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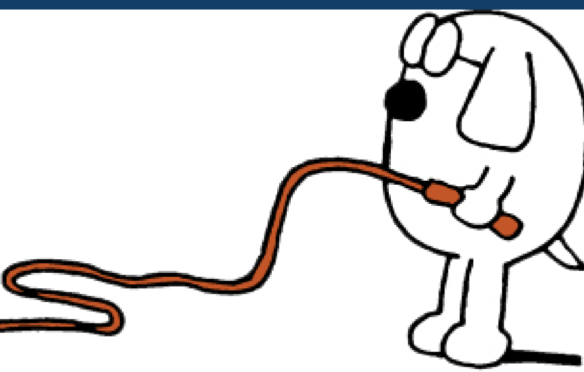

$$\tau(U) = ch^2 |F'(U)| \frac{|U_x U_{xx}|}{U_x}$$

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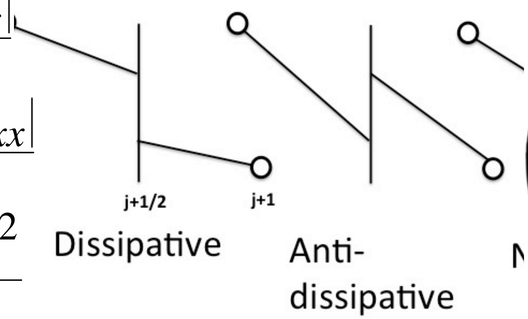

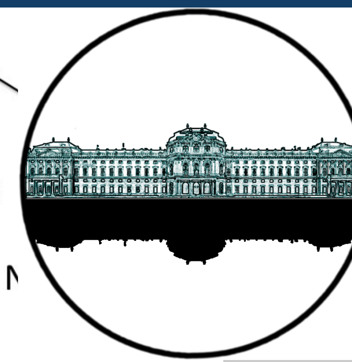

Evolution Equations for Developing Improved High-Resolution Schemes

Bill Rider

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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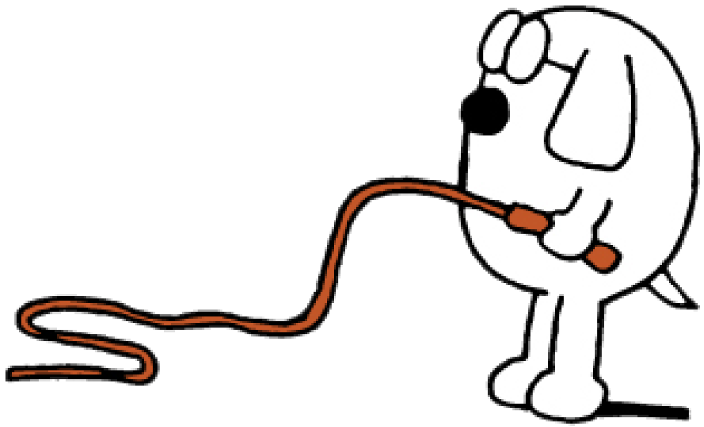
The Three Goals for this Talk

- **Goal 1:** Why have second-order monotonicity-preserving method been so dominant and remain so?
- **Goal 2:** What can the method of modified equations teach us about these numerical methods?
- **Goal 3:** What is needed to move beyond monotonicity preserving methods to something better and more accurate?

High-Resolution Methods

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



- **The Dogbert Principle (Scott Adams of Dilbert fame) : *"Logically all things are created by a combination of simpler, less capable components"***

(see Laney in Computational Gasdynamics)

Three reasons why the second-order methods were so dominantly successful.

- **Reason 1:** Robustness without inducing a viscosity that implicitly renders all solutions laminar and a stable hyperviscous regularization that provides turbulent "looking" solutions.
- **Reason 2:** A very robust nonlinear stability principle (that even allows linearly unstable methods to be used).
- **Reason 3:** "Huge" gains in accuracy over previous methods.

All these conclusions come from modified equation analysis!

If one uses a method based on conservation, a control volume method, a model is implied.

- Use modified equation analysis where the effective PDE is derived.
- Use a second-order centered difference for the flux

$$F(U)_{j+1/2} = \left(F(U)_j + F(U)_{j+1}\right)/2 \qquad U_t + F(U)_x = 0 \rightarrow = \tau(U)_x$$

- The nonlinear truncation error induces a dissipative effect on compression consistent with Bethe's asymptotic entropy law

$$\tau_{\text{numerical}}(U) = \frac{1}{6}h^2\left[F'U_{xx} + F''(U_x)^2\right] \Rightarrow \tau_{3D}(U) = C_{\text{CV}} h^2 F''_{i,j} \frac{\partial u_i}{\partial u_k}\frac{\partial u_j}{\partial u_k}$$

  - For LES, It can generate backscatter,often performs well in *a priori* comparisons of subgrid stress, except for its inherent stability problems.
  - The high resolution numerical methods cure the stability problems!

Three principles for high resolution methods from Bell, Colella, Trangenstein 1989.

- **Principle 1:** Use a high-order foundational method that is upstream centered, or at least fourth-order centered
- **Principle 2:** Use an entropy satisfying Riemann solver for computing fluxes
- **Principle 3:** Apply additional dissipation mechanisms at strongly nonlinear or degenerate discontinuities.

[BCT89] Bell, John B., Phillip Colella, and John A. Trangenstein. "Higher order Godunov methods for general systems of hyperbolic conservation laws." Journal of Computational Physics 82.2 (1989): 362-397.

A second-order Godunov method uses piecewise linear polynomials.

- A first order polynomial (PLM) or a second-order polynomial uses the cell average and the cell edge values (PPM),

$$\mathbf{P}_j(\theta) = \mathbf{P}_0 + \mathbf{P}_1\theta \qquad \mathbf{P}_0 = \mathbf{U}_j^n; \mathbf{P}_1 = S_j$$

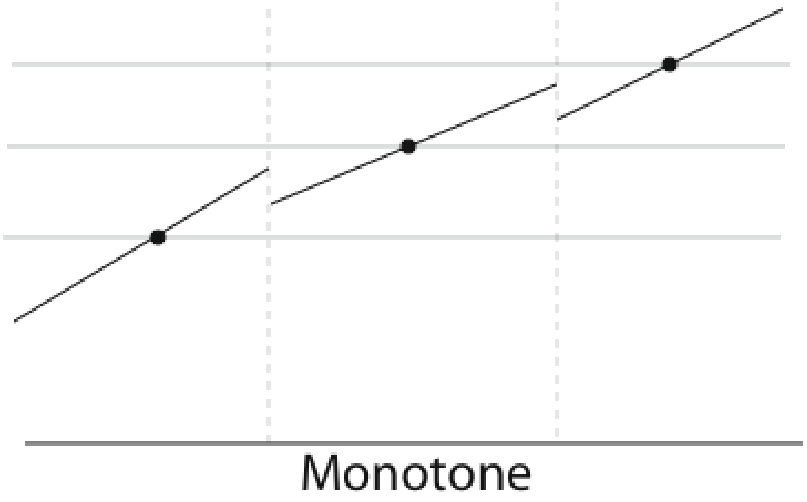
$$\mathbf{P}_j(\theta) = \mathbf{P}_0 + \mathbf{P}_1\theta + \mathbf{P}_2\theta^2$$

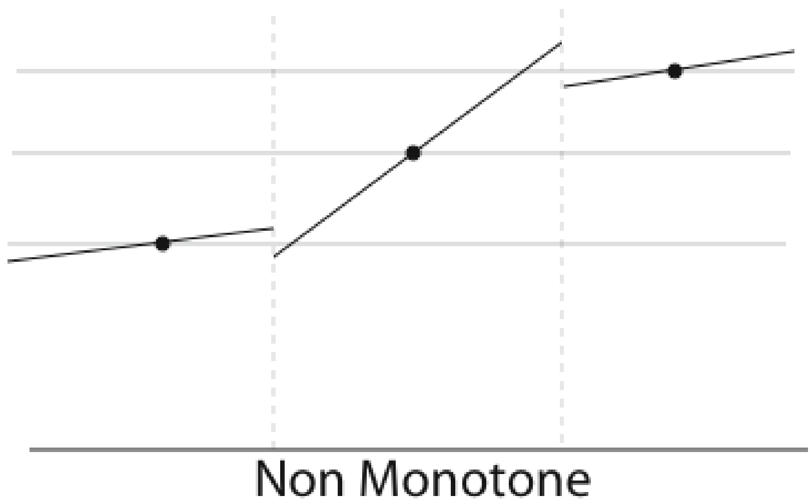
$$\mathbf{P}_0 = \mathbf{U}_j^n - \tfrac{1}{12}\mathbf{P}_2; \mathbf{P}_1 = U_{j+1/2} - U_{j-1/2}; \mathbf{P}_2 = 3\left(U_{j+1/2} + U_{j-1/2}\right) - 6U_j$$

- Several key requirements are necessary for this to useful:
  - Conservation $\mathbf{U}_j = \int \mathbf{P}_j(\theta) d\theta = \mathbf{P}_0$
  - Accuracy $\mathbf{U}_{j\pm 1/2} = \mathbf{U}\left(x_{j\pm 1/2}\right) + \mathcal{O}\left(\Delta x^n\right)$
  - Boundedness (monotonicity)

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,

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

$$\mathbf{U}_{j-1}^n \le \mathbf{U}_j^n + \tfrac{1}{2}\mathbf{S}_j \le \mathbf{U}_{j+1}^n \qquad \mathbf{U}_{j-1}^n \le \mathbf{U}_j^n - \tfrac{1}{2}\mathbf{S}_j \le \mathbf{U}_{j+1}^n$$

$$\mathbf{U}_{j-1}^n - \mathbf{U}_j^n \le \tfrac{1}{2}\mathbf{S}_j \le \mathbf{U}_{j+1}^n - \mathbf{U}_j^n \qquad \mathbf{U}_{j-1}^n - \mathbf{U}_j^n \le -\tfrac{1}{2}\mathbf{S}_j \le \mathbf{U}_{j+1}^n - \mathbf{U}_j^n$$

- Assume the data is increasing left-to-right

$$\mathbf{S}_j \le 2\left(\mathbf{U}_{j+1}^n - \mathbf{U}_j^n\right) \qquad \mathbf{S}_j \le 2\left(\mathbf{U}_j^n - \mathbf{U}_{j-1}^n\right)$$

