{2}(\varphi_N - \varphi_P)\right](\rho\mathbf{v}\cdot\mathbf{S})_f$$

Convective term approximation: 2-nd order Linear Upwind (LUD) scheme

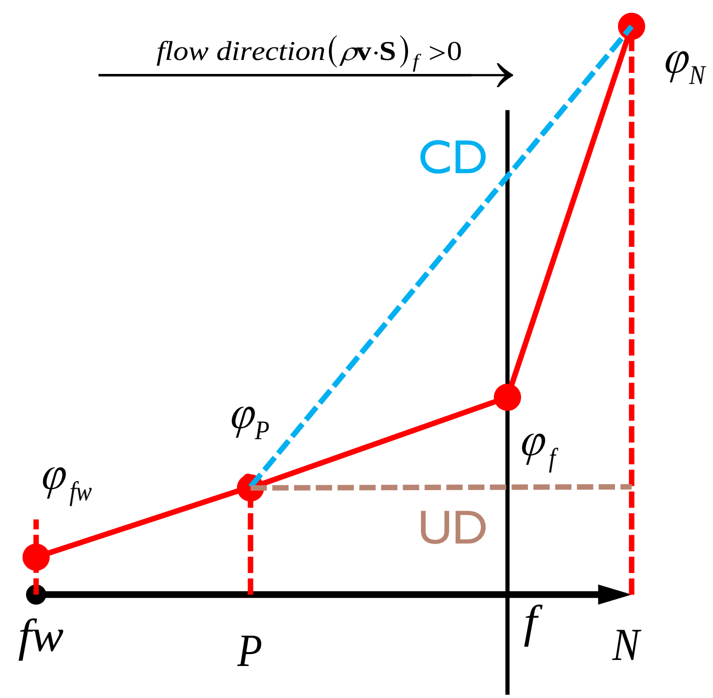
- Linear extrapolation of φ from upstream CV center yields

$$\varphi_f \left(\rho \mathbf{v} \cdot \mathbf{S}\right)_f = \varphi_f^+ m_f^+ + \varphi_f^+ m_f^-$$

$$\varphi_f^+ = \varphi_P + \left(\mathbf{r}_f - \mathbf{r}_P\right) \cdot \left(\nabla \varphi\right)_P$$

$$\varphi_f^- = \varphi_N + \left(\mathbf{r}_f - \mathbf{r}_N\right) \cdot \left(\nabla \varphi\right)_N$$

- This scheme can be considered as 2-nd order correction for UD



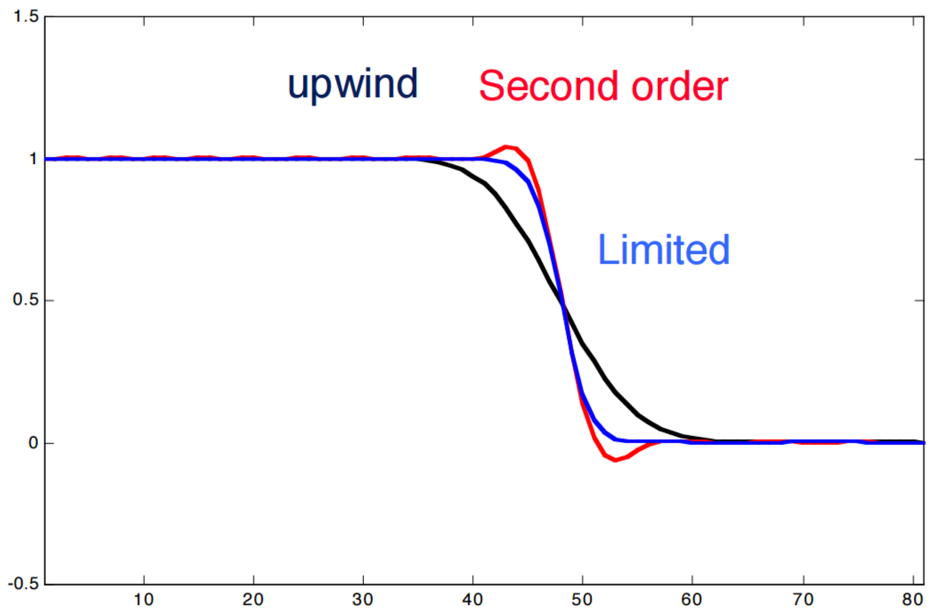
Convective term approximation: LUD features

- LUD properties
  - Conservative
  - Conditionally bounded
  - Transportive
  - Has 2-nd order of accuracy
  - May generate oscillations

- For constant γ effect of such combination is restricted by Godunov theorem: *Linear numerical schemes, having the property of not generating new extrema (monotone scheme), can be at most first-order accurate.*

