

Sharif University of Technology
School of Mechanical Engineering
Center of Excellence in Energy Conversion

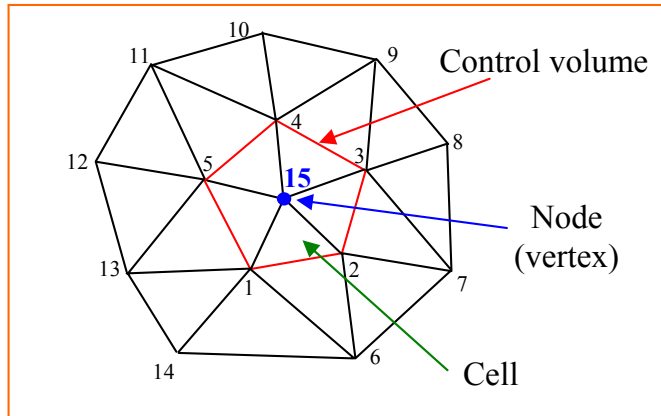
Computational Fluid Dynamics

Finite Volume Method

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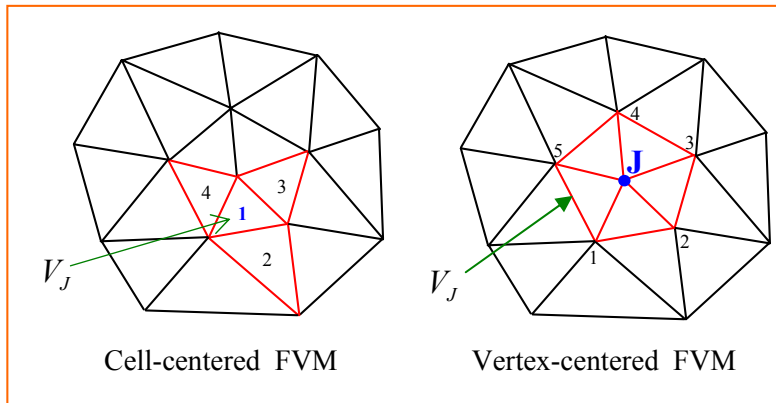
FVM: Basics

- The finite volume method was introduced by McDonald (1971) and McCormack & Paullay (1972) into the field of CFD.
- The method works with the conservation laws in the integral form and tries to preserve the conservation property.
- It is applicable to a general non-orthogonal and unstructured grid.



FVM: Basics

- There are two types of popular data structures: **cell-centered** and **vertex-centered**.
- In cell-centered form, variables are averaged values over the cell and can be considered as representative of some point inside the cell. (**mesh cell=control volume**)
- In the vertex-centered form, the variables are attributed to the mesh points (vertices). The choice of the control volume can be very flexible.



FVM: Basics

- Consider a general conservation law in its integral form

$$\frac{\partial}{\partial t} \int_V \mathbf{U} dV + \oint_S \mathbf{F} \cdot d\mathbf{S} = \int_V \mathbf{Q} dV$$

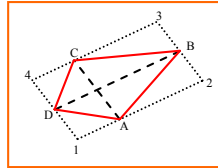
- When applied to a control volume V_J , we get

$$\frac{\partial}{\partial t} (\mathbf{U}_J V_J) + \sum_{sides} (\mathbf{F} \cdot \mathbf{S}) = \mathbf{Q}_J V_J$$

- The first term in this formulation is calculated using an average value for \mathbf{U} inside V_J .
- The source term \mathbf{Q} is also treated in the same way using a uniform value inside V_J .

Two dimensional FVM

- Consider the 2D cell ABCD.



- For this cell, with $\mathbf{F} = \mathbf{F}^x \vec{i} + \mathbf{F}^y \vec{j}$, we get

$$\frac{\partial}{\partial t} \int_V \mathbf{U} dV + \oint_{ABCD} (\mathbf{F}^x dy - \mathbf{F}^y dx) = \int_V \mathbf{Q} dV$$

- Or equivalently

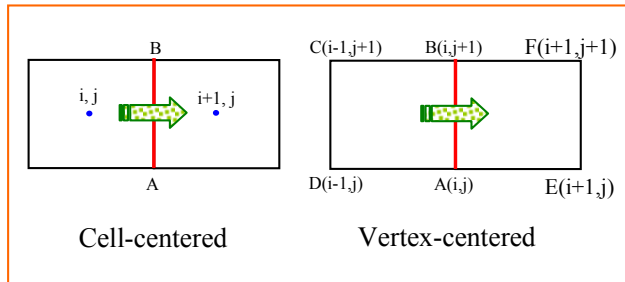
$$\frac{\partial}{\partial t} (\mathbf{U}V) + [\mathbf{F}_{AB}^x (y_B - y_A) - \mathbf{F}_{AB}^y (x_B - x_A)] + [\mathbf{F}_{BC}^x (y_C - y_B) - \mathbf{F}_{BC}^y (x_C - x_B)] + [\mathbf{F}_{CD}^x (y_D - y_C) - \mathbf{F}_{CD}^y (x_D - x_C)] + [\mathbf{F}_{DA}^x (y_A - y_D) - \mathbf{F}_{DA}^y (x_A - x_D)] = \mathbf{Q}V$$