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

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

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 $$\mathbf{S}_j = \min\bmod\left[\Delta_{j-1/2}, \Delta_{j+1/2}\mathbf{U}\right]$$
  - Van Leer $$\mathbf{S}_j = \frac{\left|\Delta_{j+1/2}\mathbf{U}\right|\Delta_{j-1/2}\mathbf{U} + \left|\Delta_{j-1/2}\mathbf{U}\right|\Delta_{j+1/2}\mathbf{U}}{\left|\Delta_{j-1/2}\mathbf{U}\right| + \left|\Delta_{j+1/2}\mathbf{U}\right|}$$
  - Fromm $$\mathbf{S}_j = \min\bmod\left[\tfrac{1}{2}\left(\Delta_{j-1/2}\mathbf{U} + \Delta_{j+1/2}\mathbf{U}\right), 2\Delta_{j-1/2}\mathbf{U}, 2\Delta_{j+1/2}\mathbf{U}\right]$$
  - Van Albada $$\mathbf{S}_j = \frac{\left(\Delta_{j+1/2}\mathbf{U}\right)^2\Delta_{j-1/2}\mathbf{U} + \left(\Delta_{j-1/2}\mathbf{U}\right)^2\Delta_{j+1/2}\mathbf{U}}{\left(\Delta_{j-1/2}\mathbf{U}\right)^2 + \left(\Delta_{j+1/2}\mathbf{U}\right)^2}$$
  - And so on,

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

$$\mathbf{S}_j \coloneqq \min\mathrm{mod}\left[\mathbf{S}_j, 2\,\Delta_{j-1/2}\mathbf{U}, 2\,\Delta_{j+1/2}\mathbf{U}\right]$$

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

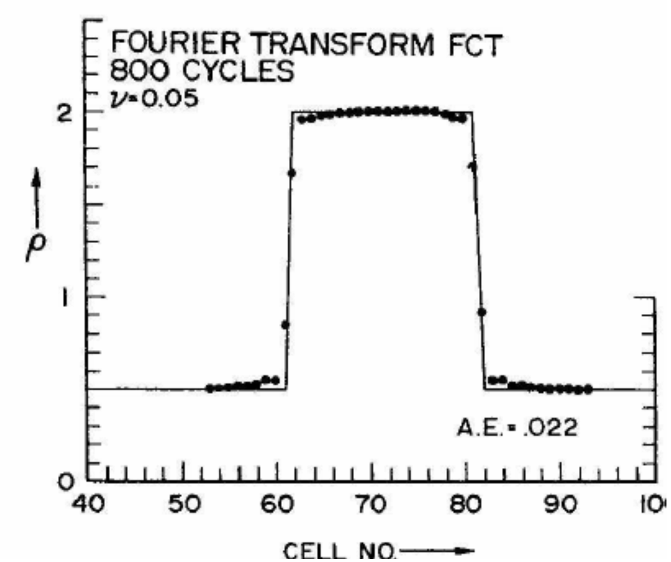
$$\mathbf{U}^n_{j+1/2} = \tfrac{2}{60}\mathbf{U}^n_{j-2} - \tfrac{13}{60}\mathbf{U}^n_{j-1} + \tfrac{47}{60}\mathbf{U}^n_j + \tfrac{27}{60}\mathbf{U}^n_{j+1} - \tfrac{3}{60}\mathbf{U}^n_{j+2}$$

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

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

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.*



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

The fundamental law of computer science: As machines become more powerful, the efficiency of algorithms grows more important, not less. – Nick Trefethen

Results' oriented methods

- Based on the chosen measure, solution error
  - not convergence rate *which are nearly the same*) a better method can be designed.
- Combine/**hybridize** the different approaches to get the best of each
- Increases the level of nonlinearity in the methods beyond that found in previous methods
- Efficiency cannot be ignored (h)

Linearity breeds contempt - Peter Lax

Verification of Hydrodynamic Methods

- The key tool is *mesh refinement* and convergence testing
  - Error ansatz - $$\|E\| = \|S - A\| = Ch^{\alpha}$$
- Two main results come from the analysis
  - Convergence Rate, *a* $$\alpha < 1; \bar{\alpha} \approx 0.8$$
  - Size of the error (local and normed), E
- Our problems intrinsically contain shocks - 1st order convergence (at best!), the size of the error is most important

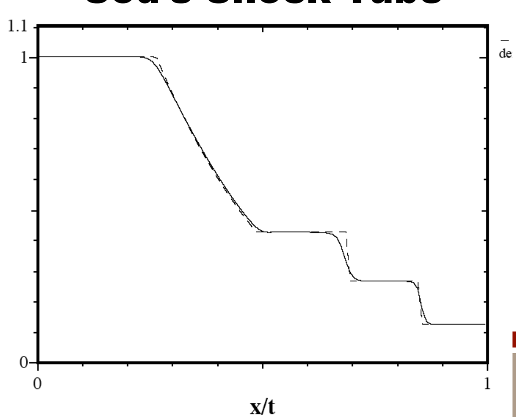
" Definition: Anyone who publishes a calculation without checking it against an identical computation with a smaller h… is an IDIOT"
John Boyd in Chebyshev and Fourier Spectral Methods

A summary of Greenough-Rider's* results on "off-the-shelf" methods

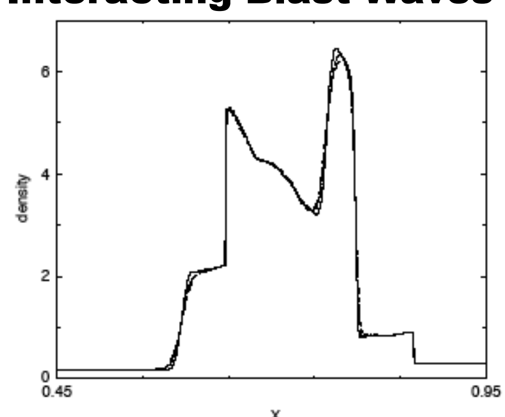
*Greenough & Rider, *J. Comp. Phys*. 196(1), 259-281, 2004.

- **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 Δx), but worse than PLM at fixed computational expense**

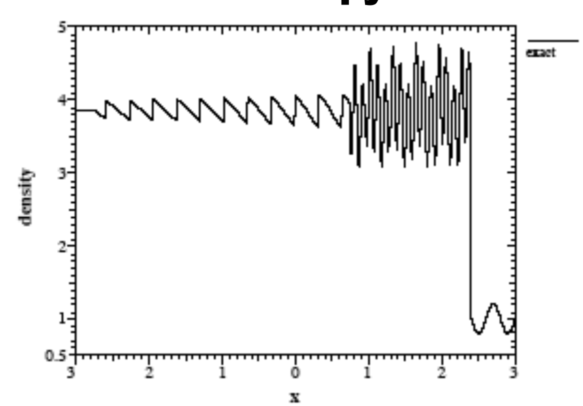
Sod's Shock Tube



Interacting Blast Waves



Shu-Osher Entropy Wave



“All Methods” are 1st Order - Relative Errors and Efficiency are Important

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Relative Errors

Method	Sod’s	Blast	Shu-Osher	CPU Cost	Efficiency 1-D,
1st order	6.28	2.25	4.19	0.85	31.5
sPLMmm	1.96	1.71	2.03	1.00	4.97
sPLM2	1.00	1.00	1.00	1.00	1.00
sPLM4	0.73	0.84	0.92	1.01	**0.63**
WENO3	2.13	1.55	2.03	3.76	18.8
WENO5	1.43	0.78	0.72	5.37	**5.06**