Monotonic and oscillating schemes

- Linear schemes produce either oscillation or smooths the solution
- There is no monotonic scheme of 2-nd order
- Combining good properties of schemes in non-Linear manner
- Flux limiter is required



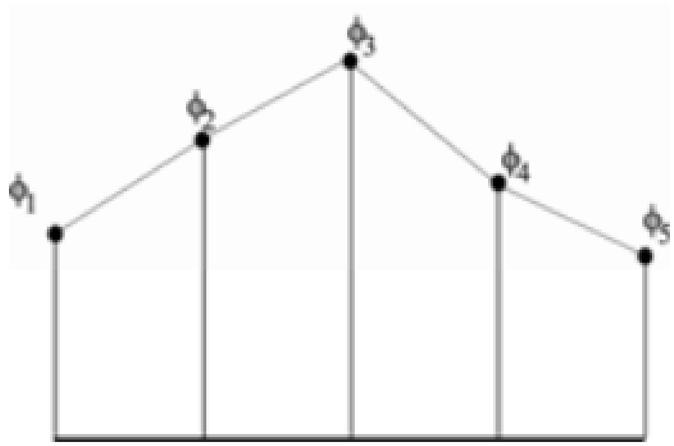
$$\varphi_f(\rho\mathbf{v}\cdot\mathbf{S})_f = \left[\varphi_P + \frac{\psi}{2}(\varphi_N - \varphi_P)\right](\rho\mathbf{v}\cdot\mathbf{S})_f$$

TVD schemes

- UD scheme is the most stable scheme (no wiggles)
- CD and LUD have higher order accuracy but give rise wiggles under certain conditions
- Our aim is to find a convection scheme with higher-order accuracy but without wiggles
- The desirable property for a stable, non-oscillatory, higher order scheme is monotonicity preserving
- For scheme to preserve monotonicity
  - It must not create local extrema
  - The value of an existing local minimum must not decrease, and value of local maximum must not increase
- Monotonicity preserving schemes do not create new undershoots and overshoots

TVD schemes

- Consider the discrete data set shown in the figure



- The total variation of this data is

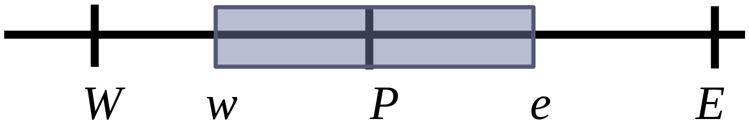
$$TV(\varphi) = |\varphi_2 - \varphi_1| + |\varphi_3 - \varphi_2| + |\varphi_4 - \varphi_3| + |\varphi_5 - \varphi_4| = |\varphi_3 - \varphi_1| + |\varphi_5 - \varphi_3|$$

- For monotonicity TV must not increase with time

TVD schemes

- In other words TV must diminish in time
- Hence, the term Total Variation Diminishing or TVD
- Originally TVD was developed for time-dependent flows
- For TVD:

$$TV\left(\varphi^{n+1}\right) \leq TV\left(\varphi^{n}\right)$$



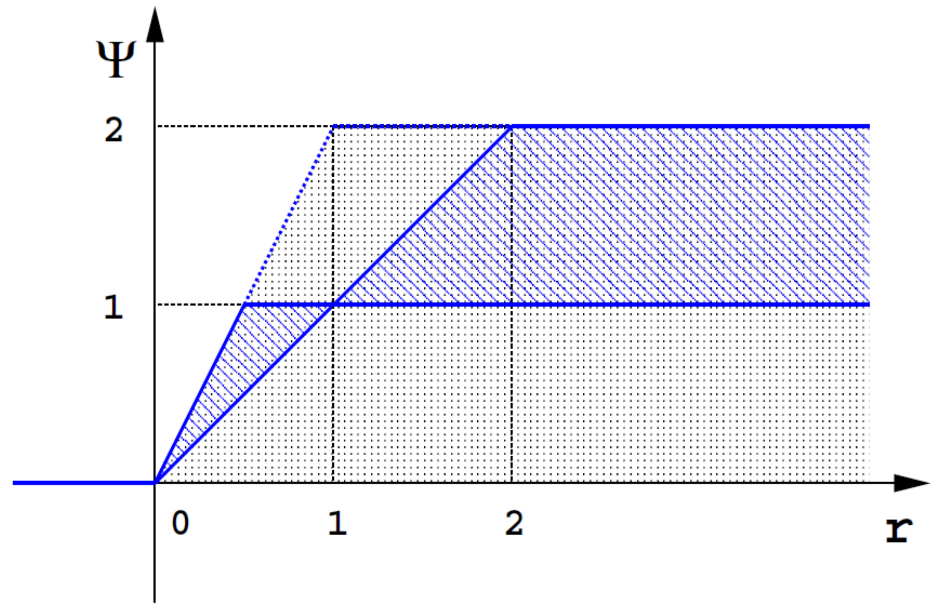
- Let

$$\gamma_f = \frac{\left(\partial\varphi/\partial x\right)_{fw}}{\left(\partial\varphi/\partial x\right)_{fe}} = \frac{\left(\varphi_W - \varphi_P\right)/\left(x_W - x_P\right)}{\left(\varphi_P - \varphi_E\right)/\left(x_P - x_E\right)}$$ - ratio of upwind gradient to downwind gradient

$$\varphi_f\left(\rho\mathbf{v}\cdot\mathbf{S}\right)_f = \left[\varphi_P + \frac{\psi\left(\gamma_f\right)}{2}\left(\varphi_N - \varphi_P\right)\right]\left(\rho\mathbf{v}\cdot\mathbf{S}\right)_f$$

TVD schemes

- Necessary and sufficient condition for scheme to be TVD:
  - For 0<r<1 $\psi(r) \leq 2r$
  - For $\mathrm{r} \geq 1$ $\psi(r) \leq 2$



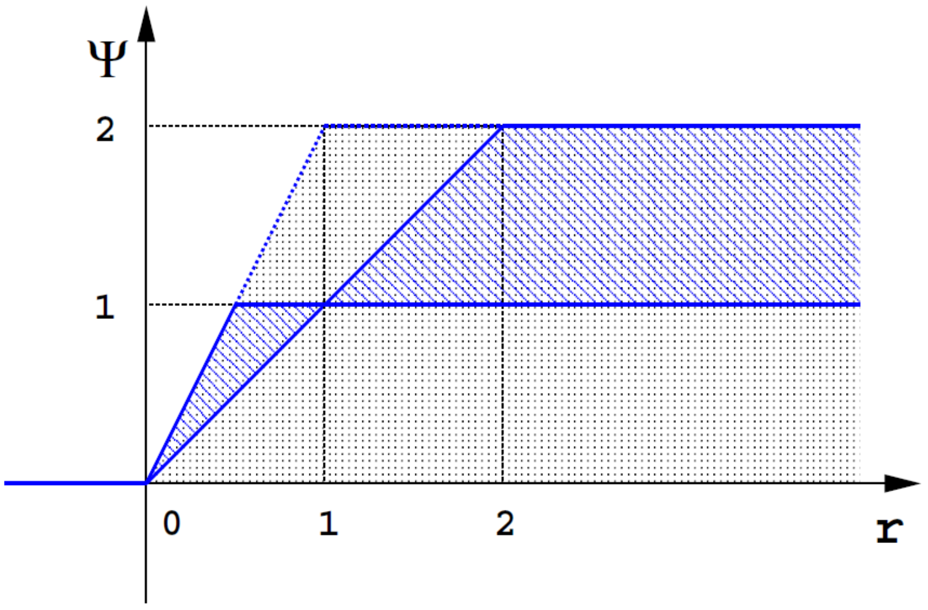
- UD scheme is TVD
- LUD scheme isn't TVD for r>2
- CD scheme isn't TVD for r<0.5
- QUICK scheme isn't TVD for r<3/7 and r>5

TVD schemes

- For second order accuracy flux limiter function should pass through (1,1)
- Range of possible second-order schemes is bounded by the CD and LUD schemes:
  - For 0<r<1 $r \leq \psi(r) \leq 1$
  - For $r \geq 1$ $1 \leq \psi(r) \leq r$
- Symmetry property for limiter function

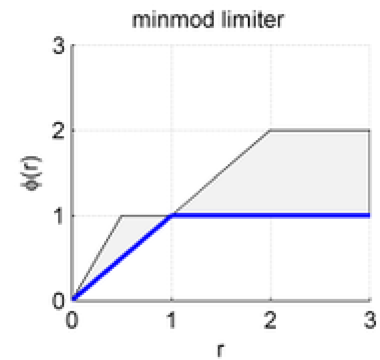
$$\psi(r)/r = \psi(1/r)$$

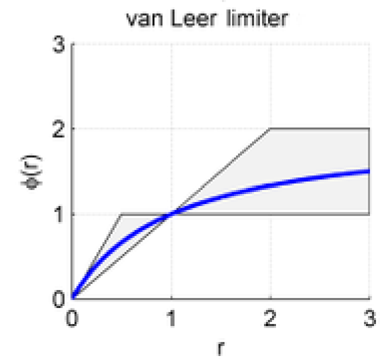
ensures that backward and forward facing gradients are treated in the same fashion

