HIGHER ORDER UPWIND SCHEMES (1)

a) Variable Extrapolation

Key Idea:

- From (Constant) u_i: Recover Higher Order Curves
- Extrapolate u to Cell Boundaries
- Use Riemann Solver With Extrapolated Values

1st Order Schemes Used Average

$$u_i = \frac{1}{\Delta x} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} u dx$$

HIGHER ORDER UPWIND SCHEMES (2)

Generalized to:

$$u = u_i + (x - x_i)u_{,x}|_i + \frac{3k}{2}\left[(x - x_i)^2 - \frac{\Delta x^2}{12}\right]u_{,xx}|_i + HOT$$

Remarks:

- $k = 1/3 \Rightarrow$ 3rd Order (From Taylor Series)
- When Averaging, Both 1st and 2nd Extrapolation Intergrals Vanish (Homework Excercise)
- Data Point u_i and Unknown at x_i In General Not the Same

$$u(x_i) = u_i + \frac{k}{8}\Delta x^2 u_{,xx}|_i$$

  - Unlike FEM

HIGHER ORDER UPWIND SCHEMES (3)

Need to Define: $u_{,x}, u_{,xx}|_i$

Simplest Way:

$$u_{,x}|_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} \quad ; \quad u_{,xx}|_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

Extrapolation to Cell Boundaries

$$u^L_{i+1/2} = u_i + \frac{\Delta x}{2} u_{,x}|_i + \frac{\Delta x^2}{4} k u_{,xx}|_i$$

$$= u_i + \frac{1}{4}(u_{i+1} - u_{i-1}) + \frac{k}{4}(u_{i+1} - 2u_i + u_{i-1})$$

$$= u_i + \frac{1}{4}(1-k)(u_i - u_{i-1}) + \frac{1}{4}(1+k)(u_{i+1} - u_i)$$

$$u^R_{i-1/2} = u_i - \frac{\Delta x}{2} u_{,x}|_i + \frac{\Delta x^2}{4} k u_{,xx}|_i$$

$$= u_i - \frac{1}{4}(1+k)(u_i - u_{i-1}) - \frac{1}{4}(1-k)(u_{i+1} - u_i)$$

HIGHER ORDER UPWIND SCHEMES (4)

Special Cases

$k = -1$: Linear, One-Sided Approximation

$$u^L_{i+1/2} = u_i + \frac{1}{2}\left(u_i - u_{i-1}\right)$$

$$u^R_{i+1/2} = u_{i+1} - \frac{1}{2}\left(u_{i+2} - u_{i+1}\right)$$

$k = 0$: Linear, One-Upstream, One Downstream

$$u^L_{i+1/2} = u_i + \frac{1}{4}\left(u_{i+1} - u_{i-1}\right)$$

$$u^R_{i+1/2} = u_{i+1} - \frac{1}{4}\left(u_{i+2} - u_i\right)$$

$k = +1$: Linear, Arithmetic Mean
(No Upwind Character)

$$u^L_{i+1/2} = u_i + \frac{1}{2}\left(u_{i+1} - u_i\right)$$

$$u^R_{i+1/2} = u_{i+1} - \frac{1}{2}\left(u_{i+1} - u_i\right)$$

$\Rightarrow u^L_{i+1/2} = u^R_{i+1/2}$ (Same !)

HIGHER ORDER UPWIND SCHEMES (5)

Residual Dissipation

$$-(u^R_{i+1/2} - u^L_{i+1/2}) =$$

$$u_i \quad + \frac{1}{4}\left[(1-k)(u_i - u_{i-1} + (1+k)(u_{i+1} - u_i\right]$$

$$-u_{i+1} + \frac{1}{4}\left[(1+k)(u_{i+1} - u_i + (1-k)(u_{i+2} - u_{i+1}\right]$$

$$= \frac{1-k}{4}\left(u_{i+2} - 3u_{i+1} + 3u_i - u_{i-1}\right)$$

$$= -\frac{1-k}{4}\Delta x^3 \frac{\partial^3 u}{\partial x^3} + O(\Delta x^4)$$

$\Rightarrow$

- $k \neq 1$: Residual 4th Order Dissipation
- $k = 1$: (No Upwinding) Higher Order Dissipation

HIGHER ORDER UPWIND SCHEMES (6)

b) Flux Extrapolation

Key Idea:

- For Flux-Split Schemes: Extrapolate Directly the Fluxes

$$f^+_{i+1/2} = f^+_i + \frac{1}{4}(1-k)(f^+_i - f^+_{i-1}) + \frac{1}{4}(1+k)(f^+_{i+1} - f^+_i)$$

$$f^-_{i-1/2} = f^-_i - \frac{1}{4}(1+k)(f^-_i - f^-_{i-1}) - \frac{1}{4}(1-k)(f^-_{i+1} - f^-_i)$$

Comparison of Variable vs. Flux Extrapolation

Anderson, Thomas and vanLeer AIAA J., 24, 1453-1460 (1986)

Variable Extrapolation Better

EXPLICIT SECOND ORDER IN TIME AND SPACE (1)

Key Idea: 2-Step, With 1st Step Only 1st Order Accurate

S1 : Advance to Half-Step With First Order in Space Fluxes

$$\tilde{u}_i = u_i - \frac{\Delta t}{2\Delta x}\left[f^{(1)}_{i+1/2} - f^{(1)}_{i-1/2}\right]$$

S2 : Obtain Interface Values By Recovery of $\tilde{u}$-Values

$$u^L_{i+1/2} = \tilde{u}_i + \frac{1}{4}(1-k)(\tilde{u}_i - \tilde{u}_{i-1}) + \frac{1}{4}(1+k)(\tilde{u}_{i+1} - \tilde{u}_i)$$

$$u^R_{i+1/2} = \tilde{u}_{i+1} - \frac{1}{4}(1+k)(\tilde{u}_{i+1} - \tilde{u}_i) - \frac{1}{4}(1-k)(\tilde{u}_{i+2} - \tilde{u}_{i+1})$$

S3 : Obtain Interface Fluxes From Riemann Problem

$$\tilde{f}^{(2)}_{i+1/2} = f(u^R_{i+1/2}, u^L_{i+1/2})$$

S4 : Advance the Solution to Next Time Level

$$\Delta u_i = -\frac{\Delta t}{\Delta x}\left[\tilde{f}^{(2)}_{i+1/2} - \tilde{f}^{(2)}_{i-1/2}\right]$$

Remark:

- Steps 1/2 Do Not Need to be Conservative

HIGH RESOLUTION SCHEMES (1)

Property of Scalar Conservation Laws:

$$u_{,t} + f_{,x} = 0$$

Total Variation:

$$TV := \int |u_{,x}| dx$$

Does Not Increase in Time (Lax (1973))

Numerically:

$$TV := \sum |u_{i+1} - u_i|$$

Total Variation Diminishing (TVD) iff:

$$TV(u^{n+1}) \leq TV(u^n)$$

HIGH RESOLUTION SCHEMES (2)

TVD $\Rightarrow$ Monotonicity Properties:

- No New Extrema in x Over Time
- No Accentuation of Existing Extrema

Godunov Theorem (1959):

No Linear Scheme of Order Higher Than One is Monotonicity Preserving

Homework:

- Take Shock Profile and Advect One Timestep by Hand With:
    - 1st Order Upwind
    - Explicit in Time, Central in Space

HIGH RESOLUTION SCHEMES (3)

Conditions for 3-Point TVD Schemes

$$\frac{du_i}{dt} = -\frac{1}{\Delta x}(f_{i+1/2} - f_{i-1/2})$$

$$:= -\frac{1}{\Delta x}\left(C^-_{i+1/2}\delta u_{i+1/2} + C^+_{i-1/2}\delta u_{i-1/2}\right)$$

TVD Only Iff: $C^+_{i+1/2} \geq 0 \quad , \quad C^-_{i+1/2} \leq 0$

Define: $s = sgn(\delta u)$

Then:

$$\frac{dTV}{dt} = \sum s_{i+1/2} \frac{d(u_{i+1} - u_i)}{dt}$$

$$= \frac{1}{\Delta x} \sum s_{i+1/2} \Big[(C^-_{i+1/2} - C^+_{i+1/2})\delta u_{i+1/2}$$

$$-C^-_{i+3/2}\delta u_{i+3/2} + C^+_{i-1/2}\delta u_{i-1/2} \Big]$$

HIGH RESOLUTION SCHEMES (4)

$$\frac{dTV}{dt} = \frac{1}{\Delta x} \sum \Big[s_{i+1/2} (C^-_{i+1/2} - C^+_{i+1/2})$$

$$- s_{i-1/2} C^-_{i+1/2} + s_{i+3/2} C^+_{i+1/2} \Big] \, \delta u_{i+1/2}$$

TVD $\Rightarrow$

$$[..]_{i+1/2} \, \delta u_{i+1/2} \leq 0$$

In Particular, For:

$$\delta u_{i+1/2} = 1 \quad , \quad \delta u_{i+3/2} = \delta u_{i-1/2} = 0$$

$\Rightarrow$

$$C^+_{i+1/2} \geq 0 \quad , \quad C^-_{i+1/2} \leq 0$$

<u>Homework</u>:

- Prove That 1st Order Upwind Scheme for Linear Advection Satisfies TVD Condition

HIGH RESOLUTION SCHEMES (5)

Lax-Wendroff

Define: Courant-Number: $\sigma = a\Delta t/\Delta x$

$$\Delta u_i = -\frac{\sigma}{2}(u_{i+1} - u_{i-1}) + \frac{\sigma^2}{2}(u_{i+1} - 2u_i + u_{i-1})$$

$$= -\frac{\sigma}{2}(1+\sigma)(u_i - u_{i-1}) - \frac{\sigma}{2}(1-\sigma)(u_{i+1} - u_i)$$

$\Rightarrow$ For:

$$\Delta u_i = -\frac{\Delta t}{\Delta x}\left(C^-_{i+1/2}\delta u_{i+1/2} + C^+_{i-1/2}\delta u_{i-1/2}\right)$$

We Have:

$$C^+_{i-1/2} = \frac{a(1+\sigma)}{2} \quad , \quad C^-_{i+1/2} = \frac{a(1-\sigma)}{2}$$

SECOND ORDER TVD SCHEMES (1)

Modus Operandi:

1) Select a 1st Order Monotone Numerical Flux
2) Extend Numerical Flux to 2nd Order
3) Restrict Reconstruction via non-Linear Limitors to Ensure TVD
4) Select Time-Integration Scheme
   - May Impose Further TVD Conditions
5) Check, If Possible, Entropy Condition

SECOND ORDER TVD SCHEMES (2)

Linear Advection

$$u_{,t} + a u_{,x} = 0$$

2nd Order Upwind Scheme

$$\frac{du_i}{dt} = -\frac{a^+}{2\Delta x}\left[3\delta u_{i-1/2} - \delta u_{i-3/2}\right] - \frac{a^-}{2\Delta x}\left[3\delta u_{i+1/2} - \delta u_{i+3/2}\right]$$

Introduce Limitor Ψ:

$$\frac{du_i}{dt} = -\frac{a^+}{\Delta x}\left[\delta u_{i-1/2} + \frac{1}{2}\Psi^+_{i-1/2}\delta u_{i-1/2} - \frac{1}{2}\Psi^+_{i-3/2}\delta u_{i-3/2}\right]$$

$$-\frac{a^-}{\Delta x}\left[\delta u_{i+1/2} + \frac{1}{2}\Psi^-_{i+1/2}\delta u_{i+1/2} - \frac{1}{2}\Psi^-_{i+3/2}\delta u_{i+3/2}\right]$$

SECOND ORDER TVD SCHEMES (3)

Express Ψ As A Function of Ratios:

$$r^{+}_{i+1/2} := \frac{\delta u_{i+3/2}}{\delta u_{i+1/2}} \quad ; \quad r^{-}_{i+1/2} := \frac{\delta u_{i-1/2}}{\delta u_{i+1/2}}$$

Then:

$$\frac{du_i}{dt} = -\frac{a^{+}}{\Delta x}\left[1 + \frac{1}{2}\Psi^{+}_{i-1/2} - \frac{1}{2}\frac{\Psi^{+}_{i-3/2}}{r^{+}_{i-3/2}}\right]\delta u_{i-1/2}$$

$$-\frac{a^{-}}{\Delta x}\left[1 + \frac{1}{2}\Psi^{-}_{i+1/2} - \frac{1}{2}\frac{\Psi^{-}_{i+3/2}}{r^{-}_{i+3/2}}\right]\delta u_{i+1/2}$$

TVD Condition Imposes:

$$1 + \frac{1}{2}\Psi^{+}_{i-1/2} - \frac{1}{2}\frac{\Psi^{+}_{i-3/2}}{r^{+}_{i-3/2}} \geq 0$$

$$1 + \frac{1}{2}\Psi^{-}_{i+1/2} - \frac{1}{2}\frac{\Psi^{-}_{i+3/2}}{r^{-}_{i+3/2}} \geq 0$$

SECOND ORDER TVD SCHEMES (4)

In Principle, Very General Class of Ψ-Functions Possible !

