Discretization of Convection Diffusion type Equation

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Presentation Outline

- Introduction
- Finite Volume Method
- Spatial discretization
- Source term discretization
- Temporal discretization
- Convergence
- False diffusion
Introduction

General transport equation for the conservation of property $\phi$:

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

- Here $\phi$ is the general variable, $\Gamma$ is diffusion constant corresponding to $\phi$, $S$ is source term.
- We shall look into different schemes for formulating set of linear equation to solve it numerically, numerical stability of formulation and false diffusion.
Finite Volume Method

Basic methodology

Divide domain into control volumes

- Integrate the differential equation over the control volume and apply divergence theorem.
- To evaluate the derivative term, values at face of control volume are needed, assume a profile.
- Result is set of linear algebraic equation: one for each control volume.
- Solve them iteratively or simultaneously.
Control volumes do not overlap.

Net flux through control volume is the sum of flux through all four faces (6 in 3D).

Values at faces are not known in general and found by interpolation.
So finally we get equation for cell P like

\[ a_p \phi = a_w \phi + a_e \phi + a_n \phi + a_s \phi + b \]
Finite Volume Method

4 basic rules

- For solutions to be physically realistic and satisfy overall balance (conservative) There are some basic rules that need to be satisfied by the discretization equations.
  1. Flux consistency at CV faces
  2. Positive coefficients
  3. Negative slope linearization of source term
     \[ \bar{S} = S_c + S_p \phi_p \quad S_p \text{ should be negative} \]
  4. Sum of neighbor coefficients
     \[ a_p = \sum a_{nb} \]
Spatial discretization
(central difference and upwind)

To start with we shall consider simplest case 1D steady state
(with no source term)

\[
\frac{d}{dx} (\rho u \phi) = \frac{d}{dx} (\Gamma \frac{d \phi}{dx})
\]

It should also satisfy continuity equation

\[
\frac{d (\rho u)}{dx} = 0 \text{ or } \rho u = \text{constant}
\]
Spatial discretization
(central difference and upwind)

- Consider the 1-dimensional grid system ($\Delta y$ and $\Delta z = 1$):

\[
\left(\delta x\right)_w \quad \Delta x \quad \left(\delta x\right)_e
\]

We integrate diffusion convection over control volume

\[
(\rho u \phi)_e - (\rho u \phi)_w = \left( \Gamma \frac{d\phi}{dx} \right)_e - \left( \Gamma \frac{d\phi}{dx} \right)_w
\]
Spatial discretization
(central difference and upwind)

Face values of $\phi$ and $\partial \phi / \partial x$ are found by making assumptions about variation of $\phi$ between cell centers.

Central Differencing Scheme

If we assume linear profile

$$
\left( \Gamma \frac{d\phi}{dx} \right)_e - \left( \Gamma \frac{d\phi}{dx} \right)_w = \frac{\Gamma_e (\phi_E - \phi_P)}{(\delta x)_e} - \frac{\Gamma_w (\phi_P - \phi_W)}{(\delta x)_w}
$$

$$
(\rho u \phi)_e - (\rho u \phi)_w = \frac{1}{2} (\rho u)_e (\phi_E + \phi_P) - \frac{1}{2} (\rho u)_w (\phi_P + \phi_W)
$$
Spatial discretization
(central difference and upwind)

Now we use following notation

\[ F_w = (\rho u)_w, \quad F_e = (\rho u)_e \]

\[ D_w = \frac{\Gamma_w}{\delta x_w}, \quad D_e = \frac{\Gamma_e}{\delta x_e} \]

Our equation becomes

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

Discretization equation can be written as

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

where

<table>
<thead>
<tr>
<th>( a_W )</th>
<th>( a_E )</th>
<th>( a_P )</th>
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<tbody>
<tr>
<td>( D_w + \frac{F_w}{2} )</td>
<td>( D_e - \frac{F_e}{2} )</td>
<td>( a_W + a_E + (F_e - F_w) )</td>
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</tbody>
</table>
Spatial discretization
(central difference and upwind)