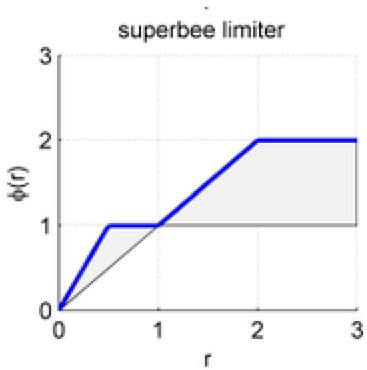


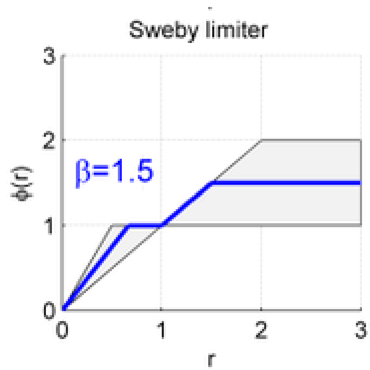
TVD schemes

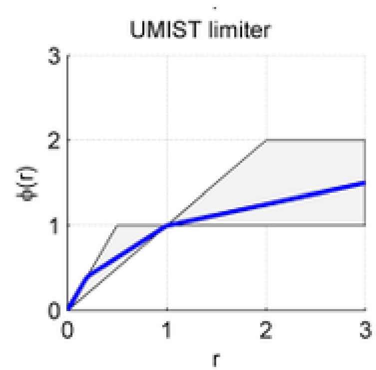
Name	**Limiter function**	**Source**
Van Leer	$\dfrac{r+\lvert r\rvert}{1+r}$	Van Leer (1974)
Van Albada	$\dfrac{r+r^2}{1+r^2}$	Van Albada *et al*. (1982)
Min-Mod	$\psi(r)=\begin{cases}\min(r,1) & \text{if } r>0\\ 0 & \text{if } r\le 0\end{cases}$	Roe (1985)
SUPERBEE	$\max[0,\min(2r,1),\min(r,2)]$	Roe (1985)
Sweby	$\max[0,\min(\beta r,1),\min(r,\beta)]$	Sweby (1984)
QUICK	$\max[0,\min(2r,(3+r)/4,2)]$	Leonard (1988)
UMIST	$\max[0,\min(2r,(1+3r)/4,(3+r)/4,2)]$	Lien and Leschziner (1993)

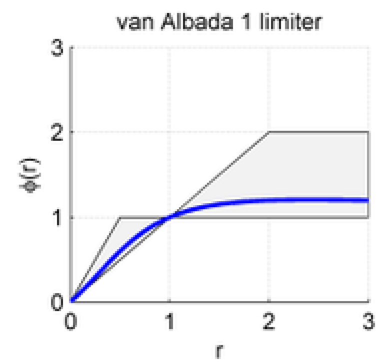






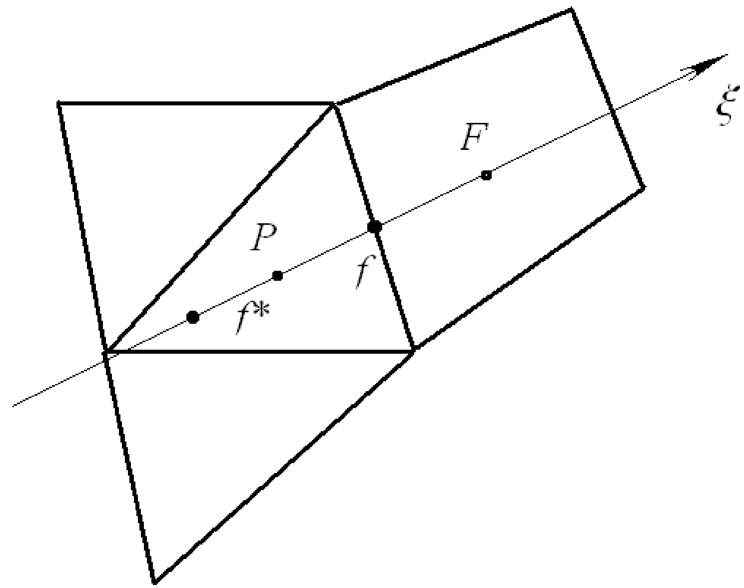






Discretization of the convective term
TVD approach in case of unstructured grids

$$\varphi_f(\rho\mathbf{v}\cdot\mathbf{S})_f \approx m_f^+\left[\varphi_P + \frac{d_f(\gamma_{f+})}{2}(\varphi_N-\varphi_P)\right] + m_f^-\left[\varphi_N + \frac{d_f(\gamma_{f-})}{2}(\varphi_P-\varphi_N)\right]$$