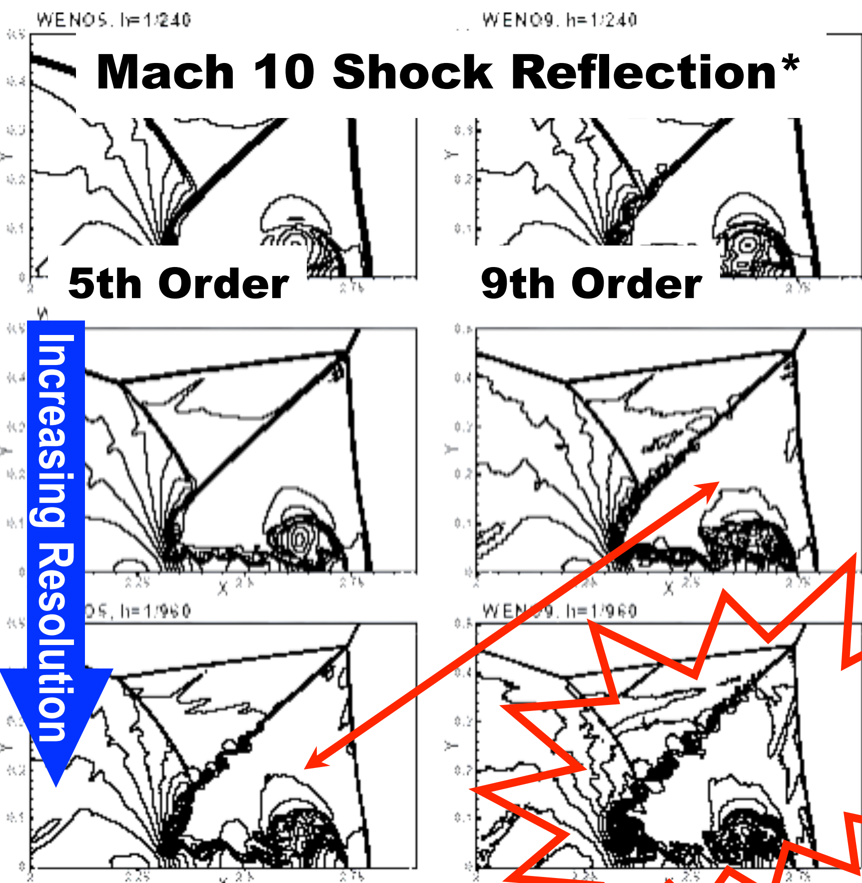
increasing linear accuracy

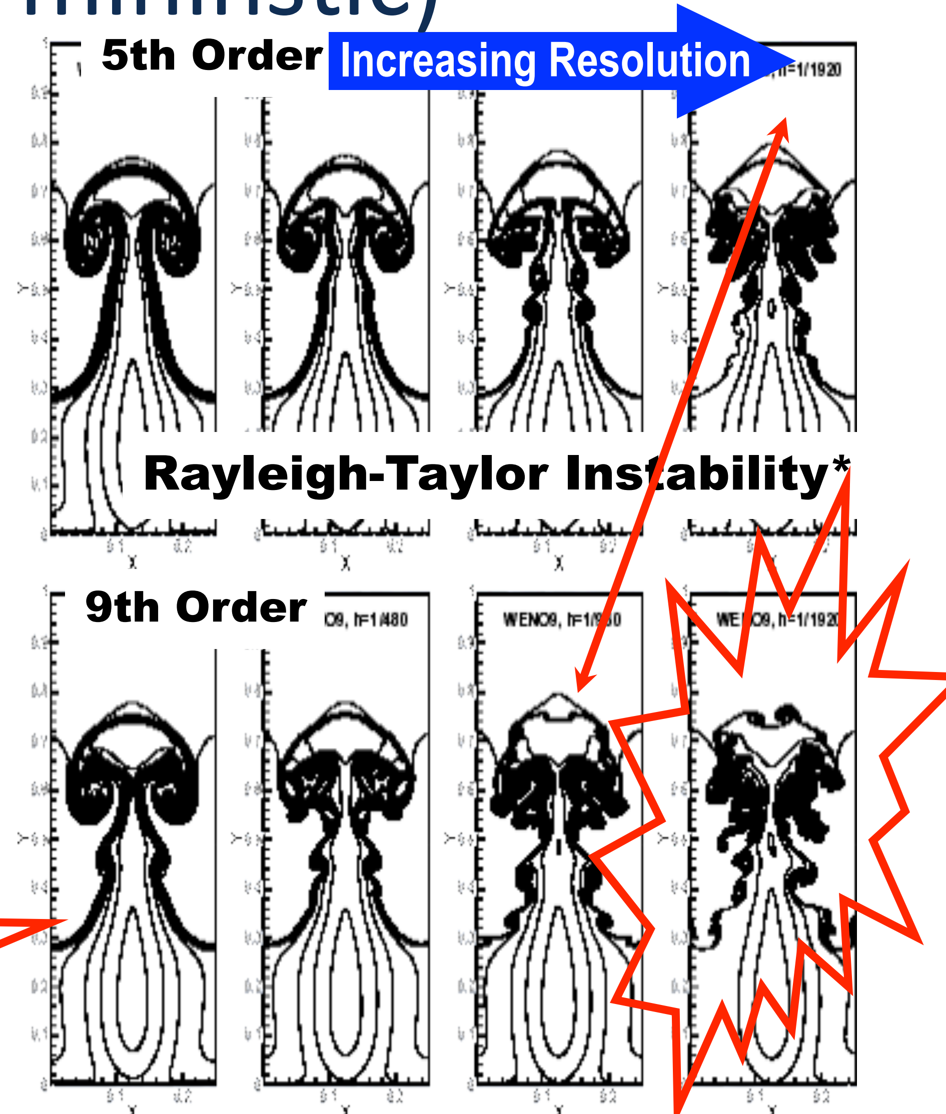
Smaller is Better

$$\eta_{1D} = \mathrm{cost}(\mathrm{R.E.})^{5/2} \quad \text{for } \alpha = 0.8$$

Multidimensional Problems Are Difficult (non-determininstic)

- What's the metric?





*Resolution of High Order WENO Schemes for Complicated Flow Structures
Shi, Zhang & Shu, J. Comp. Phys. **186**, 2003.

Role of modified equation analysis

- HHL ’76 established positivity of coefficients and prelude to TVD, and entropy conditions via vanishing viscosity
- The entropy condition was derived via the modified equation analysis, first order produces a viscous term as the leading truncation error.
- This mode of analysis largely disappeared with the focus moving to discrete conditions providing nonlinear stability
- Can modified equation analysis provide more benefits?
- I will explore here.

A Modified Equation Approach

- The modified equation is the effective differential equation for a given numerical method
  - Reproduces the original PDE
  - And effective models (error terms)
  - Surprisingly effective even with under-resolved solutions
- Derived via Taylor series expansion
- Compliments standard numerical analysis
  - Provides the nonlinear errors as well

Model for Analysis

- The chosen discrete form is not essential (other forms will do as well)
- Use a slope-based Godunov method:

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x}\left[F\left(U_{j+1/2}\right) - F\left(U_{j-1/2}\right)\right]$$

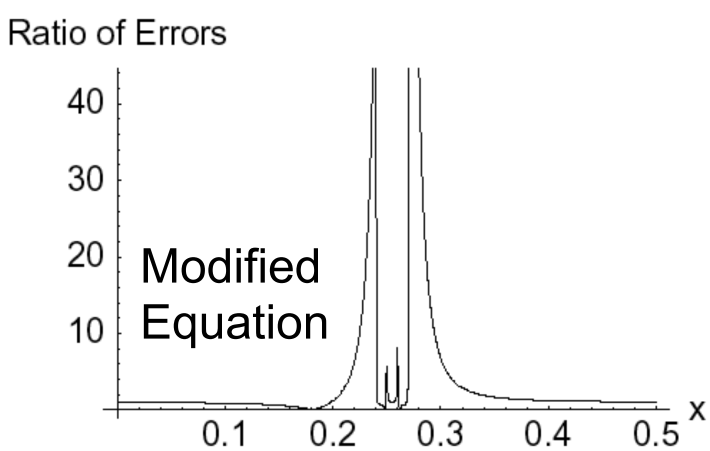
$$F\left(U_{j+1/2}\right) = \frac{1}{2}\left[F\left(U_{j+1/2;L}\right) + F\left(U_{j+1/2;R}\right)\right] - \frac{\left|F\left(\overline{U}\right)\right|}{2}\left(U_{j+1/2;R} - U_{j+1/2;L}\right)$$

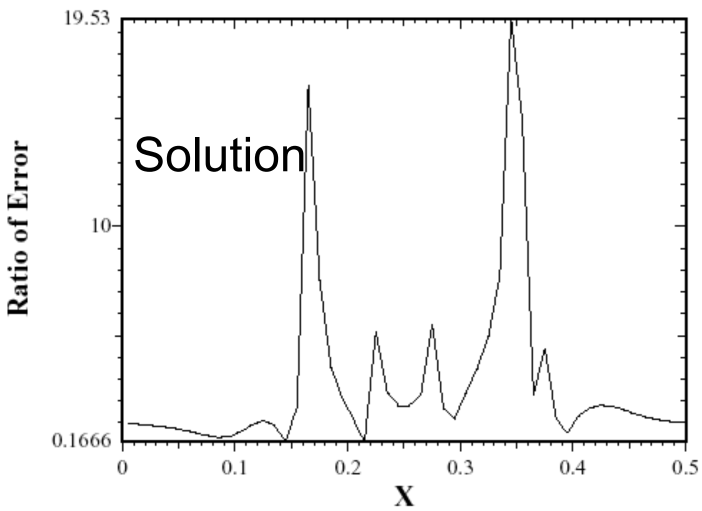
- Plug into Mathematica…

$$U_{j+1/2;L} = U_j + \frac{1}{2}S_j(U) \quad U_{j+1/2;R} = U_{j+1} - \frac{1}{2}S_{j+1}(U)$$

How Well Do Modified Equations Work?

Compare Fromm and van Leer for Linear Advection of a square wave, and estimate the error via the modified equation





The difference between the two methods is the limiter as a fourth order term,

$$\tau(U) = \frac{|F'(U)|(U_{xx})^2}{8U_x}$$

Implicit LES' s Modified Equation

- The modified equation has two parts:
  - Linear Error terms

CV term!

$$\tau(U) = c_1 h^2 F'(U) U_{xx} + \underbrace{c_2 h^2 F''(U)(U_x)^2}_{\text{CV term!}}$$

$$\tau(U) = c_3 h^3 F'(U) U_{xxx}$$

  - Nonlinear terms - associated with the limiters

$$\tau(U) = c_4 h^2 F'(U) |U_x| U_x$$ ← MPDATA

$$\tau(U) = c_5 h^3 |F'(U)| \frac{(U_{xx})^2}{U_x}$$ ← van Leer or van Albada slopes

Implicit LES' s Modified Equation (cont.)

- Nonlinear terms - associated with the limiters (cont.)

$$\tau(U) = ch^2 |F'(U)| \frac{|U_x U_{xx}|}{U_x}$$

minmod, or mineno

$$\tau(U) = ch^3 |F'(U)| \frac{|U_x U_{xxx}|}{U_x}$$

UNO

$$\tau(U) = ch^3 |F'(U)| \frac{(U_{xx})^2}{U_x}$$

WENO-3rd

$$\tau(U) = ch^5 |F'(U)| \frac{(U_{xxx})^2}{U_x}$$

WENO-5th

A Framework for Analysis and Understanding

- Analyze energy,

$$U \cdot (U_t + \nabla \cdot [F(U) - \tau(U)]) = 0$$

$$E_t + \nabla \cdot U[F(U) - \tau(U)] = [F(U) - \tau(U)]\nabla U$$

- Total variation- 1D

$$|V|_t + F' \frac{\partial}{\partial x}\left[|V| - \tau\left(V\right)\right] + HOT = 0 \qquad V = \frac{\partial U}{\partial x}$$

We will stick to linear equations for TV analysis

(Kinetic) Energy Analysis $O(\Delta x)^2$

- Stick with 1-D for simplicity's sake

$$(\tau(U))_x = \left(c|U_x|U_x\right)_x$$

$$\rightarrow \quad U(\tau(U))_x = \left(cU|U_x|U_x\right)_x - c|U_x|(U_x)^2$$

$$(\tau(U))_x = \left(c(U_x)^2\right)_x$$

$$\rightarrow \quad U(\tau(U))_x = \left(cU(U_x)^2\right)_x - c(U_x)^3$$

$$(\tau(U))_x = (U_{xx})_x$$

$$\rightarrow \quad U(\tau(U))_x = (cUU_{xx})_x - \frac{1}{2}\left(c(U_x)^2\right)_x$$

(Kinetic) Energy Analysis (cont.)

$$O(\Delta x)^3$$

- The term that comes up with monotonicity, again sticking with 1-D

$$(\tau(U))_x = \left(c\frac{(U_{xx})^2}{U_x} \right)_x$$

$$\rightarrow \quad U(\tau(U))_x = \left(cU\frac{(U_{xx})^2}{U_x} \right)_x - c(U_{xx})^2$$

$$(\tau(U))_x = (cU_{xxx})_x$$

$$\rightarrow \quad U(\tau(U))_x = (cUU_{xxx})_x - (cU_x U_{xx})_x + c(U_{xx})^2$$

Analysis results, energy, TV

- Variation results all share a common theme. Variation is conserved except at sign changes in the derivatives.
- Easily shown for first order upwind.