- Conservativeness: Uses consistent expressions to evaluate convective and diffusive fluxes at CV faces. Hence Unconditionally Conservative

- Boundedness: $a_W$ or $a_E$ will become negative if $P_e > 2$

  \[ P_e = \frac{F_e}{D_e} \]

  Scheme is conditionally bounded for $P_e < 2$

- Transportiveness: The CDS uses influence at node P from all directions. Does not recognize direction of flow or strength of convection relative to diffusion. Does not possess Transportiveness at high Peclet Numbers
Spatial discretization
(central difference and upwind)

- Accuracy: Second Order in terms of Taylor series Stable and accurate only if \( P_e < 2 \)

Now

\[
P_e = \frac{F_e}{D_e} = \frac{(\rho u)_e \partial x_e}{\Gamma_e}
\]

Hence, for stability and accuracy, either velocity should be very low or grid spacing should be small.
Spatial discretization
(central difference and upwind)

- First order upwind scheme

\[ \phi_e = \phi_P \quad \text{if } F_e > 0 \]
\[ \phi_e = \phi_E \quad \text{if } F_e < 0 \]

Similarly for \( \phi_W \)

If \( [A, B] = Max(A, B) \)

Then discretization equation

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

<table>
<thead>
<tr>
<th>( a_W )</th>
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<th>( a_P )</th>
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<tr>
<td>( D_W + [F_W, 0] )</td>
<td>( D_e + [-F_e, 0] )</td>
<td>( a_W + a_E + (F_e - F_W) )</td>
</tr>
</tbody>
</table>
Spatial discretization
(central difference and upwind)

First order upwind scheme

• Conservativeness: It is conservative
• Boundedness: When flow satisfies continuity equation, all coefficients are positive.
• Transportiveness: Direction of flow inbuilt in the formulation, thus accounts for transportiveness.
• Accuracy: When flow is not aligned with the grid lines, it produces false diffusion, which will form last part of our discussion.
Spatial discretization
(exact solution)

- The governing transport equation:

\[
\frac{d}{dx} (\rho u \phi) = \frac{d}{dx} \left( \Gamma \frac{d\phi}{dx} \right)
\]

- This can be exactly solved if \( \Gamma \) is constant.

- Boundary conditions: at \( x = 0 \) \( \phi = \phi_0 \), at \( x = L \) \( \phi = \phi_L \)

Solution: \[
\frac{\phi - \phi_0}{\phi_L - \phi_0} = \frac{P x}{L} \left( e^{P x/L} - 1 \right) / (e^P - 1)
\]

Where \( P = \rho u L / \Gamma \)
Spatial discretization

Example

- Consider following convection diffusion equation

\[-\frac{d^2 u}{dx^2} + w \frac{du}{dx} = f(x), \quad 0 < x < 1 \quad \text{with} \quad u(0) = 1, \ u(1) = 0.\]

- Suppose \( f = 0 \); then exact solution is

\[
\frac{(\exp w - \exp (wx))}{(\exp w - 1)}.
\]
Spatial discretization

Example

Exact solutions for \( w = 1, 5, 10, 20 \)
Suppose we choose $N=4$ on interval $[0,1]$ then

$$x_0 = 0, x_1 = \frac{1}{4}, x_2 = \frac{2}{4}, x_3 = \frac{3}{4}, x_4 = 1$$

Here $\Delta x = \frac{1}{4}$ Hence

$$F_e = F_w = \frac{w}{\Delta x}; D_e = D_w = \frac{1}{\Delta x^2}$$

Hence we get 3 equation as

$$
\left( -\frac{1}{\Delta x^2} - \frac{w}{2\Delta x} \right) u_{i-i} + \left( \frac{1}{\Delta x^2} \right) u_i + \left( -\frac{1}{\Delta x^2} + \frac{w}{2\Delta x} \right) u_{i+1} = 0; i = 1, 2, 3
$$
Spatial discretization

