

# Rethinking Advection and Remap

William J. Rider

Computational Shock and Multiphysics

Sandia National Laboratories, Albuquerque, NM

E-mail: [wjrider@sandia.gov](mailto:wjrider@sandia.gov)

MultiMat 2013

San Francisco, CA, September 2, 2013



Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.



# Outline

- ❑ Reasoning
- ❑ Lessons from history
- ❑ Current state
- ❑ Classes of new methods
- ❑ Results

**Note: I'm going to look at methods associated with advection synonymous with remap. In reality these are methods for hyperbolic conservation (balance) laws.**

# Van Leer introduced the PLM (and PPM) method in his 1977 paper

JOURNAL OF COMPUTATIONAL PHYSICS 23, 276–299 (1977)

## Towards the Ultimate Conservative Difference Scheme. IV. A New Approach to Numerical Convection

BRAM VAN LEER

Geometric  
Limiters!

*Leiden Observatory, Leiden, The Netherlands*

Received April 30, 1976; revised July 30, 1976

An approach to numerical convection is presented that exclusively yields upstream-centered schemes. It starts from a meshwise approximation of the initial-value distribution by simple basic functions, e.g., Legendre polynomials. In this way, the integral of the distribution is conserved. The overall approximation is continuous. The weights of the basic functions are computed by finite difference fitting. In the latter scheme, independent state quantities and third-order schemes are given, and the accuracy of these schemes is indicated. Numerical examples are given of linear and nonlinear wave propagation, also regarding monotonicity.

Hybrid  
FV-FD

Hermite

Discontinuous  
Galerkin!

PLM!

PPM!

# Reasoning for rethinking advection & remap

- ❑ For the most part this community has focused upon a single method (Van Leer's slope limiter) for remap
- ❑ That method was introduced in a 1977 paper that includes six different methods.
- ❑ We look at this paper and the method's contained therein for opportunities.
  - ✓ The method favored for remap is the “worst” of the six
- ❑ Some of these methods may be much better on modern computing platforms due to their compact nature.
- ❑ For example, Paul Woodward's PPB scheme is based on Van Leer's scheme VI
  - ✓ Not described in the '77 paper

# The six schemes introduced in Van Leer's paper

- I – The standard slope limited method
  - ✓ You know all about it
- II – The evolved slope scheme (Hermite)
  - ✓ Described briefly here
- III – Piecewise linear DG (moment method)
  - ✓ Focus of lots of recent effort
- IV – Piecewise parabolic on three points
  - ✓ Basis for the famous PPM scheme
- V – Piecewise parabolic with evolving edge values
  - ✓ Reintroduced as the PPM-L scheme
- VI – Piecewise parabolic DG
  - ✓ Woodward's PPB scheme

Van Leer's 1979 paper provided the true successor to Godunov's method.

JOURNAL OF COMPUTATIONAL PHYSICS 135, 229–248 (1997)  
ARTICLE NO. CP975704

# Lagrange- Remap

# Towards the Ultimate Conservative Difference Scheme V. A Second-Order Sequel to Godunov's Method

Bram van Leer

*University Observatory, Leiden, The Netherlands*

Received October 18, 1977; revised October 17, 1978

A method of second-order accuracy is described for integrating the equations of ideal compressible flow. The method is based on the integral conservation laws and is dissipative, so that it can be used across shocks. The heart of the method is a one-dimensional Lagrangean scheme that may be regarded as a second-order sequel to Godunov's method. The second-order accuracy is achieved by taking the distributions of the state quantities inside a gas slab to be linear, rather than uniform as in Godunov's method. The Lagrangean results are remapped with least-squares accuracy onto the desired Euler grid in a separate step. Several monotonicity algorithms are applied to ensure positivity, monotonicity, and nonlinear stability. Higher dimensions are covered through time splitting. Numerical results for one-dimensional and two-dimensional flows are presented, demonstrating the efficiency of the method. The paper concludes with a summary of the results of the whole series "Towards the Ultimate Conservative Difference Scheme." © 1979 Academic Press

tions, with due care taken to account for the discontinuities in the interaction flow. The convective difference scheme hidden in the Lagrangean scheme, for integrating the characteristic equations is a so-called upstream-centered (upwind) scheme and has been discussed as "scheme II" in the previous paper [1] of this series. The Lagrangean results onto the Euler equations are obtained by the upstream-centered scheme III.

A substantial improvement of the Lagrangean step, the Euler scheme III.

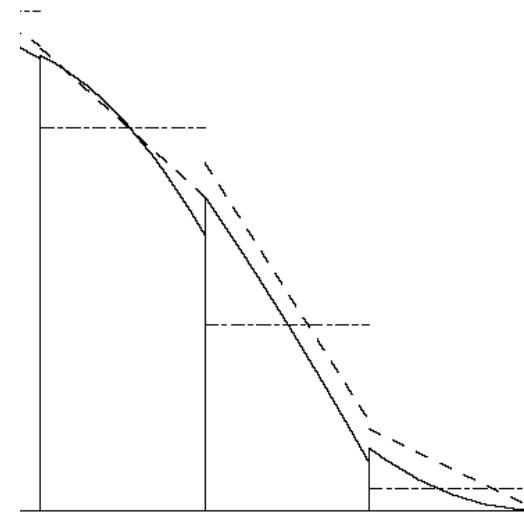
Answering the questions, (MUSCL) is a numerical method for solving hyperbolic partial differential equations. It is a finite difference scheme that uses a piecewise linear reconstruction of the solution at each cell interface. The method is second-order accurate in space and time. It is a Godunov-type scheme, meaning it preserves the total variation of the solution. The name 'MUSCL' is derived from the fact that it uses a 'Monotonic Upstream Scheme for Conservation Laws'. The method is widely used in computational fluid dynamics for its ability to handle discontinuities and shocks accurately. It is also used in other fields such as magnetohydrodynamics and astrophysics. The method is implemented in various software packages, including OpenFOAM, Fluent, and ANSYS.

# PLM for the Euler Equations (MUSCL)



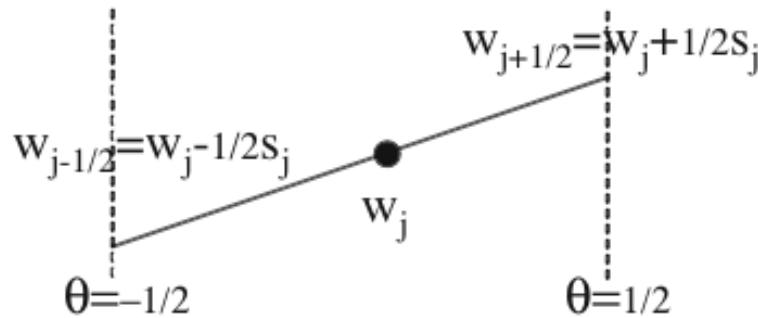
# Godunov methods use a geometric approach to developing the method.

- ◆ One of the key aspects of Godunov's methods is the development of the numerical method through interpolation - the reconstruction of the dependent variables in a finite zone.
- ◆ Because the geometry is clear often the methods (or the differences between them) can be easy to understand.

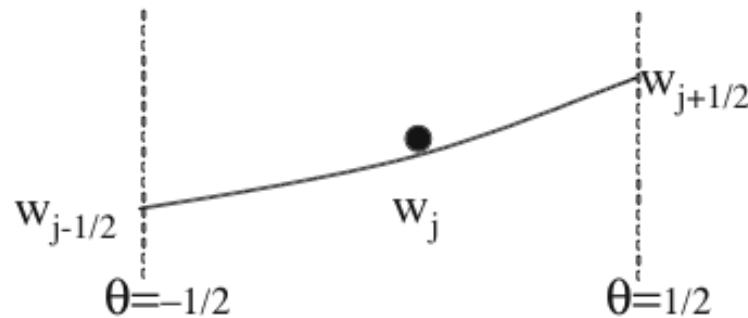


Now we will spend time looking at **linear** and **parabolic** reconstruction procedures.

**PLM**



**PPM**



- ◆ PLM is the piecewise linear method (Van Leer I)
- ◆ PPM is the piecewise parabolic method (Van Leer IV)
- ◆ Both methods produce high quality methods

# A second-order Godunov method uses piecewise linear polynomials.

- ◆ The second-order polynomial uses the cell average and a first-derivative (often called a **slope**),

$$\mathbf{P}_j(\theta) = \mathbf{P}_0 + \mathbf{P}_1\theta; \mathbf{P}_0 = \mathbf{U}_j; \mathbf{P}_1 = \mathbf{S}_j$$

- ◆ Several key requirements are necessary for this to be useful:

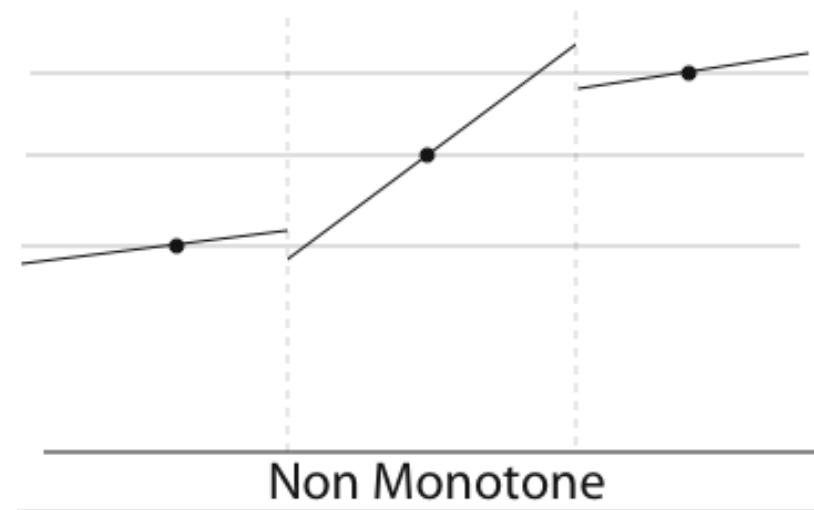
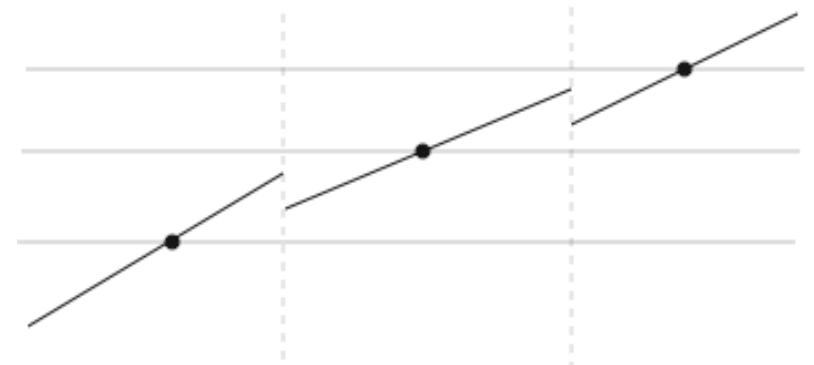
✓ Conservation  $\mathbf{U}_j = \int \mathbf{P}_j(\theta) d\theta = \mathbf{P}_0$

✓ Accuracy  $\mathbf{S}_j = \mathbf{P}_1 = \frac{\partial \mathbf{P}}{\partial \theta} = \frac{\partial \mathbf{U}}{\partial x} \Delta x$

✓ Boundedness (monotonicity)-the next few slides!

# The key to using these reconstructions is keeping the polynomials monotone.

- ◆ The original statement is heuristic: the reconstruction should be bounded by the neighboring data.
- ◆ Later, time-dependence will be entertained, the time integrated edge values must be bounded.