- Note that, for example,

$$\begin{aligned} \mathbf{S}_{AB} &= \Delta y_{AB} \vec{n}_x - \Delta x_{AB} \vec{n}_y = (y_B - y_A) \vec{n}_x - (x_B - x_A) \vec{n}_y \\ V_{ABCD} &= \frac{1}{2} \left| \vec{AC} \times \vec{BD} \right| = \frac{1}{2} [(x_C - x_A)(y_D - y_B) - (x_D - x_B)(y_C - y_A)] \\ &= \frac{1}{2} (\Delta x_{AC} \Delta y_{BD} - \Delta x_{BD} \Delta y_{AC}) \end{aligned}$$

Evaluation of Fluxes

- An important step in producing a successful FVM method is devising good approximations for fluxes crossing the boundary of a control volume.
- This can be done in two major fashions:
 - Central schemes
 - Upwind schemes
- Note that in each method either a cell-centered or vertex-centered approach may be used.
- Let us consider the flux F which crosses a side AB .



Evaluation of Fluxes...

- **Central scheme and cell-centered:** Here, there are three choices to make:

$$\begin{aligned} F_{AB}^x &= \frac{1}{2}(F_{ij}^x + F_{i+1,j}^x) \\ F_{AB}^x &= \frac{1}{2}(F_A^x + F_B^x) \quad \text{with} \quad \begin{cases} F_A^x = F^x(\mathbf{U}_A) = \frac{1}{4}(F_{ij}^x + F_{i+1,j}^x + F_{i+1,j-1}^x + F_{i,j-1}^x) \\ F_B^x = F^x(\mathbf{U}_B) = \frac{1}{4}(F_{ij}^x + F_{i+1,j}^x + F_{i+1,j+1}^x + F_{i,j+1}^x) \end{cases} \\ F_{AB}^x &= F^x\left(\frac{\mathbf{U}_{ij} + \mathbf{U}_{i+1,j}}{2}\right) \end{aligned}$$

- **Central scheme and vertex-centered:**

$$F_{AB}^x = F^x\left(\frac{\mathbf{U}_{ij} + \mathbf{U}_{i+1,j}}{2}\right) \quad \text{or} \quad F_{AB}^x = \frac{1}{2}(F_A^x + F_B^x)$$

Evaluation of Fluxes...

- Upwind scheme and cell-centered:

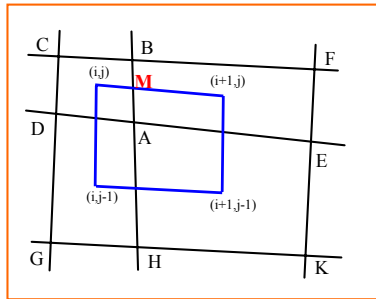
$$\mathbf{A} = \frac{\partial \mathbf{F}}{\partial \mathbf{U}} = \frac{\partial \mathbf{F}^x}{\partial \mathbf{U}} \vec{n}_x + \frac{\partial \mathbf{F}^y}{\partial \mathbf{U}} \vec{n}_y$$
$$\left\{ \begin{array}{ll} (\mathbf{F} \cdot \mathbf{S})_{AB} = (\mathbf{F} \cdot \mathbf{S})_{ij} & \text{if } (\mathbf{A} \cdot \mathbf{S})_{AB} > 0 \\ (\mathbf{F} \cdot \mathbf{S})_{AB} = (\mathbf{F} \cdot \mathbf{S})_{i+1,j} & \text{if } (\mathbf{A} \cdot \mathbf{S})_{AB} < 0 \end{array} \right.$$

- Upwind scheme and vertex-centered:

$$\mathbf{A} = \frac{\partial \mathbf{F}}{\partial \mathbf{U}} = \frac{\partial \mathbf{F}^x}{\partial \mathbf{U}} \vec{n}_x + \frac{\partial \mathbf{F}^y}{\partial \mathbf{U}} \vec{n}_y$$
$$\left\{ \begin{array}{ll} (\mathbf{F} \cdot \mathbf{S})_{AB} = (\mathbf{F} \cdot \mathbf{S})_{CD} & \text{if } (\mathbf{A} \cdot \mathbf{S})_{AB} > 0 \\ (\mathbf{F} \cdot \mathbf{S})_{AB} = (\mathbf{F} \cdot \mathbf{S})_{EF} & \text{if } (\mathbf{A} \cdot \mathbf{S})_{AB} < 0 \end{array} \right.$$

Non-uniform Grids

- The effect of non-uniformity in the mesh will decrease the order of accuracy of the method.