Solution by CDS

- Further we need boundary condition, in this case it is
  \[ u_0 = 1; u_4 = 0 \]

\[
\begin{pmatrix}
32 & -16+2w & 0 \\
-16-2w & 32 & -16+2w \\
-16-2w & 32 & -16-2w
\end{pmatrix}
\begin{pmatrix}
u_1 \\
u_2 \\
u_3
\end{pmatrix}
= 
\begin{pmatrix}
16+2w \\
0 \\
0
\end{pmatrix}
\]

- Now we solve it to get values of \( u_1, u_2 \) and \( u_3 \)
Exact and numerical solution for $u(x), w=40, N=5, 10, 15$ and $20$
Solution by First order upwind

- Here coefficients are different from CDS

\[
\left( -\frac{1}{\Delta x^2} - \frac{w}{\Delta x} \right) u_{i-i} + \left( \frac{2}{\Delta x^2} + \frac{w}{\Delta x} \right) u_i + \left( -\frac{1}{\Delta x^2} \right) u_{i+1} = 0; i = 1, 2, 3
\]

- Boundary condition \( u_0 = 1; u_4 = 0 \)

\[
\begin{pmatrix}
32 + 4w & -16 & 0 \\
-16 - 4w & 32 + 4w & -16 \\
-16 - 4w & 32 + 4w & 0
\end{pmatrix}
\begin{pmatrix}
u_1 \\
u_2 \\
u_3
\end{pmatrix} =
\begin{pmatrix}
16 + 4w \\
0 \\
0
\end{pmatrix}
\]
Spatial discretization

Solution by first order upwind

Exact and numerical solution for $u(x), w=40, N=5, 10, 15$ and $20$
Exponential scheme

(exponential)

- Define
  \[ J = \rho u \phi - \Gamma \frac{d\phi}{dx} \]

- Our transport equation becomes
  \[ \frac{dJ}{dx} = 0 \]

- integrating over CV
  \[ J_e - J_w = 0 \]

- The exact solution derived above can be used as profile assumption with
  \[ \phi_0 \rightarrow \phi_P, \phi_L \rightarrow \phi_E, L \rightarrow \delta x_e \]

- Substitution gives
  \[ J_e = F_e (\phi_P + \frac{\phi_P - \phi_E}{e^{Pe} - 1}) \]

- Where
  \[ Pe = \frac{(\rho u)_e \delta x_e}{\Gamma_e} = \frac{F_e}{D_e} \]
Exponential scheme
(exponential)

- After substitution of similar expression for $J_w$, equation in our standard form can be written as:

$$a_P \phi_P = a_W \phi_W + a_E \phi_E \quad a_P = a_W + a_E + (F_e - F_w)$$

<table>
<thead>
<tr>
<th>$a_W$</th>
<th>$a_E$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_w e^{F_w/D_w} / (e^{F_w/D_w} - 1)$</td>
<td>$F_e / (e^{F_e/D_e} - 1)$</td>
</tr>
</tbody>
</table>

- Merit: Guaranteed to produce exact solution for any Peclet number for 1-D steady convection-diffusion
- Demerits: 1. exponentials expensive to compute
  2. not exact for 2-D, 3-D
Hybrid Scheme

- In exponential scheme
  \[ \frac{a_E}{D_e} = \frac{P_e}{e^{P_e} - 1} \]

- Hence
  \[ \text{For } P_e \to \infty, \quad \frac{a_E}{D_e} \to 0 \]
  \[ \text{For } P_e \to -\infty, \quad \frac{a_E}{D_e} \to -P_e \]
  \[ \text{At } P_e = 0, \quad \frac{a_E}{D_e} = 1 - \frac{P_e}{2} \]

