Finite Volume Method for Convection Derivatives II

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Mechanical Engineering 692

Computational Fluid Dynamics

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Outline

- Review finite-volume convection
  - Note need for average ϕ value at cell faces for convection terms
  - Examine use of arithmetic mean as average value and show its problems
- Look at other schemes
  - Upwind differencing
  - Hybrid and power law
  - Total variation diminishing (TVD)

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Review Convection Terms

- Steady equation with convection and diffusion terms in one dimension $\frac{d\rho u\varphi}{dx} = \frac{d}{dx}\Gamma\frac{d\varphi}{dx}$
- Steady continuity equation in one dimension $\frac{d\rho u}{dx} = 0$
- Apply finite volume approach to integrate small volume

$$\int \frac{d\rho u\varphi}{dx}dV = \int \frac{d}{dx}\Gamma\frac{d\varphi}{dx}dV \qquad \int \frac{d\rho u}{dx}dV = 0$$

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Review Integrated PDE

- Constant area result
  - Define F = ρu and D = Γ/δx

$$F_e\varphi_e - F_w\varphi_w = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

- Use (second-order accurate) arithmetic mean for face values

$$F_e\frac{\varphi_E + \varphi_P}{2} - F_w\frac{\varphi_P + \varphi_W}{2} = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

$$a_E = D_e + \frac{F_e}{2} \quad a_W = D_w + \frac{F_w}{2} \quad a_P = a_E + a_W + F_e - F_w$$

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$$a_W\varphi_W - a_P\varphi_P + a_E\varphi_E = 0$$

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Review Example Problem

- Constant ρ, u, and Γ with $\phi = \phi_0$ at x = 0 and $\phi = \phi_L$ at x = L

$$\frac{d\rho u\varphi}{dx} = \frac{d}{dx}\Gamma\frac{d\varphi}{dx} \Rightarrow \frac{\rho u}{\Gamma}\frac{d\varphi}{dx} = \frac{d}{dx}\frac{d\varphi}{dx}$$

- Exact solution below with plot on next slide

$$\frac{\varphi(x) - \varphi_0}{\varphi_L - \varphi_0} = \frac{e^{\frac{\rho u x}{\Gamma}} - 1}{e^{\frac{\rho u L}{\Gamma}} - 1}$$

Pe = ρuL/Γ

Pe_{cell} = ρuδx/Γ = F/D

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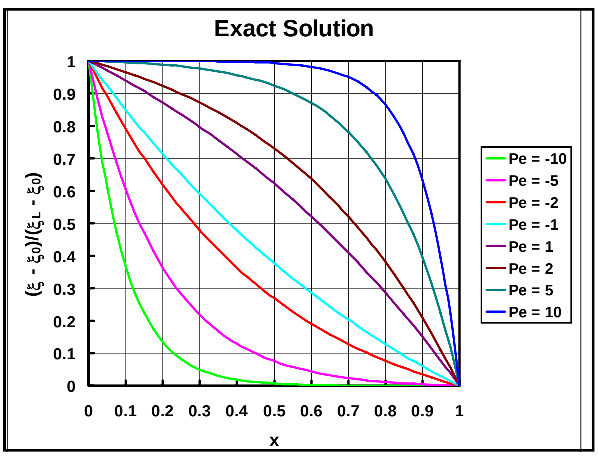

Review Numerical Solution

- Here δx, ρu and Γ are constants
  - $F_e = F_w = \rho u = F$ $D_e = D_w = \Gamma / \delta x = D$

$$a_W \varphi_W - a_P \varphi_P + a_E \varphi_E = \left(F + \frac{D}{2}\right)\varphi_W - 2F\varphi_P + \left(F - \frac{D}{2}\right)\varphi_E = 0$$

|-----●-----|-----●-----|-----●-----|-----●-----|-----●-----|-----●-----|

left 1 2 3 4 5 6 right

- Boundary conditions at x = 0 and x = L

$$-\left(\frac{F}{2} + 3D\right)\varphi_1 + \left(D - \frac{F}{2}\right)\varphi_2 = -(F + 2D)\varphi_{left}$$

$$\left(D + \frac{F}{2}\right)\varphi_{N-2} - \left(3D - \frac{F}{2}\right)\varphi_{N-1} = -(2D - F)\varphi_{right}$$

