SAND 2013-7318

Reconsidering Remap Methods

William J. Rider

Computational Shock and Multiphysics

Sandia National Laboratories, Albuquerque, NM

E-mail: 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.

NNSA National Nuclear Security Administration

Sandia National Laboratories

Outline

- Lessons from history – an inspiration for this talk
- The core of what is done for remap has a very simple basis
- Classes of new methods found in old places.
- Results of basic accuracy and stability analysis.

Note: I'm going to look at methods associated with advection synonymous with remap. One useful perspective is that these are simply general methods for hyperbolic conservation (balance) laws.

Sandia National Laboratories

There was a symposium in June honoring three CFD greats – Van Leer, Roe and Jameson

- It was a really interesting few days and it provided some perspective on the history of our field.

“Read the Classics!” Don’t just cite them, a way of summarizing Van Leer’s talk there.

COMMUNICATIONS ON PURE AND APPLIED MATHEMATICS, VOL. XIII, 217–237 (1960)

Systems of Conservation Laws*

PETER LAX and BURTON WENDROFF
New York University and Los Alamos Scientific Laboratory

Introduction

In this paper a wide class of difference equations is described for approximating discontinuous time dependent solutions with prescribed initial data of hyperbolic systems of nonlinear conservation laws. Among these schemes we determine the best ones, i.e., those which have the smallest truncation error and in which the discontinuities are confined to a narrow band of 2–3 meshpoints. These schemes are tested for stability and are found to be stable under a mild strengthening of the Courant-Friedrichs-Lewy criterion. Test calculations of one-dimensional flows of compressible fluids with shocks, rarefaction waves and contact discontinuities show excellent agreement with exact solutions. When Lagrange coordinates are used, there is no smearing of interfaces.

The additional terms introduced into the difference scheme for the purpose of keeping the shock transition narrow, when computed specifically for the equations of hydrodynamics, are reminiscent of the artificial viscosity terms introduced by Richtmyer and von Neumann and similar devices considered by other workers in the field. In particular, the methods proposed in this paper have some features similar to the methods proposed and used by Godunov [14].

1. Difference Schemes for Conservation Laws

In this paper we consider systems of conservation laws, i.e., equations of the form

$$u_t = f_x, \tag{1.1}$$

where u is an unknown vector function of x and t with n components, and f a given vector function of u, depending in general nonlinearly on u. When the differentiation on the right side of (1.1) is carried out a quasi-linear system results:

$$u_t = A u_x. \tag{1.1'}$$

*This paper represents results obtained under the sponsorship of the U. S. Atomic Energy Commission, Contract W-7405-ENG 36. Reproduction in whole or in part permitted for any purpose of the United States Government.

A Method for the Numerical Calculation of Hydrodynamic Shocks

J. VonNeumann and R. D. Richtmyer
Institute for Advanced Study, Princeton, New Jersey
(Received September 26, 1949)

The equations of hydrodynamics are modified by the inclusion of additional terms which greatly simplify the procedures needed for stepwise numerical solution of the equations in problems involving shocks. The quantitative influence of these terms can be made as small as one wishes by choice of a sufficiently fine mesh for the numerical integrations. A set of difference equations suitable for the numerical work is given, and the condition that must be satisfied to insure their stability is derived.

I. INTRODUCTION

IN the investigation of phenomena arising in the flow of a compressible fluid, it is frequently desirable to solve the equations of fluid motion by stepwise numerical procedures, but the work is usually severely complicated by the presence of shocks. The shocks manifest themselves mathematically as surfaces on which density, fluid velocity, temperature, entropy and the like have discontinuities; and clearly the partial differential equations governing the motion require boundary conditions connecting the values of these quantities on the two sides of each such surface. The necessary boundary conditions are, of course, supplied by the Rankine-Hugoniot equations, but their application is complicated because the shock surfaces are in motion relative to the network of points in space-time used for the numerical work, and the differential equations and boundary conditions are non-linear. Furthermore, the motion of the surfaces is not known in advance but is governed by the differential equations and boundary conditions themselves. In consequence, the treatment of shocks requires lengthy computations (usually by trial and error) at each step, in time, of the calculation.

We describe here a method for automatic treatment of shocks which avoids the necessity for application of any such boundary conditions. The approximations in it can be rendered as accurate as one wishes, by suitable choice of interval sizes and other parameters occurring in the method. It treats all shocks, correctly and automatically, whenever and wherever they may arise.

The method utilizes the well-known effect on shocks of dissipative mechanisms, such as viscosity and heat conduction.[1] When viscosity is taken into account, for example, the shocks are seen to be smeared out, so that the mathematical surfaces of discontinuity are replaced by thin layers in which pressure, density, temperature, etc. vary rapidly but continuously. Our idea is to introduce (artificial) dissipative terms into the equations so as to give the shocks a thickness comparable to (but preferably somewhat larger than) the spacing of the points of the network. Then the differential equations (more accurately, the corresponding difference equations) may be used for the entire calculation, just as though there were no shocks at all. In the numerical results obtained, the shocks are immediately evident as near-discontinuities that move through the fluid with very nearly the correct speed and across which pressure, temperature, etc. have very nearly the correct jumps.

It will be seen that for the assumed form of dissipation (and, indeed, for many others as well), the Rankine-Hugoniot equations are satisfied, provided the thickness of the shock layers is small in comparison with other physically relevant dimensions of the system. We then consider one way in which the transition from differential to finite-difference equations can be made and we discuss the mathematical stability of these equations. It will be seen that the dissipative terms have the effect of making the stability condition more stringent than the familiar one of Courant, Friedrichs, and Lewy,[2] but not seriously so if the amount of dissipation introduced is only enough to produce a shock thickness comparable with the spatial interval length of the network used.

The method has been applied, so far, only to one-dimensional flows, but it appears to be equally suited to the study of more complicated flows; where, indeed, shock calculations by direct application of the Hugoniot equations would ordinarily be prohibitively difficult, even for rapid, automatic computers.

The discussions which follow are primarily intended to give a complete picture of the ideas and mathematical procedures involved. In some places (Chapter VII, also the essential inferences from some of the material of Chapters IV, V) the mathematical discussions are, however, carried through only with a view to give a complete chain of the necessary procedure, but not with all the detail that rigorous proofs in a primarily mathematical paper would require. The reason for doing this was partly desire to avoid inconvenient length, partly that of not wishing to have to select now the precise degree of generality for the

[1] Lord Rayleigh (Proc. Roy. Soc. A84, 247 (1910)) and G. I. Taylor (Proc. Roy. Soc. A84, 371 (1910)) showed, on the basis of general thermodynamical considerations, that dissipation is necessarily present in shock waves. Later, R. Becker (Zeits. f. Physik 8, 321 (1922)) gave a detailed discussion of the effects of heat conduction and viscosity. Recently, L. H. Thomas (J. Chem. Phys. 12, 449 (1944)) has investigated these effects further in terms of the kinetic theory of gases.

[2] Courant, Friedrichs, and Lewy, Math. Ann. 100, 32 (1928). It is in this important paper that these authors first published their discovery of the conditional stability of the difference-equation integration method for partial differential equations.

COMMUNICATIONS ON PURE AND APPLIED MATHEMATICS, VOL. VII, 159–193 (1954)

Weak Solutions of Nonlinear Hyperbolic Equations and Their Numerical Computation

By PETER D. LAX
New York University

Introduction

This paper describes a finite difference scheme for the calculation of *time dependent* one-dimensional compressible fluid flows containing *strong shocks*. This method is closely related to one proposed by J. von Neumann and modified more recently by him and R. D. Richtmyer (see [13]), inasmuch as the path of the shock is *not* regarded as an interior boundary.* The novel feature of the method described here is the use of the *conservation form* of the hydrodynamic equations and, to a lesser extent, the particular way of differencing the equations.

Although the method was designed to deal with hydrodynamic problems, it can be used to construct solutions of discontinuous initial value problems for any hyperbolic system of first order nonlinear conservation laws (to be defined below) in any number of space variables. The evidence for the convergence of the method is a number of calculations carried out on high speed computing machines that show every sign of convergence. Although the flows calculated so far all belong to a somewhat special class, I fully believe that the method will reproduce the most general type of flow. The question of *accuracy* of the approximate solution with a given mesh-size, specifically the detrimental effect of *contact discontinuities* on accuracy, is discussed at the end of Section 1.

In addition to the numerical evidence, I succeeded in proving the convergence of the scheme for arbitrary bounded measurable initial data, for the single conservation law

$$u_t - [\log(a + be^{u})]_x = 0,$$

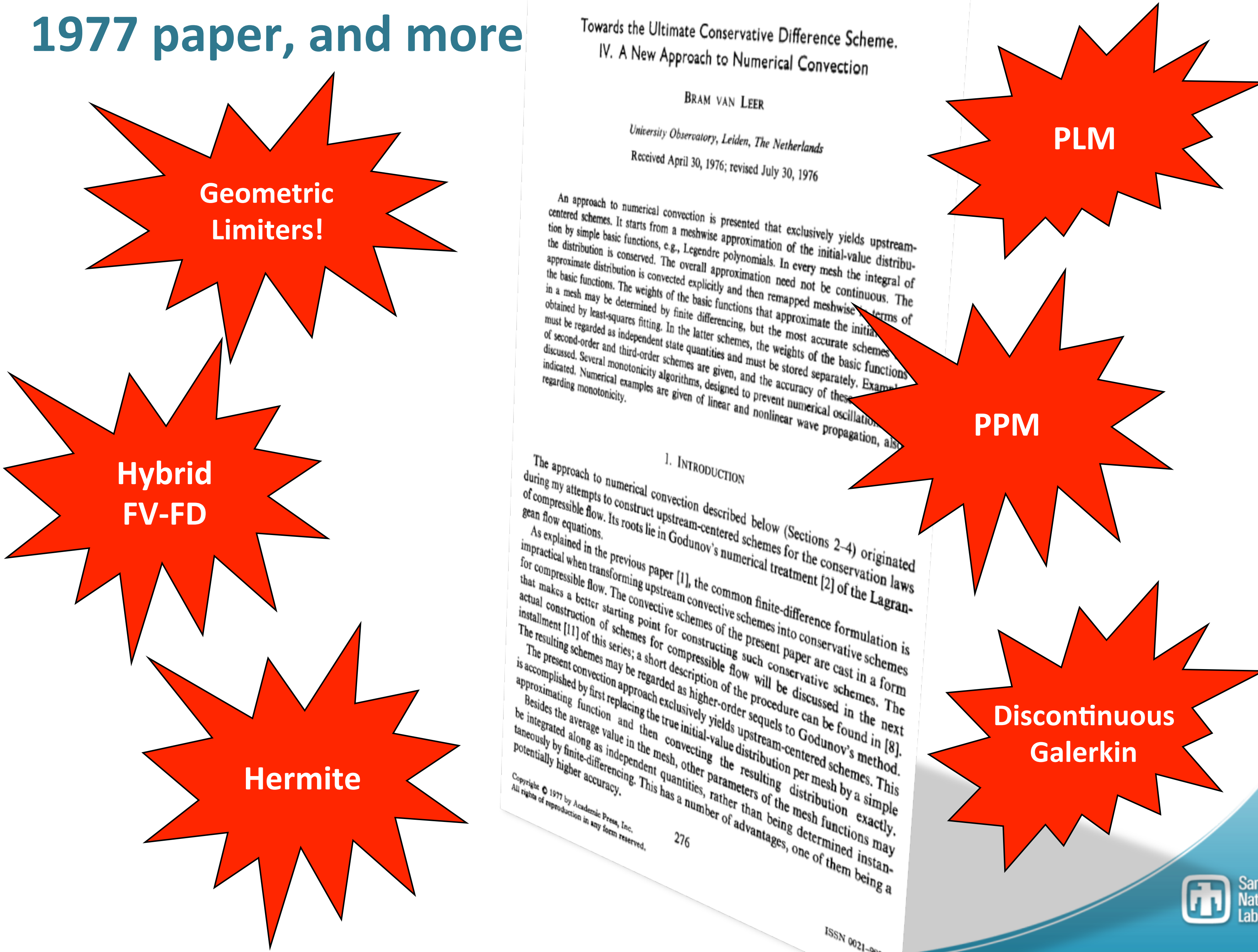
a and b being arbitrary positive constants (or even functions depending on x and t). The proof, modeled after a procedure of E. Hopf, see [8], will be published in a separate note.