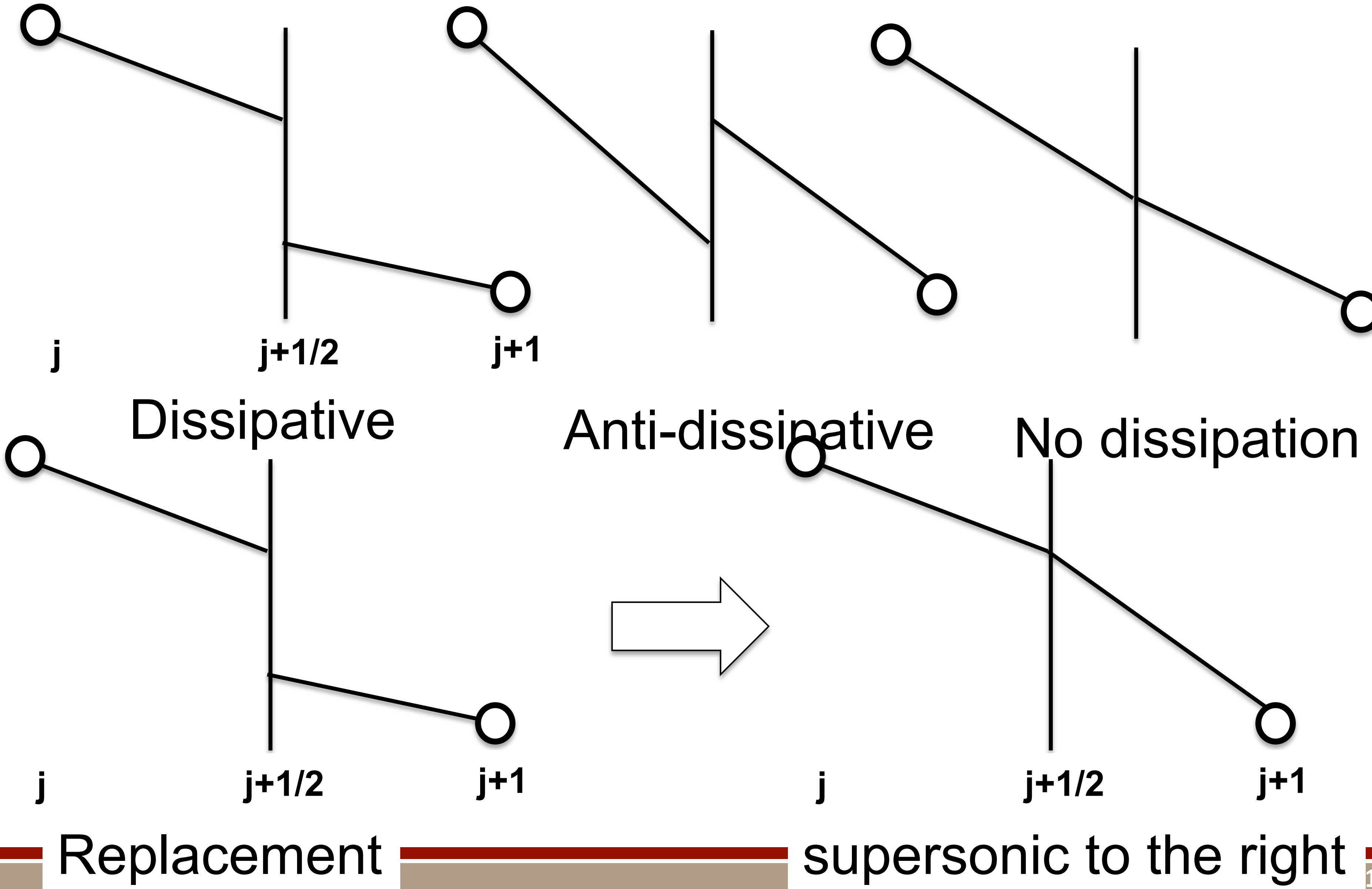
$$|V|_t + |V|_x = \left(\lambda |V|_x\right)_x ; \lambda = |F'| \frac{\Delta x}{2} \quad \left(\lambda |V|_x\right)_x = \lambda |V|_{xx} + \lambda sign'\left(V_x\right)^2$$

- The variation is conserved except at sign changes then dissipated proportional to the second derivative

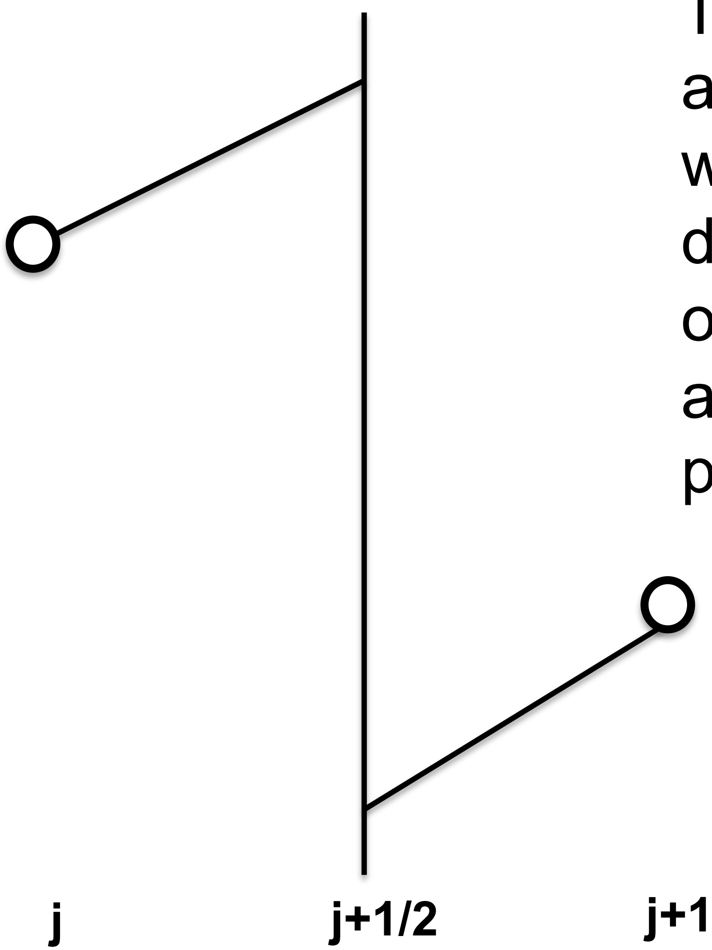
Form for the artificial viscosities

- 1st order $\tau(U)=ch\left|F'(U)\right|$
- 2nd order $\tau(U)=ch^2\left|F'(U)\right|\left|\frac{U_{xx}}{U_x}\right|$
- 3rd order $\tau(U)=ch^3\left|F'(U)\right|\left|\frac{U_{xxx}}{U_x}\right|$ $\tau(U)=ch^3\left|F'(U)\right|\left(\frac{U_{xx}}{U_x}\right)^2$
- 5th order $\tau(U)=ch^5\left|F'(U)\right|\frac{\left(U_{xxx}\right)^2}{\left(U_x\right)^2}$
- Implications – Limiters are needed to control the size of the viscosity. Schemes without limiters (ENO-WENO) may have too large a viscosity when the solution highly under-resolved.
- As I will discuss this may produce robustness issues for these schemes and can be "easily" seen by examining edge values.

Edge swapping: dissipation, steepening, recovery – an under utilized technique



A reason why entropy-stable ENO schemes might actually have fragile non-robust side



This circumstance is "entropy stable" and a recipe for disaster especially with a Lax-Friedrichs flux. Too much dissipation can yield instability and oscillations. ENO schemes can do this and there is no extra nonlinear stability principle being applied to rescue it.

Three reasons why methods have stalled.

- **Reason 1:** lack of smoothness in real problems and failed utility for formally high-order accurate methods
- **Reason 2:** Removal of the first-order method as a path for achieving robustness
- **Reason 3:** Use of much weaker nonlinear stability mechanisms with new instabilities

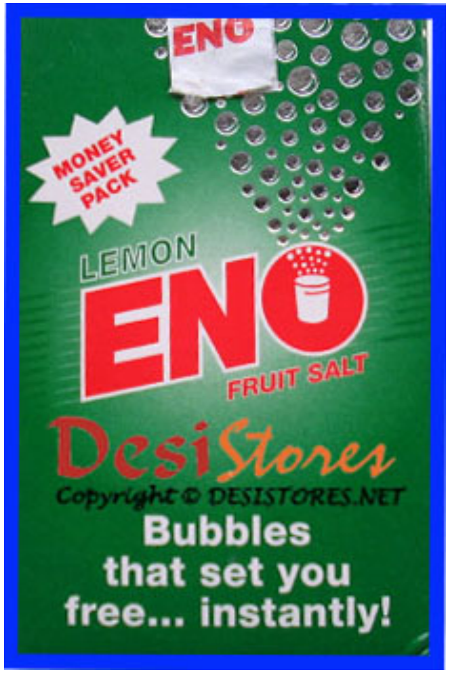
“Change almost never fails because it's too early. It almost always fails because it's too late.” — Seth Godin

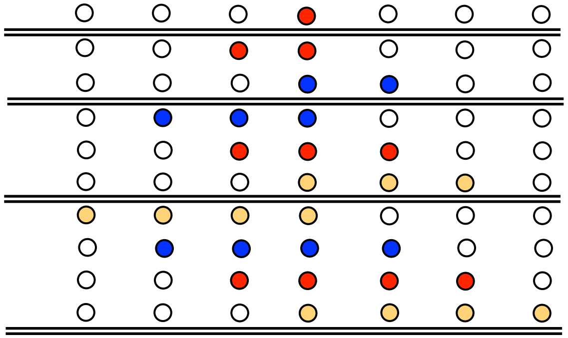
Three proposed principles for moving beyond monotonicity preservation in production codes.

- **Principle 1:** Use a nonlinear stability mechanism that detects extrema and carefully relaxes from monotonicity preservation
- **Principle 2:** Continue to use the high-order base scheme unless it violates monotonicity
- **Principle 3:** Apply additional dissipation at strongly nonlinear discontinuities. If the solution is under-resolved give up high-order accuracy and degenerate to first-order.

Introduction to ENO and WENO

- The starting point for modern methods are 1st order monotone methods.
- These were extended to 2nd order with TVD methods.
- *TVD methods degenerate to 1st order at extrema.*
  - UNO methods moved the TVD methods to uniform 2nd order accuracy.
- ENO methods moved methods to arbitrarily high order.
- WENO methods moved ENO methods toward greater practicality.
- Not really extending TVD!