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Review Numerical Solution II

- Data: L = 1 m, u = 0.1 m/s, Γ = 0.1 kg/m·s, δx = 0.2 m, ρ = 1 kg/m^3
  - F = ρu = (1 kg/m^3)(0.1 m/s) = 0.1 kg/m^2·s
  - D = $\Gamma/\delta x$ = (0.1 kg/m·s)(0.2 m) = 0.5 kg/m^2·s
  - Ratio F/D = 0.2
- Second case: change from 0.1 m/s to 2.5 m/s changing F/D from 0.2 to 5
- Third case: leave u at 0.1 m/s; change dx from 0.2 to 0.05 changing F/D to 1.25

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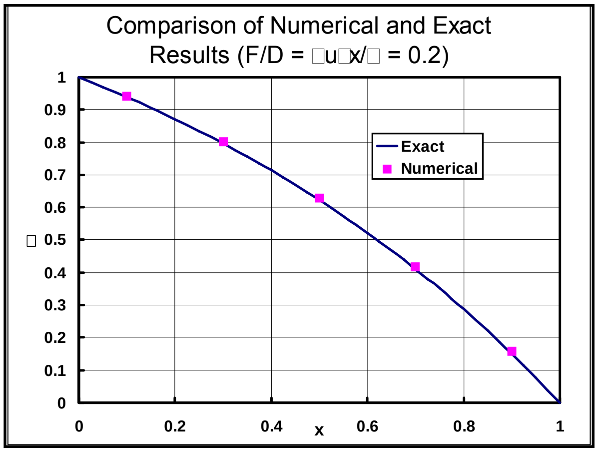

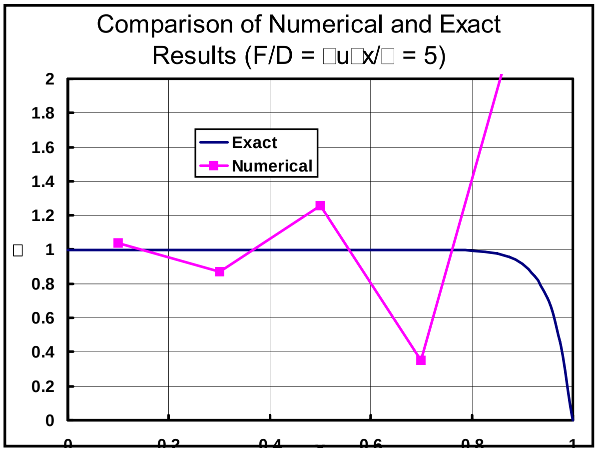

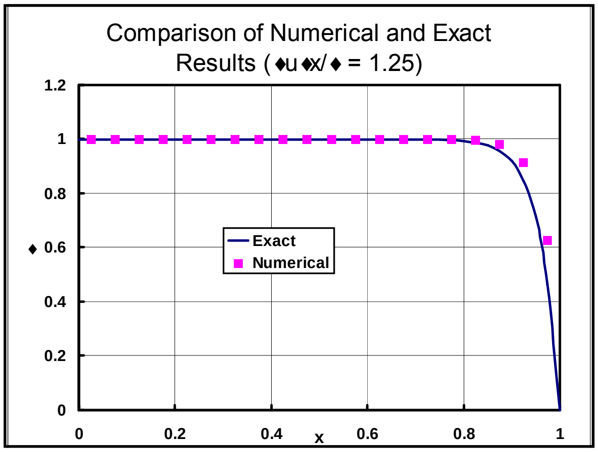

What is Happening Here?

- When flow term F = ρu is large compared to diffusion term D = $\delta x/\Gamma$ the use of average values does not recognize the directionality of the flow
- Keeping the F/D ratio small allows use of average values in convection terms
  - Requires small δx for large flow rates
- How can we use larger δx for large flow rates and keep accuracy?