For the discussion of the difference scheme presented here I found it useful to develop the theory of weak solutions of nonlinear conservation laws a little more systematically than customary. The theory and the numerical evidence supporting it is presented in Section 1. Section 2 contains some remarks, plus

*Added in proof: See also Ludford, Polachek and Seeger, [18], who employ a linear viscosity term but one which is artificially large. The difference scheme employed in [18] is implicit and is solved by iteration. The difference equations are centered in time.

Sandia National Laboratories

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


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

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

BRAM VAN LEER

University 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 every mesh the integral of the distribution is conserved. The overall approximation need not be continuous. The approximate distribution is convected explicitly and then remapped meshwise in terms of the basic functions. The weights of the basic functions that approximate the initia in a mesh may be determined by finite differencing, but the most accurate schemes obtained by least-squares fitting. In the latter schemes, the weights of the basic functions must be regarded as independent state quantities and must be stored separately. Exampl of second-order and third-order schemes are given, and the accuracy of thes discussed. Several monotonicity algorithms, designed to prevent numerical oscillatio indicated. Numerical examples are given of linear and nonlinear wave propagation, als regarding monotonicity.

1. INTRODUCTION

The approach to numerical convection described below (Sections 2–4) originated during my attempts to construct upstream-centered schemes for the conservation laws of compressible flow. Its roots lie in Godunov's numerical treatment [2] of the Lagrangean flow equations.

As explained in the previous paper [1], the common finite-difference formulation is impractical when transforming upstream convective schemes into conservative schemes for compressible flow. The convective schemes of the present paper are cast in a form that makes a better starting point for constructing such conservative schemes. The actual construction of schemes for compressible flow will be discussed in the next installment [11] of this series; a short description of the procedure can be found in [8]. The resulting schemes may be regarded as higher-order sequels to Godunov's method.

The present convection approach exclusively yields upstream-centered schemes. This is accomplished by first replacing the true initial-value distribution per mesh by a simple approximating function and then convecting the resulting distribution exactly. Besides the average value in the mesh, other parameters of the mesh functions may be integrated along as independent quantities, rather than being determined instantaneously by finite-differencing. This has a number of advantages, one of them being a potentially higher accuracy.

ISSN 0021-9

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 that 1977 paper, which also includes six different methods (of three basic types).
- ❑We will look at this paper and the method's contained therein for opportunities that we might have missed.
  - ✓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
  - ✓Scheme VI is not described in detail in the '77 paper

Sandia National Laboratories

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 scheme)
  - ✓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
  - ✓Used for ALEGRA these days in the three point form.
- ❑V – Piecewise parabolic with evolving edge values
  - ✓Reintroduced as the PPM-L scheme
- ❑VI – Piecewise parabolic DG
  - ✓Woodward's PPB scheme

Sandia National Laboratories

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

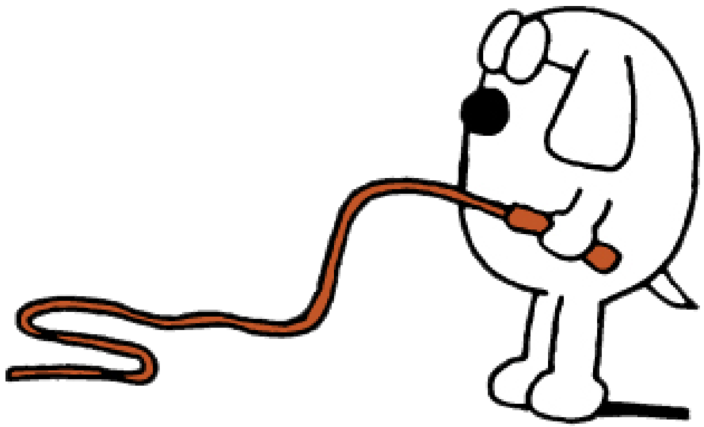
- Before taking the time to code a scheme one should know exactly what to expect from the method. It also makes a good time to state the design principles:

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

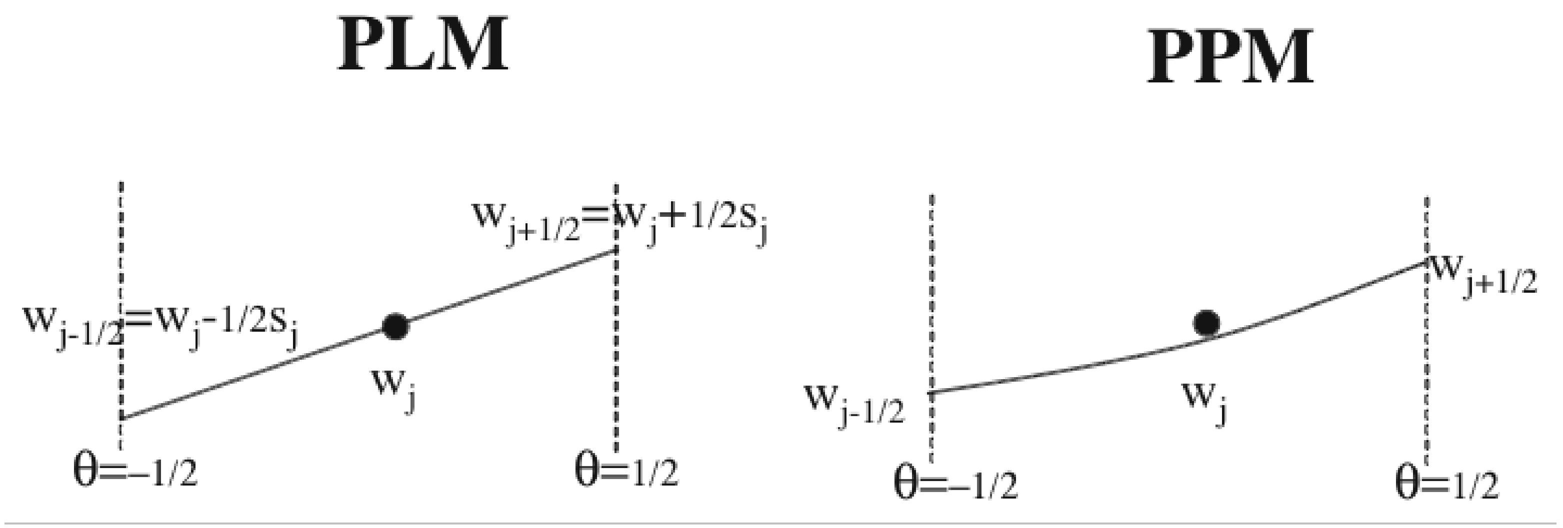
- **Provide an introduction to *high-resolution* schemes including some ideas about motivation and implementation**

  - ✓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)

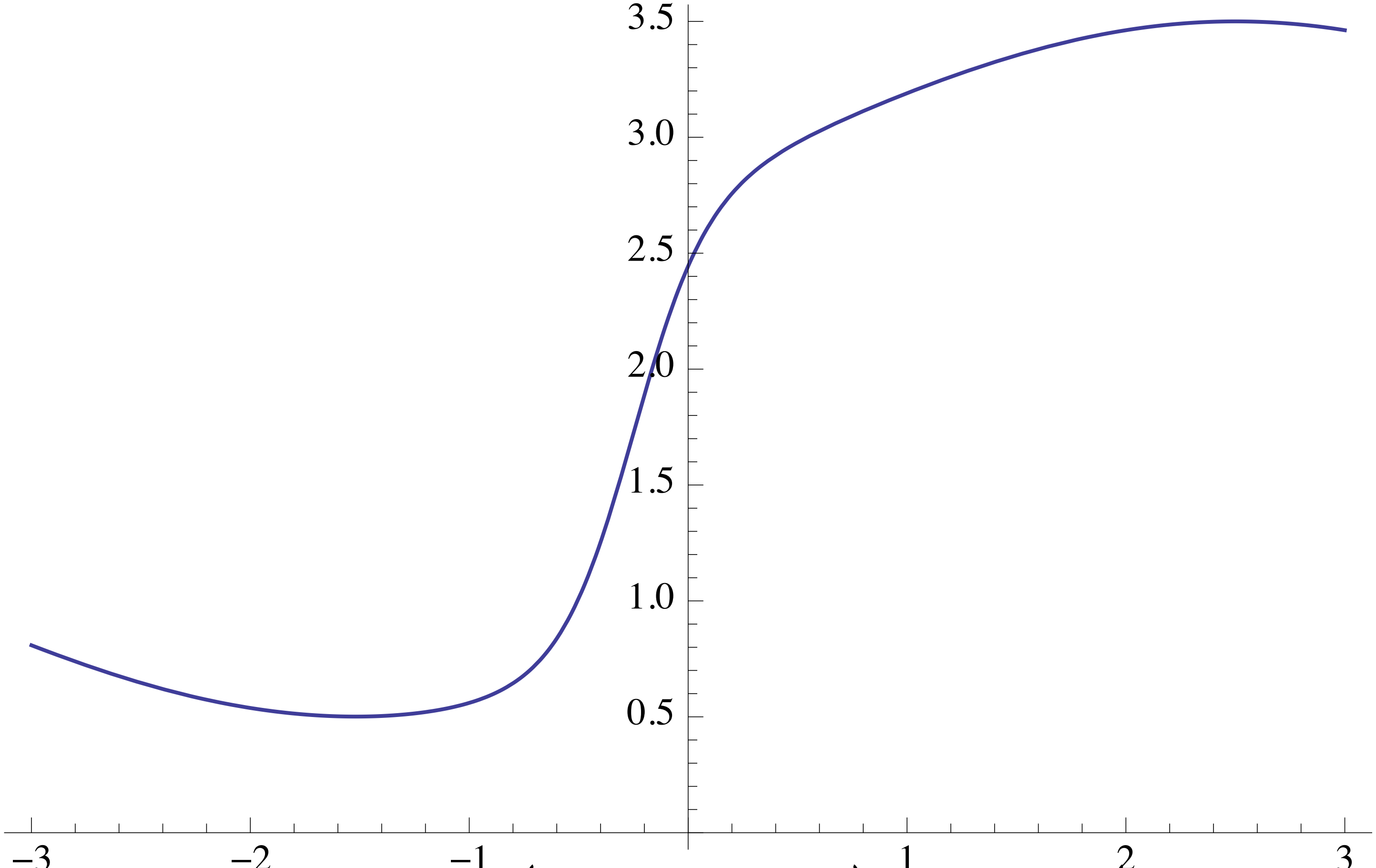
Now we will spend time looking at linear and parabolic reconstruction procedures.