# We can derive the monotonicity conditions using geometric arguments.

- ◆ Take the PLM reconstruction and derive the monotonicity conditions,

$$\mathbf{U}_{j-1}^n \leq \mathbf{P}(1/2) \leq \mathbf{U}_{j+1}^n$$

$$\mathbf{U}_{j-1}^n \leq \mathbf{U}_j^n + \frac{1}{2}\mathbf{S}_j \leq \mathbf{U}_{j+1}^n$$

$$\mathbf{U}_{j-1}^n - \mathbf{U}_j^n \leq \frac{1}{2}\mathbf{S}_j \leq \mathbf{U}_{j+1}^n - \mathbf{U}_j^n$$

$$\mathbf{U}_{j-1}^n \leq \mathbf{P}(-1/2) \leq \mathbf{U}_{j+1}^n$$

$$\mathbf{U}_{j-1}^n \leq \mathbf{U}_j^n - \frac{1}{2}\mathbf{S}_j \leq \mathbf{U}_{j+1}^n$$

$$\mathbf{U}_{j-1}^n - \mathbf{U}_j^n \leq -\frac{1}{2}\mathbf{S}_j \leq \mathbf{U}_{j+1}^n - \mathbf{U}_j^n$$

- ◆ Assume the data is increasing left-to-right

$$\mathbf{S}_j \leq 2(\mathbf{U}_{j+1}^n - \mathbf{U}_j^n)$$

$$\mathbf{S}_j \leq 2(\mathbf{U}_j^n - \mathbf{U}_{j-1}^n)$$

- ◆ Test the alternate case and you see the minmod limiter does the trick,

$$\mathbf{S}_j := \text{minmod}[\mathbf{S}_j, 2\Delta_{j-1/2} \mathbf{U}, 2\Delta_{j+1/2} \mathbf{U}]$$

# Making PLM second-order in time is relatively simple.

- ◆ Taking the definition of the time-averaged value from the integral we can find a second-order time-accurate value,

$$\frac{1}{-C} \int_{1/2}^{1/2-C} \mathbf{P}(\theta) d\theta = \frac{1}{-C} \int_{1/2}^{1/2-C} (\mathbf{P}_0 + \mathbf{P}_1 \theta) d\theta = \mathbf{P}_0 + \frac{1}{2} (1 - C) \mathbf{P}_1$$

$$\mathbf{U}_j^n + \frac{1}{2} (1 - C) \mathbf{S}_j^n$$

$$\frac{1}{-C} \int_{-1/2}^{-1/2-C} \mathbf{P}(\theta) d\theta = \frac{1}{-C} \int_{-1/2}^{-1/2-C} (\mathbf{P}_0 + \mathbf{P}_1 \theta) d\theta = \mathbf{P}_0 - \frac{1}{2} (1 + C) \mathbf{P}_1$$

$$C = \frac{\lambda \Delta t}{\Delta x}$$

Courant Number

**There is a wide variety of slopes that can be used with PLM (many from the TVD schemes).**

◆ **Here is a slew of different recipes**

✓ **Minmod**

$$S_j = \min \text{mod} \left[ \Delta_{j-1/2} U, \Delta_{j+1/2} U \right]$$

✓ **Van Leer**

$$S_j = \frac{|\Delta_{j+1/2} U| \Delta_{j-1/2} U + |\Delta_{j-1/2} U| \Delta_{j+1/2} U}{|\Delta_{j-1/2} U| + |\Delta_{j+1/2} U|}$$

✓ **Fromm**

$$S_j = \min \text{mod} \left[ \frac{1}{2} \left( \Delta_{j-1/2} U + \Delta_{j+1/2} U \right), 2 \Delta_{j-1/2} U, 2 \Delta_{j+1/2} U \right]$$

✓ **Van Albada**

$$S_j = \frac{\left( \Delta_{j+1/2} U \right)^2 \Delta_{j-1/2} U + \left( \Delta_{j-1/2} U \right)^2 \Delta_{j+1/2} U}{\left( \Delta_{j-1/2} U \right)^2 + \left( \Delta_{j+1/2} U \right)^2}$$

There's more, the slope before limiting can be chosen more broadly.

◆ High-order slopes can improve the performance of the method,

✓ An example would be a fourth-order choice,

$$S_j^n = \frac{8(U_{j+1}^n - U_{j-1}^n) - (U_{j+2}^n - U_{j-2}^n)}{12}$$

✓ Or a sixth-order choice

$$S_j^n = \frac{45(U_{j+1}^n - U_{j-1}^n) - 9(U_{j+2}^n - U_{j-2}^n) + (U_{j+3}^n - U_{j-3}^n)}{60}$$

✓ Or whatever you like...

✓ It can be used in conjunction with the limiter

$$S_j := \min \text{mod} [S_j, 2 \Delta_{j-1/2} U, 2 \Delta_{j+1/2} U]$$

**Its always important to start with a stability analysis to make sure you're on the right path.**

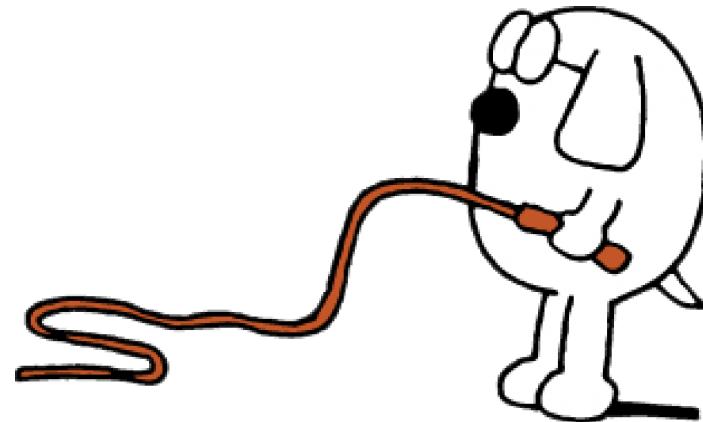
◆ **Before taking the time to code a scheme one should know exactly what to expect from the method. It also makes a good time to state the design principles:**

- 1. Have a stable dissipative (entropy condition satisfying) monotone method as a foundation,**
- 2. Blend it with a stable (upsteam-centered) high-order method**
- 3. Define the blending via monotonicity or some other nonlinear stability principle .**
- 4. Test, test, test**

# High-Resolution Methods

- ◆ Provide an introduction to *high-resolution* schemes including some ideas about motivation and implementation

- ✓ These methods have provided an enormous upgrade in computational performance over the previous generation of methods.



- ✓ The Dogbert Principle: “*Logically all things are created by a combination of simpler, less capable components*” (see Laney in Computational Gasdynamics)

# High Resolution Methods and Accuracy and order of convergence

- ❑ Linear versus nonlinear error
- ❑ For high order (unsplit) schemes getting nonlinear high order is very expensive (lots of quadrature points)
- ❑ If there is a discontinuity then the order of accuracy is first order
- ❑ A good question to ask, what is required for practical accuracy for discontinuous problems?
- ❑ What is the important design point... I think the linear accuracy is a good guide.

# What is a high-resolution method? Or the role of method nonlinearity

- ◆ The need for method nonlinearity is a consequence of Godunov's theorem:
  - ✓ No *linear* method can be second-order and monotone... **but a *nonlinear* method can be second-order and monotone (TVD, FCT, PLM, PPM, ENO, WENO...)!\***
- ◆ These methods hybridized the (classical) linear schemes (**capitalizing on** the best of each!)
  - ✓ To achieve **higher order** and **physically relevant** solutions e.g. **LxW** and **upwind**

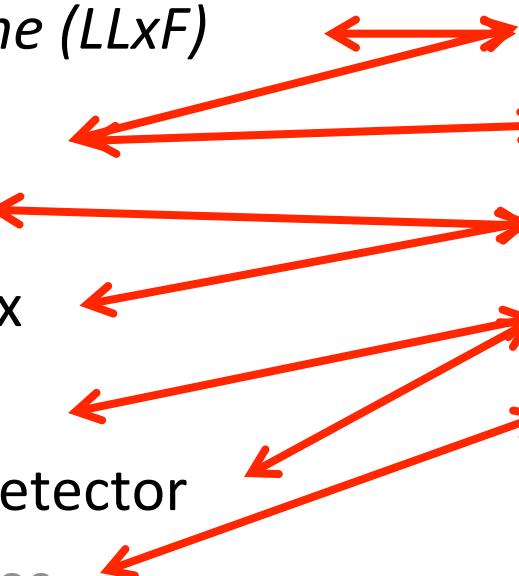
# Basic Elements of Methods

## Weighted ENO Method

- *Entropy scheme (LLxF)*
- Flux Splitting
- Base fluxes
- High-order flux
- Weights
- Smoothness detector
- Method-of-lines

## High-Order Godunov

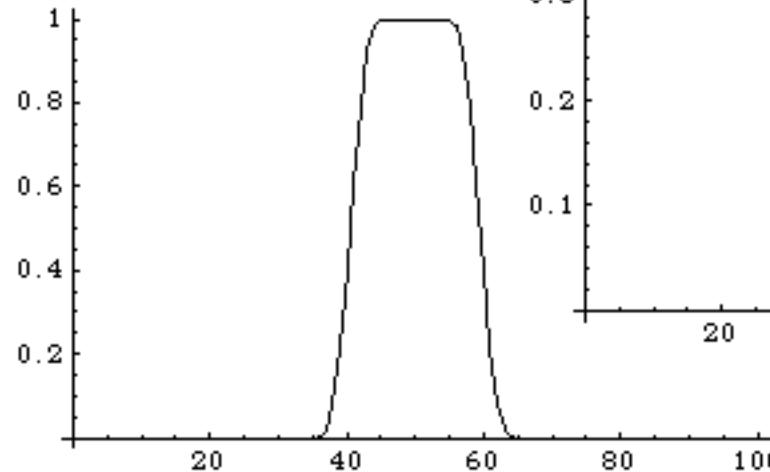
- Riemann solver (upwind)
- *Characteristic Projection*
- High-order differencing
- Limiter
- Time-centering



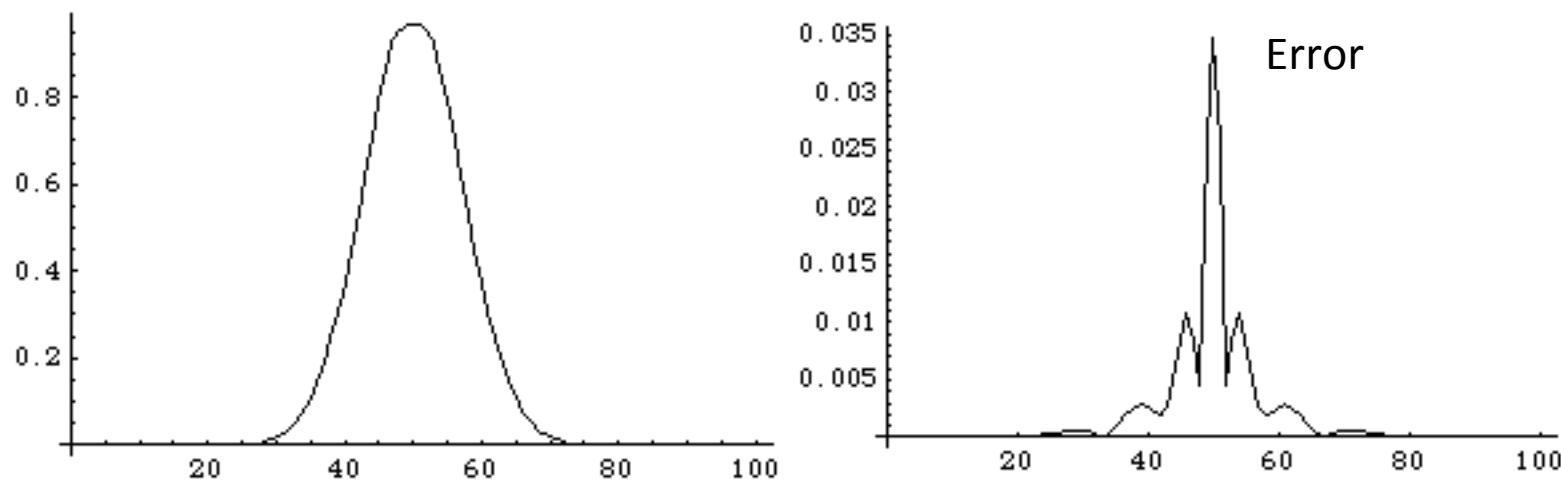
- The key to these methods is successfully ***hybridizing*** high-order and entropy satisfaction