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Algorithm Properties

- Conservative schemes – conserve properties in finite difference equations
  - Requires exit flux from one face to be same as input flux in adjacent cell
- Transportive schemes – have correct balance between diffusion and convection
- Accuracy – need schemes that have a good truncation error

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Algorithm Properties II

- Limit on coefficient magnitude for iteration schemes (boundedness)
  - Absolute value of diagonal coefficient must be greater than the sum of absolute values of all other coefficients
    - For simple equations here $|a_P| \geq |a_E| + |a_W|$
  - Deferred correction separates coefficients into two parts
    - Adjustment leaves $|a_P| \geq |a_E| + |a_W|$
    - Places part removed from adjusted coefficients into source term

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Upwind Convection Term

- Models directionality of flow

W w P e E

- Previously we replaced $F_e\phi_e$ by $F_e(\phi_E + \phi_P)/2$ in convection term
- Upwind difference uses $\phi_e = \phi_P$ if F_e is positive and $\phi_e = \phi_E$ if F_e is negative
- Start with basic finite volume equation

$$F_e\varphi_e - F_w\varphi_w = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

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Positive F Terms

- If F_e and F_w are both positive then $\phi_e = \phi_P$ and $\phi_w = \phi_W$

W w P e E

$$F_e\varphi_e - F_w\varphi_w = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

$$F_e\varphi_P - F_w\varphi_W = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

$$0 = D_e\varphi_E - (D_e + F_e + D_w)\varphi_P + (D_w + F_w)\varphi_W$$

$$a_P = D_e + F_e + D_w + F_w - F_w = D_e + D_w + F_w + F_e - F_w$$

$$a_E = D_e \quad a_W = D_w + F_w \quad a_P = a_E + a_W + F_e - F_w$$

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Negative F Terms

- If F_e and F_w are both negative then $\phi_e = \phi_E$ and $\phi_w = \phi_P$

W w P e E

$$F_e\varphi_e - F_w\varphi_w = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

$$F_e\varphi_E - F_w\varphi_P = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W)$$

$$0 = (D_e - F_e)\varphi_E - (D_e - F_w + D_w)\varphi_P + D_w\varphi_W$$

$$a_P = D_e - F_w + D_w + F_e - F_e = D_e - F_e + D_w + F_e - F_w$$

$$a_E = D_e - F_e \quad a_W = D_w \quad a_P = a_E + a_W + F_e - F_w$$

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Computational Formulas

- Positive F terms

$$a_E = D_e \quad a_W = D_w + F_w \quad a_P = a_E + a_W + F_e - F_w$$

- Negative F terms

$$a_E = D_e - F_e \quad a_W = D_w \quad a_P = a_E + a_W + F_e - F_w$$

- Computational formulas

$$a_W = D_w + \max(F_w, 0) \quad a_E = D_e + \max(-F_e, 0)$$

$$a_P = a_E + a_W + F_e - F_w$$

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Upwind Solution

- Case III for previous problem
  - L = 1 m
  - u = 0.1 m/s
  - Γ = 0.1 kg/m·s
  - δx = 0.05 m
  - ρ = 1 kg/m^3
- F = ρu = (1 kg/m^3)(2.5 m/s) = 2.5 kg/m^2·s
- D = $\Gamma/\delta x$ = (0.1 kg/m·s) / (0.05 m) = 2 kg/m^2·s
- Ratio F/D = 1.25 = Pe_{cell}

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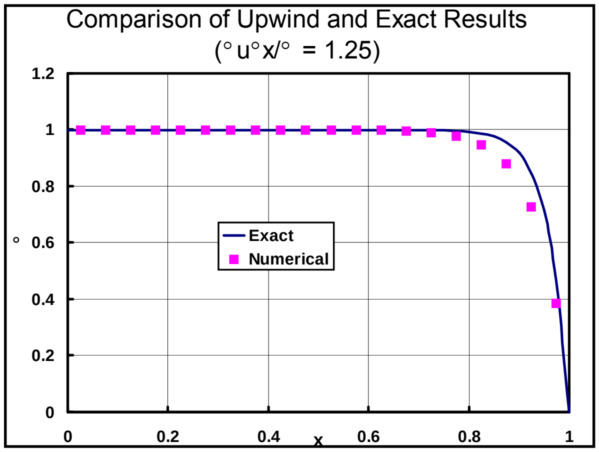