$$\gamma_f = (\partial\varphi/\partial\boldsymbol{\xi})_{f*}/(\partial\varphi/\partial\boldsymbol{\xi})_f$$

$$(\partial\varphi/\partial\boldsymbol{\xi})_f \approx (\varphi_N-\varphi_P)/|\mathbf{r}_N-\mathbf{r}_P|$$

$$\left.\begin{aligned}\left(\frac{\partial\varphi}{\partial\xi}\right)_P &= \frac{1}{2}\left[\left(\frac{\partial\varphi}{\partial\xi}\right)_{f*} + \left(\frac{\partial\varphi}{\partial\xi}\right)_f\right]\\ (\partial\varphi/\partial\boldsymbol{\xi})_P &= (\nabla\varphi)_P\cdot\boldsymbol{\xi}\end{aligned}\right\} \Rightarrow \left(\frac{\partial\varphi}{\partial\xi}\right)_{f*} = 2(\nabla\varphi)_P\cdot\boldsymbol{\xi} - \left(\frac{\partial\varphi}{\partial\xi}\right)_f \Rightarrow$$

$$\Rightarrow \gamma_f = 2\frac{(\nabla\varphi)_P\cdot\boldsymbol{\xi}}{(\partial\varphi/\partial\boldsymbol{\xi})_f} - 1$$

Unsteady term discretization

- Integrate transport equation over time

$$\int_{t}^{t+\Delta t}\left(\frac{\partial}{\partial t}\int_{\Omega_P}\rho\varphi dV+\int_{S}\rho\mathbf{v}_f\varphi_f\cdot\mathbf{n}dS-\int_{S}\Gamma_f\left(\nabla\varphi\right)_f dS\right)dt=\int_{t}^{t+\Delta t}\left(\int_{\Omega_P}q_P dV\right)dt$$

- Rewrite in semidiscretized form

$$\int_{t}^{t+\Delta t}\left[\left(\frac{\partial\rho\varphi}{\partial t}\right)_P\Omega_P\right]dt=\int_{t}^{t+\Delta t}\underbrace{\left[\sum_f\Gamma_f\left(\nabla\varphi_f\cdot\mathbf{S}_f\right)-\sum_f\varphi_f\left(\rho\mathbf{v}_f\cdot\mathbf{S}_f\right)+q_P\Omega_P\right]dt}_{L(\varphi,t)}$$

- Time derivative approximation

$$\left(\frac{\partial\rho\varphi}{\partial t}\right)_P\approx\frac{\left(\rho_P\varphi_P\right)^{n+1}-\left(\rho_P\varphi_P\right)^n}{\Delta t}$$

Unsteady term discretization: Explicit scheme

- 1. Explicit scheme:

$$\int_{t}^{t+\Delta t} \varphi(t)dt \approx \varphi^n \Delta t \quad \Rightarrow \quad \frac{(\rho_P \varphi_P)^{n+1} - (\rho_P \varphi_P)^n}{\Delta t} \Omega_P = L(\varphi^n, t)$$

$$\frac{(\rho_P \varphi_P)^{n+1} - (\rho_P \varphi_P)^n}{\Delta t} \Omega_P = \left[\sum_f \Gamma_f \left(\nabla \varphi_f \cdot \mathbf{S}_f \right) - \sum_f \varphi_f \left(\rho \mathbf{v}_f \cdot \mathbf{S}_f \right) + q_P \Omega_P \right]^n$$

- Conditionally stable

$$CFL = \max_f |\mathbf{v}|_f \frac{\Delta t}{\min_{P,N} |\mathbf{r}_N - \mathbf{r}_P|} < 1$$

- Has 1-st order of accuracy in time
- Easy for implementation

Unsteady term discretization: Implicit scheme

- 2. Implicit scheme:

$$\int_{t}^{t+\Delta t} \varphi(t)dt \approx \varphi^{n+1}\Delta t \quad \Rightarrow \quad \frac{(\rho_P \varphi_P)^{n+1} - (\rho_P \varphi_P)^{n}}{\Delta t}\Omega_P = L(\varphi^{n+1}, t+\Delta t)$$

$$\frac{(\rho_P \varphi_P)^{n+1} - (\rho_P \varphi_P)^{n}}{\Delta t}\Omega_P = \left[\sum_f \Gamma_f \left(\nabla \varphi_f \cdot \mathbf{S}_f \right) - \sum_f \varphi_f \left(\rho \mathbf{v}_f \cdot \mathbf{S}_f \right) + q_P \Omega_P \right]^{n+1}$$