- If we had an orthogonal grid with a and b being the distance of M from point (i, j) and $(i+1, j)$ then we could write:

$$\mathbf{F}_{AB}^x = \frac{b}{a+b} \mathbf{F}_{ij}^x + \frac{a}{a+b} \mathbf{F}_{i+1,j}^x$$

or

$$\mathbf{F}_{AB}^x = \mathbf{F}^x \left(\frac{b}{a+b} \mathbf{U}_{ij} + \frac{a}{a+b} \mathbf{U}_{i+1,j} \right)$$

Computation of Gradients

- In some applications it is required to approximate gradients of the dependent variables. This can be done as follows:

$$\left(\frac{\partial U}{\partial x}\right)_V = \frac{1}{V} \int_V \frac{\partial U}{\partial x} dV = \frac{1}{V} \oint_S U \bar{n}_x \cdot d\mathbf{S} = -\frac{1}{V} \oint_S y dU$$
$$\left(\frac{\partial U}{\partial y}\right)_V = \frac{1}{V} \int_V \frac{\partial U}{\partial y} dV = \frac{1}{V} \oint_S U \bar{n}_y \cdot d\mathbf{S} = -\frac{1}{V} \oint_S U dx = \frac{1}{V} \oint_S x dU$$

- On a structured grid, we get

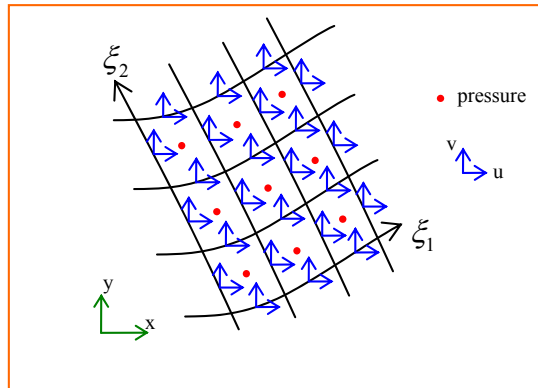
$$\begin{aligned} \left(\frac{\partial U}{\partial x}\right)_V &= \frac{1}{2V} \sum_I (U_I + U_{I+1})(y_{I+1} - y_I) \\ &= \frac{-1}{2V} \sum_I (U_{I+1} - U_I)(y_{I+1} + y_I) \\ &= \frac{1}{2V} \sum_I U_I (y_{I+1} - y_{I-1}) \\ &= \frac{-1}{2V} \sum_I y_I (U_{I+1} - U_{I-1}) \end{aligned}$$

- A similar equation can be written for the y -direction by interchanging x and y :

$$\left(\frac{\partial U}{\partial y}\right)_V = \frac{1}{2V} \sum_I (U_{I+1} - U_I)(x_{I+1} + x_I) = \frac{-1}{2V} \sum_I U_I (x_{I+1} - x_{I-1}) = \frac{1}{2V} \sum_I x_I (U_{I+1} - U_{I-1})$$

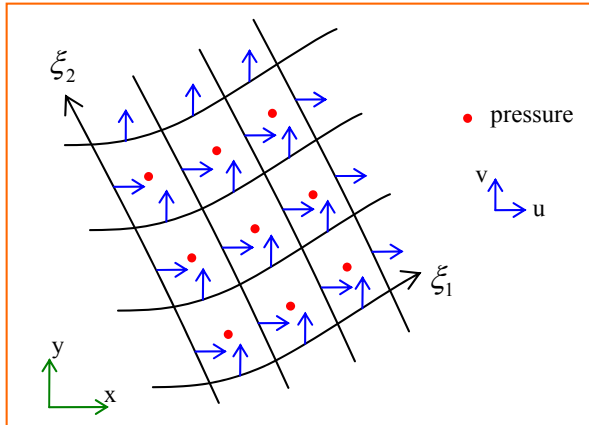
Layout of Dependent Variables

- A sensitive part of FVM design is to choose an appropriate form for the dependent variables.
- The following choices are possible:
 - Methods without interpolation
 - Methods with interpolation
- **Methods without interpolation:**
 - **Partial staggering:** variables located on $\xi_1 = cte$ are connected to $\xi_2 = cte$ only through the pressure field.