- Hybrid scheme is piecewise linear approximation of exponential scheme
  \[ P_e < -2 \quad \frac{a_E}{D_e} = -P_e; \quad -2 < P_e < 2 \quad \frac{a_E}{D_e} = 1 - \frac{P_e}{2}; \quad P_e > 2 \quad \frac{a_E}{D_e} = 0 \]
Power Law scheme

- Another approximation to exponential scheme
- Diffusion is set equal to zero for $P_e > 10$ or $P_e < -10$
- Otherwise calculated as follows

\begin{align*}
For P_e < -10, \quad \frac{a_E}{D_e} &= -P_e \\
For -10 \leq P_e < 0, \quad \frac{a_E}{D_e} &= (1 + 0.1P_e)^5 - P_e, \\
For 0 \leq P_e \leq 10, \quad \frac{a_E}{D_e} &= (1 - 0.1P_e)^5 \\
For P_e > 10, \quad \frac{a_E}{D_e} &= 0
\end{align*}
Second order upwind scheme

We determine the value of $\phi$ from the cell values in the two cells upstream of the face.

More accurate than the first order upwind scheme, but in regions with strong gradients it can result in face values that are outside of the range of cell values. It is then necessary to apply limiters to the predicted face values.
QUICK stands for Quadratic Upwind Interpolation for Convective Kinetics.

A quadratic curve is fitted through two upstream nodes and one downstream node. This is a very accurate scheme, but in regions with strong gradients, overshoots and undershoots can occur. This can lead to stability problems in the calculation.
Accuracy of different scheme

- Each of the previously discussed numerical schemes assumes some shape of the function $\phi$. These functions can be approximated by Taylor series polynomials:

$$
\phi(x_e) = \phi(x_p) + \frac{\phi'(x_p)}{1!}(x_e - x_p) + \frac{\phi''(x_p)}{2!}(x_e - x_p)^2 + \ldots + \frac{\phi^{(n)}(x_p)}{n!}(x_e - x_p)^n + \ldots
$$

- The first order upwind scheme only uses the constant and ignores the first derivative and consecutive terms. This scheme is therefore considered first order accurate.

- For high Peclet numbers the power law scheme reduces to the first order upwind scheme, so it is also considered first order accurate.

- The central differencing scheme and second order upwind scheme do include the first order derivative, but ignore the second order derivative. These schemes are therefore considered second order accurate. QUICK does take the second order derivative into account, but ignores the third order derivative. This is then considered third order accurate.
Spatial Discretization 2-D and 3-D

Discretization in 2D

\[ a_P \phi_P = a_W \phi_W + a_E \phi_E + a_S \phi_S + a_N \phi_N \]
\[ a_P = a_W + a_E + a_S + a_N + \Delta F \]

Discretization in 3D

\[ a_P \phi_P = a_W \phi_W + a_E \phi_E + a_S \phi_S + a_N \phi_N + a_B \phi_B + a_T \phi_T \]
\[ a_P = a_W + a_E + a_S + a_N + a_B + a_T + \Delta F \]
## Spatial Discretization 2-D and 3-D

Coefficients for 2-D, 3-D(HDS)