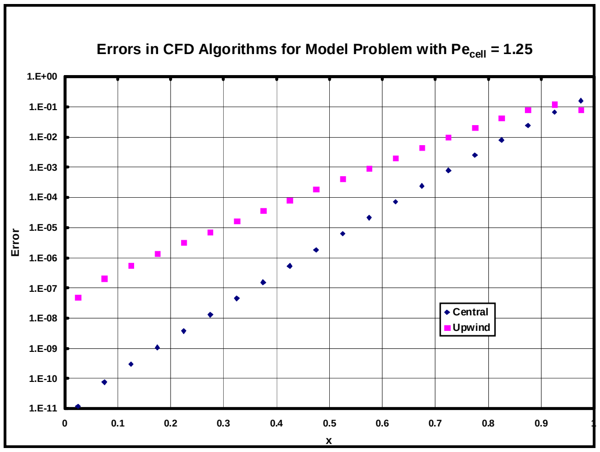

Other Algorithms

- Hybrid algorithm
  - Combination of central difference for $Pe_{cell} < 2$ and upwind for $Pe_{cell} \geq 2$

$$a_W = \max\left[F_w, \left(D_w + \frac{F_w}{2}\right), 0\right] \qquad a_E = \max\left[-F_e, \left(D_e + \frac{F_e}{2}\right), 0\right]$$

$$a_P = a_E + a_W + F_e - F_w$$

- Power-law algorithm
  - Similar to hybrid
  - Sets D = 0 for $|Pe_{cell}| > 10$
  - Uses power law formula for $|Pe_{cell}| \leq 10$

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Other Algorithms II

- Power law formula $a_P = a_E + a_W + F_e - F_w$

$$a_W = D_w \max\left[0, \left(1 - |Pe_w|^5\right)\right] + \max[F_w, 0] \qquad Pe_w = F_w / D_w$$

$$a_E = D_e \max\left[0, \left(1 - |Pe_e|^5\right)\right] + \max[-F_e, 0] \qquad Pe_e = F_e / D_e$$

- QUICK – Quadratic Upstream Interpolation for Convective Kinetics
  - Uses quadratic intrepolation formula
  - Choose nodes to use for interpolation depending on velocity

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Other Algorithms III

- QUICK formulas for central node P involve five nodes instead of three

WW ww W w P e E ee EE

$$a_{WW}\varphi_{WW} + a_W\varphi_W - a_P\varphi_P + a_E\varphi_E + a_{EE}\varphi_{EE} = 0$$

$$a_W = D_w + \frac{6\alpha_w F_w + 3(1-\alpha_w)F_w + \alpha_e F_e}{8} \qquad a_{WW} = -\frac{\alpha_w F_w}{8}$$

$$a_E = D_e - \frac{3\alpha_e F_e + 6(1-\alpha_e)F_e + (1-\alpha_w)F_w}{8} \qquad a_{EE} = \frac{(1-\alpha_e)F_e}{8}$$

$\alpha_w = 1$ if $F_w > 0$ and $\alpha_e = 1$ if $F_e > 0$

$\alpha_w = 0$ if $F_w < 0$ and $\alpha_e = 0$ if $F_e < 0$

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Homework for March 3

- Download the Excel workbook from the course web site for the sample convection problem with Pe_{cell} = 1.25
  - Shows results for Central and Upwind on separate worksheets
- Add similar worksheets to get results for Hybrid, Power Law, and QUICK
- Add error results for these algorithms to the error chart

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TVD Algorithms

- Total Variation Diminishing schemes
  - Designed to maintain both accuracy and stability with no unphysical "wiggles"
  - Consider set of different differencing schemes for ϕ_e with positive u velocity

|----------•----------|----------•----------|----------•----------|
W w P e E

- Upwind: $\phi_e = \phi_P$
- Linear Upwind: $\phi_e = \phi_P + \frac{\phi_P - \phi_W}{x_P - x_W}(x_e - x_P)$
  - For constant δx: $\phi_e = \phi_P + \frac{\phi_P - \phi_W}{2}$

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TVD Algorithms II

|----------•----------|----------•----------|----------•----------|
W w P e E

- QUICK: $\phi_e = \phi_P + \frac{3\phi_E - 2\phi_P - \phi_W}{8}$
- Second order: $\phi_e = \phi_P + \frac{\phi_E - \phi_P}{2}$
- General form is $\phi_e = \phi_P$ + Correction
- Correction can always be written as a correction (ψ/2) times $\phi_E - \phi_P$
- Correction function ψ depends on $(\phi_P - \phi_W)/(\phi_E - \phi_P)$

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Why TVD?