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

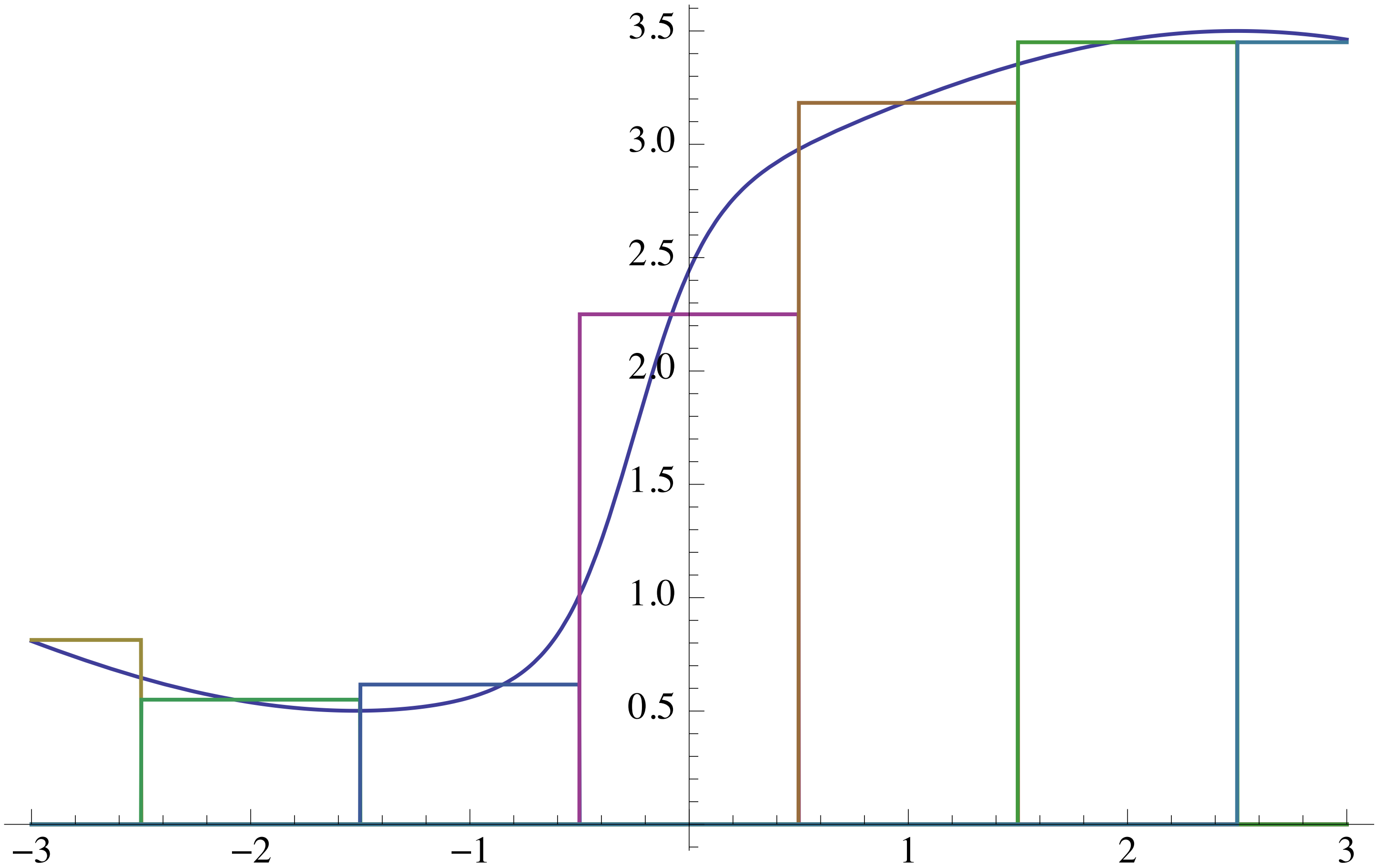
How does accuracy change with polynomial order and approach?

- **We will move through a series of polynomial descriptions of different type and order looking at interpolatory accuracy.**



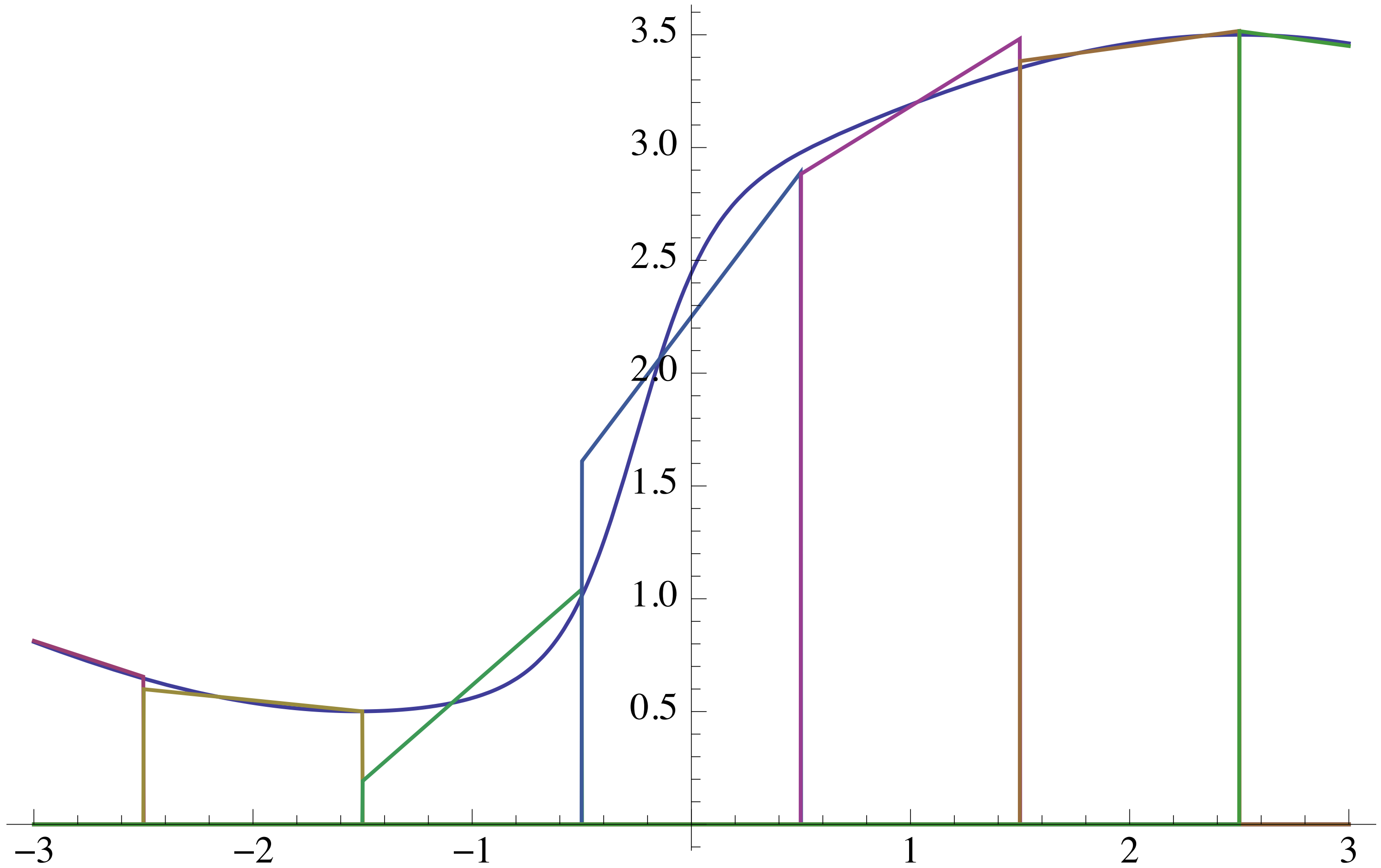
$$f(x) = 2 + \tfrac{1}{2}\sin\left(\tfrac{1}{4}\pi\left(x - \tfrac{1}{2}\right)\right) + \tanh\left(3\left(x + \tfrac{1}{4}\right)\right)$$

Piecewise Constant is the basis of first-order Godunov or donor cell



Integrated Error = 0.882

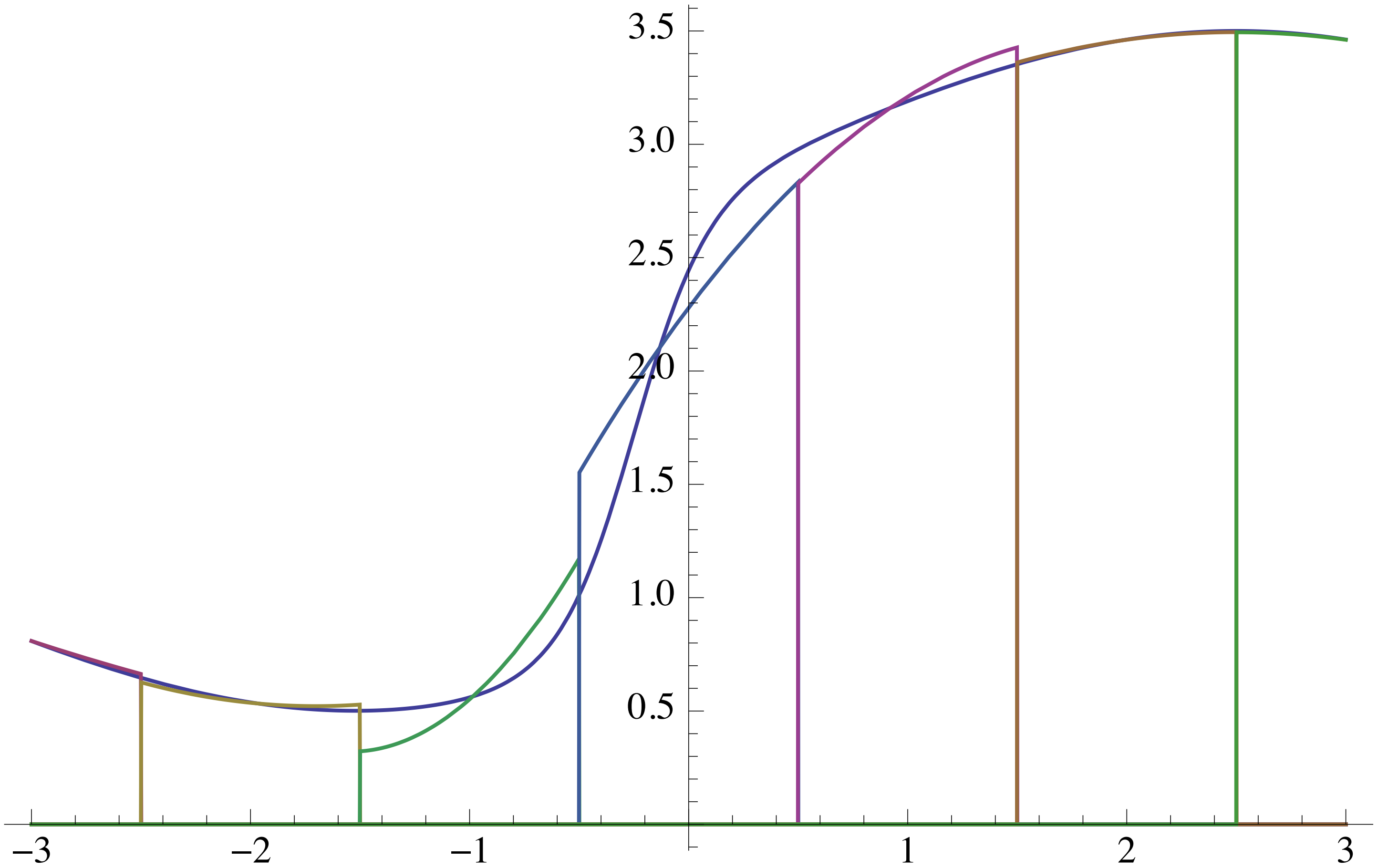
Piecewise linear is the basis of second-order methods, and remap (Scheme I).



Integrated Error = 0.448

We are going to examine a couple of different parabolic reconstructions (Scheme IV).