# How does the method do?

## ◆ Square wave -

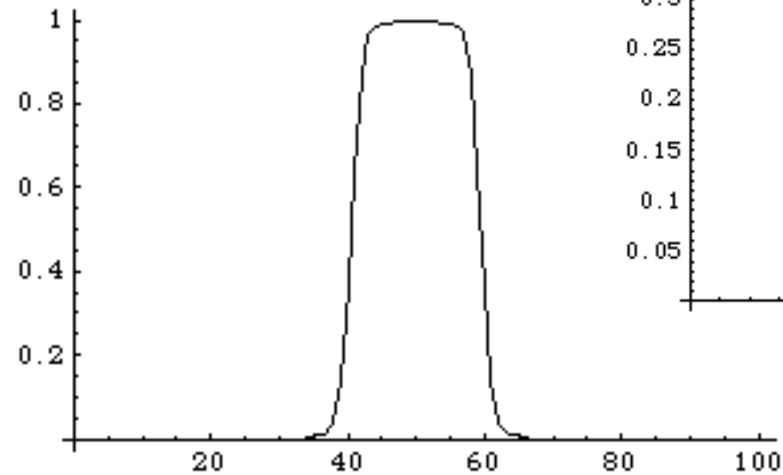


## ◆ Gaussian -

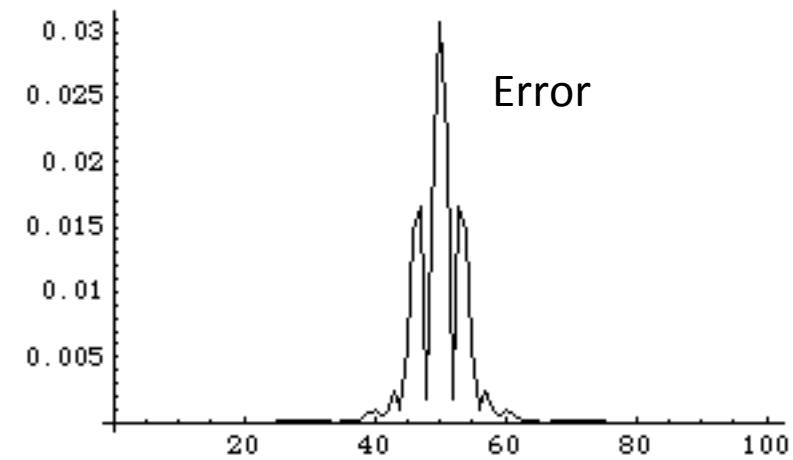
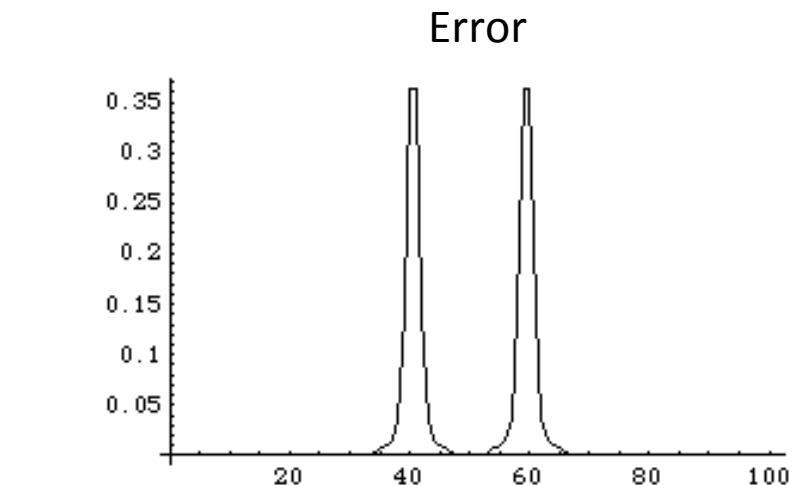
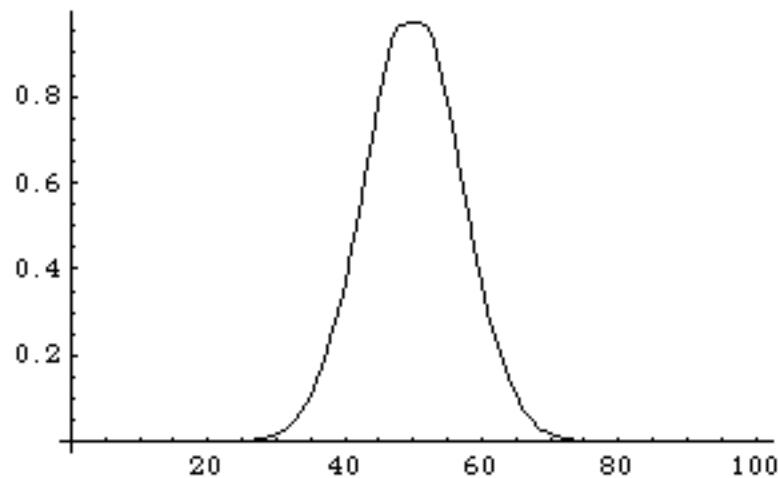


# What about 4th order slopes

## ◆ Square wave

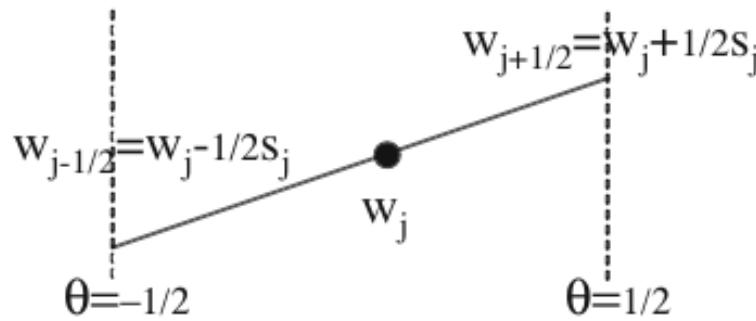


## ◆ Gaussian

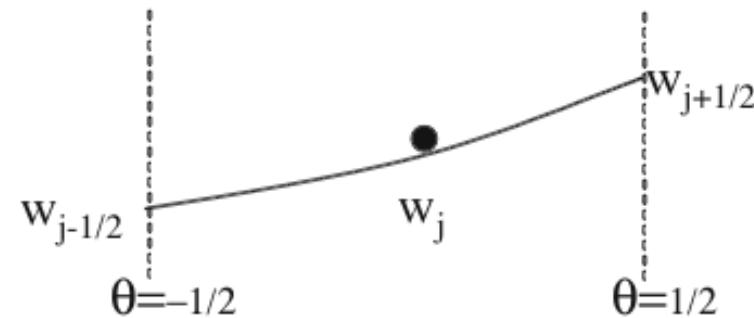


Now we will spend time looking at linear and parabolic reconstruction procedures.

**PLM**



**PPM**



- ◆ PLM is the piecewise linear method (Van Leer I)
- ◆ PPM is the piecewise parabolic method (Van Leer IV)
- ◆ Both methods produce high quality methods

# The PPM method first studied by Van Leer in '77 appeared in Colella & Woodward's paper.

JOURNAL OF COMPUTATIONAL PHYSICS 54, 174–201 (1984)

## The Piecewise Parabolic Method (PPM) for Gas-Dynamical Simulations

PHILLIP COLELLA

*Lawrence Berkeley Laboratory, University of California,  
Berkeley, California, 94720*

AND

PAUL R. WOODWARD

*Lawrence Livermore National Laboratory, University of California,  
Livermore, California 94550*

Received August 3, 1982; revised August 25, 1983

We present the piecewise parabolic method, a higher-order extension of Godunov's method. There are several new features of this method which distinguish it from other higher-order Godunov-type methods. We use a higher-order spatial interpolation than previously used, which allows for a steeper representation of discontinuities, particularly contact discontinuities. We introduce a simpler and more robust algorithm for calculating the nonlinear wave interactions used to compute fluxes. Finally, we recognize the need for additional dissipation in any higher-order Godunov method of this type, and introduce it in such a way so as not to degrade the quality of the results.

# A second-order Godunov method uses piecewise linear polynomials.

- ◆ The second-order polynomial uses the cell average and the cell edge values,

$$P_j(\theta) = P_0 + P_1\theta + P_2\theta^2$$

$$P_0 = U_j^n - \frac{1}{12}P_2; P_1 = U_{j+1/2}^n - U_{j-1/2}^n; P_2 = 3(U_{j+1/2}^n - 2U_j^n + U_{j-1/2}^n)$$

- ◆ Several key requirements are necessary for this to be useful:

✓ Conservation  $U_j = \int P_j(\theta) d\theta = P_0$

✓ Accuracy  $U_{j \pm 1/2} = U(x_{j \pm 1/2}) + \mathcal{O}(\Delta x^n)$

✓ Boundedness (monotonicity)-the next few slides!

# First, a new function to simplify programming

- ◆ Remember the minmod function, using it we can define a median function

$$\text{median}(a, b, c) = a + \text{min mod}(b - a, c - a)$$

- ◆ The median will return whatever argument that is bounded by the other two.
- ◆ The median also has some other useful properties that we will exploit in a later lecture (for getting high-order accuracy)

# We can derive the monotonicity conditions using geometric arguments.

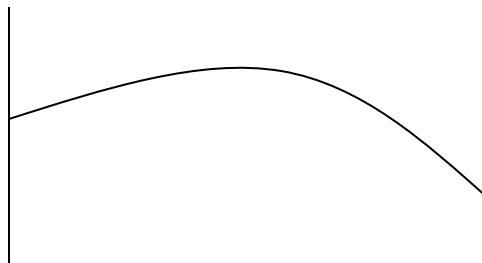
- ◆ Just as PLM we start with the same basic conditions,

$$\mathbf{U}_{j-1}^n \leq \mathbf{P}(1/2) \leq \mathbf{U}_{j+1}^n \quad \mathbf{U}_{j-1}^n \leq \mathbf{P}(-1/2) \leq \mathbf{U}_{j+1}^n$$

- ◆ We can enforce this condition with two operations that put the interface value between the cell values bounding them.

$$\mathbf{U}_{j+1/2}^n := \text{median}(\mathbf{U}_j^n, \mathbf{U}_{j+1/2}^n, \mathbf{U}_{j+1}^n) \quad \mathbf{U}_{j-1/2}^n := \text{median}(\mathbf{U}_{j-1}^n, \mathbf{U}_{j-1/2}^n, \mathbf{U}_j^n)$$

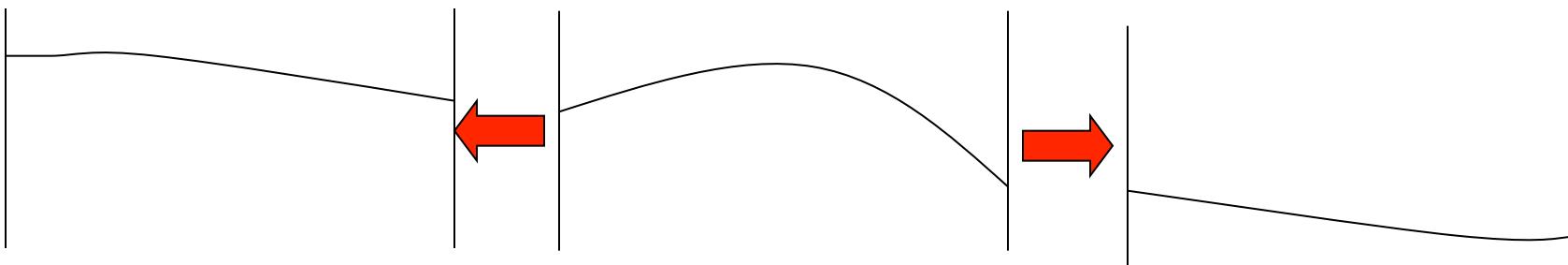
- ◆ The only problem now is an local extrema inside the zone.