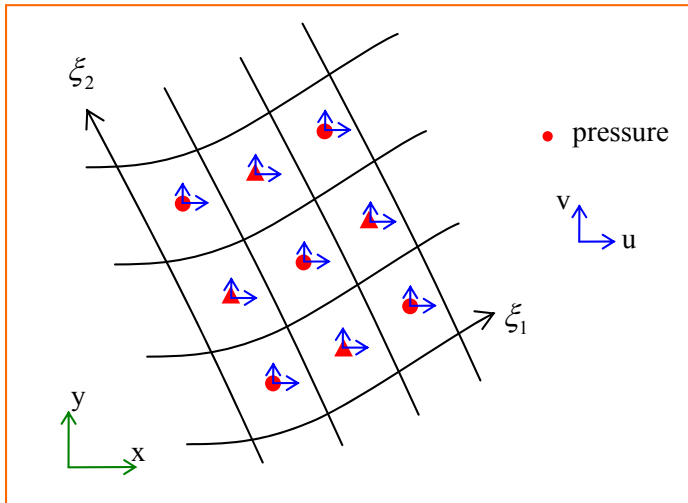
Layout of Dependent Variables...

- Staggered grid with contra-variant velocities and pressure field. (Kwak 1986): computations become costly.



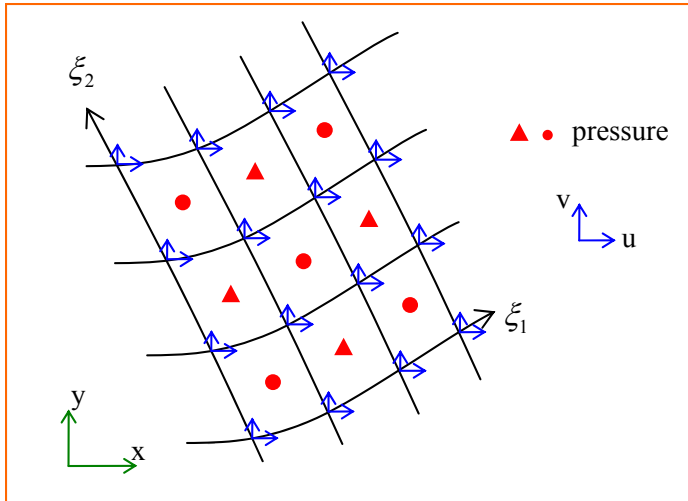
Layout of Dependent Variables...

- **Methods with interpolation:**
 - **Collocated grid:** the pressure field at circle points is decoupled from triangle points showing checkerboard.



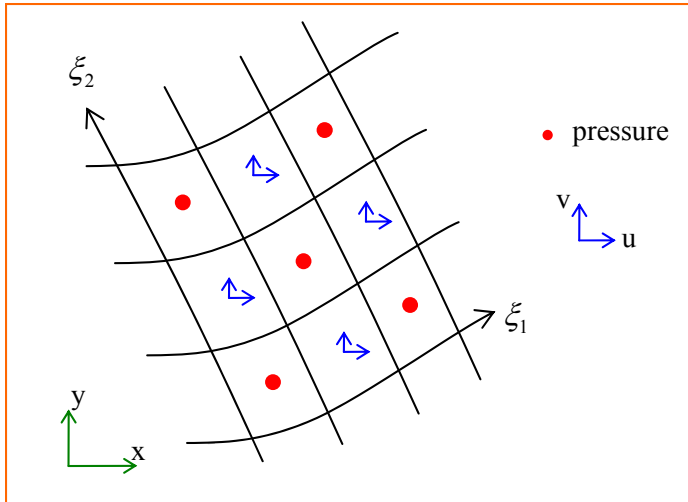
Layout of Dependent Variables...

- Partial staggering of ICED-ALE technique.



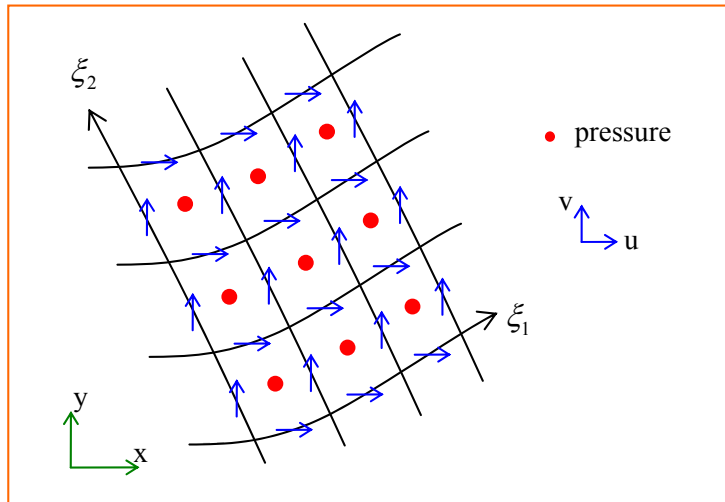
Layout of Dependent Variables...