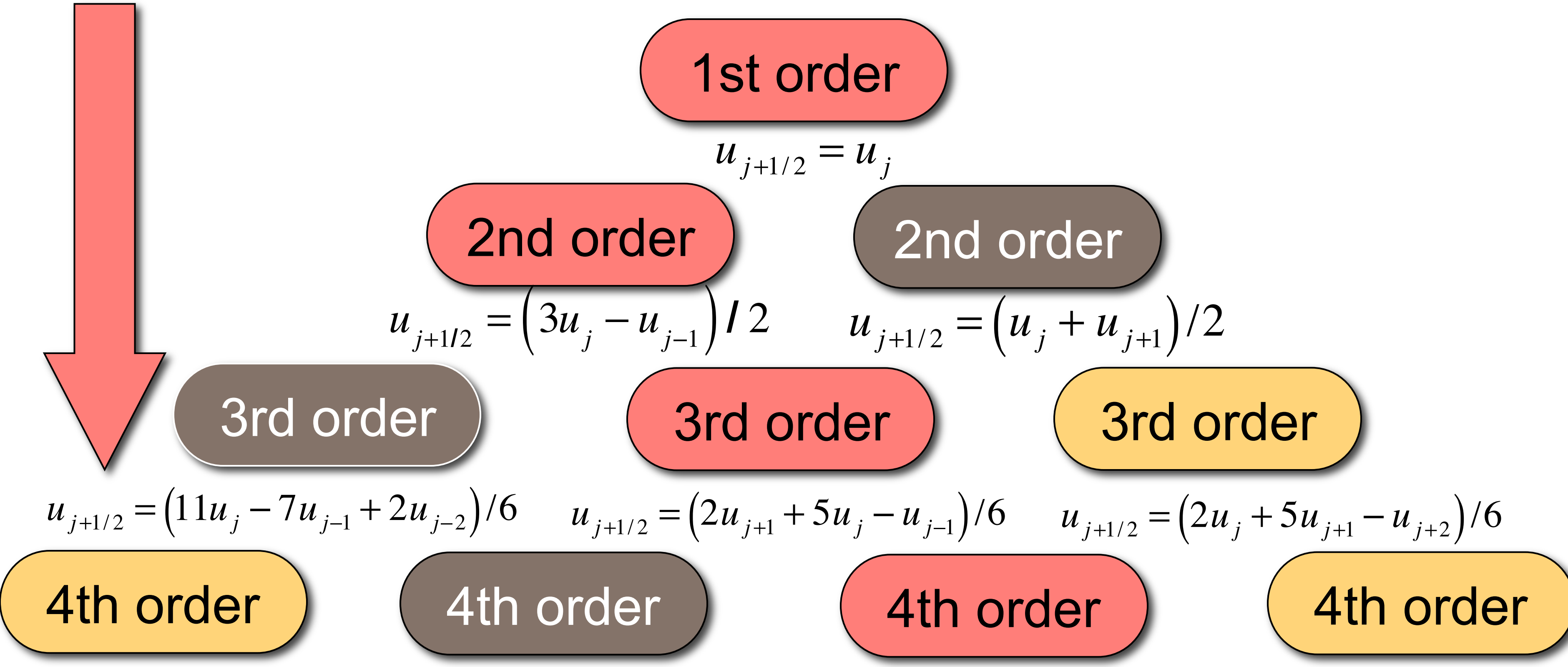


ENO Design Principles

- Divide the methods into three main steps:
  - Reconstruction or spatial differencing.
  - Evolution (solution in the small) or Riemann solution.
  - Integration or time advance.
- The evolution step and integration are TVD (analytically at least), but the reconstruction might not be,…
- *… thus a focus on the reconstruction step.*
- In monotone and TVD methods, the reconstruction is TVD, ENO methods allow variation to potentially increase, although in a controlled bounded manner.
  - Keeping the variation controlled can lead to convergent methods (compactness).

$$\mathrm{TV}\left(u^{n+1}\right) \leq C\,\mathrm{TV}\left(u^{n}\right)$$

ENO Methods use smoothness to adaptively choose a stencil.



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

The same differencing may be arrived at through a different path.

1st order

$$u_{j+1/2} = u_j$$

2nd order | 2nd order

$$u_{j+1/2} = \left(3u_j - u_{j-1}\right)/2 \qquad u_{j+1/2} = \left(u_j + u_{j+1}\right)/2$$

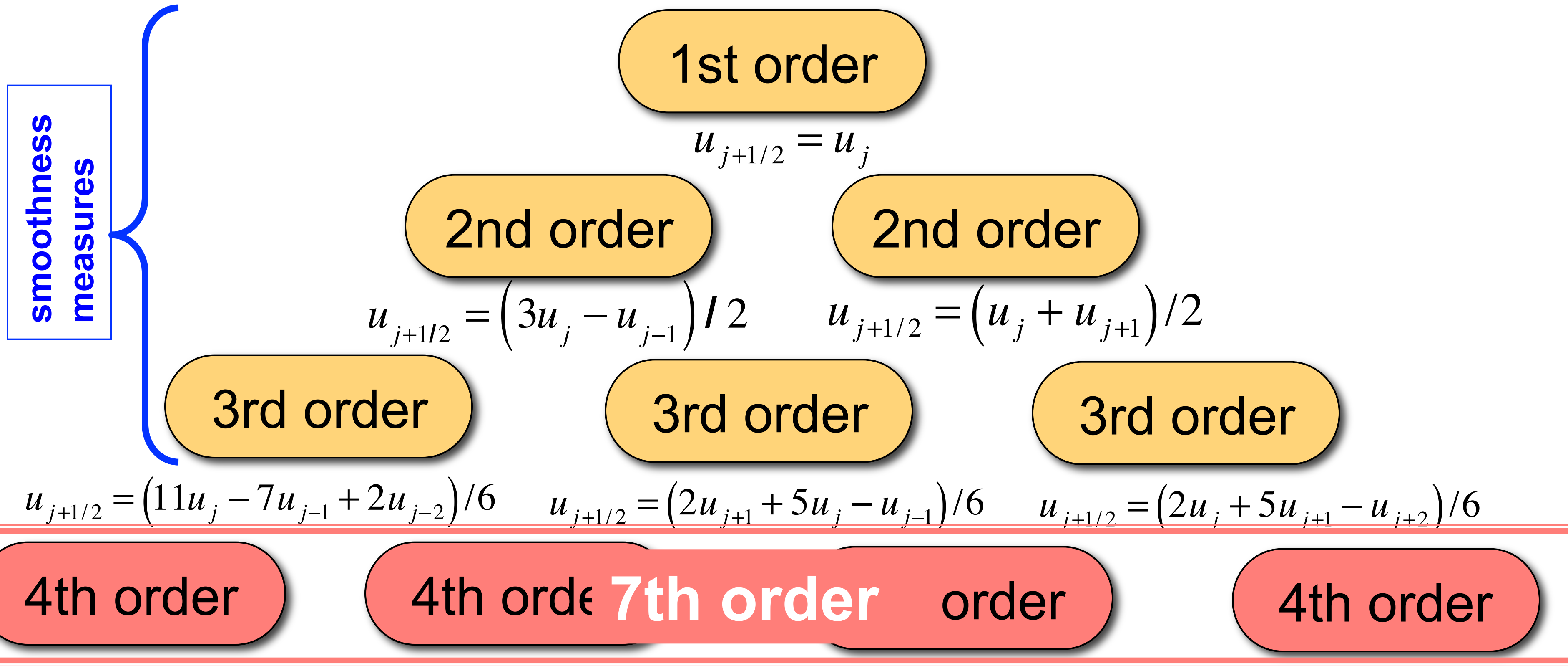
3rd order | 3rd order | 3rd order

$$u_{j+1/2} = \left(11u_j - 7u_{j-1} + 2u_{j-2}\right)/6 \qquad u_{j+1/2} = \left(2u_{j+1} + 5u_j - u_{j-1}\right)/6 \qquad u_{j+1/2} = \left(2u_j + 5u_{j+1} - u_{j+2}\right)/6$$

4th order | 4th order | 4th order | 4th order

- The high-order stencils are evaluated pair-wise. This characteristic also hints at one of ENO's pathologies.

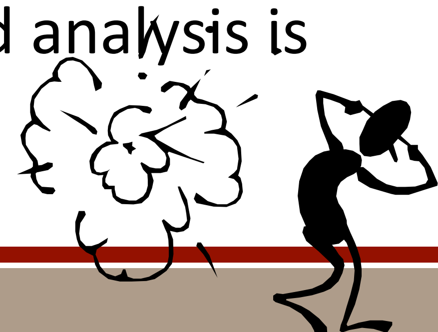
Weighted ENO methods are different in their approach, but the result is similar.



- These methods evaluate ***all*** the high-order stencils and compare them (and combine them) algebraically.
- Weights can be chosen to achieve *2m-1* order schemes.