# We can derive the monotonicity conditions using geometric arguments.

- ◆ We can observe that the PPM reconstruction can introduce local extrema within a zone. This is clearly NOT monotone so it must be excluded.
- ◆ A local extrema occurs when the derivative of the polynomial is zero, if we force this to occur at or outside (no problem) we are monotone.

$$d\mathbf{P}(\theta)/d\theta = \mathbf{P}_1 + 2\mathbf{P}_2\theta$$



# We can now finish the monotonicity derivation

◆ Force zero in the derivative to the edges if they occur in the cell

$$0 = \mathbf{P}_1 + 2\mathbf{P}_2\theta$$

$$0 = \mathbf{P}_1 + \mathbf{P}_2 = \mathbf{U}_{j+1/2}^n - \mathbf{U}_{j-1/2}^n + 3(\mathbf{U}_{j+1/2}^n - 2\mathbf{U}_j^n + \mathbf{U}_{j-1/2}^n)$$

$$4\mathbf{U}_{j+1/2}^n - 2\mathbf{U}_{j-1/2}^n - 6\mathbf{U}_j^n = 0 \quad \rightarrow \quad \mathbf{U}_{j-1/2}^n = 3\mathbf{U}_j^n - 2\mathbf{U}_{j+1/2}^n$$

$$0 = \mathbf{P}_1 - \mathbf{P}_2 = \mathbf{U}_{j+1/2}^n - \mathbf{U}_{j-1/2}^n - 3(\mathbf{U}_{j+1/2}^n - 2\mathbf{U}_j^n + \mathbf{U}_{j-1/2}^n)$$

$$-2\mathbf{U}_{j+1/2}^n - 4\mathbf{U}_{j-1/2}^n + 6\mathbf{U}_j^n = 0 \quad \rightarrow \quad \mathbf{U}_{j+1/2}^n = 3\mathbf{U}_j^n - 2\mathbf{U}_{j-1/2}^n$$

◆ Summarize the algorithm

$$\mathbf{U}_{j\pm 1/2}^n \coloneqq \text{median}(\mathbf{U}_j^n, \mathbf{U}_{j\pm 1/2}^n, \mathbf{U}_{j\pm 1}^n)$$

$$\mathbf{U}_{j\pm 1/2}^n \coloneqq \text{median}(\mathbf{U}_j^n, \mathbf{U}_{j\pm 1/2}^n, 3\mathbf{U}_j^n - 2\mathbf{U}_{j\mp 1/2}^n)$$

## Making PPM third-order in time more complex.

◆ Taking the definition of the time-averaged value from the integral we can find a second-order time-accurate value,

$$\frac{1}{-C} \int_{1/2}^{1/2-C} \mathbf{P}(\theta) d\theta = \int_{1/2}^{1/2-C} (\mathbf{P}_0 + \mathbf{P}_1\theta + \mathbf{P}_2\theta^2) d\theta$$

$$\bar{\mathbf{U}}_{j+1/2} = \mathbf{P}_0 + \mathbf{P}_1\left(\frac{1}{2} - \frac{C}{2}\right) + \mathbf{P}_2\left(\frac{1}{4} - \frac{C}{2} + \frac{C^2}{3}\right)$$

$$\frac{1}{-C} \int_{-1/2}^{-1/2-C} \mathbf{P}(\theta) d\theta = \int_{-1/2}^{-1/2-C} (\mathbf{P}_0 + \mathbf{P}_1\theta + \mathbf{P}_2\theta^2) d\theta$$

$$\bar{\mathbf{U}}_{j-1/2} = \mathbf{P}_0 + \mathbf{P}_1\left(-\frac{1}{2} - \frac{C}{2}\right) + \mathbf{P}_2\left(\frac{1}{4} + \frac{C}{2} + \frac{C^2}{3}\right)$$

# Woodward & Colella's special edge value

- ◆ The method is designed to make sure the edge lies between the adjacent cell values,

$$\mathbf{U}_{j+1/2}^n = \frac{1}{2} \left( \mathbf{U}_j^n + \mathbf{U}_{j+1}^n \right) - \frac{1}{6} \left( \delta \mathbf{U}_{j+1}^n - \delta \mathbf{U}_j^n \right)$$

$$\delta \mathbf{U}_j^n = \min \text{mod} \left[ \frac{1}{2} \left( \mathbf{U}_{j+1}^n - \mathbf{U}_{j-1}^n \right), 2 \left( \mathbf{U}_j^n - \mathbf{U}_{j-1}^n \right), 2 \left( \mathbf{U}_{j+1}^n - \mathbf{U}_j^n \right) \right]$$

- ◆ This sort of procedure can be derived for other high-order approximations to the edges.
- ◆ This approach has a significantly positive impact on the magnitude of error associated with the solution.

There's more, the initial edge values need to be chosen.

◆ Colella and Woodward chose fourth-order values\*.

$$\mathbf{U}_{j+1/2}^n = \frac{7}{12}(\mathbf{U}_j^n + \mathbf{U}_{j+1}^n) - \frac{1}{12}(\mathbf{U}_{j-1}^n + \mathbf{U}_{j+2}^n)$$

◆ Higher-order edges can improve the performance of the method, a sixth-order choice

$$\mathbf{U}_{j+1/2}^n = \frac{37}{60}(\mathbf{U}_j^n + \mathbf{U}_{j+1}^n) - \frac{8}{60}(\mathbf{U}_{j-1}^n + \mathbf{U}_{j+2}^n) + \frac{1}{60}(\mathbf{U}_{j-2}^n + \mathbf{U}_{j+3}^n)$$

✓ Or a fifth-order upwind choice

$$\mathbf{U}_{j+1/2}^n = \frac{2}{60}\mathbf{U}_{j-2}^n - \frac{13}{60}\mathbf{U}_{j-1}^n + \frac{47}{60}\mathbf{U}_j^n + \frac{27}{60}\mathbf{U}_{j+1}^n - \frac{3}{60}\mathbf{U}_{j+2}^n$$

✓ Or whatever you like, a least third-order or its not worth it!

\* C&W actually use a special fourth-order method

# High-Order Edge Values – Tremendous flexibility!

◆ First compute the edge values: Sixth-order centered

$$U_{j+1/2} = \frac{37(U_j + U_{j+1}) - 8(U_{j-1} + U_{j+2}) + (U_{j-2} + U_{j+3})}{60}$$

◆ Seventh-order upwind

$$U_{j+1/2} = \frac{-3U_{j-3} + 25U_{j-2} - 101U_{j-1} + 319U_j + 214U_{j+1} - 38U_{j+2} + 4U_{j+3}}{420}$$

◆ Seventh-order parabolic

$$U_{j+1/2} = \frac{-111U_{j-3} + 849U_{j-2} - 3010U_{j-1} + 8510U_j + 6645U_{j+1} - 1349U_{j+2} + 148U_{j+3}}{11520}$$

◆ Six-point optimal stencil [0,3p/4]

$$U_{j+1/2} = a(U_j + U_{j+1}) + b(U_{j-1} + U_{j+2}) + c(U_{j-2} + U_{j+3})$$

$$a = 0.681056...; b = -0.229918..., c = 0.048816..$$

# Scheme Stability & Truncation Error is exceptional

## ◆ Using Fourier analysis:

✓ All stable to CFL=1

## ◆ Fourth-order truncation error

✓ Amplitude  $A \approx 1 + \left( -\frac{c^2}{24} + \frac{c^3}{12} - \frac{c^4}{24} \right) \theta^4 + O(\theta^6)$

✓ Phase  $P \approx 1 + \left( -\frac{1}{30} + \frac{c}{12} - \frac{c^3}{12} + \frac{c^4}{30} \right) \theta^4 + O(\theta^6)$

## ◆ Sixth-order truncation error

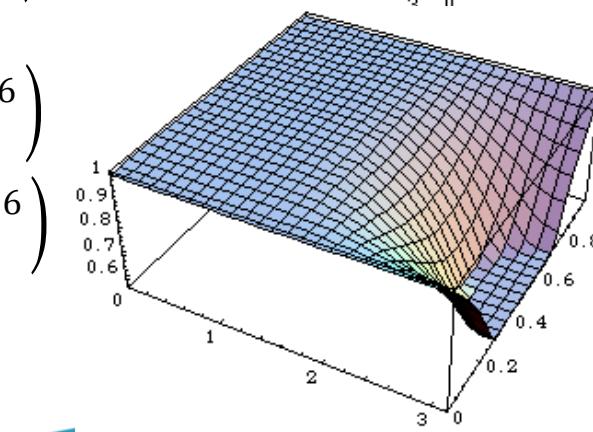
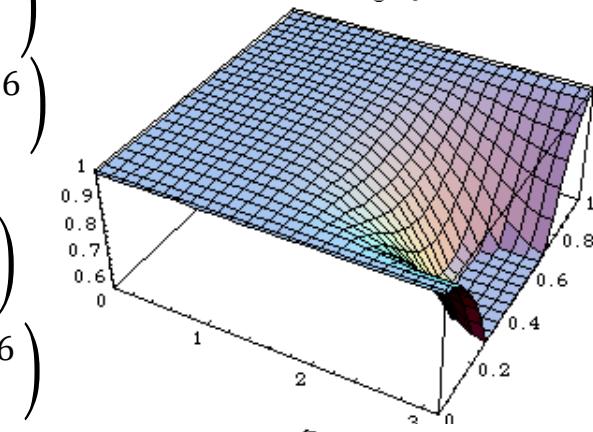
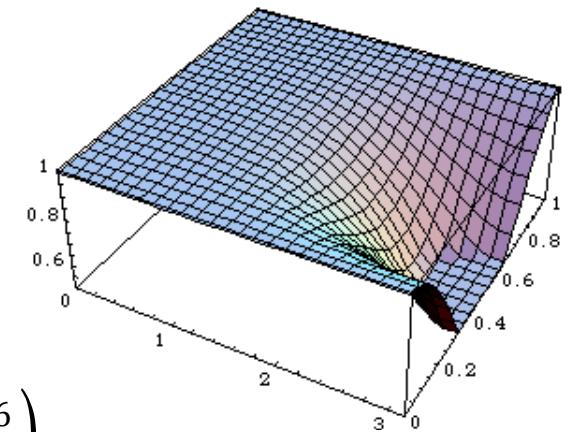
✓ Amplitude  $A \approx 1 + \left( -\frac{c^2}{24} + \frac{c^3}{12} - \frac{c^4}{24} \right) \theta^4 + O(\theta^6)$

✓ Phase  $P \approx 1 + \left( -\frac{c}{60} + \frac{c^2}{15} - \frac{c^3}{12} + \frac{c^4}{30} \right) \theta^4 + O(\theta^6)$

## ◆ Seventh-order truncation error

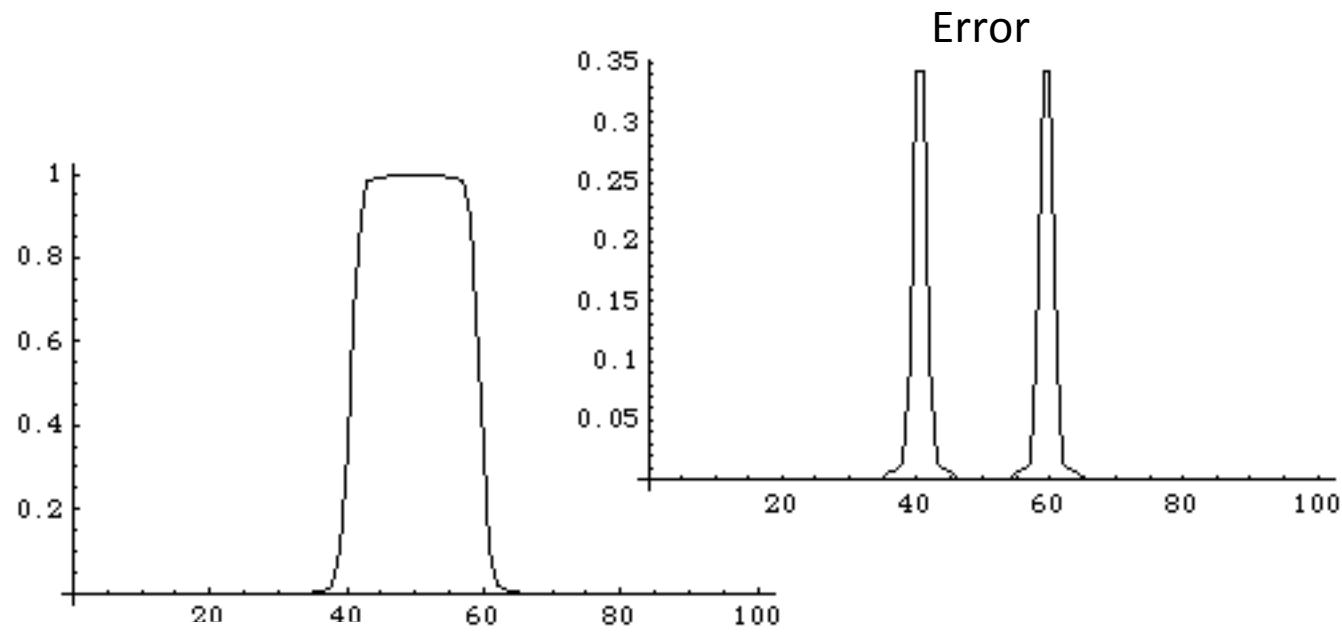
✓ Amplitude  $A \approx 1 + \left( \frac{c}{48} - \frac{c^2}{16} + \frac{c^3}{12} - \frac{c^4}{24} \right) \theta^4 + O(\theta^6)$

✓ Phase  $P \approx 1 + \left( \frac{1}{120} - \frac{c}{24} + \frac{c^2}{12} - \frac{c^3}{12} + \frac{c^4}{30} \right) \theta^4 + O(\theta^6)$

