

Finite Volume Methods

Introduction

- Integral form of the conservation equation

$$\int_S \rho \phi \mathbf{v} \cdot \mathbf{n} \, dS = \int_S \Gamma \operatorname{grad} \phi \cdot \mathbf{n} \, dS + \int_{\Omega} q_{\phi} \, d\Omega . \quad (4.1)$$

- The solution domain is subdivided into a finite number of small CVs by a grid, which defines the CV boundaries, not the computational nodes.
- 2 Approaches
 - Define CVs by a suitable grid and assign the computational node to the CV center → Usual approach
 - Define nodal locations first and construct CVs around them, so that CV faces lie midway between nodes.

Introduction – Cont.

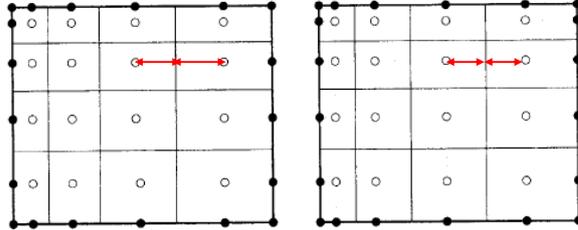


Fig. 4.1. Types of FV grids: nodes centered in CVs (left) and CV faces centered between nodes (right)

■ Advantages

- 1st approach: nodal values represents the mean over the CV to higher accuracy (2nd order)
- 2nd approach: CDS approximations of derivatives at CV faces are more accurate when the face is midway between 2 nodes.

Introduction – Cont.

■ Variants of FVM

- Cell-vertex schemes
- Dual-grid schemes
- Details in Chap 8 and references
- To obtain an algebraic equation for a particular CV, the surface and volume integrals need be approximated using quadrature formulae.

Flux Vector

- In the study of **transport phenomena** (**heat transfer**, **mass transfer** and **fluid dynamics**), flux is defined as the amount that flows through a unit area *per unit time*. Flux in this definition is a **vector**.

■ Flux definition and theorems

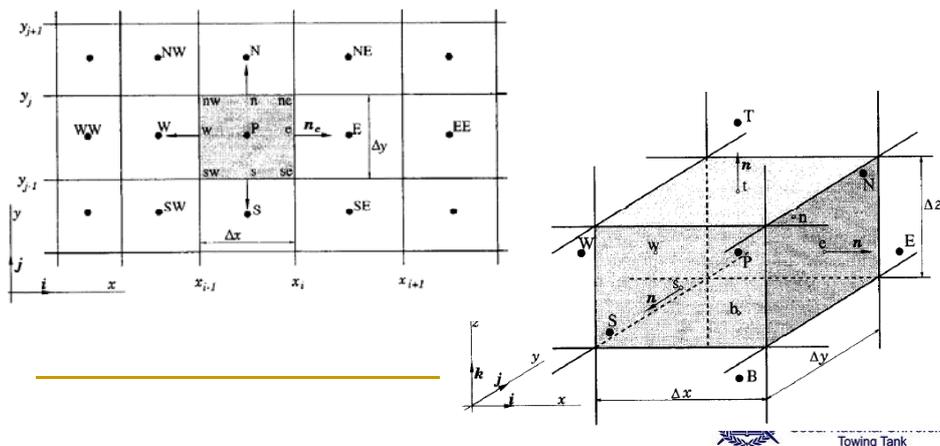
- Flux is surface bombardment rate. There are many fluxes used in the study of transport phenomena. Each type of flux has its own distinct unit of measurement along with distinct physical constants. Six of the most common forms of flux from the transport literature are defined as:
 - **Momentum flux**, the rate of transfer of **momentum** across a unit area ($\text{N}\cdot\text{s}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$). (**Newton's law of viscosity**)
 - **Heat flux**, the rate of **heat** flow across a unit area ($\text{J}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$). (**Fourier's law of conduction**)
 - **Chemical flux**, the rate of movement of molecules across a unit area ($\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$). (**Fick's law of diffusion**)
 - **Volumetric flux**, the rate of **volume** flow across a unit area ($\text{m}^3\cdot\text{m}^{-2}\cdot\text{s}^{-1}$). (**Darcy's law of groundwater flow**)
 - **Mass flux**, the rate of **mass** flow across a unit area ($\text{kg}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$). (Either an alternate form of Fick's law that includes the molecular mass, or an alternate form of Darcy's law that includes the density)
 - **Energy flux**, the rate of transfer of **energy** through a unit area ($\text{J}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$). The radiative flux and heat flux are specific cases of energy flux.
- These fluxes are vectors at each point in space, and have a definite magnitude and direction. Also, one can take the **divergence** of any of these fluxes to determine the accumulation rate of the quantity in a control volume around a given point in space. For **incompressible flow**, the divergence of the volume flux is zero.