- Elimination of half of the variables over a collocated grid.



Layout of Dependent Variables...

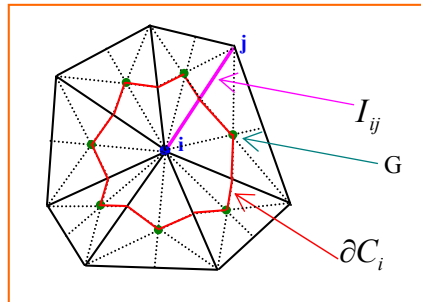
- **Fully staggered grid:** The model works well when the grid lines are aligned with the Cartesian velocity components (the effect of interpolation is minimum). When the interpolated part of the flux becomes dominant, the system becomes ill-conditioned or even singular.



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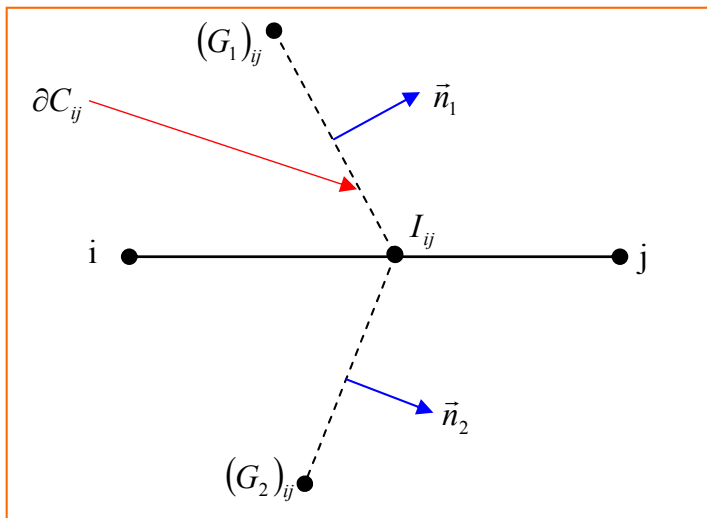
Unstructured Grids

- For 2D FVM discretization, we first create a normal finite element triangulation.
 - Then a dual FEM mesh is created by defining a cell C_i for each vertex S_i where $i = 1, 2, \dots, n$.
 - The procedure is as follows:
 - Every triangle having S_i as a vertex is subdivided in six sub-triangles by means of medians.
 - The cell C_i is the union of the sub-triangles having S_i as a vertex.
- The boundary of C_i is denoted by ∂C_i .



Unstructured Grids...

- The unit vector $\vec{n}_i = (n_x, n_y)_i$ is defined as the outward normal to ∂C_i .
- We split ∂C_i into panels ∂C_{ij} separating i and j .



Unstructured Grids...

- The flux integrals becomes:

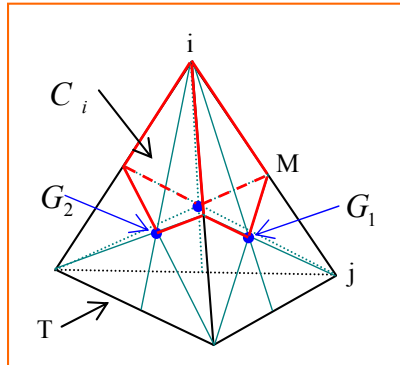
$$\int_{\partial C_i} \mathbf{F} \cdot \vec{n}_i dS = \sum_{j \in k(i)} \int_{\partial C_{ij}} \mathbf{F} \cdot \vec{n}_i dS$$

- Where $k(i)$ denotes the set of indices of neighboring nodes of S_i .
- The flux function for a segment ∂C_{ij} is given by:

$$\int_{\partial C_{ij}} \mathbf{F} \cdot \vec{n}_i dS = m_{ij}^x F_{ij}^x + m_{ij}^y F_{ij}^y \quad \text{with} \quad \vec{m}_{ij} = \int_{\partial C_{ij}} \vec{n}_i dS$$

3D Cases

The concept used in 2D case can be easily extended to 3D cases as follows:



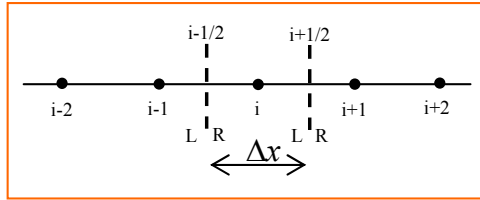
- The computational domain Ω is assumed to be discretized using standard FEM tetrahedrons.
- A dual FVM mesh is derived from the construction of median plans. For every vertex S_i we define a cell C_i around it.