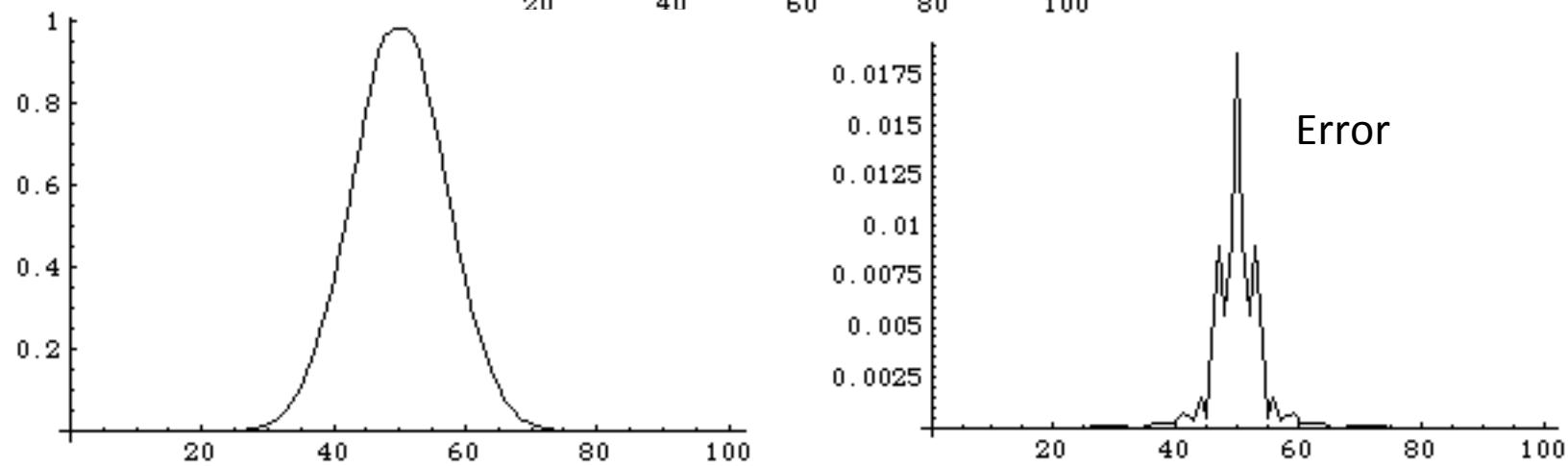


# What about 6th order edge values?

## ◆ Square wave



## ◆ Gaussian



# The observation that high-order is best is rather old.

◆ Boris and Book's most accurate method was based on a spectral flux for the high-order method. It produced the lowest absolute error in their square wave test.\*

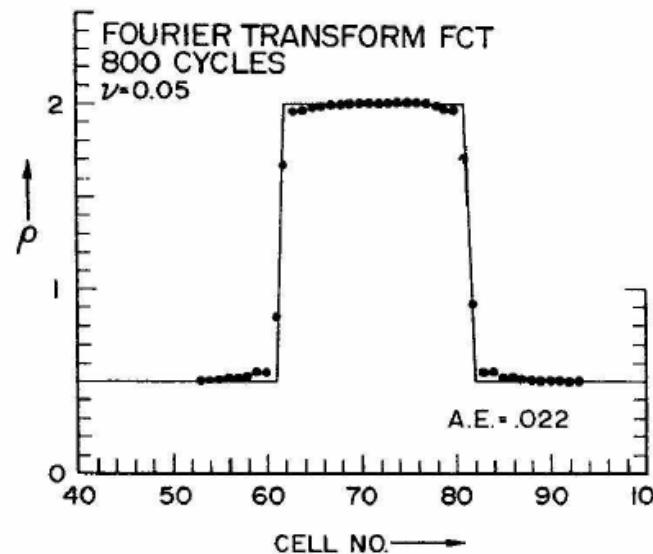
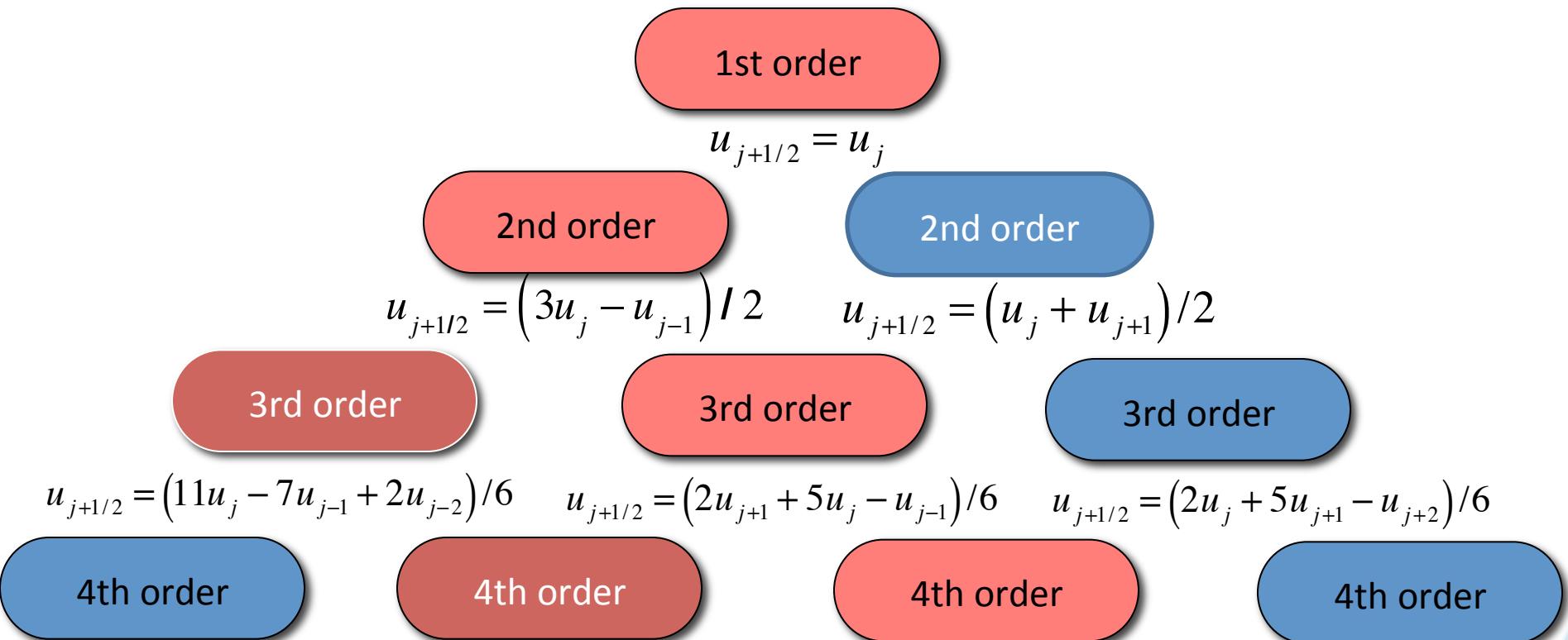


Fig. 13. The optimum FCT algorithm.

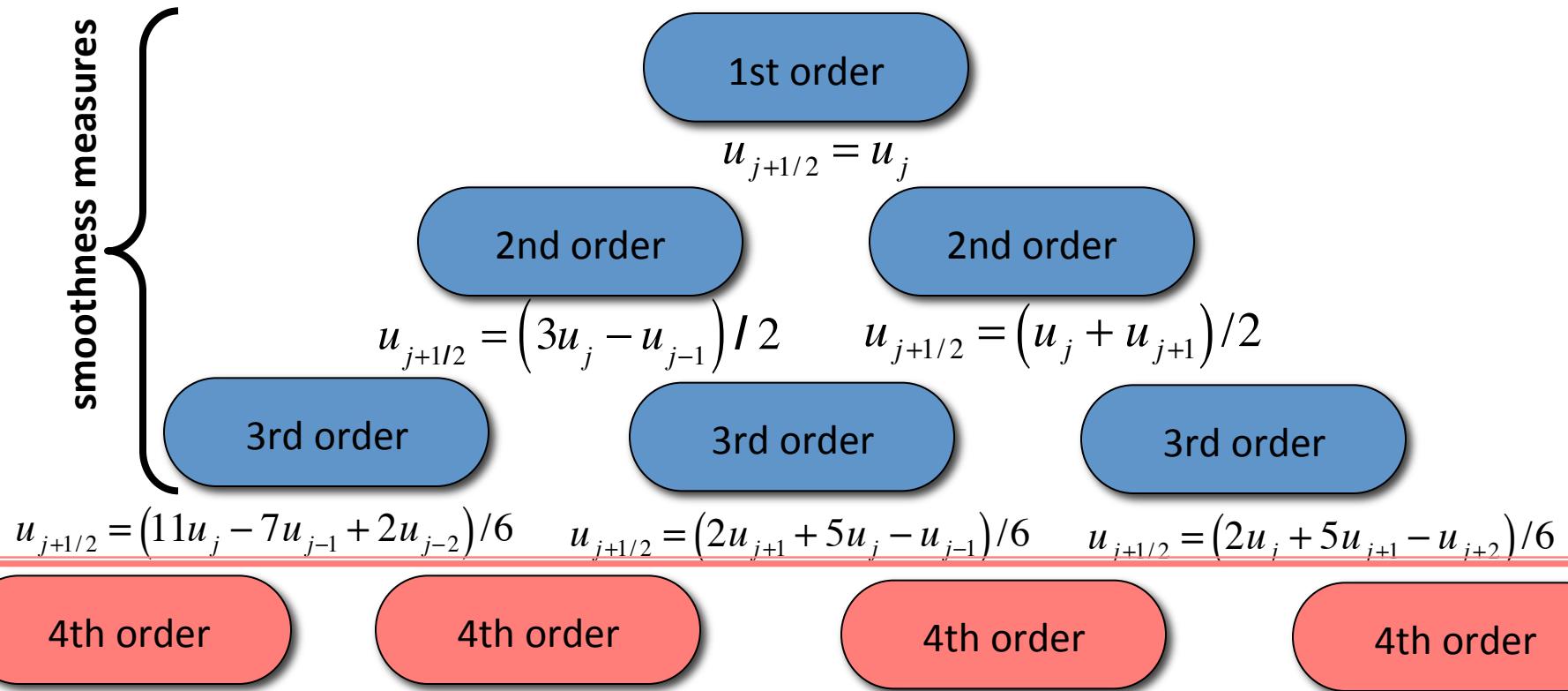
\* Boris & Book, "Methods in Computational Physics" Volume 16, 1976

ENO Methods use an adaptive stencil that chooses the “smoother” stencil locally, its formally higher order.



◆ ENO selects stencils *adaptively* by choosing the one that is closest to the next lower order.

# Weighted ENO methods are different in their approach, but the result is similar



- ◆ These methods evaluate *all* the high-order stencils and compare them algebraically.

These methods also have a few more “bells and whistles” that you’ll find in reading.

◆ Steeper slopes or edges - You’ll often see modifications of the slope or edge values that look like “pre-limiting” to make the reconstruction steeper. This can also be done for any sharp interface.

$$\chi = \frac{\partial_{xxx} u}{\partial_x u} \rightarrow \xi = \eta \max \left[ 0, \min \left( 1, 20 \left( \chi - 0.01 \right) \right) \right]$$

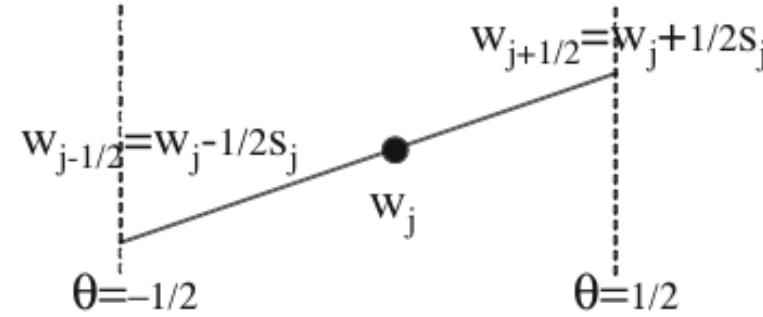
$$\tilde{u}_{j-1/2} = u_{j-1} + \frac{1}{2} \mathbf{minmod} \left( u_{j-1} - u_{j-2}, u_j - u_{j-1} \right)$$

$$\tilde{u}_{j+1/2} = u_{j+1} - \frac{1}{2} \mathbf{minmod} \left( u_{j+2} - u_{j+1}, u_{j+1} - u_j \right)$$

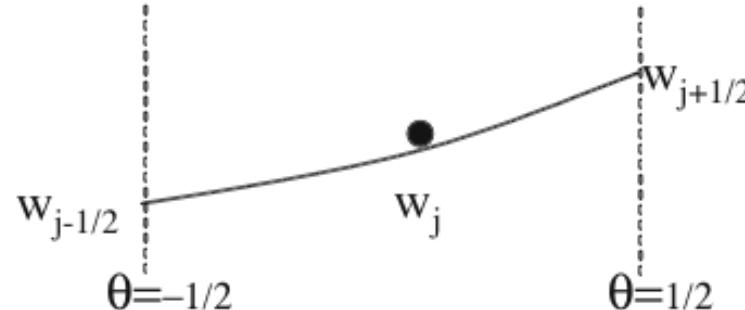
$$u_{j-1/2} := (1 - \xi) u_{j-1/2} + \xi \tilde{u}_{j-1/2} \quad u_{j+1/2} := (1 - \xi) u_{j+1/2} + \xi \tilde{u}_{j+1/2}$$

# The next couple of schemes are different

PLM



PPM



- The evolution for  $w_j$ 's will be the same using the integral (weak) form

$$\frac{\partial}{\partial t} \int w dx + \oint w dS = 0 \rightarrow \frac{\partial}{\partial t} \bar{w} = -\frac{1}{\Delta x} (w_{j+1/2} - w_{j-1/2})$$

- For the PLM now we evolve the “ $S_j$ 's” using the strong form of the PDE

$$\frac{\partial}{\partial x} \left( \frac{\partial w}{\partial t} + \frac{\partial w}{\partial x} \right) = 0 \rightarrow \frac{\partial}{\partial t} \frac{\partial w}{\partial x} + \frac{\partial}{\partial x} \frac{\partial w}{\partial x} = 0 \rightarrow \frac{\partial s}{\partial t} + \frac{\partial s}{\partial x} = 0$$

- For PPM we now evolve the edge  $w_{j\pm 1/2}$ 's ” using the strong form of the PDE

$$\frac{\partial w}{\partial t} + \frac{\partial w}{\partial x} = 0$$

If the method is higher than second-order this matter a lot!

