Finite Volume Discretization

MMVN05

ROBERT SZASZ
Goal & Outline

Partial Differential Equation(s)

- 1D Cartesian
  - Diffusion
  - Source
  - Convection
  - Time dependent

Set of Algebraic Equations

- 2D Cartesian
- 2D Unstructured
The Finite Volume Method

• Generic transport equation

\[
\frac{\partial \rho \phi}{\partial t} + \text{div}(\rho u \phi) = \text{div}(\Gamma \text{grad } \phi) + S
\]

Time evolution  Convection  Diffusion  Source term

• Integrate over a control volume

\[
\int_V \frac{\partial \rho \phi}{\partial t} \, dV + \int_V \text{div}(\rho u \phi) \, dV = \int_V \text{div}(\Gamma \text{grad } \phi) \, dV + \int_V S \, dV
\]
Discretization in 1D

Control volume boundaries

Control volume

W

P

E

δx_{WP}

δx_{Pe}

Δx

δx_{PE}
Diffusion problems in 1D

\[ \text{div} (\Gamma \text{grad } \phi) + S = 0 \]

\[ \int_V \text{div} (\Gamma \text{grad } \phi) \, dV + \int_V S \, dV = 0 \]

\[
\int_A n. (\Gamma \text{grad } \phi) \, dA + \int_V S \, dV = 0
\]

\[
\left( \Gamma A \frac{\partial \phi}{\partial x} \right)_e - \left( \Gamma A \frac{\partial \phi}{\partial x} \right)_w + \bar{SV} = 0
\]

\[
\Gamma_e A_e \left( \frac{\partial \phi}{\partial x} \right)_e - \Gamma_w A_w \left( \frac{\partial \phi}{\partial x} \right)_w + S_u + S_p \phi_P = 0
\]
Diffusion problems in 1D

\[ \Gamma_e A_e \frac{\partial \phi}{\partial x}_e - \Gamma_w A_w \frac{\partial \phi}{\partial x}_w + S_u + S_p \phi_P = 0 \]

\[ \Gamma_e = \frac{\Gamma_W + \Gamma_P}{2}, \quad \Gamma_w = \frac{\Gamma_E + \Gamma_P}{2}, \quad \frac{\partial \phi}{\partial x}_e = \frac{\phi_E - \phi_P}{\delta x_{PE}}, \quad \frac{\partial \phi}{\partial x}_w = \frac{\phi_P - \phi_W}{\delta x_{WP}} \]

These are usually stored

\[ \phi_P \left( \frac{\Gamma_e A_e}{\delta x_{PE}} + \frac{\Gamma_w A_w}{\delta x_{WP}} - S_P \right) = \phi_W \frac{\Gamma_w A_w}{\delta x_{WP}} + \phi_E \frac{\Gamma_e A_e}{\delta x_{PE}} + S_u \]

\[ \phi_P a_P = \phi_W a_W + \phi_E a_E + S_u \]
Boundaries

Case 1: $\phi_w = F_w$ is known

$$\Gamma_e A_e \left( \frac{\partial \phi}{\partial x} \right)_e - \Gamma_w A_w \left( \frac{\partial \phi}{\partial x} \right)_w + S_u + S_p \phi_P = 0$$

$$\left( \frac{\partial \phi}{\partial x} \right)_w = \frac{\phi_P - F_w}{\delta x_{wp}}$$

Case 2: $\left( \frac{\partial \phi}{\partial x} \right)_w = G_w$ is known

$$\phi_P a_P = \phi_E a_E + S_u$$

Eastern boundary similarly
Building the system of equations

\[ \phi_P a_P = \phi_W a_W + \phi_E a_E + S_u \]

\[ \phi_1 a_{1,1} = \phi_2 a_{2,1} + S_1 \]
Building the system of equations

\[
\phi_p a_p = \phi_W a_W + \phi_E a_E + S_u
\]

\[
\phi_1 a_{1,1} = \phi_2 a_{2,1} + S_1
\]

\[
\phi_2 a_{2,2} = \phi_1 a_{1,2} + \phi_3 a_{3,2} + S_2
\]
Building the system of equations

\[ \phi_P a_P = \phi_W a_W + \phi_E a_E + S_u \]
\[ \phi_1 a_{1,1} = \phi_2 a_{2,1} + S_1 \]
\[ \phi_2 a_{2,2} = \phi_1 a_{1,2} + \phi_3 a_{3,2} + S_2 \]
\[ \phi_3 a_{3,3} = \phi_2 a_{2,3} + \phi_4 a_{4,3} + S_3 \]
Building the system of equations