Restrict:

- Dependency on Just <u>One</u> Upwind Gradient
- Only Closest Gradient

$\Rightarrow$

$$\Psi^+_{i-1/2} = \Psi^+_{i-1/2}(r^+_{i-1/2}) \quad ; \quad \Psi^-_{i+1/2} = \Psi^-_{i+1/2}(r^-_{i+1/2})$$

Re-Write TVD Conditions:

$$\frac{\Psi^+_{i-3/2}}{r^+_{i-3/2}} - \Psi^+_{i-1/2} \leq 2$$

$$\frac{\Psi^-_{i+3/2}}{r^-_{i+3/2}} - \Psi^-_{i+1/2} \leq 2$$

Or:

$$\frac{\Psi(r)}{r} - \Psi(s) \leq 2 \quad \forall r, s$$

SECOND ORDER TVD SCHEMES (5)

Still, Very General $\Rightarrow$ Impose Constraints

a) Restrict Ψ to be Positive

$$r \geq 0 \Rightarrow \Psi(r) \geq 0$$

b) Revert to 1st Order at Extrema ($r < 0$)

$$r \leq 0 \Rightarrow \Psi(r) = 0$$

c) Ensure TVD for $s = 0$

$$0 \leq \Psi(r) \leq 2r$$

d) Advect Exactly Linear Profile ($r = 1$)

$$r = 1 \Rightarrow \Psi(r) = 1$$

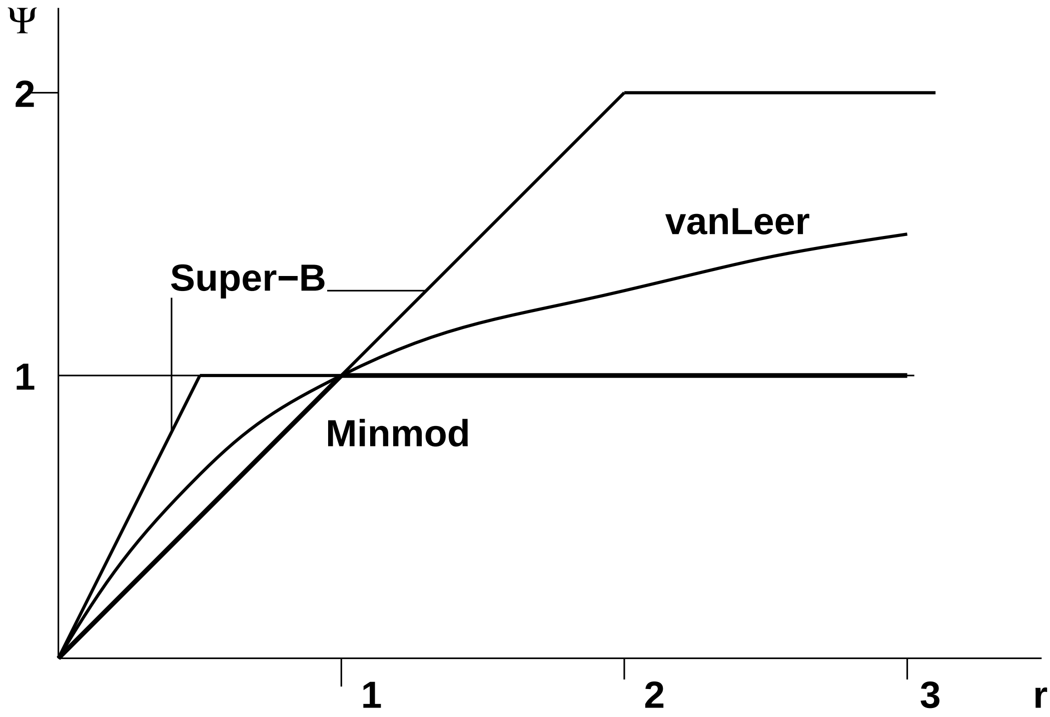
e) Stability Analysis:

$$0 \leq \Psi(r) \leq 2$$

$\Rightarrow$ General Conditions:

$$0 \leq \Psi(r) \leq min(2r, 2) \quad , \quad \Psi(1) = 1$$

SECOND ORDER TVD SCHEMES (6)



SECOND ORDER TVD SCHEMES (7)

Possibilities:

- van Leer

$$\Psi(r) = \frac{r + |r|}{1 + r}$$

- van Albada

$$\Psi(r) = \frac{r^2 + r}{1 + r^2}$$

- Minmod

$$\Psi(r) = \begin{cases} min(r, 1) & r \geq 0 \\ 0 \quad r < 0 \end{cases}$$

- Superbee

$$\Psi(r) = max(0, min(2r, 1), min(r, 2))$$

Note: All of These Satisfy:

$$\frac{\Psi(r)}{r} = \Psi(\frac{1}{r})$$

$\Rightarrow$ Symmetry With Respect to Gradients

SECOND ORDER TVD SCHEMES (8)