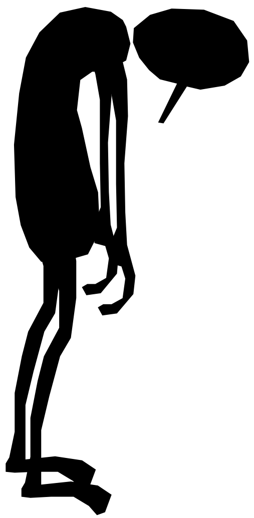
Issues with ENO and WENO

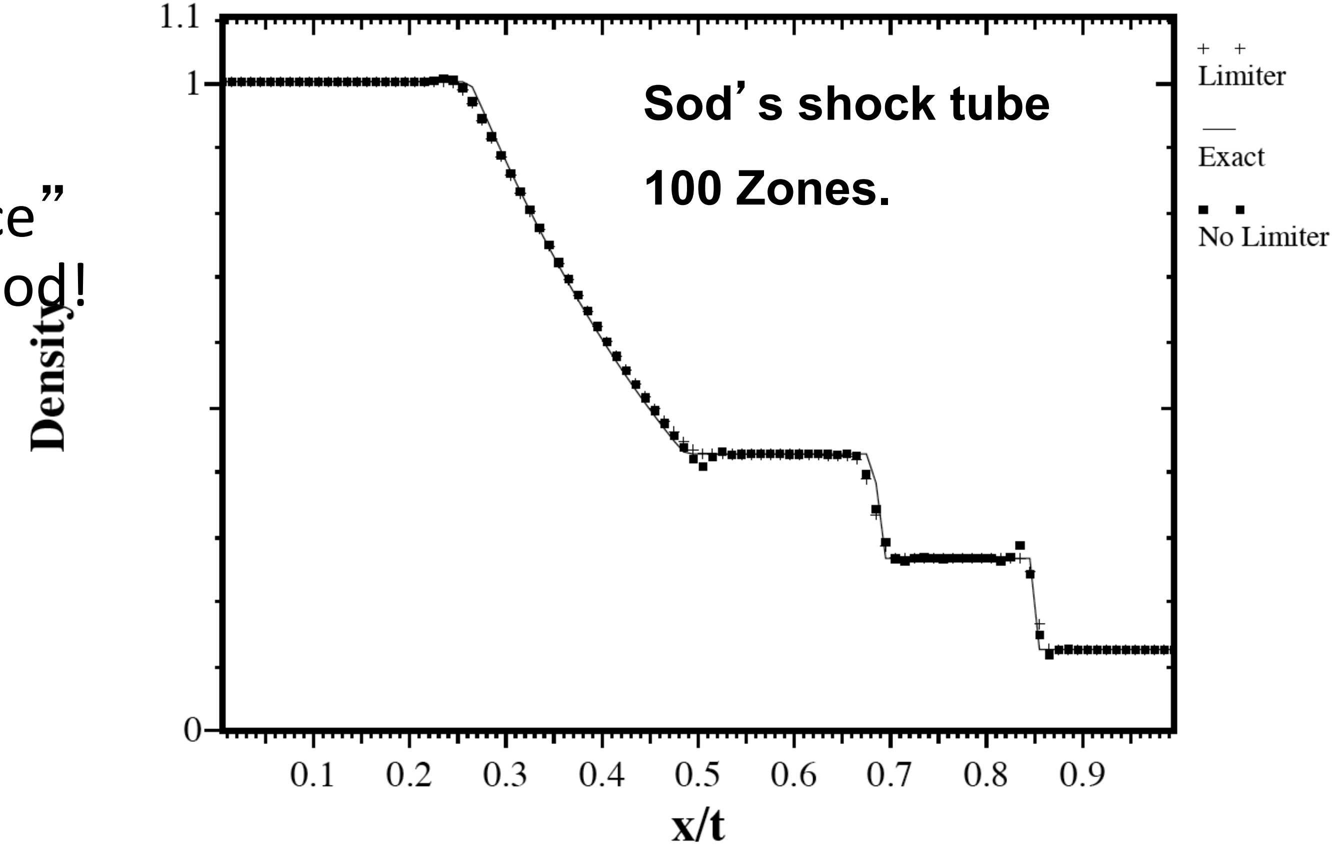
- ENO can produce biased stencils that are linearly unstable (one reason for WENO).
    - Unstable dissipation due to poor edge value selction
- WENO methods are still somewhat oscillatory for very high-order (7th order and higher using a monotone limiter to control these oscillations, *inelegant*).
- The methods are still excessively dissipative compared with other high-resolution methods.
- These methods are somewhat difficult to code (especially the smoothness detectors for >7th order), and analysis is even worse.



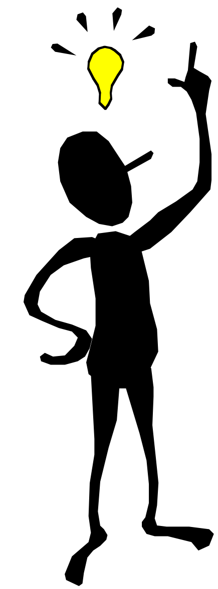
Issues with Results - oscillations or limiters?

- Sod's shock tube and 11th order WENO
  - Oscillations w/o limiter!
  - The limiter destroys the "elegance" of the method!

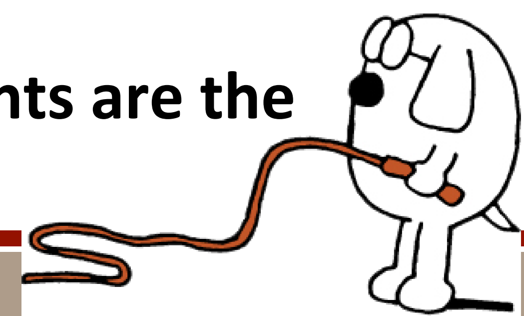




Algorithm idea 1: Combine different high resolution methods.



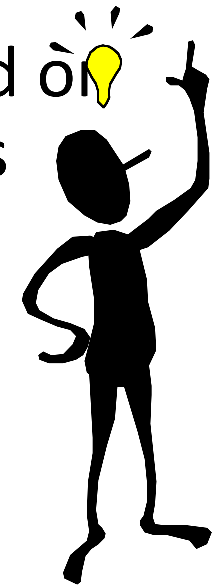
- *Can we have the best of each type of method?*
- Hybridize the nonlinear monotone/non-oscillatory methods*
  - Start with a nonlinear monotone method: high-order + monotonicity test
  - If the flow is not monotone use the median of the original high-order, monotone limiting value and an ENO/WENO value (new methods have an "x" designation in the following slides)
- Again quoting Dogbert: "*Logically all things are created by a combination of simpler, less capable components*"
  - **Now the simpler, less capable components are the older high-resolution methods**



Algorithm Idea 2: ENO methods based on the Comparison Principle

- The current ENO (and WENO) algorithms are based on the adaptive stencil approach that *recursively* finds the "smoothest" stencil.
- I'm proposing using a different principle than the smoothest stencil - **Using a comparison with TVD schemes to choose the high-order stencil.**

$$\mathbf{TV}\left(\mathbf{R}\left(u^n\right)\right) \le \mathbf{TV}\left(u^n\right) + O\left(h^r\right)$$



- In other words, one would begin with a TVD stencil and choose the higher-order stencil that is closest to that TVD stencil in some sense (to be defined) .
- This leads to schemes similar to existing ENO and WENO schemes, *but with somewhat better properties*.

A general form for limiters

- Introduced by Rider and Margolin 2001

$$\tilde{p}_j(\theta) = U_j + \phi\left[p_j(\theta) - U_j\right] \qquad \phi = \min\left[1, \frac{U_{\max} - U_j}{U_{MAX} - U_j}\right]$$

- Extended to positivity-preserving (bounded) limiters by Shu and collaborators (accuracy-preserving)

$$\tilde{U}_{j+1/2} = U_j + \phi\left[U_{j+1/2} - U_j\right] \qquad \phi = \min\left[1, \frac{U_{\min} - U_j}{U_{MIN} - U_j}\right]$$

- Can be used more broadly to preserve other properties
  - Monotonicity
  - Extrema
  - Other choices

$$\phi = \min\left[1, \frac{\text{standard}}{\text{choice}}\right]$$

Total variation is used to define methods

- Define **TV**=total variation $\mathbf{TV} = \sum \left| u_{j+1} - u_j \right|$
- TVD means the *total variation diminishing*

$$\mathrm{TV}\left(u^{n+1}\right) \leq \mathrm{TV}\left(u^{n}\right) \text{ or } \mathrm{TV}\left(\mathrm{R}\left(u^{n}\right)\right) \leq \mathrm{TV}\left(u^{n}\right)$$

  - Here **R**(*u*) is a reconstruction (interpolation) of *u*
  - TVD is a manner of making nonlinear schemes monotone
- ENO is closely related conceptually

$$\mathbf{TV}\left(\mathbf{R}\left(u^{n}\right)\right) \leq \mathbf{TV}\left(u^{n}\right) + O\left(h^{r}\right)$$

  - Thus ENO is almost monotone, but allows oscillations of a size $O\left(h^{r}\right)$

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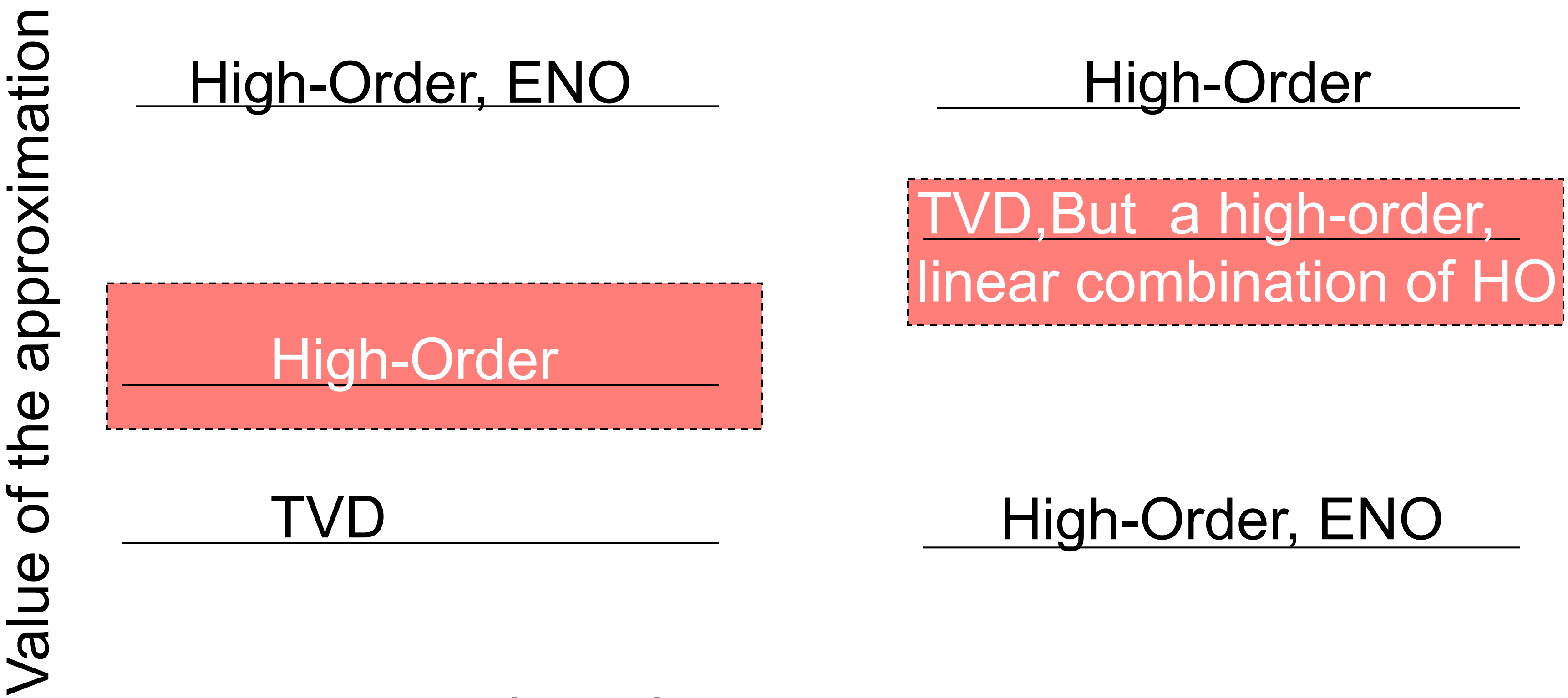
$$O\left(h^{r}\right)$$

The median function bounds the different approximations.