Surface Integrals

■ CV surfaces

- 2D: four (e, w, n, s)
- 3D: six (e, w, n, s, t, b)



Surface Integrals – Cont.

- net flux through CV boundary = sum of integrals over CV faces

$$\square \int_S f \, dS = \sum_k \int_{S_k} f \, dS, \quad (4.2)$$

- f : component of convective ($\rho\phi\mathbf{v}\cdot\mathbf{n}$) or diffusive ($\Gamma\text{grad}\phi\cdot\mathbf{n}$) flux vector in the direction normal to CV face.
- CVs do not overlap, each CV face is unique to 2 CVs which lie on either side of it.
- Let's consider a typical CV face, e .



Surface Integrals – Cont.

- To calculate the surface integral in Eq. (4.2), we need to know f everywhere on S_e . However, only the nodal (CV center) values are calculated. Use 2 levels of approximation:

- The integral is approximated in terms of the variable values at one or more locations on the cell face.
- The cell-face values are approximated in terms of the nodal (CV center) values.

- Midpoint rule - simplest

- Integral is approximated as a product of f at cell-face center and cell-face area. The cell-face center value is in itself an approximation to the mean value over the surface.
- 2nd order accuracy

$$F_e = \int_{S_e} f \, dS = \bar{f}_e S_e \approx f_e S_e. \quad (4.3)$$



Surface Integrals – Cont.

- Trapezoidal rule
 - Need to evaluate the flux at CV corners
 - 2nd order accuracy

$$F_e = \int_{S_e} f \, dS \approx \frac{S_e}{2} (f_{ne} + f_{se}) . \quad (4.4)$$

- Simpson's rule
 - 4th order accuracy

$$F_e = \int_{S_e} f \, dS \approx \frac{S_e}{6} (f_{ne} + 4f_e + f_{se}) . \quad (4.5)$$

- In order to preserve the accuracy level, the values of f have to be computed with the same level of accuracy.



Volume Integrals

- Simplest 2nd order accurate approximation
 - Product of mean value (approximated as CV center value) and CV volume

$$Q_P = \int_{\Omega} q \, d\Omega = \bar{q} \Delta\Omega \approx q_P \Delta\Omega , \quad (4.6)$$

- Eq. (4.6) is exact if q is either constant or varies linearly within the CV; otherwise, it contains a 2nd order error.
- Higher order approximation requires q at more locations. These values have to be obtained by interpolating nodal values or by using shape functions.



Volume Integrals – Cont.

- In 2D

- 4th order approximation by bi-quadratic shape function

$$q(x, y) = a_0 + a_1 x + a_2 y + a_3 x^2 + a_4 y^2 + a_5 xy + a_6 x^2 y + a_7 xy^2 + a_8 x^2 y^2 . \quad (4.7)$$

- The coefficients are obtained by fitting the function to q 's at nine locations (nw, w, sw, n, P, s, ne, e, se).
- In 2D for Cartesian grids,

$$Q_P = \int_{\Omega} q \, d\Omega \approx \Delta x \Delta y \left[a_0 + \frac{a_3}{12} (\Delta x)^2 + \frac{a_4}{12} (\Delta y)^2 + \frac{a_8}{144} (\Delta x)^2 (\Delta y)^2 \right] . \quad (4.8)$$

- On a uniform Cartesian grid,

$$Q_P = \frac{\Delta x \Delta y}{36} (16 q_P + 4 q_s + 4 q_n + 4 q_w + 4 q_e + q_{se} + q_{sw} + q_{ne} + q_{nw}) . \quad (4.9)$$



Interpolation & Differentiation

- The approximations to the integrals require the variable values at locations other than CV centers.
- The integrand f involves the product of several variables and/or variable gradients at those locations
 - Convective flux $f^c = \rho \phi \mathbf{v} \cdot \mathbf{n}$
 - Diffusive flux $f^d = \Gamma \bar{\text{grad}} \phi \cdot \mathbf{n}$
- To calculate the convective and diffusive fluxes, the value of ϕ and its gradient normal to the cell face at one or more locations on the CV surface are needed.