\[ \phi_P a_P = \phi_W a_W + \phi_E a_E + S_u \]

\[ \phi_1 a_{1,1} = \phi_2 a_{2,1} + S_1 \]

\[ \phi_2 a_{2,2} = \phi_1 a_{1,2} + \phi_3 a_{3,2} + S_2 \]

\[ \phi_3 a_{3,3} = \phi_2 a_{2,3} + \phi_4 a_{4,3} + S_3 \]

\[ \phi_N a_{N,N} = \phi_{N-1} a_{N-1,N} + S_N \]
Convection-Diffusion problems in 1D

\[ \text{div}(\rho u \phi) = \text{div}(\Gamma \text{grad} \phi) \]

(source terms not considered for simplicity)

\[ \int_V \text{div}(\rho u \phi) dV = \int_V \text{div}(\Gamma \text{grad} \phi) dV \]

\[ \int_A n. (\rho \phi u) dA = \int_A n. (\Gamma \text{grad} \phi) dA \]

\[ (\rho u A \phi)_e - (\rho u A \phi)_w = \left( \Gamma A \frac{\partial \phi}{\partial x} \right)_e - \left( \Gamma A \frac{\partial \phi}{\partial x} \right)_w \]

Assume \( A_e = A_w = A \) and denote fluxes as:

\[ F_w = (\rho u)_w \quad F_e = (\rho u)_e \quad D_w = \frac{\Gamma_w}{\delta x_{WP}} \quad D_e = \frac{\Gamma_e}{\delta x_{PE}} \]

\[ F_e \phi_e - F_w \phi_w = D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W) \]
Convection-Diffusion problems in 1D

The continuity equation must be also fulfilled:

\[ \frac{\partial (\rho u)}{\partial x} = 0 \]

\[ (\rho u A)_e - (\rho u A)_w = 0 \]

\[ F_e - F_w = 0 \]
Convection-Diffusion problems in 1D

\[ F_e \phi_e - F_w \phi_w = D_e (\phi_E - \phi_P) - D_w (\phi_P - \phi_W) \]

How to estimate \( \phi_e, \phi_w \)?

Central difference scheme:

\[ \phi_e = \frac{\phi_P + \phi_E}{2} \quad \phi_w = \frac{\phi_W + \phi_P}{2} \]

\[ \left( D_w + \frac{F_w}{2} + D_e - \frac{F_e}{2} \right) \phi_P = \left( D_w + \frac{F_w}{2} \right) \phi_W + \left( D_e - \frac{F_e}{2} \right) \phi_E \]

\[ a_P \phi_P = a_W \phi_W + a_E \phi_E \]
Fig. 5.4. $N=5$, $u=0.1 \text{ m/s}$, $F=0.1$, $D=0.5$

Fig. 5.5. $N=5$, $u=2.5 \text{ m/s}$, $F=2.5$, $D=0.5$

Fig. 5.6. $N=20$, $u=2.5 \text{ m/s}$, $F=2.5$, $D=2.0$

WHY?
Properties of discretization schemes

• Conservativeness
  – Estimate the fluxes in a consistent manner!
Properties of discretization schemes

• **Boundedness**
  
  – In the absence of sources, the value of a property should be bounded by its boundary values
  
  – Requirements:
    
    » All coefficients the same sign
    
    » \[ \frac{\sum |a_{nb}|}{|a_{p'}|} \leq 1 \text{ at all nodes}, < 1 \text{ at one node at least} \]
Properties of discretization schemes

• **Transportiveness**
  – Where is the information transported?

Fig. 5.9
Assessment of the central differencing scheme

- Conservativeness: OK
- Boundedness:
  \[
  \left( D_w + \frac{F_w}{2} + D_e - \frac{F_e}{2} \right) \phi_P = \left( D_w + \frac{F_w}{2} \right) \phi_W - \left( D_e - \frac{F_e}{2} \right) \phi_E
  \]
  \( a_e < 0 \) for \( \text{Pe}_e = F_e / D_e > 2 \) !!!
- Transportiveness: Not OK!
- Accuracy: 2\textsuperscript{nd} order
Upwind differencing scheme

• Compute the convective term depending on the flow direction:

\[ \phi_e = \phi_P \quad \phi_w = \phi_W \]

\[ \phi_e = \phi_E \quad \phi_w = \phi_P \]
Upwind differencing scheme

- Assessment:
  - Conservativeness: OK
  - Boundedness: OK
  - Transportiveness: OK
  - Accuracy: 1\(^{\text{st}}\) order