The median(a,b,c) returns the value bounded by the other two values. Preserves the accuracy given by at least two arguments.

The median function has some key properties.

- One can use a median, or bounding function, **median**(a,b,c) that returns the middle argument of the three.
  - The one that is bounded by the other two
  - Theorem (Huynh): If two arguments are $O(h^n)$ the median is too!
  - If one argument is $O(h^n)$ and a second is $O(h^m)$ with $m<n$, the median is $O(h^m)$
  - Conjecture: If two arguments produce a linearly stable method, the **median** will as well.

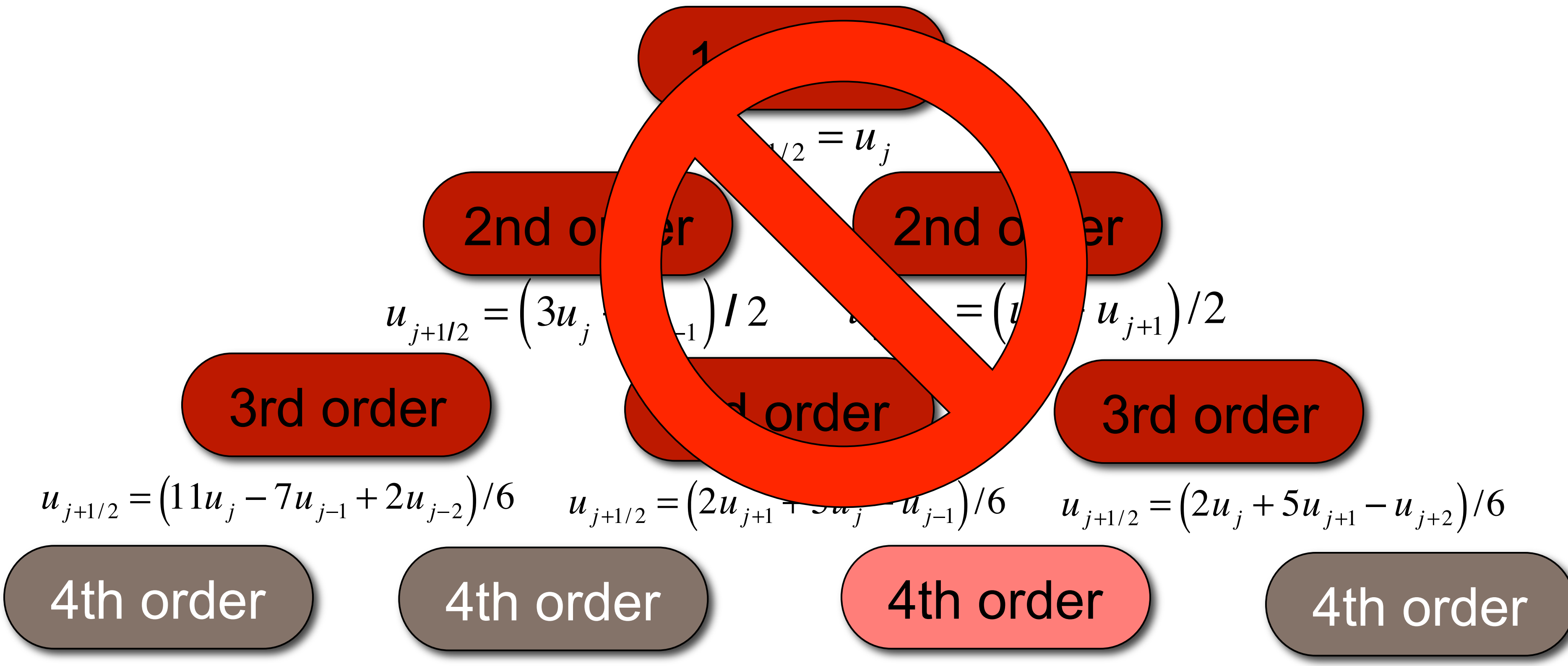
Applying the Comparison Principle

- The basis of the approach is the following definition for the ENO schemes,

$$\mathrm{TV}\left(\mathrm{R}\left(u^n\right)\right) \leq \mathrm{TV}\left(u^n\right) + O\left(h^r\right)$$

- Thus, the proposition is that choosing the stencil that is closest to the TVD method (or the comparison scheme) will satisfy this condition.
  - No proof (yet), but the results are very similar to existing ENO & WENO method in terms of accuracy (better), and total variation behavior (nearly identical)
- *The procedure resulting from the principle is flexible allowing freedom in choosing for the method's properties.*

Examples of implementation of the comparison principle.



- One approach would pick the 4th order scheme with the smallest distance from the TVD method.

One Might Use a Median function to accomplish the task.

- An algorithm for a 4th order comparison-ENO method would look like the following (using 4-4th order fluxes as building blocks:

$$f_a = \text{median}\left(f_1, f_2, f_{TVD}\right)$$

$$f_b = \text{median}\left(f_3, f_4, f_{TVD}\right)$$

$$\boxed{f_{ENO} = \text{median}\left(f_a, f_b, f_{TVD}\right)}$$

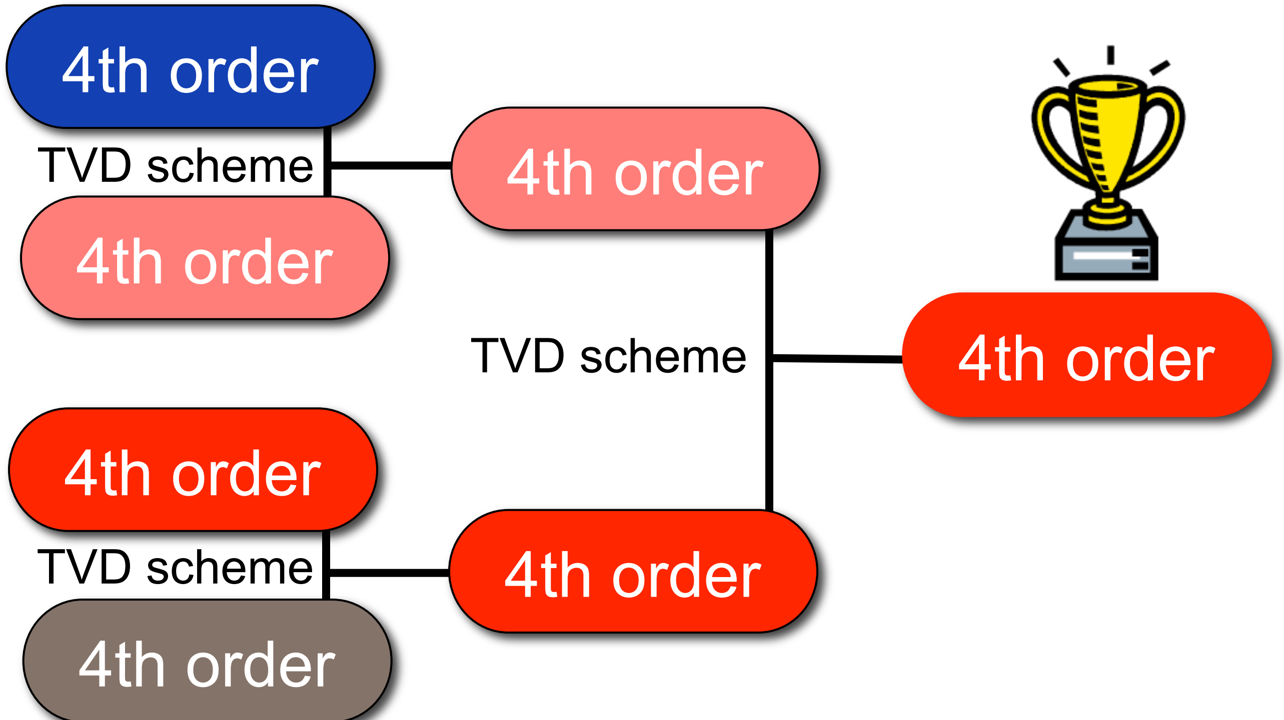
- The median(a,b,c) function chooses the function bounded by the other two and preserves accuracy

$$\text{median}\left(a,b,c\right) = a + \text{minmod}\left(b-a, c-a\right)$$

  - If two arguments are $O(h^m)$ then the median is $O(h^m)$

The comparison algorithm can be arranged more like “playoff”

- The TVD scheme chosen for comparison is used to test the “fitness” of each stencil. It’s the fitness determined by the “closeness” to the TVD method.



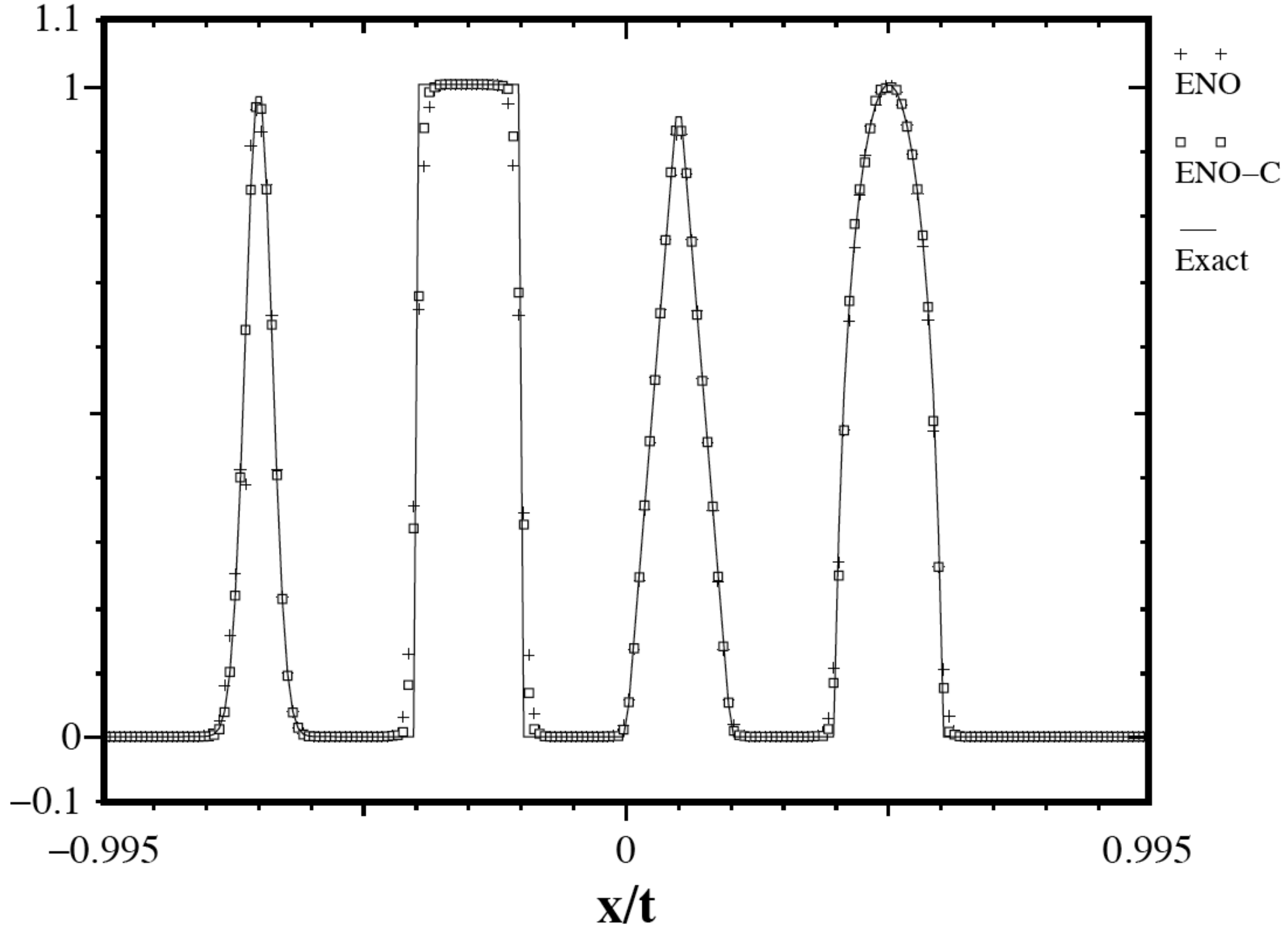
Analysis: Accuracy is unaffected.