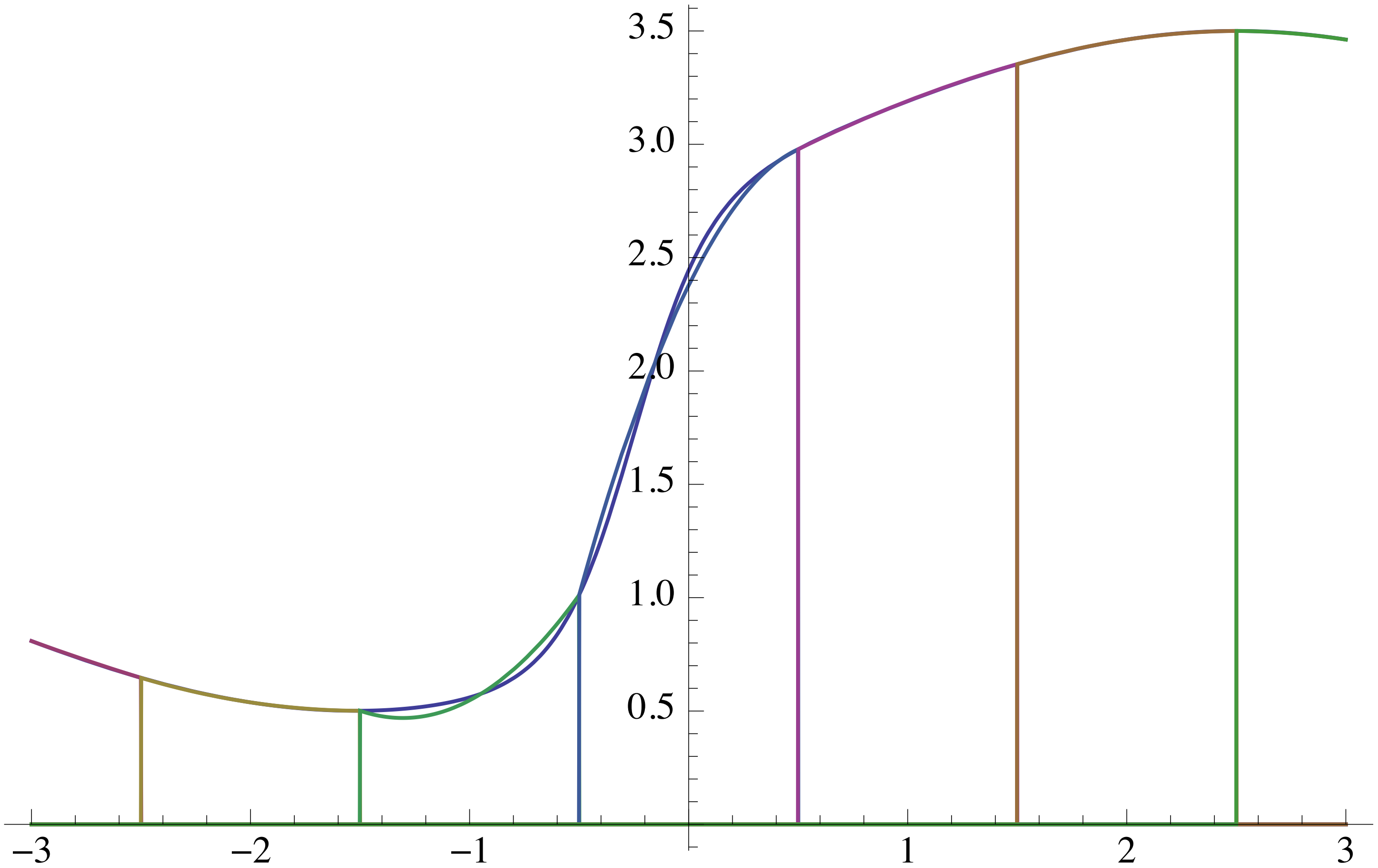
$$u_{j-1} = \int_{j-3/2}^{j-1/2} P(\theta)d\theta; u_j = \int_{j-1/2}^{j+1/2} P(\theta)d\theta; u_{j+1} = \int_{j+1/2}^{j+3/2} P(\theta)d\theta$$



Integrated Error = 0.427

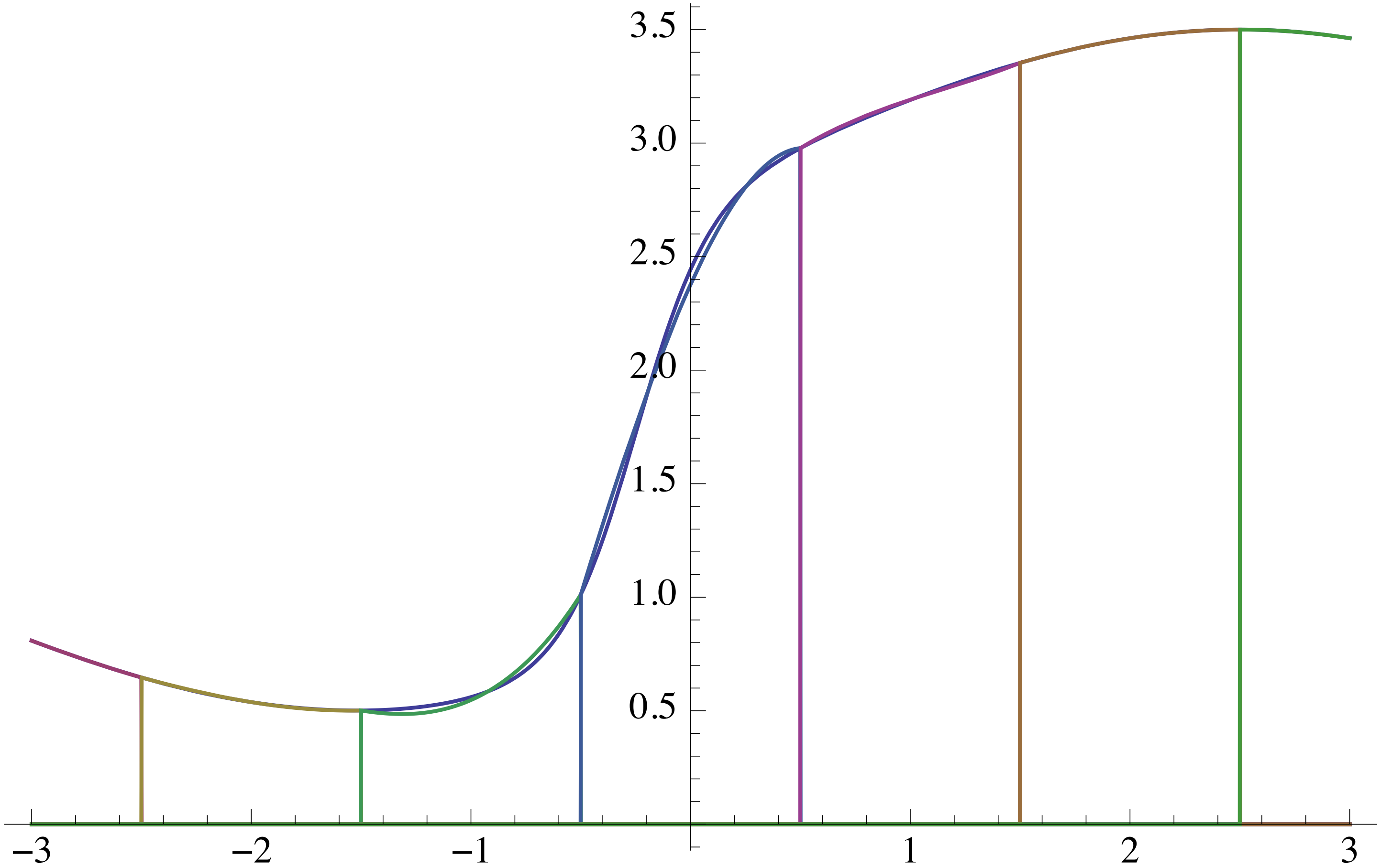
A differently constructed parabola is much better (Scheme V)

$$u_j = \int_{j-1/2}^{j+1/2} P(\theta)d\theta; u_{j-1/2} = P(-1/2); u_{j+1/2} = P(1/2)$$