# Van Leer II – The slope evolution scheme

- This scheme uses the evolution of the slope (gradient) as an extra equation, otherwise it is a “PLM” method with better accuracy,

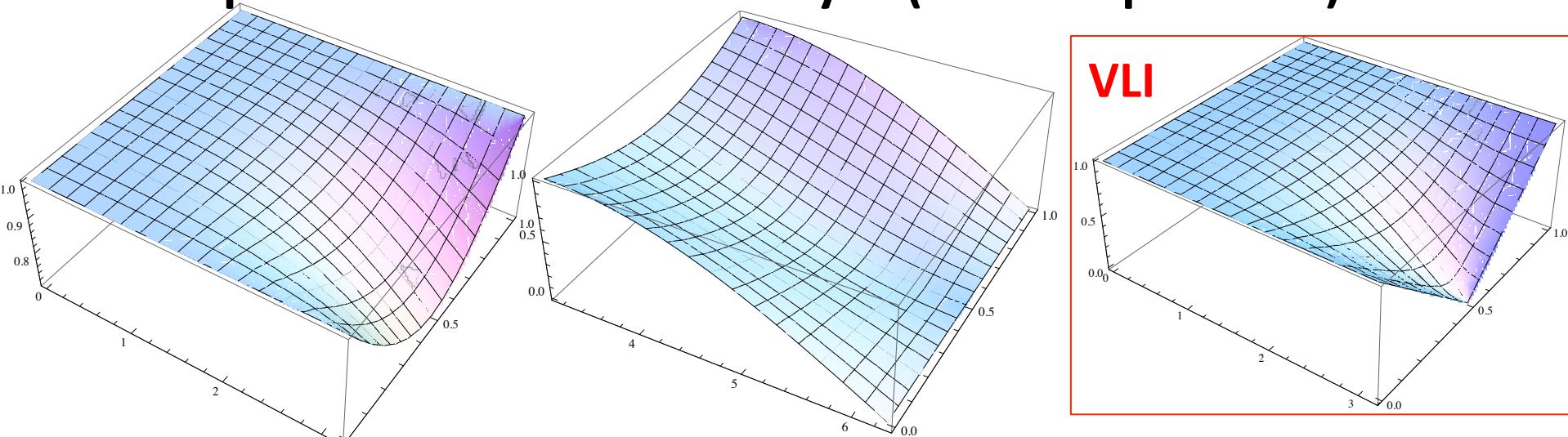
$$U_j^{n+1} = U_j^n - C \left( U_{j+1/2}^{n+1/2} - U_{j-1/2}^{n+1/2} \right) \quad U_{j+1/2}^{n+1/2} = U_j^n + \frac{1}{2} (1 - C) S_j^n$$

$$S_j^{n+1} = U_{j+1/2}^n - U_{j-1/2}^n - C \left( S_j^n - S_{j-1}^n \right) \quad U_{j+1/2}^n = U_j^n + \frac{1}{2} S_j^n$$

- This defines the simplest Hermitian method.
  - ✓ Very similar in flavor to discontinuous Galerkin except the gradient evolution is differential rather than integral
- More complex schemes can be defined by combining the data from multiple cells.
- These methods are both compact and capable of higher resolution.

# Van Leer II - Properties

- With two degrees of freedom, there are two computational modes to analyze (one is “spurious”)



- Truncation error is nice although there is an issue... basically the same as VLI (PLM), but better at  $C=1/2$

$$A \approx 1 + \left( -\frac{c^2}{8} + \frac{c^3}{4} - \frac{c^4}{8} \right) \theta^4 + O(\theta^6)$$

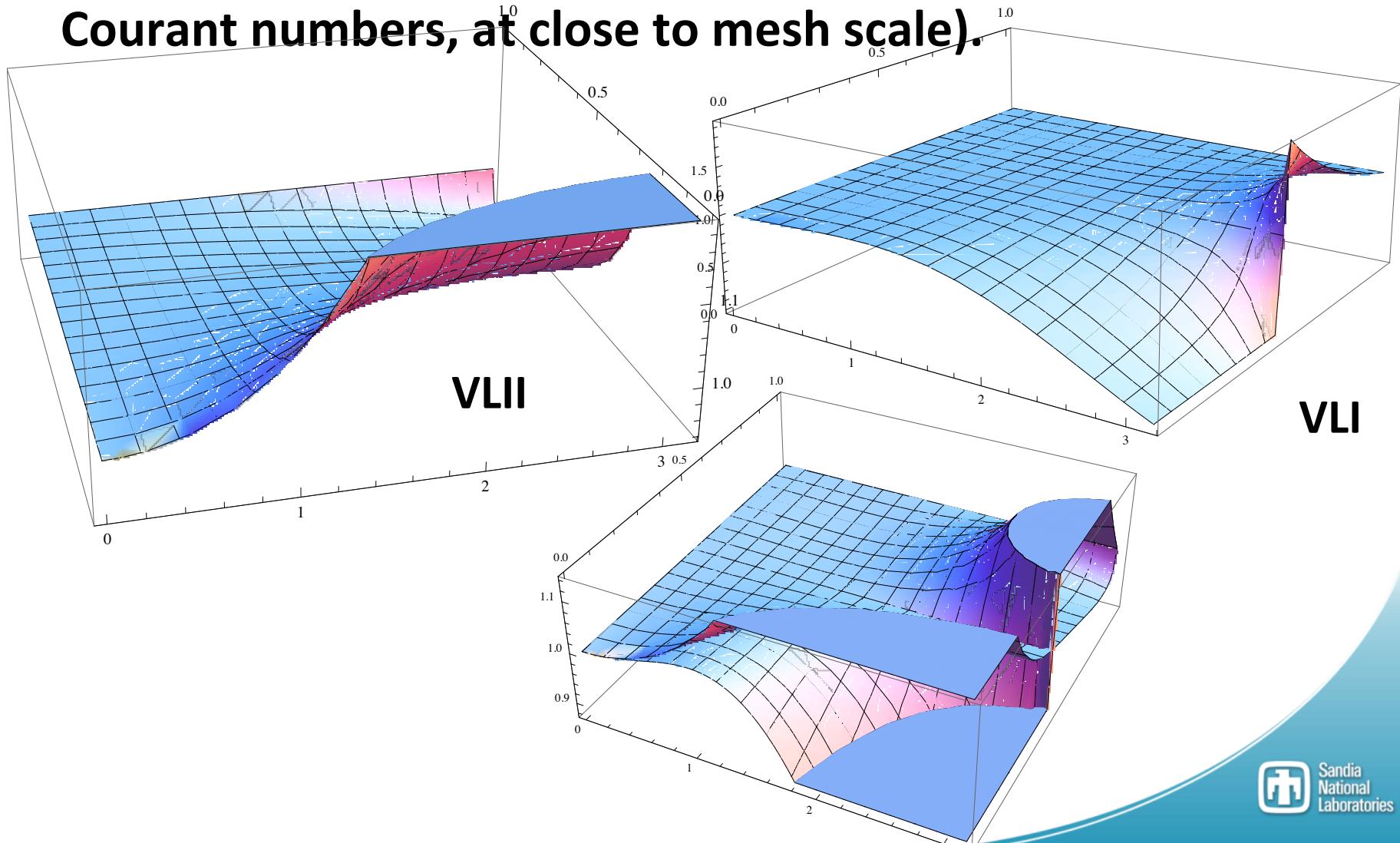
$$P \approx 1 + \left( \frac{1}{12} - \frac{c}{4} - \frac{c^2}{6} \right) \theta^2 + \left( \frac{1}{120} - \frac{c}{8} + \frac{5c^2}{12} - \frac{c^3}{2} + \frac{c^4}{5} \right) \theta^4 + O(\theta^6)$$

VLI

$$\left( -\frac{c}{8} + \frac{c^2}{4} - \frac{c^3}{4} + \frac{c^4}{8} \right) \theta^4$$

# VL II Phase Error Plots

□ The phase error show the problems with VLII (at small Courant numbers, at close to mesh scale).



# The DG method mathematically.

- ◆ It is based on the integral, weak form of the PDE
- ◆ Legendre Polynomial basis.

$$\int_V \frac{\partial U}{\partial t} w dV - \oint_S f(U) \cdot w + \int_V f(U) \cdot \nabla w dV = 0$$

$$\int P(x) dV = U dV$$


$$P_0(x) = 1; P_1(x) = x; P_2(x) = x^2 - \frac{1}{12}$$
$$\left( \partial_x U \right)_t + \frac{6}{\Delta x^2} \left[ f(U_{j-1/2}) + f(U_{j+1/2}) \right] - \frac{12}{\Delta x^2} \int_{-\Delta x/2}^{\Delta x/2} f(U) dx = 0$$

$$\left( \partial_{xx} U \right)_t + \frac{30}{\Delta x^3} \left[ f(U_{j+1/2}) - f(U_{j-1/2}) \right]$$

$$- \frac{360}{\Delta x^3} \int_{-\Delta x/2}^{\Delta x/2} f(U) (x - x_0) dx = 0$$

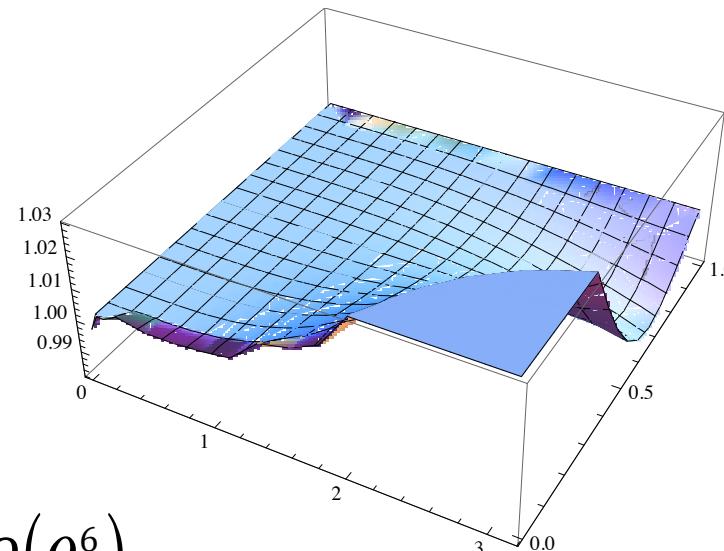
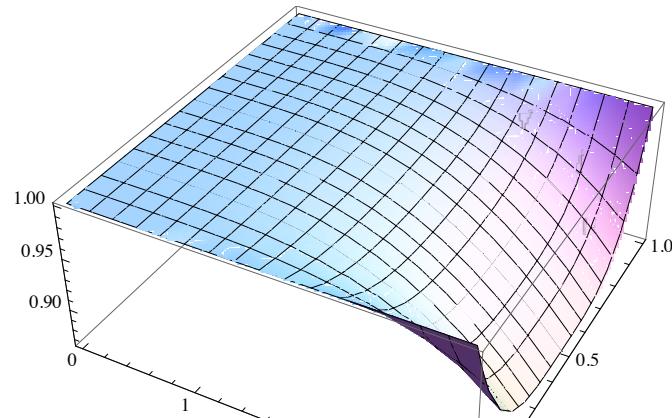
# Van Leer III – Discontinuous Galerkin (moment)