- Unconditionally stable and bounded
- 1-st order of accuracy in time
- RHS-term is non-linear in general case => requires internal iterations

Unsteady term discretization: Crank-Nicholson scheme

- 3. Crank-Nicholson scheme :

$$\int_{t}^{t+\Delta t} \varphi(t)dt \approx \frac{1}{2}\left(\varphi^{n+1} + \varphi^{n}\right)\Delta t \quad \Rightarrow \quad \frac{(\rho_P \varphi_P)^{n+1} - (\rho_P \varphi_P)^{n}}{\Delta t}\Omega_P = \frac{L(\varphi^{n}, t) + L(\varphi^{n+1}, t+\Delta t)}{2}$$

$$\frac{(\rho_P \varphi_P)^{n+1} - (\rho_P \varphi_P)^{n}}{\Delta t}\Omega_P = \frac{1}{2}\left[\sum_f \Gamma_f\left(\nabla\varphi_f \cdot \mathbf{S}_f\right) - \sum_f \varphi_f\left(\rho\mathbf{v}_f \cdot \mathbf{S}_f\right) + q_P\Omega_P\right]^{n} +$$

$$\frac{1}{2}\left[\sum_f \Gamma_f\left(\nabla\varphi_f \cdot \mathbf{S}_f\right) - \sum_f \varphi_f\left(\rho\mathbf{v}_f \cdot \mathbf{S}_f\right) + q_P\Omega_P\right]^{n+1}$$

- Unconditionally stable
- Has 2-nd order of accuracy in time
- RHS-term is non-linear in general case => requires internal iterations

Discretization of the source term

- Simplest way

$$\int_{\Omega} q d\Omega = q_P \Omega_P$$

- However if q depends on φ and (semi)implicit scheme is used it is beneficial to linearize it making the scheme more "implicit" and enforcing diagonal domination of resulting SLAE

$$\int_{\Omega_p} q(\varphi) d\Omega = \int_{\Omega_p} \left[q_0 + \varphi q_1 + q_2(\varphi)\right] d\Omega = \left[q_0(\varphi) + \varphi q_1(\varphi)\right]^{n+1} \Omega_P + q_2(\varphi)^n \Omega_P$$

Cell properties calculation

- In 3D general case of unstructured grid CV's are convex polyhedrons
  - CF square

$$S_f = \frac{1}{2}\sum_{i=3}^{Nv}\left[\left(\mathbf{r}_{v_{i-1}} - \mathbf{r}_{v_1}\right)\times\left(\mathbf{r}_{v_i} - \mathbf{r}_{v_1}\right)\right]$$

  - CF center (center of gravity)

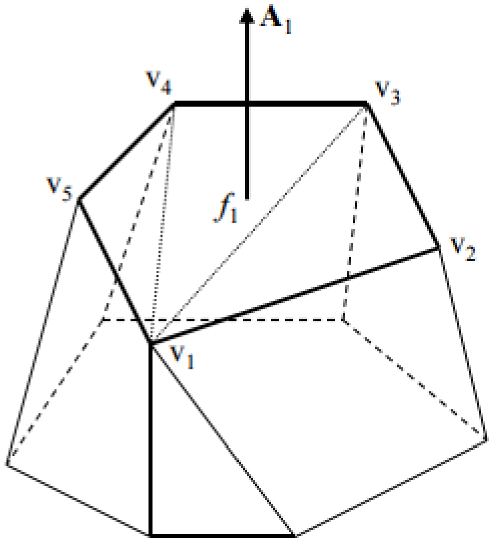
$$\mathbf{r}_f = \frac{1}{6S_f}\sum_{i=3}^{Nv}\left[\left(\mathbf{r}_{v_{i-1}} - \mathbf{r}_{v_1}\right)\times\left(\mathbf{r}_{v_i} - \mathbf{r}_{v_1}\right)\right]\left(\mathbf{r}_{v_i} + \mathbf{r}_{v_{i-1}} + \mathbf{r}_{v_{i-2}}\right)$$