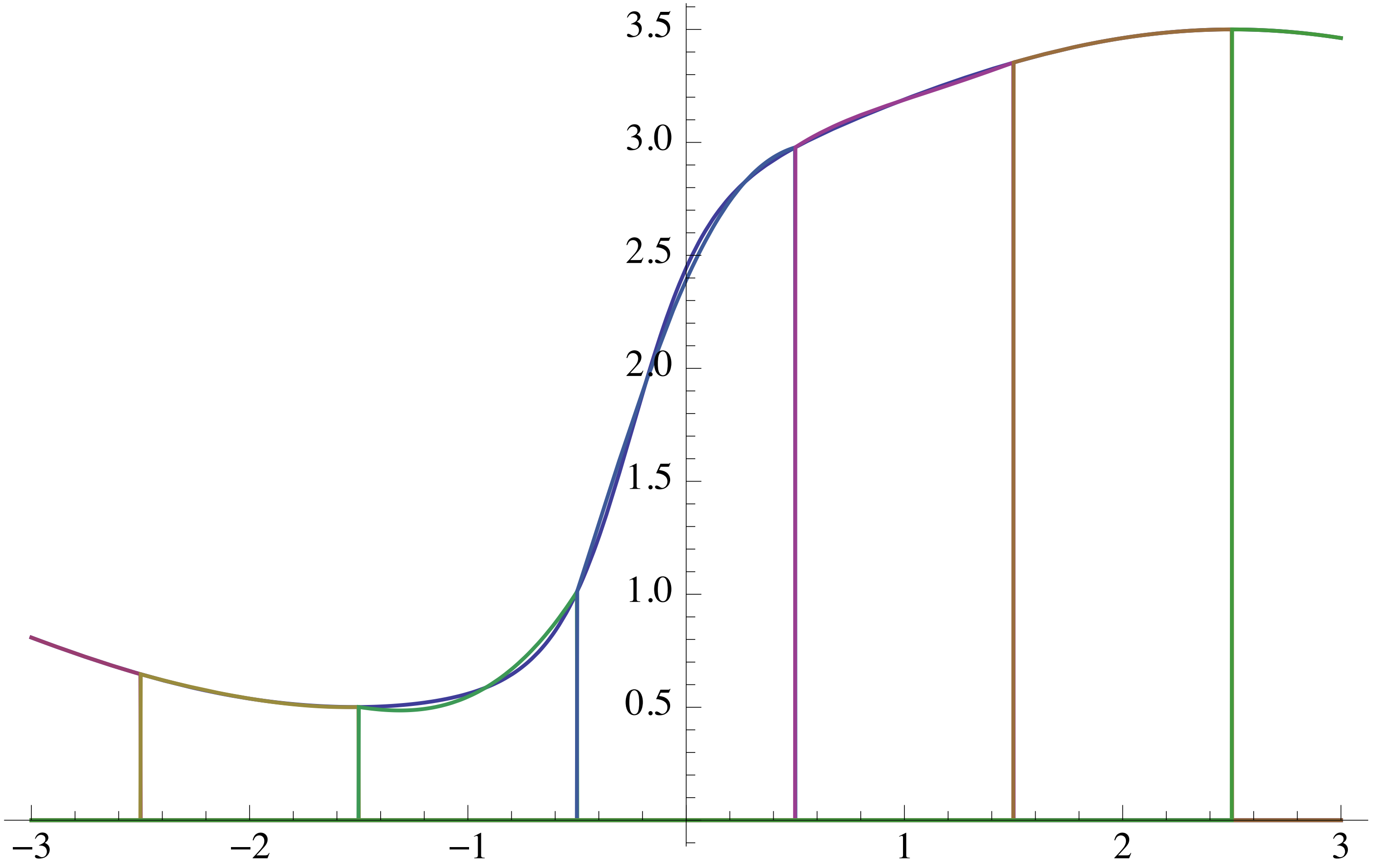
Integrated Error = 0.080

A cubic reconstruction is better still



Integrated Error = 0.065

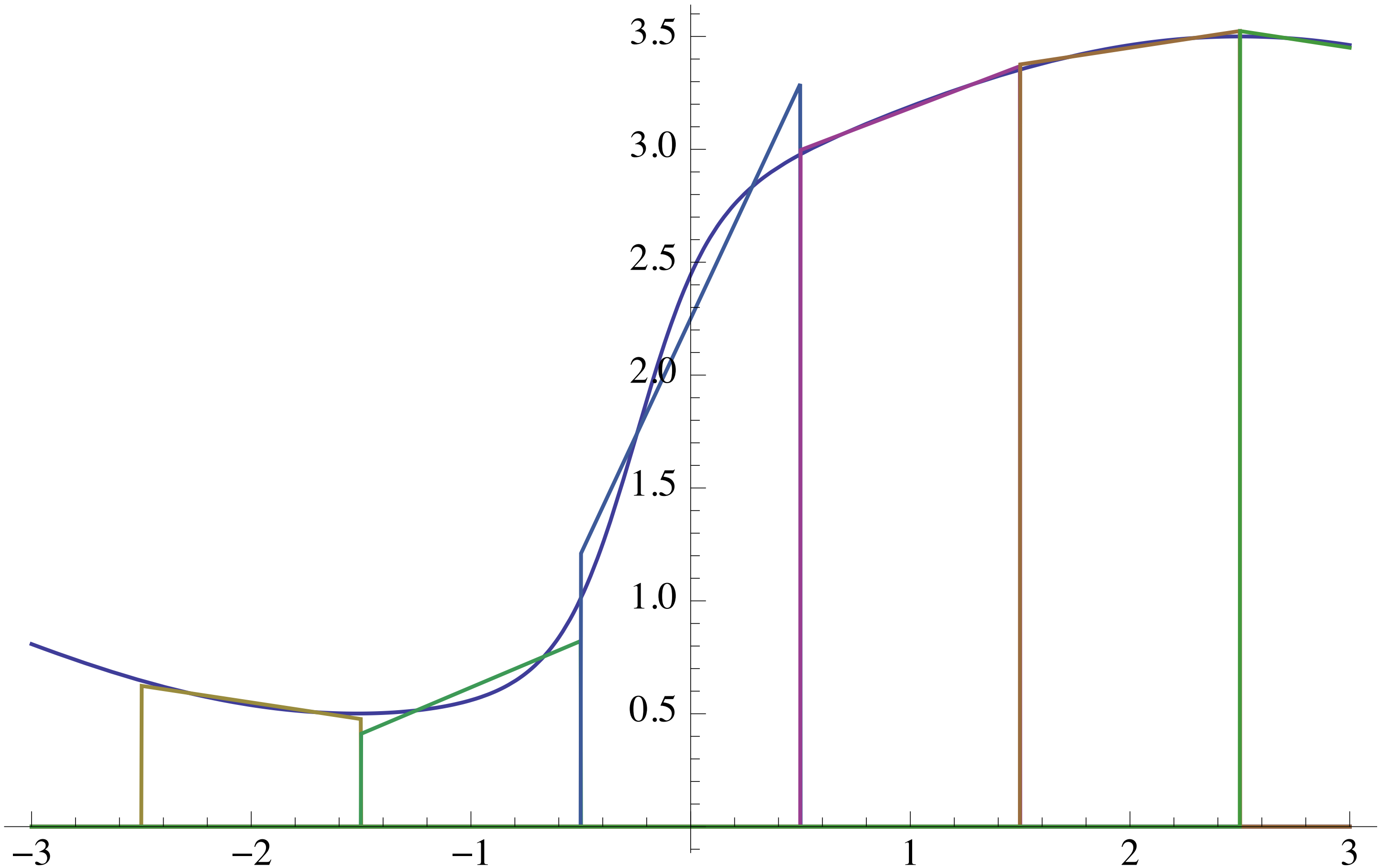
…and a quartic reconstruction improves a bit more



Integrated Error = 0.058

Just a note about moment-based methods (i.e., discontinuous Galerkin, Scheme III) – 1st moment

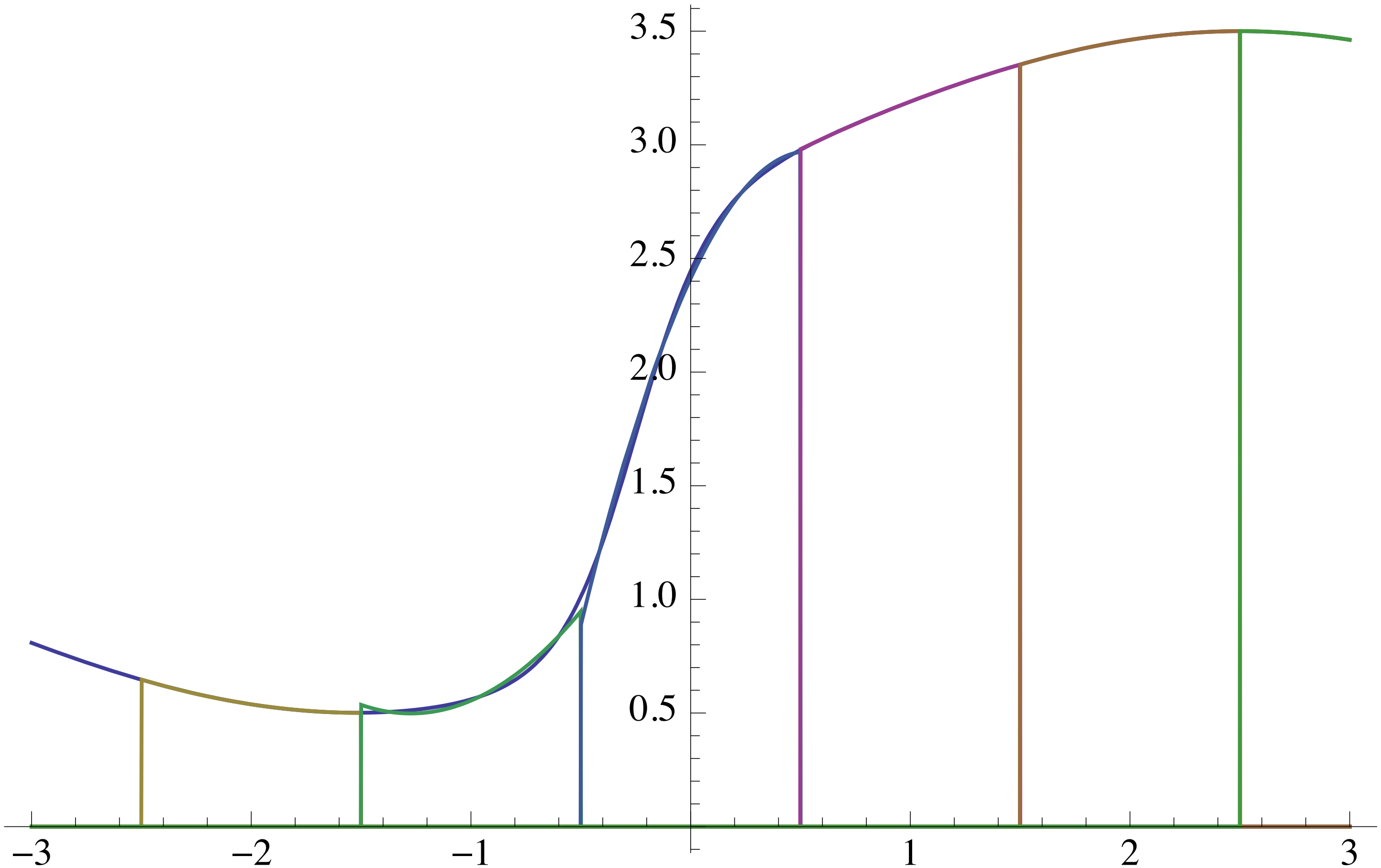
$$S_j = 12\int_{j-1/2}^{j+1/2} f(x)\,x\,dx$$



Integrated Error = 0.208

Just a note about moment-based methods (i.e., discontinuous Galerkin, Scheme VI) – 2nd moment

$$C_j = 80\int_{j-1/2}^{j+1/2} f(x)x^2 dx$$



Integrated Error = 0.042

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 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)- uses limiters and not our focus here

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,

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

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

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

$$\boxed{\mathbf{C}=\frac{\lambda\Delta t}{\Delta x}}$$ Courant Number

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,

$$\mathbf{S}_j^n = \frac{8\left(\mathbf{U}_{j+1}^n - \mathbf{U}_{j-1}^n\right) - \left(\mathbf{U}_{j+2}^n - \mathbf{U}_{j-2}^n\right)}{12}$$

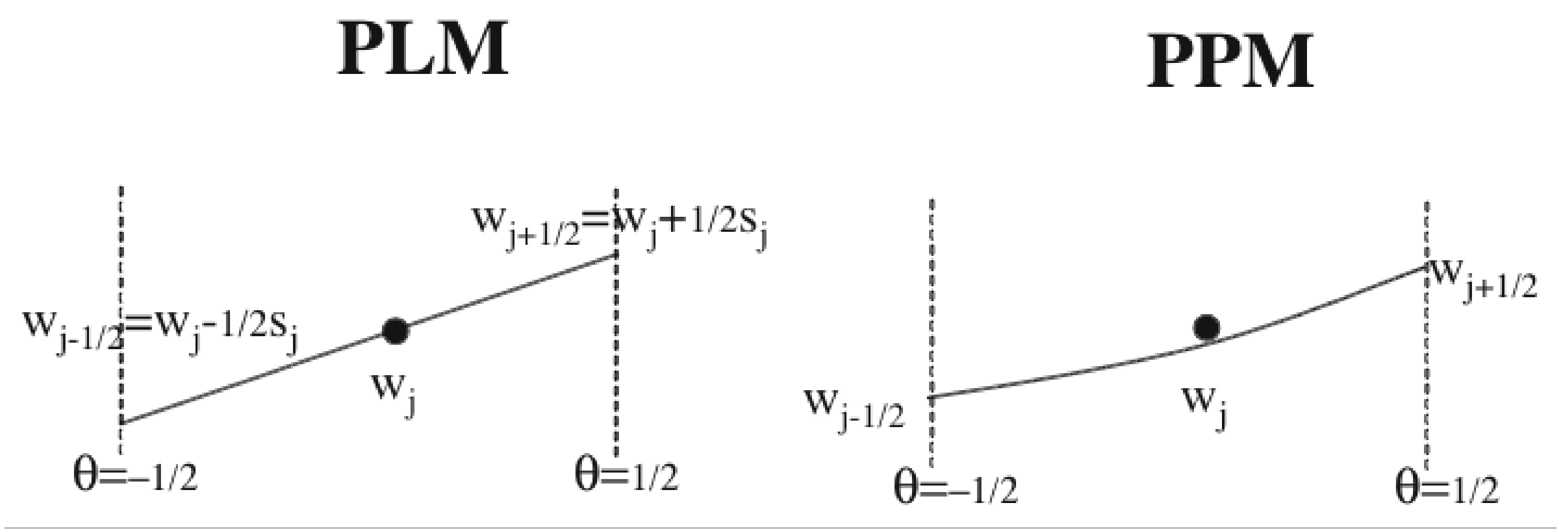
  - ✓ Or a sixth-order choice

$$\mathbf{S}_j^n = \frac{45\left(\mathbf{U}_{j+1}^n - \mathbf{U}_{j-1}^n\right) - 9\left(\mathbf{U}_{j+2}^n - \mathbf{U}_{j-2}^n\right) + \left(\mathbf{U}_{j+3}^n - \mathbf{U}_{j-3}^n\right)}{60}$$