□ This is a very good method; similar to Van Leer-II, but lower errors

$$U_j^{n+1} = U_j^n - C \left( U_{j+1/2}^{n+1/2} - U_{j-1/2}^{n+1/2} \right)$$

$$U_{j+1/2}^{n+1/2} = U_j^n + \frac{1}{2} \left( 1 - C \right) S_j^n$$

$$S_j^{n+1} = S_j^n - 6C \left( U_{j-1/2}^n + U_{j+1/2}^n \right) + 2C \left( U_j^n + 4U_{j+1/2}^{n+1/2} + U_j^{n+1} \right)$$



$$A \approx 1 + \left( -\frac{C}{72} + \frac{C^2}{36} - \frac{C^3}{36} + \frac{C^4}{72} \right) \theta^4 + O(\theta^6)$$

$$P \approx 1 + \left( \frac{1}{270} - \frac{C}{108} + \frac{C^3}{108} - \frac{C^4}{270} \right) \theta^4 + O(\theta^6)$$

# Van Leer V – Evolved edge values

- ❑ This method has largely been ignored until lately.
- ❑ Several Authors have reinvented the method without realizing it.
  - ✓ Popov's PPM-L scheme

Piecewise parabolic method on a local stencil for magnetized supersonic turbulence simulation

Sergey D. Ustyugov<sup>a</sup>, Mikhail V. Popov<sup>a</sup>, Alexei G. Krtsuk<sup>b,\*</sup>, Michael L. Norman<sup>b</sup>

<sup>a</sup> Keldysh Institute of Applied Mathematics, Miusskaya Sq. 4, 125047 Moscow, Russia

<sup>b</sup> University of California, San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0424, USA

- ✓ Zeng's hybrid differencing (FV-FD method)
- ❑ It is basically PPM using the edge values as the unknowns and advanced using a differential form.
- ❑ This is a very good scheme.

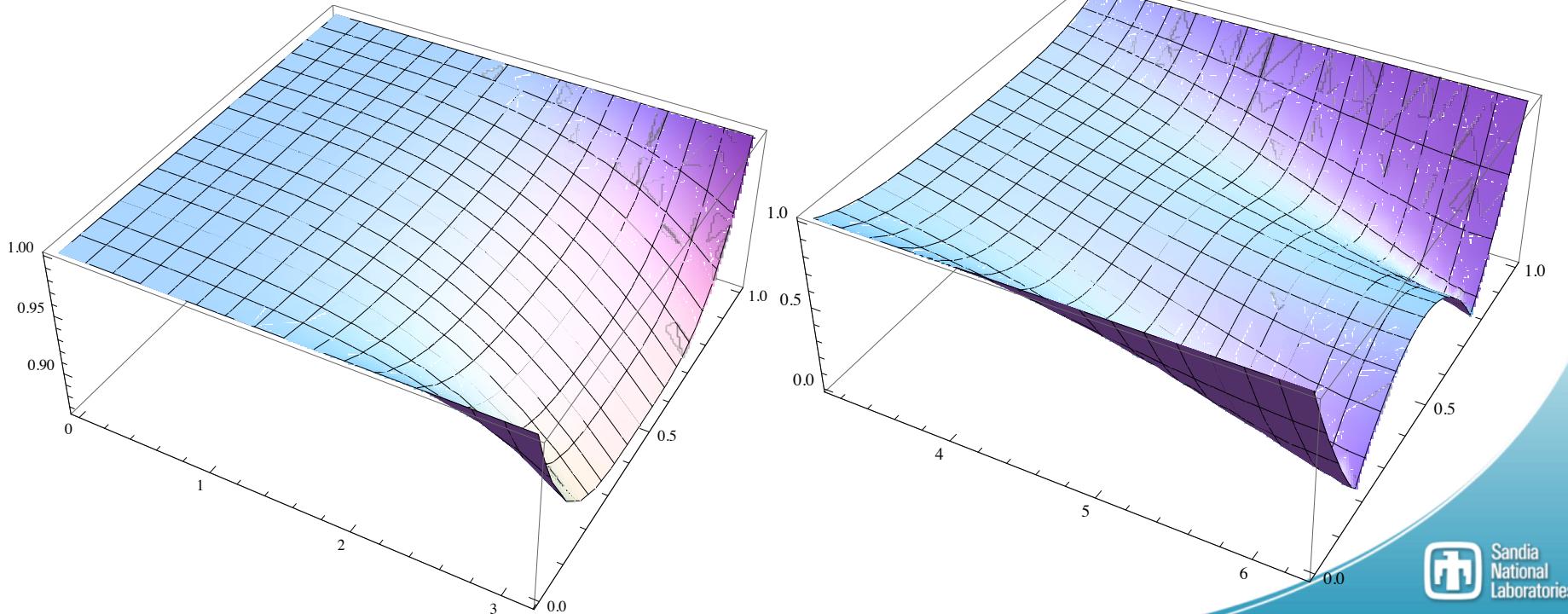
# Van Leer V as a discrete method in 1-D

## ❑ Evolve the cell-centers

$$U_j^{n+1} = U_j^n - C \left( U_{j+1/2}^{n+1/2} - U_{j-1/2}^{n+1/2} \right)$$
$$U_{j+1/2}^{n+1/2} = P_{0,j}^n + \left( \frac{1}{2} - \frac{1}{2}C \right) P_{1,j}^n + P_{2,j}^n \left( \frac{1}{4} - \frac{1}{2}C + \frac{1}{3}C^2 \right)$$

## ❑ Evolve the edges

$$U_{j+1/2}^{n+1} = U_{j+1/2}^n - CP_{1,j}^n - CP_{2,j}^n \left( 1 - C \right)$$

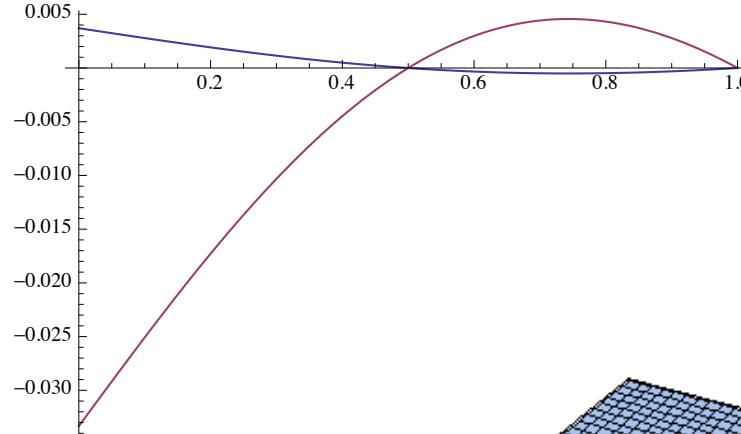
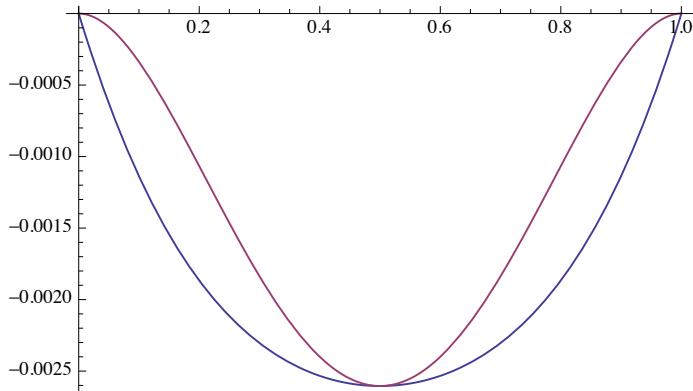


# The truncation error for Van Leer V is exciting!

□ This is a great form and equal or better than standard

PPM

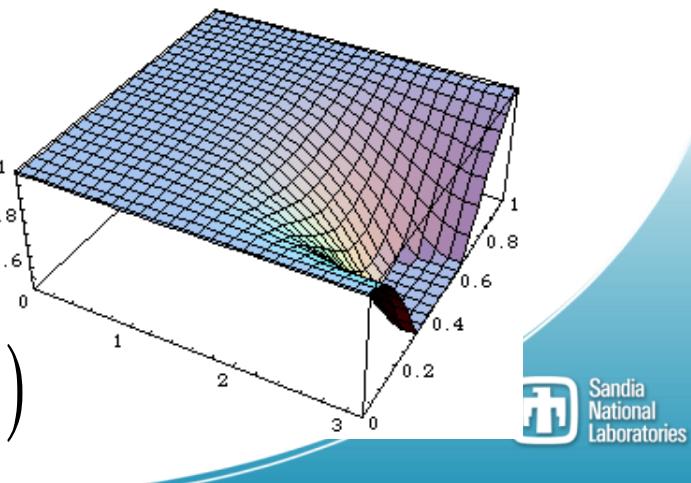
$$A \approx 1 + \left( -\frac{c}{72} + \frac{c^2}{36} - \frac{c^3}{36} + \frac{c^4}{72} \right) \theta^4 + O(\theta^6)$$
$$P \approx 1 + \left( \frac{1}{270} - \frac{c}{108} + \frac{c^3}{108} - \frac{c^4}{270} \right) \theta^4 + O(\theta^6)$$



PPM  
Errors  
For  
Comparison

$$A \approx 1 + \left( -\frac{c^2}{24} + \frac{c^3}{12} - \frac{c^4}{24} \right) \theta^4 + O(\theta^6)$$

$$P \approx 1 + \left( -\frac{1}{30} + \frac{c}{12} - \frac{c^3}{12} + \frac{c^4}{30} \right) \theta^4 + O(\theta^6)$$



# Extensions from Van Leer-V could be even better I will call it Van Leer-VII

- Fifth order – interpolate using the three cell averages and two edge values (analyzed next)

$$P_j(\theta) = P_0 + P_1\theta + P_2\theta^2 + P_3\theta^3 + P_4\theta^4$$

$$\frac{1}{-C} \int_{1/2}^{1/2-C} P(\theta) d\theta = \bar{U}_{j+1/2} = P_0 + P_1\left(\frac{1}{2} - \frac{C}{2}\right) + P_2\left(\frac{1}{4} - \frac{C}{2} + \frac{C^2}{3}\right) + P_3\left(\frac{1}{8} - \frac{3C}{4} + \frac{C^2}{2} - \frac{C^3}{4}\right) + P_4\left(\frac{1}{16} - \frac{C}{4} + \frac{C^2}{2} - \frac{C^3}{2} - \frac{C^4}{5}\right)$$

$$\frac{1}{-C} \int_{1/2}^{1/2-C} \frac{\partial P}{\partial \theta}(\theta) d\theta = P_1 + P_2\left(1 - C\right) + P_3\left(\frac{3}{4} - \frac{3C}{2} + C^2\right) + P_4\left(\frac{1}{2} - \frac{3C}{2} + 2C^2 - C^3\right)$$

- Similar to a method introduced by Xiang & Shu
- Fifth order WENO – could develop WENO versions of this scheme.
- Multidimensional extensions would be interesting with cell-centered Lagrangian.