  - CV volume

$$\Omega = \frac{1}{3}\sum_f\left(\mathbf{r}_f \cdot \mathbf{n}_f\right)S_f$$

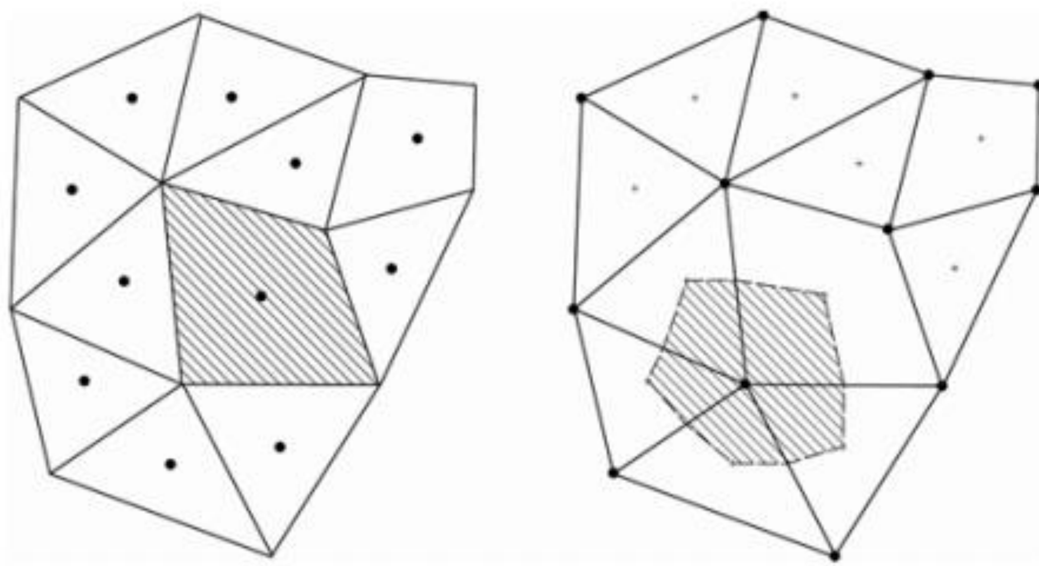
  - CV center (center of gravity)

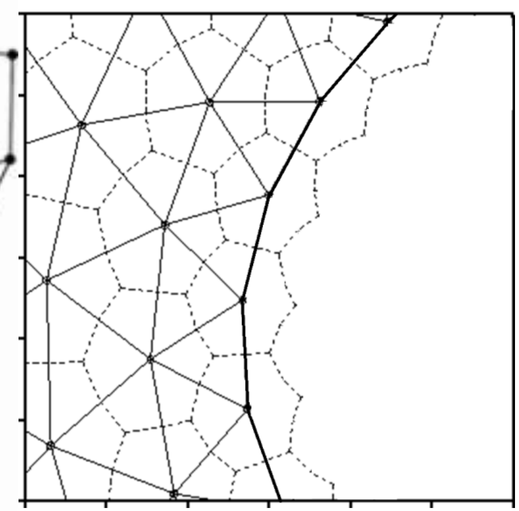
$$\int_\Omega\left(\mathbf{r} - \mathbf{r}_P\right)d\Omega = 0$$



Boundary conditions
Boundary cells

- There are two ways of defining CV's in unstructured grids:
  - Cell-centerd CV
  - Vertex centered CV





- We consider cell-centered cell volumes

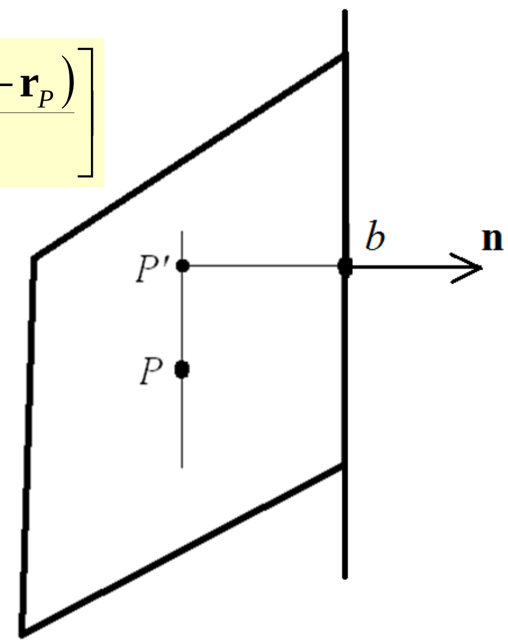
Boundary conditions

- Prescribed value φ_b :
  - Diffusive flux

$$\Gamma_b\left(\nabla\varphi_b\cdot\mathbf{S}_b\right)=\Gamma_b S_b\left(\partial\varphi/\partial\mathbf{n}\right)_b=\Gamma_b S_b\frac{\varphi_b-\varphi_P}{\left|\mathbf{r}_b-\mathbf{r}_{P'}\right|}-\Gamma_b S_b\left[\frac{\left(\nabla\varphi\right)_P\cdot\left(\mathbf{r}_{P'}-\mathbf{r}_P\right)}{\left|\mathbf{r}_b-\mathbf{r}_{P'}\right|}\right]$$