  - ✓ Or whatever you like…
  - ✓ It can be used in conjunction with the limiter

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

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



- ◆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,**

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

$$\mathbf{P}_0 = \mathbf{U}_j^n - \tfrac{1}{12}\mathbf{P}_2; \mathbf{P}_1 = \mathbf{U}_{j+1/2}^n - \mathbf{U}_{j-1/2}^n; \mathbf{P}_2 = 3\left(\mathbf{U}_{j+1/2}^n - 2\mathbf{U}_j^n + \mathbf{U}_{j-1/2}^n\right)$$

- **Several key requirements are necessary for this to useful:**

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

✓ **Accuracy** $\quad \mathbf{U}_{j\pm1/2} = \mathbf{U}\left(x_{j\pm1/2}\right) + \mathcal{O}\left(\Delta x^n\right)$

✓ **Boundedness (monotonicity)-not today.**

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,

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

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

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

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

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

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

$$\mathbf{U}^n_{j+1/2} = \tfrac{7}{12}\left(\mathbf{U}^n_j + \mathbf{U}^n_{j+1}\right) - \tfrac{1}{12}\left(\mathbf{U}^n_{j-1} + \mathbf{U}^n_{j+2}\right)$$

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

$$\mathbf{U}^n_{j+1/2} = \tfrac{37}{60}\left(\mathbf{U}^n_j + \mathbf{U}^n_{j+1}\right) - \tfrac{8}{60}\left(\mathbf{U}^n_{j-1} + \mathbf{U}^n_{j+2}\right) + \tfrac{1}{60}\left(\mathbf{U}^n_{j-2} + \mathbf{U}^n_{j+3}\right)$$

  - ✓ Or a fifth-order upwind choice

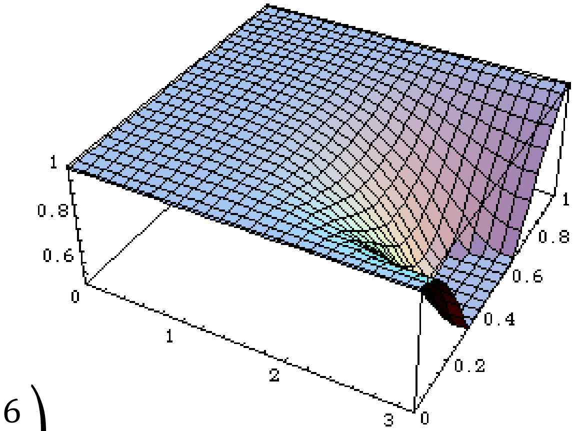
$$\mathbf{U}^n_{j+1/2} = \tfrac{2}{60}\mathbf{U}^n_{j-2} - \tfrac{13}{60}\mathbf{U}^n_{j-1} + \tfrac{47}{60}\mathbf{U}^n_j + \tfrac{27}{60}\mathbf{U}^n_{j+1} - \tfrac{3}{60}\mathbf{U}^n_{j+2}$$

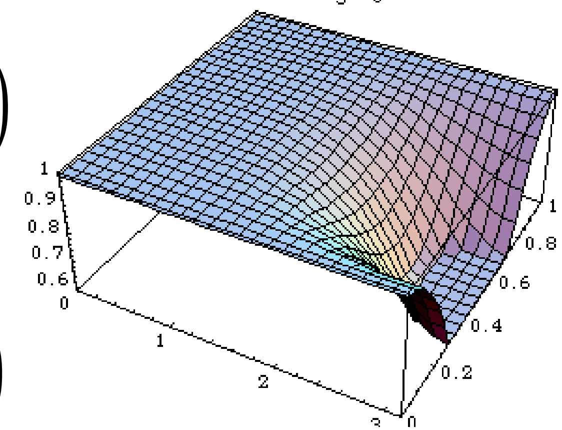
  - ✓ Or whatever you like, a least third-order or its not worth it!

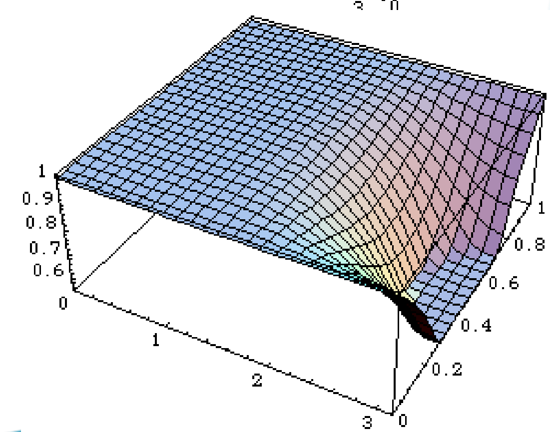
* C&W actually use a special fourth-order method

Scheme Stability & Truncation Error is exceptional

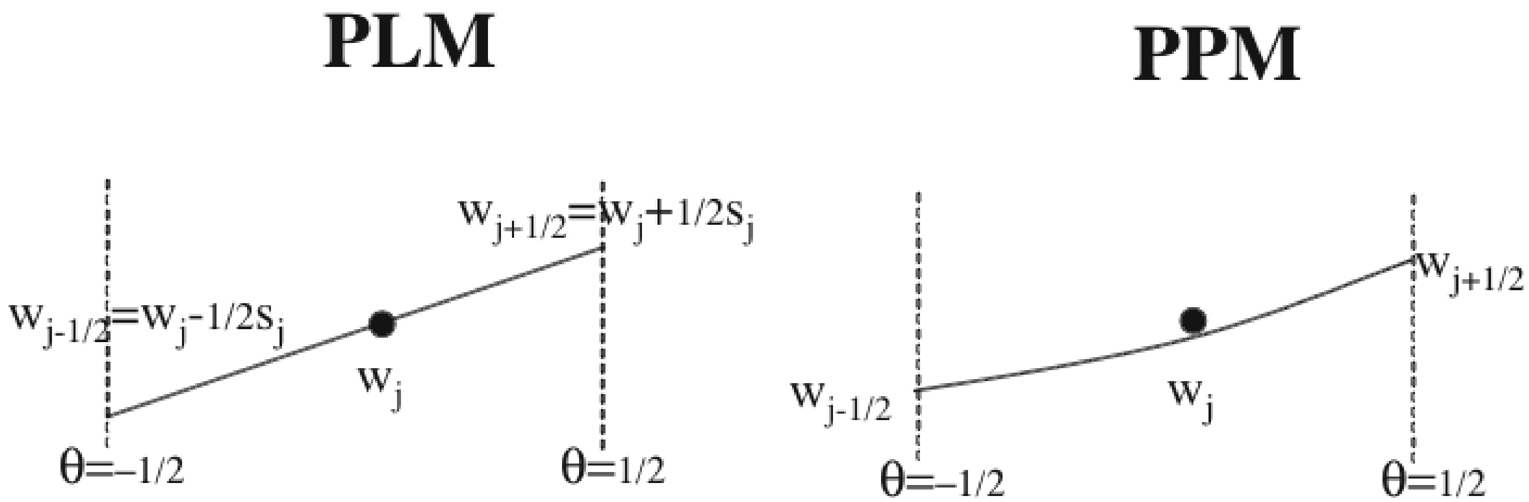
- **Using Fourier analysis:**
  - ✓ All stable to CFL=1
- **Fourth-order truncation error**
  - ✓ Amplitude $$A \approx 1+\left(-\frac{c^2}{24}+\frac{c^3}{12}-\frac{c^4}{24}\right)\theta^4+O\left(\theta^6\right)$$
  - ✓ Phase $$P \approx 1+\left(-\frac{1}{30}+\frac{c}{12}-\frac{c^3}{12}+\frac{c^4}{30}\right)\theta^4+O\left(\theta^6\right)$$
- **Sixth-order truncation error**
  - ✓ Amplitude $$A \approx 1+\left(-\frac{c^2}{24}+\frac{c^3}{12}-\frac{c^4}{24}\right)\theta^4+O\left(\theta^6\right)$$
  - ✓ Phase $$P \approx 1+\left(-\frac{c}{60}+\frac{c^2}{15}-\frac{c^3}{12}+\frac{c^4}{30}\right)\theta^4+O\left(\theta^6\right)$$
- **Seventh-order truncation error**
  - ✓ Amplitude $$A \approx 1+\left(\frac{c}{48}-\frac{c^2}{16}+\frac{c^3}{12}-\frac{c^4}{24}\right)\theta^4+O\left(\theta^6\right)$$
  - ✓ Phase $$P \approx 1+\left(\frac{1}{120}-\frac{c}{24}+\frac{c^2}{12}-\frac{c^3}{12}+\frac{c^4}{30}\right)\theta^4+O\left(\theta^6\right)$$







The next couple of schemes are different



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

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

- 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 $wj_{\pm 1/2}$'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!

Sandia National Laboratories

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,

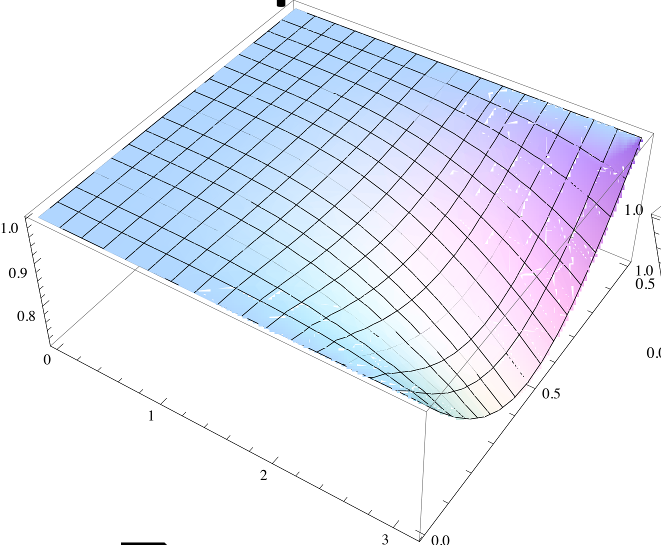
$$U_j^{n+1} = U_j^n - C\left(U_{j+1/2}^{n+1/2} - U_{j-1/2}^{n+1/2}\right) \qquad U_{j+1/2}^{n+1/2} = U_j^n + \tfrac{1}{2}\left(1 - C\right)S_j^n$$

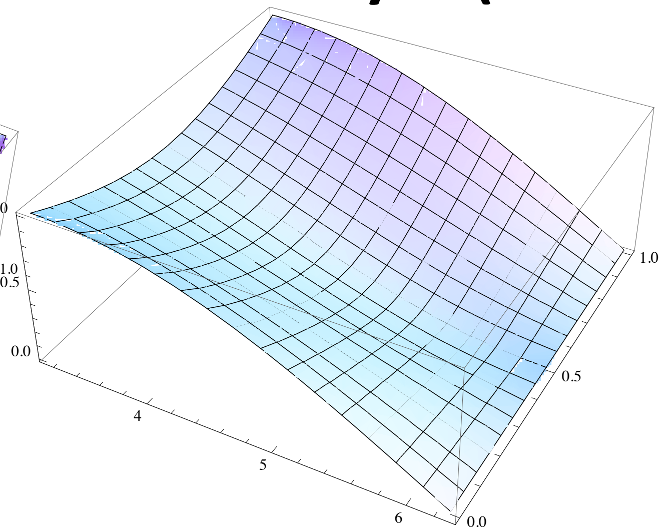
$$S_j^{n+1} = U_{j+1/2}^n - U_{j-1/2}^n - C\left(S_j^n - S_{j-1}^n\right) \qquad U_{j+1/2}^n = U_j^n + \tfrac{1}{2}S_j^n$$

- 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.