3D Cases...

- Every tetrahedron is subdivided into 24 sub-tetrahedra by means of planes containing an edge and the middle of the opposite edge. Then, the cell C_i is the union of sub-tetrahedra having S_i as a vertex.
- In particular, the boundary ∂C_i of C_i is the union of $\partial C_{ij} = \partial C_i \cap \partial C_j$ that can be defined as the union of triangles such that
 - One vertex is the middle of the edge $S_i S_j$.
 - One vertex is the centroid of tetrahedral T having $S_i S_j$ as a side.
 - One vertex is the centroid of a triangular face of T having $S_i S_j$ as a side.

An interesting Observation

- Let us consider the following 1D grid:



- In 1D case, the cell average value becomes:

$$\bar{u}_i(t) \equiv \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t) dx$$

- Now, with $\xi = x - x_i$, we can expand $u(x)$ about x_i to get:

$$\begin{aligned} \bar{u}_i &\equiv \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} \left[u_i + \xi \left(\frac{\partial u}{\partial x} \right)_i + \frac{\xi^2}{2} \left(\frac{\partial^2 u}{\partial x^2} \right)_i + \frac{\xi^3}{6} \left(\frac{\partial^3 u}{\partial x^3} \right)_i + \dots \right] d\xi \\ &= u_i + \frac{\Delta x^2}{24} \left(\frac{\partial^2 u}{\partial x^2} \right)_i + \frac{\Delta x^4}{1920} \left(\frac{\partial^4 u}{\partial x^4} \right)_i + O(\Delta x^6) \\ &= u_i + O(\Delta x^2) \end{aligned}$$

- Hence, the cell-average value and the value at the center differ by a term of second order.

Example: 1D linear Convection

- Let us consider a scalar linear convection equation:

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0 \quad \text{with} \quad f = u$$

- Applying FVM we get:

$$\frac{d\bar{u}_i}{dt} + \frac{1}{\Delta x} (f_{i+1/2} - f_{i-1/2}) = 0$$

- Now, we choose a **piecewise constant** approximation to $u(x)$ in each cell such that

$$u(x) = \bar{u}_i \quad x_{i-1/2} \leq x \leq x_{i+1/2}$$

- Therefore,

$$\begin{aligned} f_{i+1/2}^L &= f(u_{i+1/2}^L) = u_{i+1/2}^L = \bar{u}_i \\ f_{i+1/2}^R &= f(u_{i+1/2}^R) = u_{i+1/2}^R = \bar{u}_{i+1} \end{aligned}$$

- Similarly,

$$\begin{aligned} f_{i-1/2}^L &= f(u_{i-1/2}^L) = u_{i-1/2}^L = \bar{u}_{i-1} \\ f_{i-1/2}^R &= f(u_{i-1/2}^R) = u_{i-1/2}^R = \bar{u}_i \end{aligned}$$

Example: 1D linear Convection...

- Note that the fluxes are discontinuous at the cell boundaries.
- We solve this problem by taking the average of the fluxes on either side of the boundary: (numerical fluxes \hat{f})

$$\hat{f}_{i+1/2} = \frac{1}{2}(f_{i+1/2}^L + f_{i+1/2}^R) = \frac{1}{2}(\bar{u}_i + \bar{u}_{i+1})$$

$$\hat{f}_{i-1/2} = \frac{1}{2}(f_{i-1/2}^L + f_{i-1/2}^R) = \frac{1}{2}(\bar{u}_{i-1} + \bar{u}_i)$$

- We finally get:

$$\frac{d\bar{u}_i}{dt} + \frac{1}{2\Delta x}(\bar{u}_{j+1} - \bar{u}_{j-1}) = 0$$

- This formulation is equivalent to a 2nd-order centered difference scheme.

Example: More on 1D Case...