- Developed for transient compressible gas dynamics equations
- Scheme to obtain accurate compromise between false diffusion of upwinding and "wiggles" of more accurate schemes in some regions
- Basic development mathematically complex, but results useful
- Basic equation $\phi_e = \phi_P + \psi(r)(\phi_E - \phi_P)/2$
  - $r = (\phi_P - \phi_W)/(\phi_E - \phi_P)$

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What is ψ?

- Upwind: $\phi_e = \phi_P$ $\psi = 0$
- Second order arithmetic mean:

$$\phi_e = \phi_P + \frac{\phi_E - \phi_P}{2} = \frac{1}{2}1(\phi_E - \phi_P) \Rightarrow \psi = 1$$

- Linear upwind with constant δx:

$$\phi_e = \phi_P + \frac{\phi_P - \phi_W}{2} = \phi_P + \frac{1}{2}\frac{\phi_P - \phi_W}{\phi_E - \phi_P}(\phi_E - \phi_P) = \phi_P + \frac{1}{2}r(\phi_E - \phi_P) \Rightarrow \psi = r$$

- QUICK (after some algebra)

$$\phi_e = \phi_P + \frac{1}{2}\left[\frac{1}{4}\left(3 + \frac{\phi_P - \phi_W}{\phi_E - \phi_P}\right)\right](\phi_E - \phi_P) = \phi_P + \frac{1}{2}\left[\frac{3+r}{4}\right](\phi_E - \phi_P) \Rightarrow \psi = \frac{3+r}{4}$$

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TVD Region Limits on $\psi(r)$

- For $0 < r \le 1$, $\psi(r) \le 2r$
- For $r \ge 1$, $\psi(r) \le 2$
- For second-order accuracy and TVD
  - For $0 < r \le 1$, $r \le \psi(r) \le 2r$
  - For $1 \ge r \ge 2$, $1 \le \psi(r) \le r$
  - For $r > 2$, $1 \le \psi(r) \le 2$
- Implementation of TVD requires parts of coefficient terms in S_u term as deferred correction

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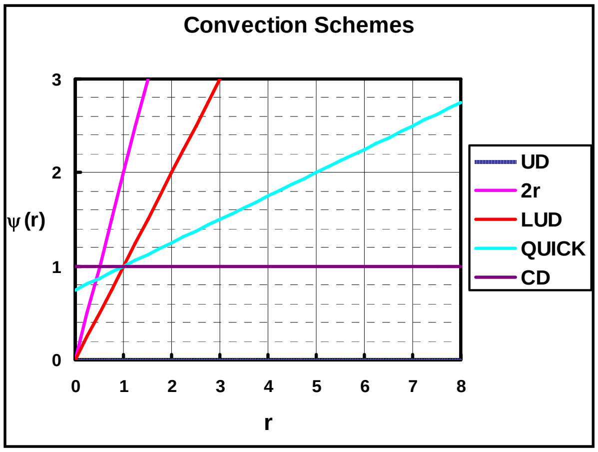
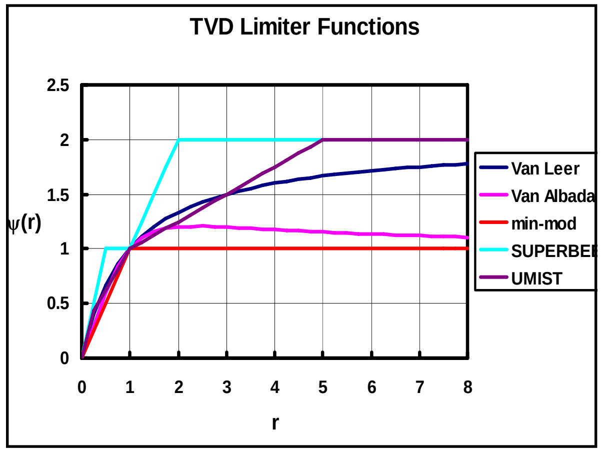

Convection Schemes
ψ(r)
r
0
1
2
3
4
5
6
7
8
UD
2r
LUD
QUICK
CD


TVD Limiter Functions
ψ(r)
r
0
0.5
1
1.5
2
2.5
Van Leer
Van Albada
min-mod
UMIST