Interpolation & Differentiation – Cont.

- Upwind interpolation (UDS)

- Approximating ϕ_e by its value at the node upstream of ‘e’
- Equivalent to using a backward- or forward difference approximation for 1st derivative

$$\phi_e = \begin{cases} \phi_P & \text{if } (\mathbf{v} \cdot \mathbf{n})_e > 0; \\ \phi_E & \text{if } (\mathbf{v} \cdot \mathbf{n})_e < 0. \end{cases} \quad (4.10)$$

- Unconditionally satisfy the boundedness condition, i.e., never yield oscillatory solutions.
- Numerically diffusive



Interpolation & Differentiation – Cont.

- Upwind interpolation (UDS) – Cont.

- Why diffusive

UDS → $\phi_e = \phi_P + (x_e - x_P) \left(\frac{\partial \phi}{\partial x} \right)_P + \frac{(x_e - x_P)^2}{2} \left(\frac{\partial^2 \phi}{\partial x^2} \right)_P + H, \quad (4.11)$

Leading truncation error

- Leading truncation error resembles a diffusive flux

$$f_e^d = \Gamma_e \left(\frac{\partial \phi}{\partial x} \right)_e. \quad (4.12)$$

with $\Gamma_e^{\text{num}} = (\rho u)_e \Delta x / 2$.

- Numerical diffusion is magnified in multidimensional problems if the flow is oblique to the grid; produces diffusion in the direction normal to the flow as well as in the streamwise direction.



Interpolation & Differentiation – Cont.

- Linear interpolation (CDS)

- Linear interpolation between two nearest points

$$\phi_e = \phi_E \lambda_e + \phi_P (1 - \lambda_e), \quad (4.13)$$

with

$$\lambda_e = \frac{x_e - x_P}{x_E - x_P}. \quad (4.14)$$

- Eq. (4.13) is 2nd order accurate (HW)

Leading truncation error

$$\phi_e = \phi_E \lambda_e + \phi_P (1 - \lambda_e) - \frac{(x_e - x_P)(x_E - x_e)}{2} \left(\frac{\partial^2 \phi}{\partial x^2} \right)_P + H. \quad (4.15)$$

- The leading truncation error term is proportional to the square of the grid spacing.
- May produce oscillatory solutions.
- Equivalent to central difference approximation of 1st derivative in FDM



Interpolation & Differentiation – Cont.

- Linear interpolation (CDS) – Cont.

- With assumption of a linear profile between P and E, it offers the simplest approximation of the gradient,

$$\left(\frac{\partial \phi}{\partial x} \right)_e \approx \frac{\phi_E - \phi_P}{x_E - x_P}. \quad (4.16)$$

with truncation error

$$\epsilon_\tau = \frac{(x_e - x_P)^2 - (x_E - x_e)^2}{2(x_E - x_P)} \left(\frac{\partial^2 \phi}{\partial x^2} \right)_e - \frac{(x_e - x_P)^3 + (x_E - x_e)^3}{6(x_E - x_P)} \left(\frac{\partial^3 \phi}{\partial x^3} \right)_e + H. \quad (4.17)$$

- When 'e' is midway between P and E, the approximation is of 2nd-order accuracy, since 1st term vanishes and leading error term is proportional to $(\Delta x)^2$.



Interpolation & Differentiation – Cont.