<table>
<thead>
<tr>
<th></th>
<th>One Dimensional Flow</th>
<th>Two Dimensional Flow</th>
<th>Three Dimensional Flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_W$</td>
<td>$\left[ F_w, \left( D_w + \frac{F_w}{2} \right), 0 \right]$</td>
<td>$\left[ F_w, \left( D_w + \frac{F_w}{2} \right), 0 \right]$</td>
<td>$\left[ F_w, \left( D_w + \frac{F_w}{2} \right), 0 \right]$</td>
</tr>
<tr>
<td>$a_E$</td>
<td>$\left[ -F_e, \left( D_e - \frac{F_e}{2} \right), 0 \right]$</td>
<td>$\left[ -F_e, \left( D_e - \frac{F_e}{2} \right), 0 \right]$</td>
<td>$\left[ -F_e, \left( D_e - \frac{F_e}{2} \right), 0 \right]$</td>
</tr>
<tr>
<td>$a_S$</td>
<td>$\left[ F_s, \left( D_s + \frac{F_s}{2} \right), 0 \right]$</td>
<td>$\left[ F_s, \left( D_s + \frac{F_s}{2} \right), 0 \right]$</td>
<td>$\left[ F_s, \left( D_s + \frac{F_s}{2} \right), 0 \right]$</td>
</tr>
<tr>
<td>$a_N$</td>
<td>$\left[ -F_n, \left( D_n - \frac{F_n}{2} \right), 0 \right]$</td>
<td>$\left[ -F_n, \left( D_n - \frac{F_n}{2} \right), 0 \right]$</td>
<td>$\left[ -F_n, \left( D_n - \frac{F_n}{2} \right), 0 \right]$</td>
</tr>
<tr>
<td>$a_B$</td>
<td>$\left[ F_b, \left( D_b + \frac{F_b}{2} \right), 0 \right]$</td>
<td>$\left[ F_b, \left( D_b + \frac{F_b}{2} \right), 0 \right]$</td>
<td>$\left[ F_b, \left( D_b + \frac{F_b}{2} \right), 0 \right]$</td>
</tr>
<tr>
<td>$a_T$</td>
<td>$\left[ -F_t, \left( D_t - \frac{F_t}{2} \right), 0 \right]$</td>
<td>$\left[ -F_t, \left( D_t - \frac{F_t}{2} \right), 0 \right]$</td>
<td>$\left[ -F_t, \left( D_t - \frac{F_t}{2} \right), 0 \right]$</td>
</tr>
<tr>
<td>$\Delta F$</td>
<td>$F_e - F_w$</td>
<td>$F_e - F_w + F_n - F_s$</td>
<td>$F_e - F_w + F_n - F_s + F_t - F_b$</td>
</tr>
</tbody>
</table>
Source term discretization

- For 1-D, Discretization equation simply becomes,

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

- If the source term is a constant then \( b = S \Delta x \)

- If Source term is dependent of \( \phi \) then linearize \( S \) about \( P \) s.t.

\[ S = S_C + S_P \phi_P \]

- Hence

\[ b = S_C \Delta x, \quad a'_P = a_P - S_P \Delta x \]

- And all other coefficients remain the same
Temporal discretization

For simplicity we consider time-dependent heat conduction:

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

We integrate in time (from \( t \) to \( t + \Delta t \)) and space:

\[ \rho c \int_0^{t+\Delta t} \int_t^{t+\Delta t} \frac{\partial T}{\partial t} \, dt \, dx = \int_0^{t+\Delta t} \int_t^{t+\Delta t} \frac{\partial}{\partial t} \left( k \frac{\partial T}{\partial x} \right) \, dx \, dt \]
Temporal discretization

If we assume the value of $T$ prevails over the entire volume:

$$
\rho c \int_{t}^{t+\Delta t} \int_{w}^{e} \frac{\partial T}{\partial t} \, dt \, dx = \rho c \Delta x (T_{P}^{1} - T_{P}^{0})
$$

For the diffusion term:

$$
\rho c \Delta x (T_{P}^{1} - T_{P}^{0}) = \int_{t}^{t+\Delta t} \left[ \frac{k_{e}(T_{E} - T_{P})}{(\delta x)_{e}} - \frac{k_{w}(T_{P} - T_{W})}{(\delta x)_{w}} \right] \, dt
$$
Temporal discretization

We need an assumption for the variation of $T$ in time (between $t$ and $t + \Delta t$):

$$\int_{t}^{t+\Delta t} T_P \, dt = \left[ f \, T_P^1 + (1 - f) \, T_P^0 \right] \Delta t$$

where $0 < f < 1$

- $f = 0$: Explicit scheme (first-order accurate)
- $f = 0.5$: Crank-Nicolson (second-order accurate)
- $f = 1$: Implicit (first-order accurate)
Temporal discretization

For stability, the *Explicit scheme* requires (on uniform grid):

\[ \Delta t < \frac{\rho (\Delta x)^2}{2\Gamma} \]

To give realistic results, the *Crank-Nicolson scheme* requires:

\[ \Delta t < \frac{\rho (\Delta x)^2}{\Gamma} \]

The *Implicit scheme* is always stable (but still only first-order)!