- Let us replace the piecewise constant approximation with a piecewise **quadratic** form as:

$$u(\xi) = a\xi^2 + b\xi + c \quad \text{where} \quad \xi = x - x_i$$

- The three parameters are chosen to satisfy the following constraints:

$$\frac{1}{\Delta x} \int_{-3\Delta x/2}^{-\Delta x/2} u(\xi) d\xi = \bar{u}_{i-1}, \quad \frac{1}{\Delta x} \int_{-\Delta x/2}^{\Delta x/2} u(\xi) d\xi = \bar{u}_i, \quad \frac{1}{\Delta x} \int_{\Delta x/2}^{3\Delta x/2} u(\xi) d\xi = \bar{u}_{i+1}$$

- which leads to:

$$a = \frac{1}{2\Delta x^2} (\bar{u}_{i+1} - 2\bar{u}_i + \bar{u}_{i-1}), \quad b = \frac{1}{2\Delta x} (\bar{u}_{i+1} - \bar{u}_{i-1}), \quad c = \frac{1}{24} (-\bar{u}_{i+1} + 26\bar{u}_i - \bar{u}_{i-1})$$

- Using the above approximation, we get

$$\begin{aligned} u_{i+1/2}^L &= \frac{1}{6} (2\bar{u}_{i+1} + 5\bar{u}_i - \bar{u}_{i-1}) & u_{i+1/2}^R &= \frac{1}{6} (-\bar{u}_{i+2} + 5\bar{u}_{i+1} + 2\bar{u}_i) \\ u_{i-1/2}^L &= \frac{1}{6} (2\bar{u}_i + 5\bar{u}_{i-1} - \bar{u}_{i-2}) & u_{i-1/2}^R &= \frac{1}{6} (-\bar{u}_{i+1} + 5\bar{u}_i + 2\bar{u}_{i-1}) \end{aligned}$$

Example: More on 1D Case...

- Recalling that $f = u$, we obtain:

$$\hat{f}_{i+1/2} = \frac{1}{2} [f(u_{i+1/2}^L) + f(u_{i+1/2}^R)] = \frac{1}{12} (-\bar{u}_{i+2} + 7\bar{u}_{i+1} + 7\bar{u}_i - \bar{u}_{i-1})$$
$$\hat{f}_{i-1/2} = \frac{1}{2} [f(u_{i-1/2}^L) + f(u_{i-1/2}^R)] = \frac{1}{12} (-\bar{u}_{i+1} + 7\bar{u}_i + 7\bar{u}_{i-1} - \bar{u}_{i-2})$$

- Substituting into the integral form, we get:

$$\frac{d\bar{u}_i}{dt} + \frac{1}{12\Delta x} (-\bar{u}_{i+2} + 8\bar{u}_{i+1} - 8\bar{u}_{i-1} + \bar{u}_{i-2}) = 0$$

- This is a 4th-order approximation to the problem.

Example: 1D Diffusion

- Let us consider the diffusion equation as:

$$\frac{\partial u}{\partial t} + \nabla \mathbf{F} = 0 \quad \text{with} \quad \mathbf{F} = -\nabla u = -\left(\frac{\partial u}{\partial x} \mathbf{i} + \frac{\partial u}{\partial y} \mathbf{j} \right)$$

- In integral form, we have

$$\frac{d}{dt} \int_A u dA = \oint_S (n_x \mathbf{i} + n_y \mathbf{j}) \cdot \left(\frac{\partial u}{\partial x} \mathbf{i} + \frac{\partial u}{\partial y} \mathbf{j} \right) ds$$

- In 1D case, we can write:

$$\frac{d\bar{u}_i}{dt} + \frac{1}{\Delta x} (f_{i+1/2} - f_{i-1/2}) = 0 \quad \text{with} \quad f = -\frac{\partial u}{\partial x}$$

- Also, note that

$$\frac{1}{\Delta x} \int_{x_i}^{x_{i+1}} \frac{\partial u}{\partial x} dx = \frac{1}{\Delta x} (u_{i+1} - u_i) \quad \text{over } x_i \leq x \leq x_{i+1}$$

Example: 1D Diffusion

- Using a **piecewise constant** approximation inside each cell, we get

$$\hat{f}_{i+1/2} = -\left(\frac{\partial u}{\partial x}\right)_{i+1/2} = -\frac{1}{\Delta x}(\bar{u}_{i+1} - \bar{u}_i) \quad \hat{f}_{i-1/2} = -\left(\frac{\partial u}{\partial x}\right)_{i-1/2} = -\frac{1}{\Delta x}(\bar{u}_i - \bar{u}_{i-1})$$

- Substituting these into the integral form, we get:

$$\frac{d\bar{u}_i}{dt} + \frac{1}{\Delta x^2}(-\bar{u}_{i-1} + 2\bar{u}_i - \bar{u}_{i+1}) = 0$$

- If we use a piecewise **quadratic** approximation as before

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \xi} = 2a\xi + b$$

- Then, we obtain:

$$f_{i+1/2}^R = f_{i+1/2}^L = -\frac{1}{\Delta x}(\bar{u}_{i+1} - \bar{u}_i) \quad f_{i-1/2}^R = f_{i-1/2}^L = -\frac{1}{\Delta x}(\bar{u}_i - \bar{u}_{i-1})$$