Illustration of Limitor Action

- Minmod Limitor
- Linear Advection
- $a > 0$

a) Flattening Profile

$$\delta u_{i+1/2} < \delta u_{i-1/2} \quad \Rightarrow \quad r < 1 \qquad \Rightarrow \quad \Psi(r) = r$$

$\Rightarrow \delta u_{i-1/2}$ Replaced by (Smaller) $\delta u_{i+1/2}$

b) Steepening Profile

$$\delta u_{i+1/2} > \delta u_{i-1/2} \quad \Rightarrow \quad r > 1 \qquad \Rightarrow \quad \Psi(r) = 1$$

$\Rightarrow \delta u_{i-1/2}$ Unchanged

LIMITORS FOR VARIABLE EXTRAPOLATION (MUSCL) (1)

Key Idea: Restrict Slopes

$$u^L_{i+1/2} = u_i +$$
$$\frac{1}{4}\left[(1-k)\Phi^+_{i-1/2}\delta u_{i-1/2} + (1+k)\Phi^-_{i+1/2}\delta u_{i+1/2}\right]$$

As Before, Impose Restrictions, e.g.

$$\Phi^+_{i-1/2} = \Phi(r^+_{i-1/2}) = \Phi(r^L) \quad , \quad r^L = \frac{\delta u_{i+1/2}}{\delta u_{i-1/2}}$$

$$\Phi^-_{i+1/2} = \Phi(r^-_{i+1/2}) = \Phi(\frac{1}{r^L})$$

$$u^L_{i+1/2} = u_i + \frac{1}{4}\left[(1-k)\Phi(r^L) + (1+k)r^L\Phi(\frac{1}{r^L})\right]\delta u_{i-1/2}$$

LIMITORS FOR VARIABLE EXTRAPOLATION (MUSCL) (2)

Define a General Limitor Ψ As:

$$u^L_{i+1/2} = u_i + \frac{1}{2}\Psi^L \delta u_{i-1/2}$$

$$\Psi^L := \frac{1}{2}\left[(1-k)\Phi(r^L) + (1+k)r^L\Phi(\frac{1}{r^L})\right]$$

$$u^R_{i+1/2} = u_i - \frac{1}{2}\Psi^R \delta u_{i+1/2} \quad , \; r^R = \frac{\delta u_{i+1/2}}{\delta u_{i+3/2}}$$

$$\Psi^R := \frac{1}{2}\left[(1-k)\frac{1}{r^R}\Phi(r^R) + (1+k)\Phi(\frac{1}{r^R})\right]$$

LIMITORS FOR VARIABLE EXTRAPOLATION (MUSCL) (3)

Introduce Limited Values for u Into Advection Scheme, e.g.

$$\frac{du_i}{dt} = -\frac{1}{\Delta x}(f_{i+1/2} - f_{i-1/2})$$

$$= -\frac{a^+}{\Delta x}\left[\tilde{u}^L_{i+1/2} - \tilde{u}^L_{i-1/2}\right] - \frac{a^-}{\Delta x}\left[\tilde{u}^R_{i+1/2} - \tilde{u}^R_{i-1/2}\right]$$

Special Case: $k = -1 \Rightarrow \Psi = \Phi \Rightarrow$ Slope Limitor = Limitor

In General: $\forall k$: If

$$\Phi(r) = r\Phi(\frac{1}{r}) \quad \Rightarrow \quad \Psi = \Phi$$

All of the Limitors Mentioned Above Satisfy This Condition
$\Rightarrow$ May be Used for Variable Extrapolation Limiting

Homework:

- Prove That All Limitors Satisfy $\Phi(r) = r\Phi(\frac{1}{r})$
- Prove The TVD Conditions for Variable Extrapolation

EXTENSIONS TO 2/3-D

Key Idea: Use 1-D Theory Wherever a 'Riemann Problem' Is Solved

- At Faces
- At Edges

$\Rightarrow$ Have: u_{i-1}, u_i

$\Rightarrow$ Need: u_{i-2}, u_{i+1}

Obtained From:

- Best 'Gridline'
  - Simple for Structured Grids
  - 'Most Aligned Edge' for Untructured Grids
- Interpolation
  - Restricted to Nearest Neighbour
  - Restricted to Equal Distance
- Gradients
  - Node Level
  - Element Level

All of These Have Pros and Cons

EXTENSIONS TO 2/3-D