Fig. 5.15
Hybrid differencing scheme

• Combine schemes:
  – Central for $\text{Pe} = F/D < 2$
  – Upwind for $\text{Pe} > 2$

• Assessment:
  – Conservativeness: OK
  – Boundedness: OK
  – Transportiveness: OK
  – Accuracy: 1\textsuperscript{st} order
Power-law scheme

• More accurate than hybrid
• Diffusion set to 0 for $\text{Pe} > 10$
• For $\text{Pe} < 10$ polynomial expression is used to evaluate the fluxes
The QUICK scheme

- Quadratic Upstream Interpolation for Convective Kinetics
- Higher order & Upwind
- Face values of \( \phi \) obtained from quadratic functions

- For \( u_w > 0 \)
  \[
  \phi_w = \frac{6}{8} \phi_W + \frac{3}{8} \phi_P - \frac{1}{8} \phi_{WW}
  \]

- For \( u_e > 0 \)
  \[
  \phi_e = \frac{6}{8} \phi_P + \frac{3}{8} \phi_E - \frac{1}{8} \phi_W
  \]

Fig. 5.17

- Diffusion terms can be evaluated from the gradient of the parabola
The QUICK scheme

• Generic form:

\[ a_P \phi_P = a_W \phi_W + a_E \phi_E + a_{WW} \phi_{WW} + a_{EE} \phi_{EE} \]

• Issues at boundaries: no second neighbours
  – Create virtual ‘mirror nodes’ by linear extrapolation

Fig.5.18
The QUICK scheme

• Assessment
  – Conservativeness: OK
  – Boundedness:
    » Only conditionally stable!
    – Reformulated versions to improve stability
  – Transportiveness: OK
  – Accuracy: better formal accuracy than upwind
  – Possible over/undershoots
General upwind-biased schemes

• ‘Pure’ upwind: \( \phi_e = \phi_P \)

• Linear upwind differencing: \( \phi_e = \phi_P + \frac{1}{2}(\phi_P - \phi_W) \)

• QUICK: \( \phi_e = \phi_P + \frac{1}{8}(3\phi_E - 2\phi_P - \phi_W) \)

• Central differencing: \( \phi_e = \phi_P + \frac{1}{2}(\phi_E - \phi_P) \)

• General: \( \phi_e = \phi_P + \frac{1}{2}\psi(\phi_E - \phi_P) \)
General upwind-biased schemes

\[ \psi = \psi(r) \]

\[ r = \frac{\phi_P - \phi_W}{\phi_E - \phi_P} \]

- UD \hspace{1cm} \psi(r) = 0
- CD \hspace{1cm} \psi(r) = 1
- LUD \hspace{1cm} \psi(r) = r
- QUICK \hspace{1cm} \psi(r) = (3 + r)/4

\[ \phi_e = \phi_P + \frac{1}{2} \psi(\phi_E - \phi_P) \]

Fig. 5.21
TVD schemes

- Total Variation Diminishing

\[ TV(\phi) = |\phi_2 - \phi_1| + |\phi_3 - \phi_2| + |\phi_4 - \phi_3| + |\phi_5 - \phi_4| \]

- Criteria:
  - Upper limit for TVD:
    \[ \psi(r) \leq 2r \quad r \leq 1 \]
    \[ \psi(r) \leq 2 \quad r > 1 \]
TVD

• For second order:
  – Must go through (1,1)
  – Limited by CD and LUD

Fig. 5.24

• To treat forward and backward differencing consistently: symmetry property:

$$\frac{\psi(r)}{r} = \psi(1/r)$$

Fig. 5.25

• Flux limiters
Unsteady flows

\[ \frac{\partial \rho \phi}{\partial t} + \text{div}(\rho u \phi) = \text{div}(\Gamma \text{grad} \phi) + S \]

\[ \int_V \frac{\partial \rho \phi}{\partial t} dV + \int_V \text{div}(\rho u \phi) dV = \int_V \text{div}(\Gamma \text{grad} \phi) dV + \int_V S dV \]

\[ \int_t^{t+\Delta t} \int_V \frac{\partial \rho \phi}{\partial t} dV dt + \int_t^{t+\Delta t} \int_V \text{div}(\rho u \phi) dV dt \]

\[ = \int_t^{t+\Delta t} \int_V \text{div}(\Gamma \text{grad} \phi) dV dt + \int_t^{t+\Delta t} \int_V S dV dt \]
Unsteady 1D heat conduction

\[ \rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + S \]