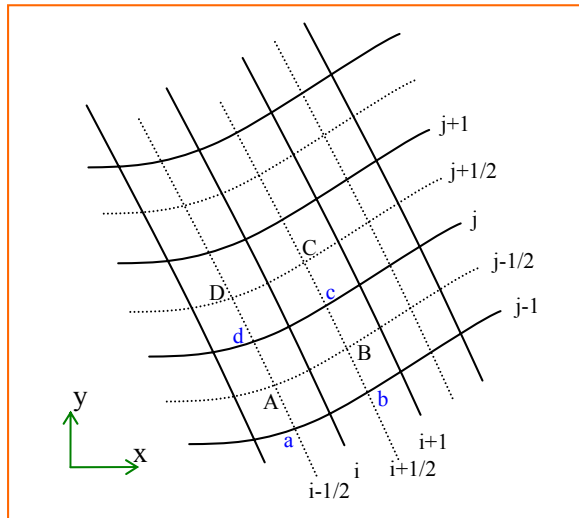
- The resulting scheme becomes exactly as before:

$$\frac{d\bar{u}_i}{dt} + \frac{1}{\Delta x^2}(-\bar{u}_{i-1} + 2\bar{u}_i - \bar{u}_{i+1}) = 0$$

2D Diffusion on Structured Grids

- Consider the transient 2D heat conduction equation:

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$



2D Diffusion on Structured Grids

- Integrating this equation over the finite volume **ABCD** (with unit dept) gives:

$$\iint_{ABCD} \frac{\partial T}{\partial t} (1) dx dy = \alpha \iint_{ABCD} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) (1) dx dy$$

- Applying the Green theorem, this becomes

$$\frac{\partial}{\partial t} \iint_{ABCD} T dx dy = \alpha \oint_{ABCD} \left(\frac{\partial T}{\partial x} \mathbf{i} + \frac{\partial T}{\partial y} \mathbf{j} \right) \cdot \mathbf{n} dS$$

- For our 2D geometry, we have

$$\frac{\partial}{\partial t} \iint_{ABCD} T dx dy = \alpha \oint_{ABCD} \left(\frac{\partial T}{\partial x} dy - \frac{\partial T}{\partial y} dx \right)$$

- Which can be approximated as

$$\begin{aligned} \frac{1}{\alpha} \left(\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} \right) S_{ABCD} &= \left(\frac{\partial T}{\partial x} \right)_{i,j-1/2} \Delta y_{AB} + \left(\frac{\partial T}{\partial x} \right)_{i+1/2,j} \Delta y_{BC} \\ &+ \left(\frac{\partial T}{\partial x} \right)_{i,j+1/2} \Delta y_{CD} + \left(\frac{\partial T}{\partial x} \right)_{i-1/2,j} \Delta y_{DA} \\ &- \left(\frac{\partial T}{\partial y} \right)_{i,j-1/2} \Delta x_{AB} - \left(\frac{\partial T}{\partial y} \right)_{i+1/2,j} \Delta x_{BC} \\ &- \left(\frac{\partial T}{\partial y} \right)_{i,j+1/2} \Delta x_{CD} - \left(\frac{\partial T}{\partial y} \right)_{i-1/2,j} \Delta x_{DA} \end{aligned}$$

2D Diffusion on Structured...

- The derivatives in the above formulation must be approximated appropriately. For example:

$$\begin{aligned}\left(\frac{\partial T}{\partial x}\right)_{i,j-1/2} &= \frac{1}{S_{abcd}} \iint \left(\frac{\partial T}{\partial x}\right) dx dy = \frac{1}{S_{abcd}} \oint T dy \\ &\cong \frac{1}{S_{abcd}} (T_{i,j-1} \Delta y_{ab} + T_b \Delta y_{bc} + T_{i,j} \Delta y_{cd} + T_a \Delta y_{da}) \\ \left(\frac{\partial T}{\partial y}\right)_{i,j-1/2} &= \frac{1}{S_{abcd}} \iint \left(\frac{\partial T}{\partial y}\right) dx dy = \frac{1}{S_{abcd}} \oint T dx \\ &\cong \frac{1}{S_{abcd}} (T_{i,j-1} \Delta x_{ab} + T_b \Delta x_{bc} + T_{i,j} \Delta x_{cd} + T_a \Delta x_{da})\end{aligned}$$

- In these equations, we have:

$$\begin{aligned}T_a &= \frac{1}{4} (T_{i,j} + T_{i-1,j} + T_{i-1,j-1} + T_{i,j-1}) \\ T_b &= \frac{1}{4} (T_{i,j} + T_{i+1,j} + T_{i+1,j-1} + T_{i,j-1})\end{aligned}$$