  - Convective flux

$$\varphi_b\left(\mathbf{v}\cdot\mathbf{S}\right)_b$$



- Prescribed gradient grad$(\varphi)_b$:
  - φ value is computed as

$$\varphi_b=\varphi_P+\left(\mathbf{r}_b-\mathbf{r}_P\right)\cdot\left(\nabla\varphi\right)_b$$

  - Diffusive flux $\Gamma_b\left(\nabla\varphi_b\cdot\mathbf{S}_b\right)$
  - Convective flux $\varphi_b\left(\mathbf{v}\cdot\mathbf{S}\right)_b$

SLAE formation

- Gathering approximations for the all terms can produce non-linear system of equations. Internal iterations or differed correction approach are able to resolve it
- To enforce convergence rate and stability we need to make method as “implicit” as possible. Non-linear terms and accuracy correction terms are in the right part

$$\left[\frac{\rho_P \Omega}{\tau} + \sum_f \left(m_f^+ + \frac{\Gamma_f S_f}{\left|\mathbf{r}_{F'} - \mathbf{r}_{P'}\right|} \right)\right]^m \varphi_P^{m+1} + \sum_f \left(m_f^- - \frac{\Gamma_f S_f}{\left|\mathbf{r}_{F'} - \mathbf{r}_{P'}\right|} \right)^m \varphi_F^{m+1} = \left(\frac{\rho_P \Omega \varphi_P}{\tau} \right)^{old} + Q_{expl}^m$$

$$Q_{expl} = \left[m_f^+ \frac{d_f(\gamma_{f+})}{2} - m_f^- \frac{d_f(\gamma_{f-})}{2} \right] (\varphi_P - \varphi_F) - \Gamma_f S_f \left[\frac{(\nabla\varphi)_F \cdot (\mathbf{r}_{F'} - \mathbf{r}_F) - (\nabla\varphi)_P \cdot (\mathbf{r}_{P'} - \mathbf{r}_P)}{\left|\mathbf{r}_{F'} - \mathbf{r}_{P'}\right|} \right] + (q)_P \Omega$$

- Add $\left[\varphi_P^{m+1} - \varphi_P^m\right] \sum_f \left(-c_f^m\right)$ to left part to enforce diagonal domination

SLAE formation

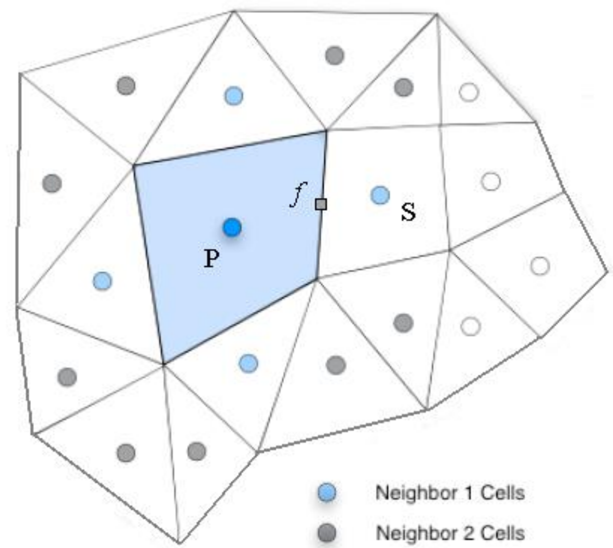
- We obtain SLAE of the form

$$A_P^m \varphi_P^{m+1} + \sum_f A_F^m \varphi_F^{m+1} = Q_P^m$$

with coefficients

$$A_P = \frac{\rho_P \Omega}{\tau} - \sum_f A_F \qquad A_F = m_f^- + \frac{\Gamma_f S_f}{\left|\mathbf{r}_{F'} - \mathbf{r}_{P'}\right|}$$

$$Q_P^m = \left(\frac{\rho_P \Omega \varphi_P}{\tau}\right)^{old} + Q_{expl}^m - \varphi_P^m \sum_f \left(m_f\right)^m$$



- Diagonal dominant sparse matrix can be solved by iteration methods

Implementation issues
Performance improvement

- Representation of the grid as graph
- There is no need to store two copies of face objects (for back and front CV)
- Loops over CFs instead of loops over CVs while calculating CF fluxes prevents double calculation of the flux for neighboring cells
- All geometrical and prescribed quantities in SLAE coefficients should be precalculated
- Use methods for sparse SLAE (in particular those which support graph representation of the grid and variables)
- Time step reduction is better than increase of number of internal iterations while solving time-dependent problems