- \( c \) – specific heat [J/(kg K)]

\[
\int _{t}^{t+\Delta t} \int _{V} \rho c \frac{\partial T}{\partial t} dV dt = \int _{t}^{t+\Delta t} \int _{V} \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) dV dt + \int _{t}^{t+\Delta t} \int _{V} S dV dt
\]

\[
\int _{V} \int _{t}^{t+\Delta t} \rho c \frac{\partial T}{\partial t} dtdV = \int _{t}^{t+\Delta t} \left[ \left( kA \frac{\partial T}{\partial x} \right) _{e} - \left( kA \frac{\partial T}{\partial x} \right) _{w} \right] dt + \int _{t}^{t+\Delta t} \tilde{S} \Delta V dt
\]
Unsteady 1D heat conduction

\[
\int_V \int_t^{t+\Delta t} \rho c \frac{\partial T}{\partial t} \, dt \, dV = \int_t^{t+\Delta t} \left[ \left( kA \frac{\partial T}{\partial x} \right)_e - \left( kA \frac{\partial T}{\partial x} \right)_w \right] \, dt + \int_t^{t+\Delta t} \bar{S} \Delta V \, dt
\]

Assume uniform T in control volume and use backward differencing

\[
\rho c (T_P - T_P^0) \Delta V = \int_t^{t+\Delta t} \left[ \left( kA \frac{T_E - T_P}{\delta x_{PE}} \right) - \left( kA \frac{T_P - T_W}{\delta x_{WP}} \right) \right] \, dt + \int_t^{t+\Delta t} \bar{S} \Delta V \, dt
\]

Use central differencing

How do \( T_E, T_W \) and \( T_P \) vary in time? Assume a linear function:

\[
I_T = \int_t^{t+\Delta t} T \, dt = (\theta T + (1 - \theta)T^0) \Delta t
\]

Lund University
Unsteady 1D heat conduction

\[ \rho c(T_P - T_P^0)\Delta V = \int_t^{t+\Delta t} \left[ \left( kA \frac{T_E - T_P}{\delta x_{PE}} \right) - \left( kA \frac{T_P - T_W}{\delta x_{WP}} \right) \right] dt + \int_t^{t+\Delta t} \tilde{S}\Delta V dt \]

Divide by A and \( \Delta t \):

\[ \frac{\rho c(T_P - T_P^0) \Delta x}{\Delta t} \]

\[ = \theta \left[ k \frac{T_E - T_P}{\delta x_{PE}} - k \frac{T_P - T_W}{\delta x_{WP}} \right] + (1 - \theta) \left[ k \frac{T_E^0 - T_P^0}{\delta x_{PE}} - k \frac{T_P^0 - T_W^0}{\delta x_{WP}} \right] + \tilde{S}\Delta x \]

\[ a_P T_P \]

\[ = a_W (\theta T_W + (1 - \theta)T_W^0) + a_E (\theta T_E + (1 - \theta)T_E^0) \]

\[ + (a_P^0 - (1 - \theta)a_W - (1 - \theta)a_E)T_P^0 + b \]
Explicit scheme

\[ \theta = 0 \]

\[ a_P T_P = a_W T_W^0 + a_E T_E^0 + (a_P^0 - a_W - a_E + S_P) T_P^0 + S_u \]

\( T_P \) can be directly computed

First order

Can be negative! To assure stability:

\[ \Delta t < \rho c \left( \frac{\Delta x}{2k} \right)^2 \]

Very small timesteps when the grid is refined!
Implicit scheme

\[ \theta = 1 \]

\[ a_P T_P = a_W T_W + a_E T_E + a^0_P T^0_P + S_u \]

Several unknowns -> System of equations

Unconditionally stable

First order
Crank-Nicolson scheme

\[ \theta = \frac{1}{2} \]

\[ a_P T_P = a_W \left( \frac{T_W + T_W^0}{2} \right) + a_E \left( \frac{T_E + T_E^0}{2} \right) + \left( \frac{a_P^0}{2} - \frac{a_W}{2} - \frac{a_E}{2} + \frac{S_P}{2} \right) T_P^0 + S_u \]

System of equations

To assure stability:

\[ \Delta t < \rho c \left( \frac{\Delta x}{k} \right)^2 \]

Very small timesteps when the grid is refined!