# Van Leer VII Polynomial Coefficients

□ All the details:

$$\mathbf{P}_j(\theta) = \mathbf{P}_0 + \mathbf{P}_1\theta + \mathbf{P}_2\theta^2 + \mathbf{P}_3\theta^3 + \mathbf{P}_4\theta^4$$

$$\mathbf{P}_0 = \mathbf{U}_j^n - \frac{1}{12}\mathbf{P}_2 + \frac{1}{80}\mathbf{P}_4$$

$$\mathbf{P}_1 = \frac{5}{4}\mathbf{U}_{j+1/2}^n - \frac{5}{4}\mathbf{U}_{j-1/2}^n - \frac{1}{8}\mathbf{U}_{j+1}^n + \frac{1}{8}\mathbf{U}_{j-1}^n$$

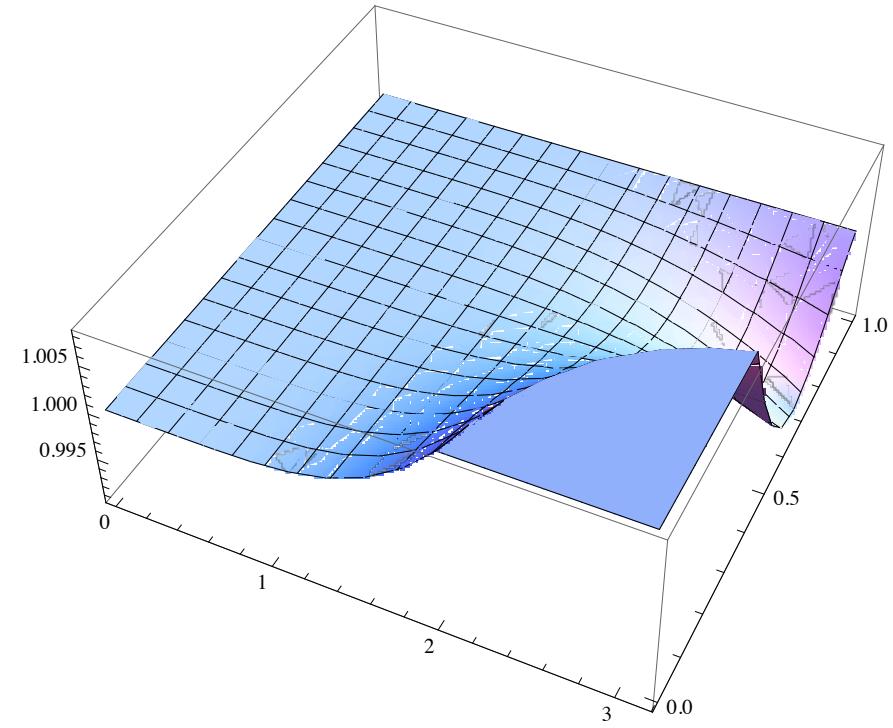
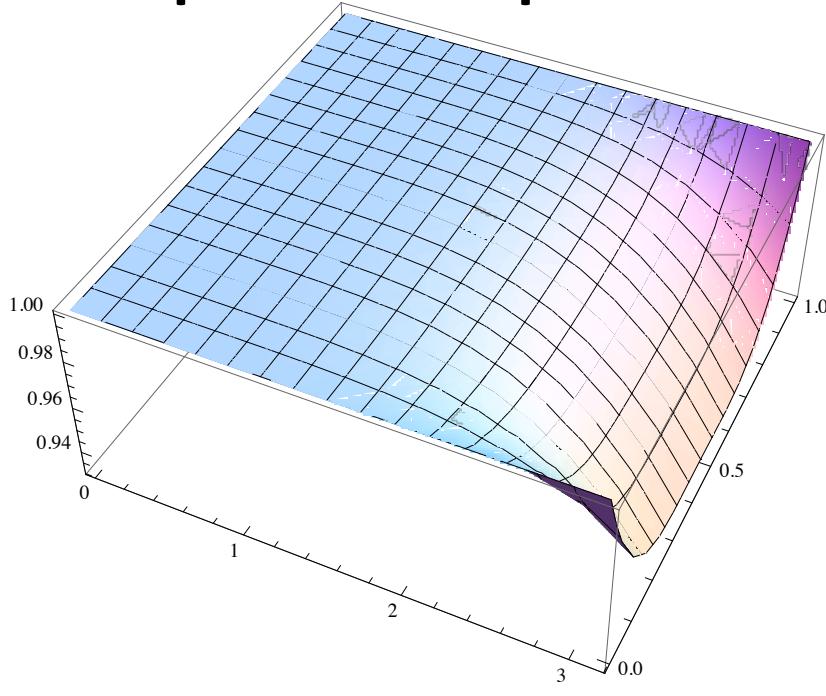
$$\mathbf{P}_2 = -\frac{1}{8}\mathbf{U}_{j-1}^n + \frac{15}{4}\mathbf{U}_{j+1/2}^n - \frac{29}{4}\mathbf{U}_j^n + \frac{15}{4}\mathbf{U}_{j-1/2}^n - \frac{1}{8}\mathbf{U}_{j+1}^n$$

$$\mathbf{P}_3 = -\frac{1}{2}\mathbf{U}_{j-1}^n - \mathbf{U}_{j+1/2}^n + \mathbf{U}_{j-1/2}^n + \frac{1}{2}\mathbf{U}_{j+1}^n$$

$$\mathbf{P}_4 = \frac{5}{12}\mathbf{U}_{j-1}^n - \frac{5}{2}\mathbf{U}_{j+1/2}^n + \frac{25}{6}\mathbf{U}_j^n - \frac{5}{2}\mathbf{U}_{j-1/2}^n + \frac{5}{12}\mathbf{U}_{j+1}^n$$

# The fifth order version Van Leer-VII has fantastic properties

## □ Amplitude and phase error



## □ Truncation errors are nice (but complex)

$$A \approx 1 + \frac{1}{7200(c^2 - c - 1)} (8c - 10c^2 - 3c^3 + 17c^4 - 13c^5 - 5c^6 + 8c^7 - 2c^8) \theta^6 + O(\theta^8)$$

$$P \approx 1 + \frac{1}{252000(c^2 - c - 1)} (104 - 170c - 223c^2 + 107c^3 + 475c^4 + 63c^5 - 678c^6 + 198c^7) \theta^8$$

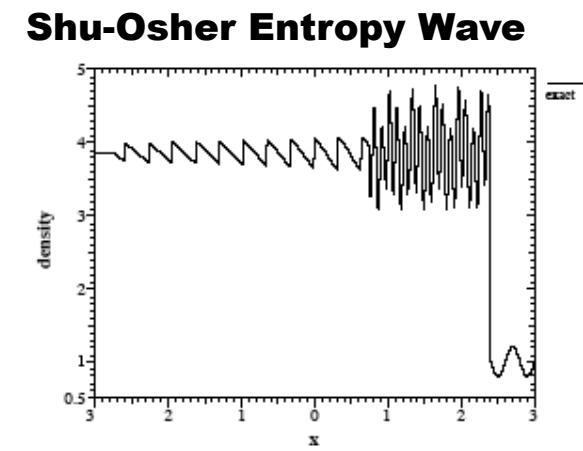
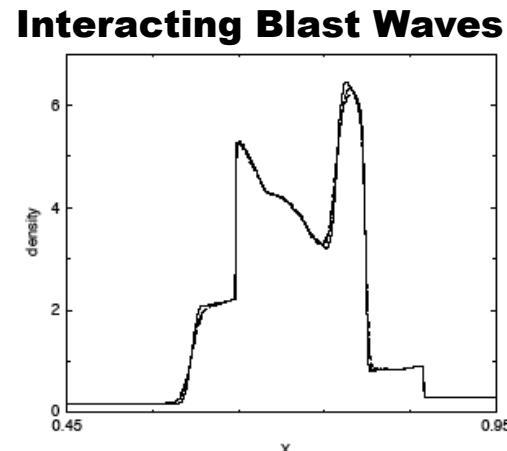
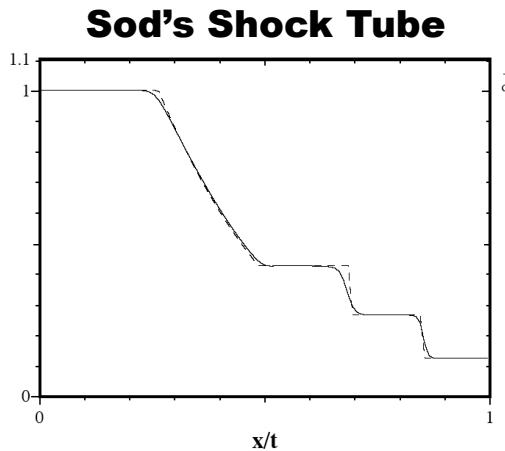
# Conclusions

- ❑ The basis of most remap is the simplest and many the worst scheme from Van Leer's classic 1977 paper
- ❑ Many extensions in resolution are possible for this scheme and its closely related PPM scheme
- ❑ The four remaining schemes have a great deal of promise:
  - ✓ Two are basically discontinuous Galerkin
  - ✓ One is a Hermite scheme
  - ✓ The other is a hybrid finite volume-finite difference method
  - ✓ These methods are accurate and compact.

# A summary of Greenough-Rider's\* results on “off-the-shelf” methods

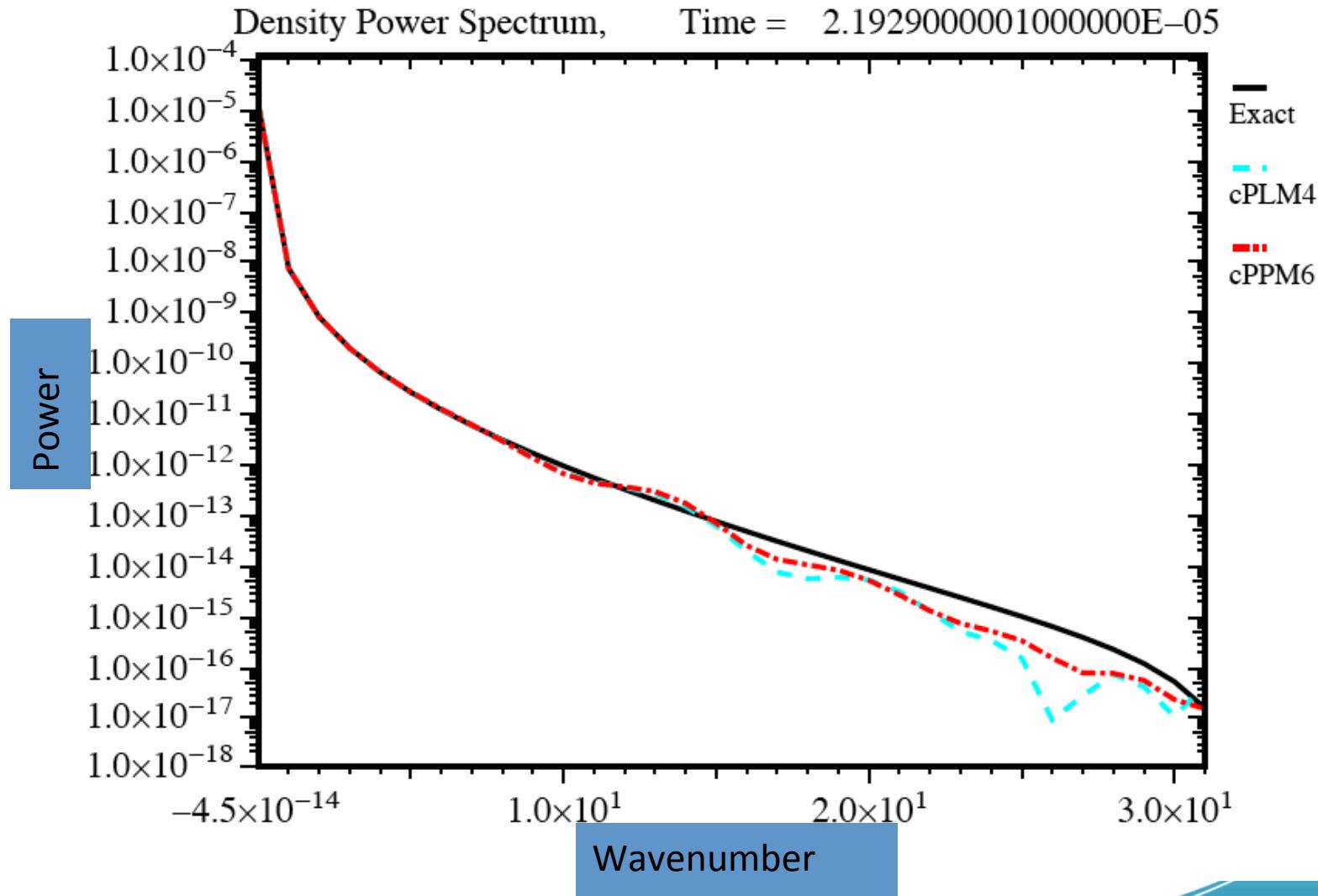
\*Greenough & Rider, *J. Comp. Phys.* 196(1), 259-281, 2004.

- ◆ **WENO5** is more efficient for linear problems
- ◆ **PLM** is more efficient than **WENO5 (6X CPU)** on all nonlinear problems (with discontinuities).
- ◆ The advantage is unambiguous for Sod's shock tube and the Interacting Blast Waves
- ◆ **WENO5** gives better answers for the Shu-Osher problem (same  $\Delta x$ ), but worse than **PLM** at fixed computational expense



# What's the impact? Look at a smooth wave-breaking problem spectrally

## Cuervo 1-D Simulation



# What's the impact? Look at a smooth wave-breaking problem spectrally

## Cuervo 1-D Simulation