**Temporal and spatial discretization are strongly coupled**
Temporal Discretization

- Schemes that are **higher-order** accurate in time exist, e.g.:

\[
\frac{\partial T}{\partial t} = \frac{1}{2\Delta t} (3T^{n+1} - 4T^n + T^{n-1})
\]
Iteration and Convergence

- At each iteration, at each cell, a new value for variable $\phi$ in cell P can then be calculated from that equation.
- It is common to apply relaxation as follows:

\[
\phi_{P,\text{new, used}} = \phi_{P,\text{old}} + U(\phi_{P,\text{new, predicted}} - \phi_{P,\text{old}})
\]

Here $U$ is the relaxation factor:
- $U < 1$ is underrelaxation. This may slow down speed of convergence but increases the stability of the calculation, i.e. it decreases the possibility of divergence or oscillations in the solutions.
- $U = 1$ corresponds to no relaxation. One uses the predicted value of the variable.
- $U > 1$ is overrelaxation. It can sometimes be used to accelerate convergence but will decrease the stability of the calculation.
Convergence

- The iterative process is repeated until the change in the variable from one iteration to the next becomes so small that the solution can be considered converged.

- At convergence:
  - All discrete conservation equations (momentum, energy, etc.) are obeyed in all cells to a specified tolerance.
  - The solution no longer changes much with additional iterations.

Residuals measure imbalance (or error) in conservation equations.

The absolute residual at point \( P \) is defined as:

\[
R_P = \left| a_P \phi_P - \sum_{nb} a_{nb} \phi_{nb} - b \right|
\]
Convergance

- Always ensure proper convergence before using a solution: unconverged solutions can be misleading!!
- Solutions are converged when the flow field and scalar fields are no longer changing.
- Determining when this is the case can be difficult.
- It is most common to monitor the residuals.
False Diffusion

- Often it is stated that the **Central difference** scheme is superior to the **Upwind** scheme because it is second-order accurate whereas the **Upwind** scheme is only first-order accurate.

If we compare the **Central difference** and **Upwind** schemes:

\[
\Gamma_{\text{Upwind}} = \Gamma + \frac{\rho u \delta x}{2}
\]

This added diffusion is considered bad, however it actually **corrects** the solution at large Peclet number (large cells)!
False Diffusion

- False diffusion is numerically introduced diffusion and arises in convection dominated flows, i.e. high Pe number flows.
- False diffusion is a multidimensional phenomenon and occurs when the flow is NOT perpendicular to the grid lines!

Consider If there is no false diffusion, the temperature will be exactly 100 °C everywhere above the diagonal and exactly 0 °C everywhere below the diagonal.
False diffusion

8 x 8

First-order Upwind

Second-order Upwind

64 x 64
False diffusion

- An approximate expression for false diffusion is given by

\[ \Gamma_{false} = \frac{\rho u \Delta x \Delta y \sin 2\theta}{4(\Delta y \sin^3 \theta + \Delta x \cos^3 \theta)} \]

- False diffusion reduction: Use smaller \( \Delta x \) and \( \Delta y \), align grid lines more in direction of flow, Enough to make false diffusion \( << \) real diffusion

- CDS is no remedy for false diffusion. At high Pe, it produces unrealistic results
Summary

- We saw different schemes of discretizing convection diffusion equation, and considered their numerical accuracy, stability, and looked into false diffusion.
References

- Numerical heat transfer, S. Pathnkar
- Computational Science, Gilbert Strang
Thank You