Second order
Unsteady 1D convection-diffusion

\[ \frac{\partial \rho \phi}{\partial t} + \frac{\partial \rho u \phi}{\partial x} = \frac{\partial}{\partial x} \left( \Gamma \frac{\partial \phi}{\partial x} \right) + S \]

- Similarly to unsteady diffusion
- Additional stability limits due to convection
Finite volume method for 2D Cartesian grids

- E.g. diffusion problem:
  \[ \frac{\partial}{\partial x} \Gamma \frac{\partial \phi}{\partial x} + \frac{\partial}{\partial y} \Gamma \frac{\partial \phi}{\partial y} + S = 0 \]

\[ \int_{\Delta V} \frac{\partial}{\partial x} \Gamma \frac{\partial \phi}{\partial x} dV + \int_{\Delta V} \frac{\partial}{\partial y} \Gamma \frac{\partial \phi}{\partial y} dV \]

\[ + \int_{\Delta V} S dV = 0 \]

\[ \Gamma_e A_e \frac{\phi_E - \phi_P}{\delta x_{PE}} - \Gamma_w A_w \frac{\phi_P - \phi_W}{\delta x_{WP}} + \Gamma_n A_n \frac{\phi_N - \phi_P}{\delta y_{PN}} - \Gamma_s A_s \frac{\phi_P - \phi_S}{\delta y_{SP}} + \bar{S} \Delta V = 0 \]

\[ a_P \phi_P = a_W \phi_W + a_E \phi_E + a_S \phi_S + a_N \phi_N + S_u = 0 \]
Finite Volume Method on unstructured grids

\[ \int_V \frac{\partial \rho \phi}{\partial t} dV + \int_V \text{div}(\rho u \phi) dV \]

\[ = \int_V \text{div}(\Gamma \text{grad} \phi) dV + \int_V S dV \]

\[ \frac{\partial}{\partial t} \int_V \rho \phi dV + \int_A n. (\rho u \phi) dA = \int_A n. (\Gamma \text{grad} \phi) dA + \int_V S dV \]

\[ \frac{\partial}{\partial t} \int_V \rho \phi dV + \sum \int_{\Delta A_i} n_i. (\rho u \phi) dA = \sum \int_{\Delta A_i} n_i. (\Gamma \text{grad} \phi) dA + \int_V S dV \]

- \( n_i \) can be computed based on grid topology
Diffusion term

- Central differencing

\[
\int_{\Delta A_i} n_i. (\Gamma \text{grad} \, \phi) dA \approx n_i. (\Gamma \text{grad} \, \phi) \Delta A_i \approx \Gamma \frac{\phi_A - \phi_P}{\Delta \xi} \Delta A_i
\]

- Only true if the grid is orthogonal
Non-orthogonal grids

• Can be computed as:

\[
\begin{align*}
n \cdot \nabla \phi \Delta A_i &= n \cdot n \Delta A_i \phi_A - \phi_P \\
&= \frac{n \cdot e_\xi \Delta \xi}{n \cdot e_\xi} \phi_b - \phi_a \\
&+ \frac{e_\xi \cdot e_\eta \Delta A_i}{n \cdot e_\xi} \frac{\phi_b - \phi_a}{\Delta \eta}
\end{align*}
\]

Fig. 11.17
Non-orthogonal grids

\[ \text{n. grad} \phi \, \Delta A_i = \frac{n \cdot n \Delta A_i \phi_A - \phi_P}{n \cdot e_\xi} \Delta \xi - \frac{e_\xi \cdot e_\eta \Delta A_i \phi_b - \phi_a}{n \cdot e_\xi} \Delta \eta \]

Direct gradient

Cross-diffusion

Can be (pre)computed (and stored) based on grid topology.

- Compare to: \[ \text{n. grad} \phi \, \Delta A_i = \frac{\phi_A - \phi_P}{\Delta \xi} \Delta A_i \]
Convective term

- Approximate as:

\[ \int_{\Delta A_i} n_i (\rho \phi u) dA \approx \phi_i \int_{\Delta A_i} n_i (\rho u) dA \approx \phi_i F_i \]

\( F_i \) = Convective flux normal to the surface element. Usually stored.
• Upwind differencing
  - $F_i > 0 \ \phi_i = \phi_P$
  - $F_i < 0 \ \phi_i = \phi_A$
• Linear upwind differencing
  \[ \phi_i = \phi_P + \nabla \phi_P \cdot \Delta r \]
  Needs to be computed!
• QUICK
• TVD
• ...