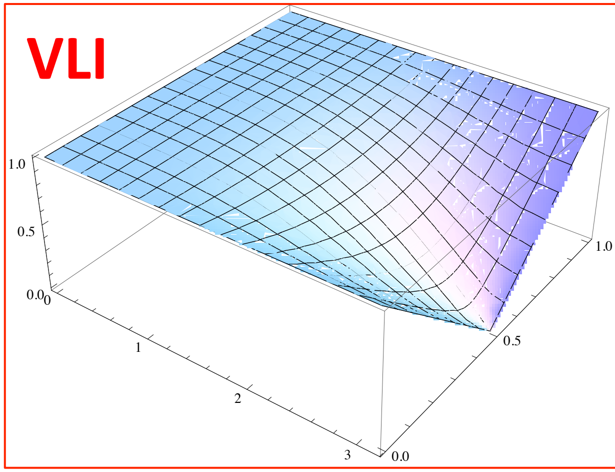
Van Leer II - Properties

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





VLI



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

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

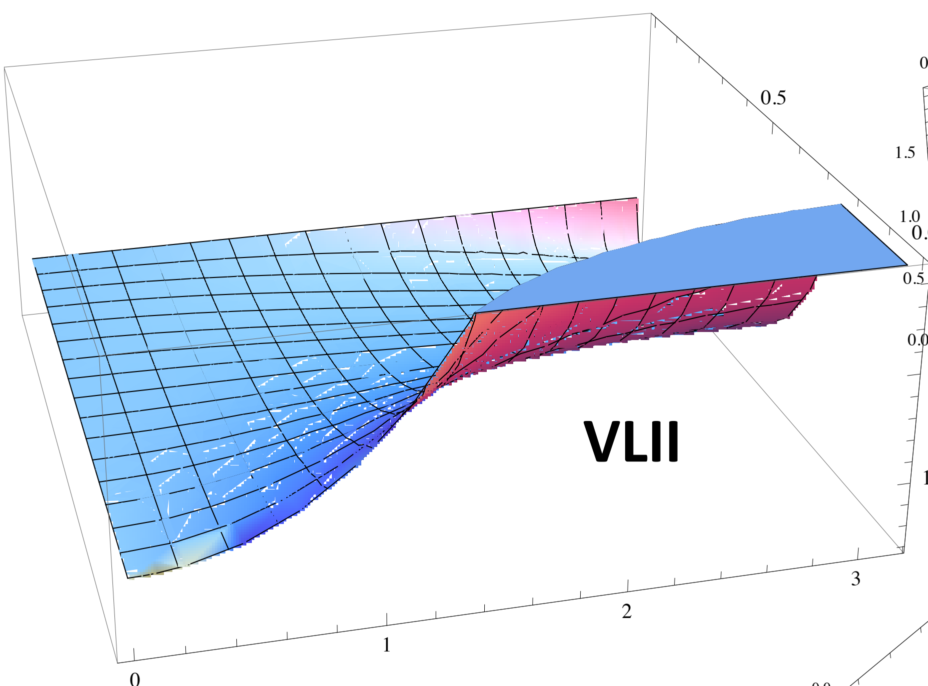
VLI $\boxed{\left(-\frac{C}{8} + \frac{C^2}{4} - \frac{C^3}{4} + \frac{C^4}{8}\right)\theta^4}$

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

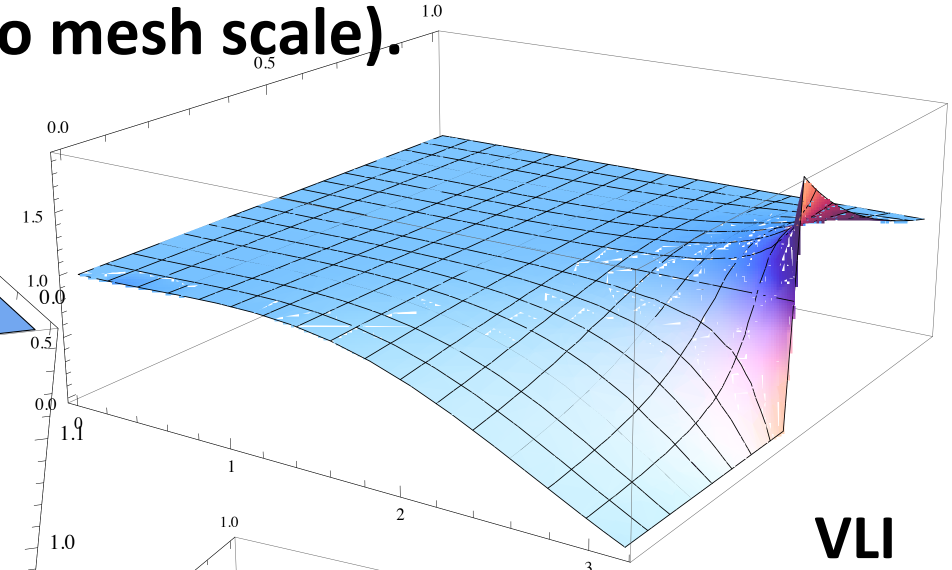
Sandia National Laboratories

VL II Phase Error Plots

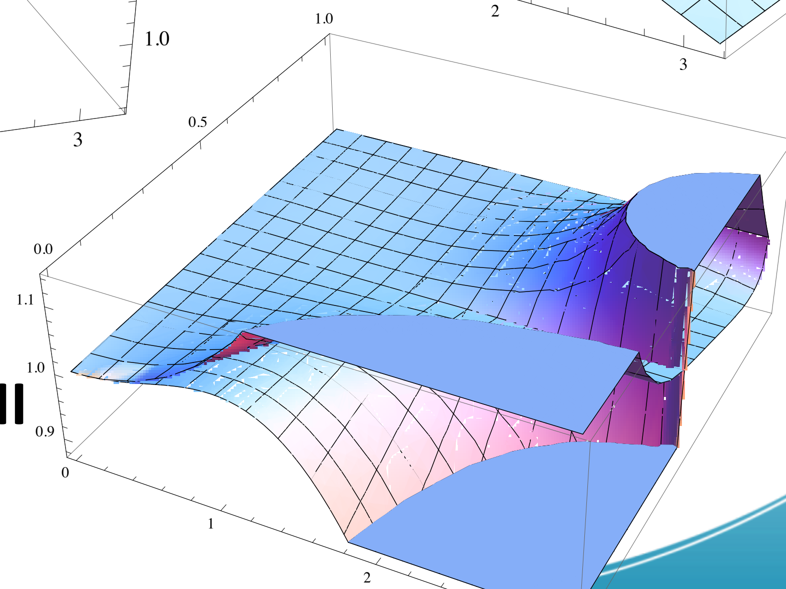
- ❑The phase error show the problems with VLII (at small Courant numbers, at close to mesh scale).



VLII



VLI



Comparing VLI & VLII On the same plot

Van Leer V – Evolved edge values

- ❑This method has largely been ignored until lately.
- ❑Several Authors have reinvented Van Leer's method without realizing it (looking at references).
  - ✓Popov's PPM-L scheme

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

Sergey D. Ustyugov[a], Mikhail V. Popov[a], Alexei G. Kritsuk[b,*], Michael L. Norman[b]

[a] *Keldysh Institute of Applied Mathematics, Miusskaya Sq. 4, 125047 Moscow, Russia*
[b] *University of California, San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0424, USA*

  - ✓Zeng's hybrid differencing (FV-FD method)
  - ✓Eymann and Roe's active flux scheme.
- ❑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

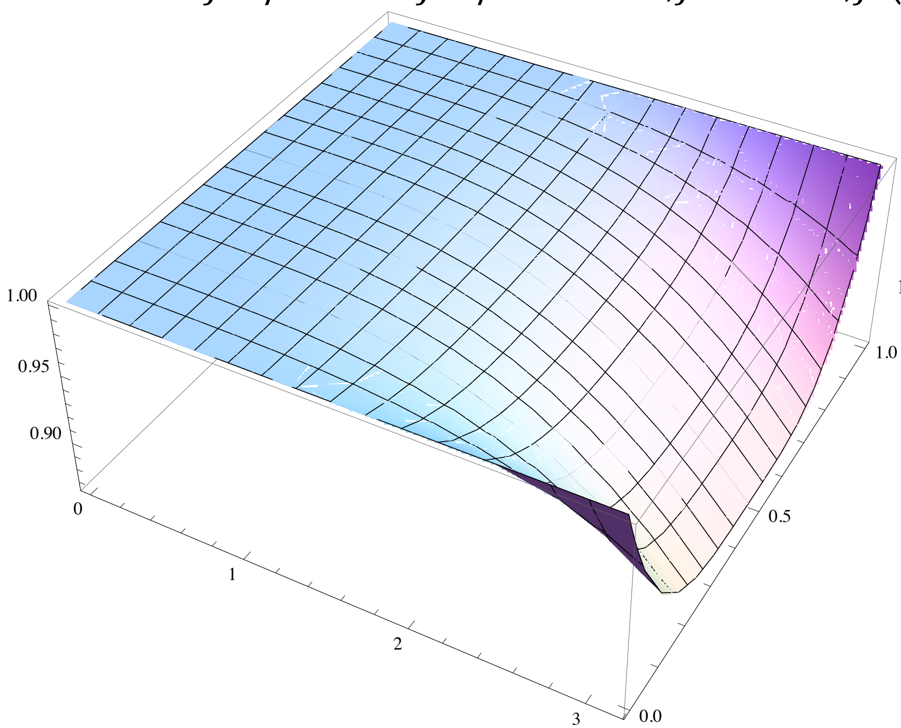
$$U_j^{n+1} = U_j^n - C\left(U_{j+1/2}^{n+1/2} - U_{j-1/2}^{n+1/2}\right)$$

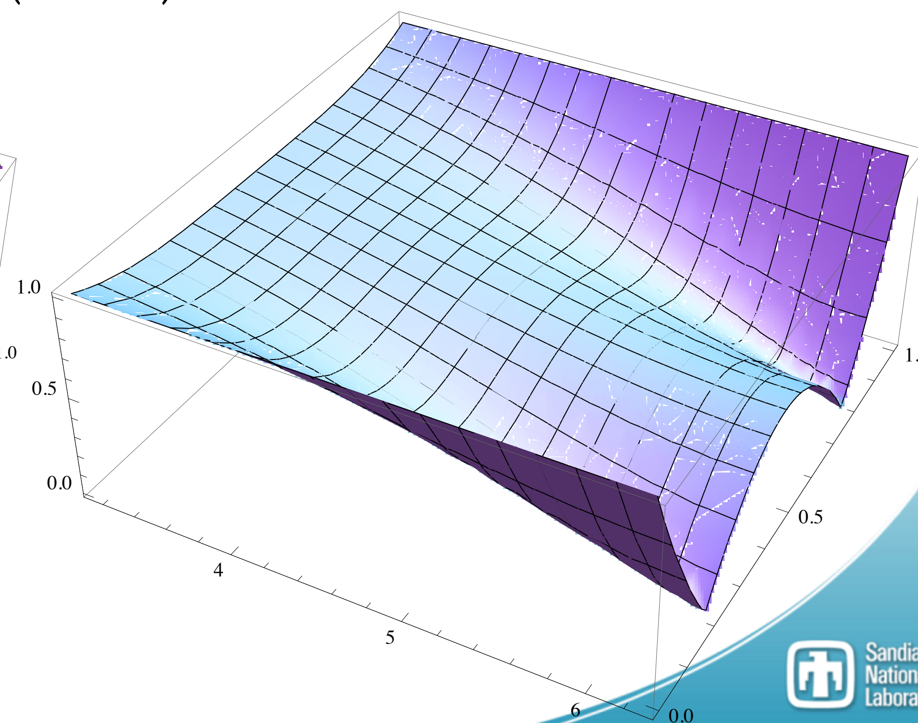
$$U_{j+1/2}^{n+1/2} = P_{0,j}^n + \left(\tfrac{1}{2} - \tfrac{1}{2}C\right)P_{1,j}^n + P_{2,j}^n\left(\tfrac{1}{4} - \tfrac{1}{2}C + \tfrac{1}{3}C^2\right)$$