■ Quadratic upwind interpolation (QUICK)

- Approximate the variable profile between P and E by a parabola → need data at one more point

$$\phi_e = \phi_U + g_1(\phi_D - \phi_U) + g_2(\phi_U - \phi_{UU}), \quad (4.18)$$

- D, U, and UU: E, P, and W or P, E, and EE

$$g_1 = \frac{(x_e - x_U)(x_e - x_{UU})}{(x_D - x_U)(x_D - x_{UU})}; \quad g_2 = \frac{(x_e - x_U)(x_D - x_e)}{(x_U - x_{UU})(x_D - x_{UU})}$$

- 3rd-order truncation error (HW), on a uniform Cartesian grid with $u_x > 0$ (flow from P to E),

$$\phi_e = \frac{6}{8} \phi_P + \frac{3}{8} \phi_E - \frac{1}{8} \phi_W - \frac{3(\Delta x)^3}{48} \left(\frac{\partial^3 \phi}{\partial x^3} \right)_P + H. \quad (4.19)$$

- Although QUICK is slightly more accurate than CDS, both converge asymptotically in a 2nd-order manner and the differences are rarely large.



Interpolation & Differentiation – Cont.

■ Higher-order schemes

- Interpolation of order higher than 3rd makes sense only if the integrals are approximated using higher-order formulae. → If one uses Simpson's rule in 2D for surface integrals, one has to interpolate with polynomials of at least degree three, which leads to interpolation errors of 4th order.

- 4th-order CDS

$$\phi(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 \quad (4.20)$$

- For a uniform Cartesian grid,

$$\phi_e = \frac{27 \phi_P + 27 \phi_E - 3 \phi_W - 3 \phi_{EE}}{48}. \quad (4.21)$$

- To determine derivative, differentiate it once

$$\left(\frac{\partial \phi}{\partial x} \right)_e = a_1 + 2 a_2 x + 3 a_3 x^2, \quad (4.22)$$



Interpolation & Differentiation – Cont.

- Higher-order schemes – Cont.

- On a uniform Cartesian grid,

$$\left(\frac{\partial \phi}{\partial x}\right)_e = \frac{27 \phi_E - 27 \phi_P + \phi_W - \phi_{EE}}{24 \Delta x}. \quad (4.23)$$

- Once variable values and its derivative are obtained at cell-face centers, one can interpolate on the cell faces to obtain values at CV corners. → 4th-order scheme produces too large a computational molecule for implicit treatment.



Interpolation & Differentiation – Cont.

- Higher-order schemes – Cont.

- Another approach is to obtain the polynomial coefficients by fitting it to the variable values and 1st derivatives at 2 nodes on either side of cell face.

$$\phi_e = \frac{\phi_P + \phi_E}{2} + \frac{\Delta x}{8} \left[\left(\frac{\partial \phi}{\partial x}\right)_P - \left(\frac{\partial \phi}{\partial x}\right)_E \right]. \quad (4.24)$$

- Approximate the derivatives at P and E

$$\left(\frac{\partial \phi}{\partial x}\right)_P = \frac{\phi_E - \phi_W}{2 \Delta x}; \quad \left(\frac{\partial \phi}{\partial x}\right)_E = \frac{\phi_{EE} - \phi_P}{2 \Delta x}$$

- The resulting approximation of the cell-face value

$$\phi_e = \frac{\phi_P + \phi_E}{2} + \frac{\phi_P + \phi_E - \phi_W - \phi_{EE}}{16} + \mathcal{O}(\Delta x)^4. \quad (4.25)$$



Interpolation & Differentiation – Cont.

- Higher-order schemes – Cont.
 - The problem is that they contain 1st derivatives at CV centers, which are not known. → Although we can replace these by 2nd-order approximations, the resulting computational molecules will be much larger.
 - One should bear in mind that a higher-order approximation does not guarantee a more accurate solution on any single grid; high accuracy is achieved only when the grid is fine enough to capture all of the essential details of the solution.



Implementation of BCs

- Fluxes through CV faces coinciding with the domain boundary require special treatment
 - Convective fluxes
 - Inflow boundary: prescribed
 - Walls and symmetry boundary: zero
 - Outflow boundary: upwind
 - Diffusive fluxes
 - Specified, e.g., adiabatic surface with zero heat flux
 - If gradient itself is specified, it is used to calculate the flux, and an approximation for the flux in terms of CV center values can be used to calculate the boundary value of the variable.



Algebraic Equation System

- By summing all the flux approximations and source terms, we produce an algebraic equation which relates the variable value at CV center to neighbor CV values.
- The algebraic equation for a particular CV has the form Eq. (3.42).

Examples

- Read through!