❑Evolve the edges

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

$$\boxed{P_{1,j}^n - P_{2,j}^n\left(1-C\right) = -\tfrac{1}{C}\int_{1/2}^{1/2-C}\left(\frac{dP}{d\theta}\right)d\theta}$$





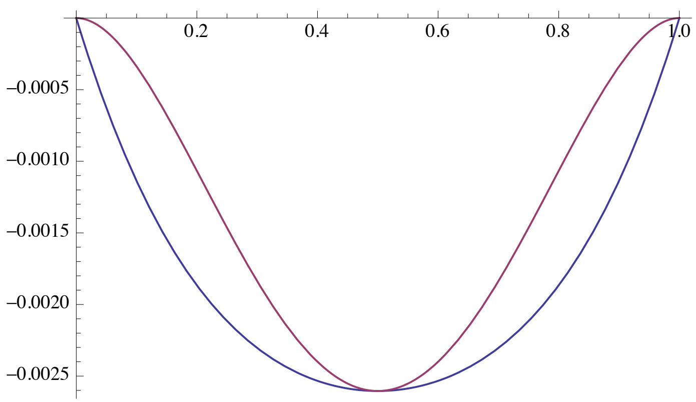
Sandia National Laboratories

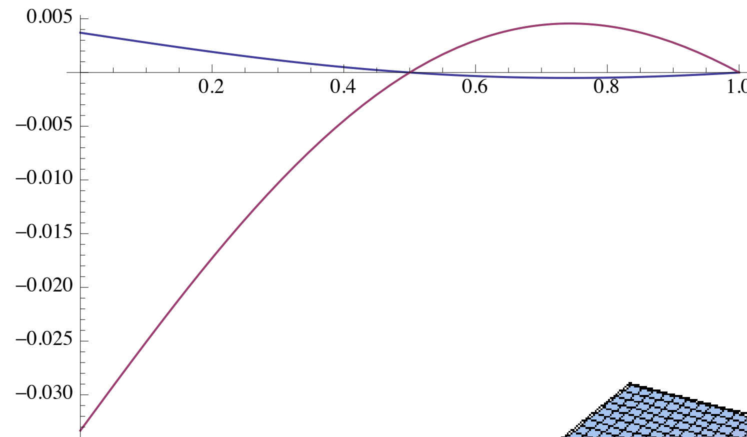
The truncation error for Van Leer V is exciting!

- This is a great form and equal or better than standard PPM

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

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

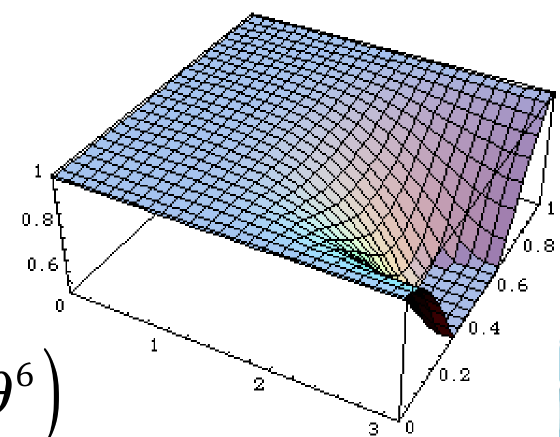




PPM Errors For Comparison

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

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



Sandia National Laboratories

We can derive the next method in the series: Van Leer VII (maybe these are VL X, XI instead)

- This might be viewed as a successor to "PPM" using a symmetric fourth-order polynomial.
- The polynomial is determined by the cell's average, its neighbors, and the edge values on the central cell.

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

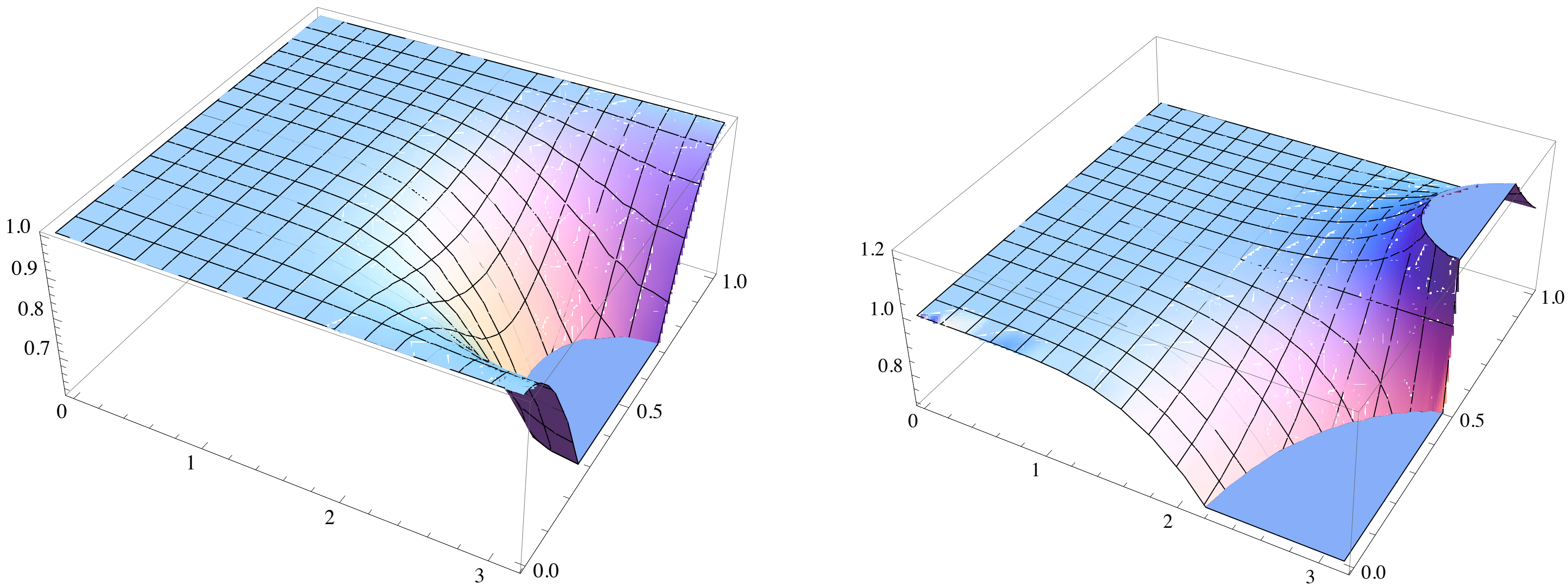
$$\frac{1}{-\mathbf{C}}\int_{1/2}^{1/2-C}\mathbf{P}(\theta)\,d\theta = \bar{\mathbf{U}}_{j+1/2} = \mathbf{P}_0 + \mathbf{P}_1\left(\tfrac{1}{2}-\tfrac{\mathbf{C}}{2}\right) + \mathbf{P}_2\left(\tfrac{1}{4}-\tfrac{\mathbf{C}}{2}+\tfrac{\mathbf{C}^2}{3}\right) + \mathbf{P}_3\left(\tfrac{1}{8}-\tfrac{3\mathbf{C}}{4}+\tfrac{\mathbf{C}^2}{2}-\tfrac{\mathbf{C}^3}{4}\right) + \mathbf{P}_4\left(\tfrac{1}{16}-\tfrac{\mathbf{C}}{4}+\tfrac{\mathbf{C}^2}{2}-\tfrac{\mathbf{C}^3}{2}-\tfrac{\mathbf{C}^4}{5}\right)$$

- We can use fifth, sixth or seventh-order edge values to determine the edges.
- Similar to a method introduced by Xiang & Shu

Van Leer VII has very nice properties.

- It is basically like a better version of PPM (6th order edges).

$$u_{j-1} = \int_{j-3/2}^{j-1/2} P(\theta) d\theta; u_j = \int_{j-1/2}^{j+1/2} P(\theta) d\theta; u_{j+1} = \int_{j+1/2}^{j+3/2} P(\theta) d\theta; u_{j-1/2} = P(-1/2); u_{j+1/2} = P(1/2)$$

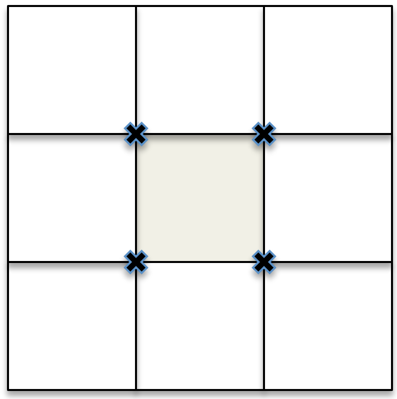


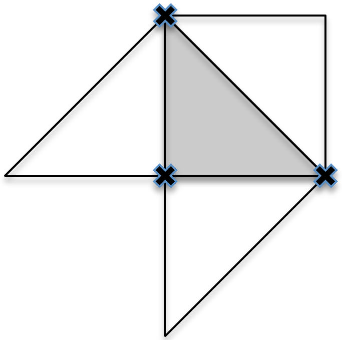
$$A \approx 1 + \tfrac{1}{720}\left(-2C^2 + 3C^3 + C^4 - 3C^5 + C^6\right)\theta^6 + O\left(\theta^8\right)$$

$$P \approx 1 + \tfrac{1}{1680}\left(-12 + 28C + 7C^2 - 35C^3 + 7C^4 + 7C^5 - 2C^6\right)\theta^6 + O\left(\theta^8\right)$$

Moving to multiple dimensions and complex meshes requires comment

- ❑ **Runge-Kutta method of lines methods are simple for complex integrators.**
  - ✓ **A downside is that these R-K methods have strict CFL stability limits.**
  - ✓ **These can alleviated to some degree by including more characteristic information.**
- ❑ **Least Squares principles can be used to derive stencils e.g., over-determined systems**





$$P(x,y)=U+U_x(x-x_0)+U_y(y-y_0)+U_{xy}(x-x_0)(y-y_0)$$
$$+U_{xx}(x-x_0)^2+U_{yy}(y-y_0)^2$$

Conclusions

- ❑The basis of most remap is the simpliest 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.

Thoughts about high-order methods

- **Accuracy per unit run time**
  - ✓ We care about discontinuous solutions with shocks or contacts determining the accuracy,
  - ✓ Think "high-resolution"
  - ✓ Define what accuracy we care about (symmetry, energy,…)
  - ✓ Test and quantify the results

$$Error = Ch^{\alpha} \rightarrow C\frac{h^{\min(\alpha,p)}}{p^{\alpha}}$$

- **Measure the work, memory, and accuracy**
  - ✓ Ullrich's work on methods for climate modeling is useful – compare resolution, memory & operations
- **Think in terms of 3-D time dependent problems**
  - ✓ A single mesh refinement costs a factor of 16 more
  - ✓ Adaptive meshes reduce this to about 8