- The previous method would produce a formally 4th order flux. *Each step produces a 4th order flux.*
- The non-oscillatory nature comes from relation of the result to the TVD comparison method.
  - Each step will choose either the TVD scheme, or the 4th order flux closest to it .
  - Results indicate that this is true. $\mathrm{TV}\left(\mathrm{R}\left(u^{n}\right)\right) \leq \mathrm{TV}\left(u^{n}\right) + O\left(h^{r}\right)$
  - *The problem is that the median function does not contain two non-oscillatory fluxes to compare. This is a concern for nonlinear stability of the results.*
  - ***At least one of the stencils would be the regular ENO stencil, which should be non-oscillatory. This resolves the nonlinear stability concern.***

Results: Accuracy on Scalar Waves

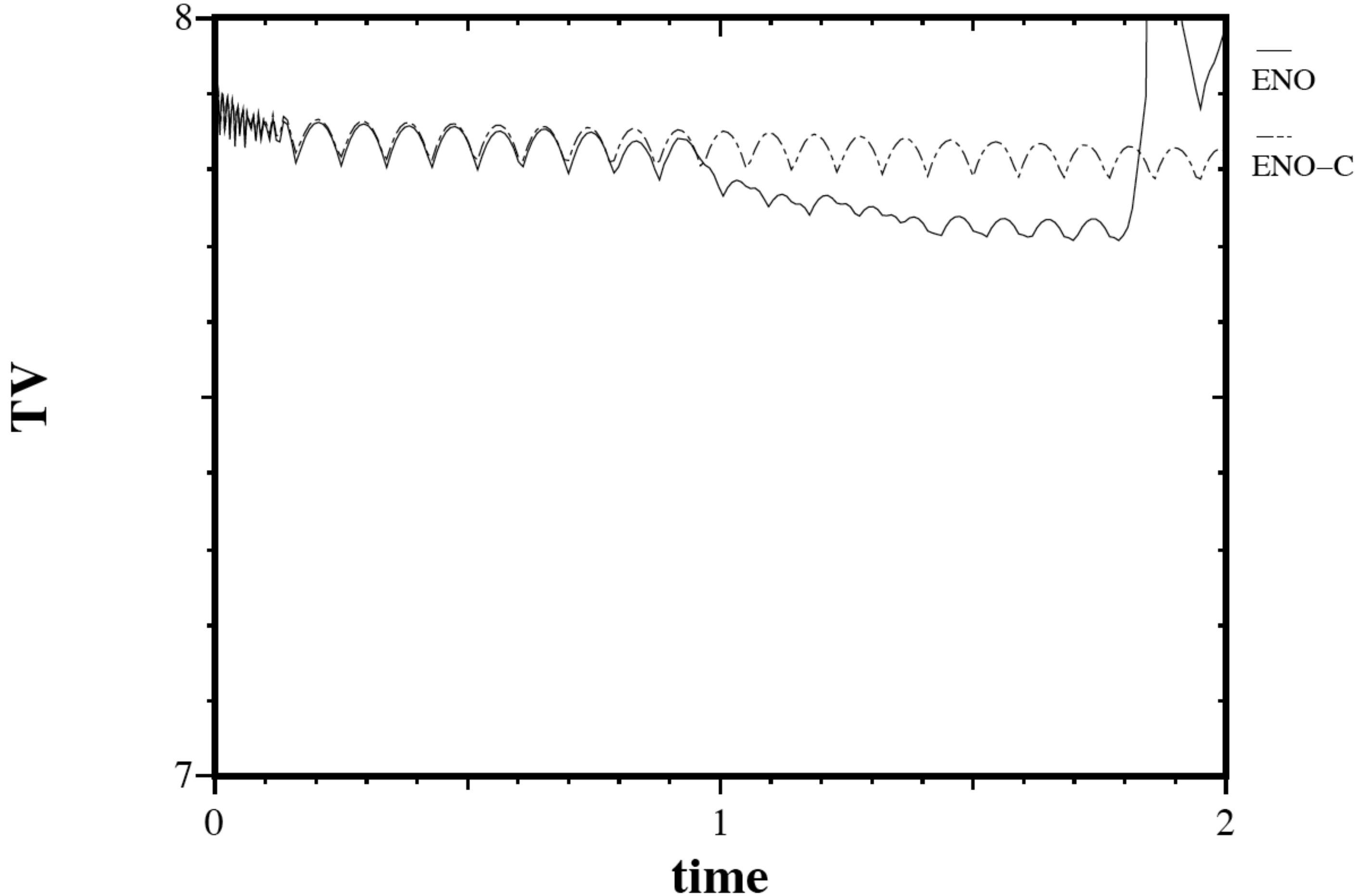
- Compare usual ENO with a comparison ENO

L1 Errors
ENO = 1.74e-02
ENO-C = 1.20e-02



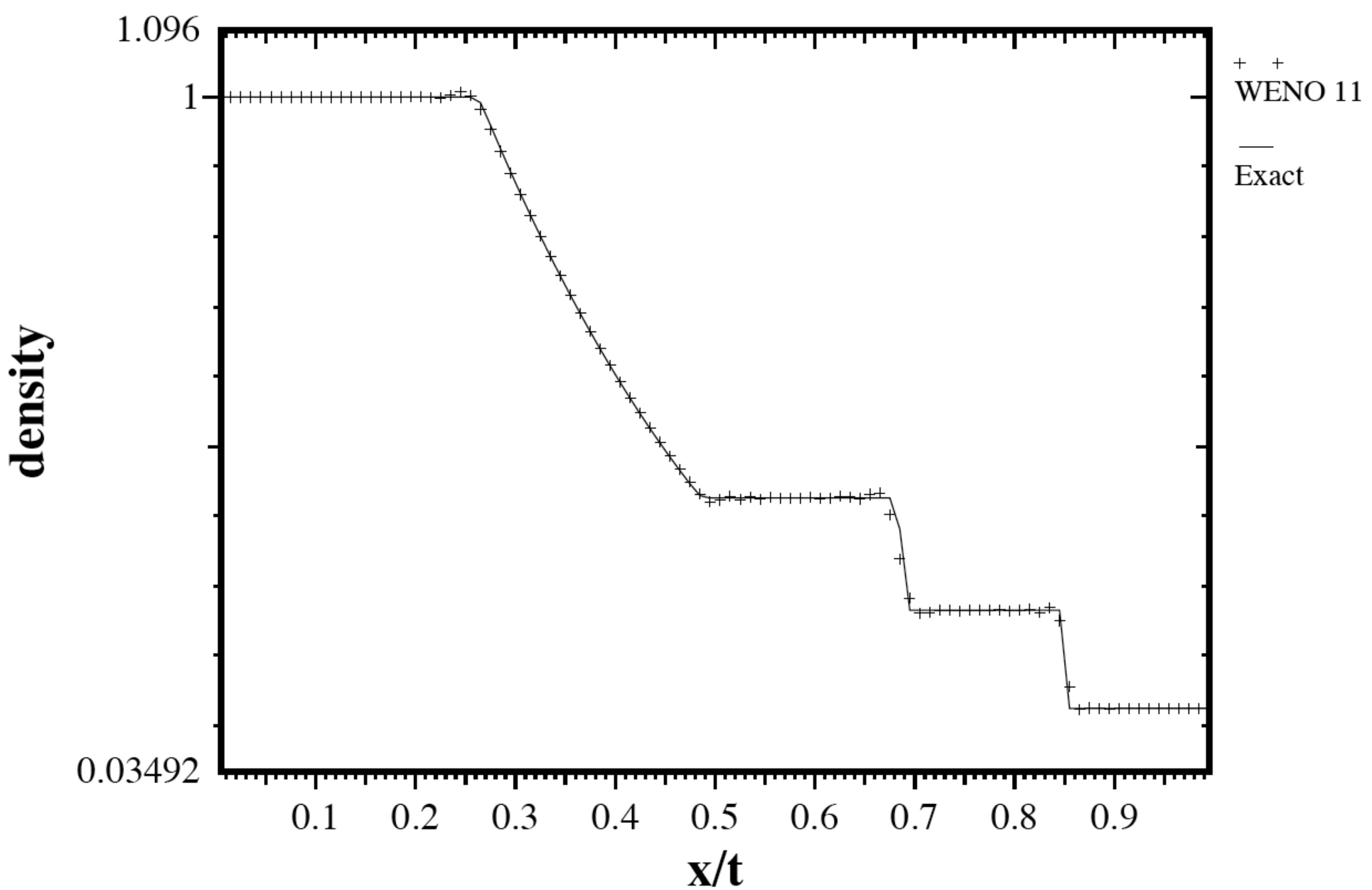
Results: Total Variation Behavior

- Look experimentally at the Total variation as a function of time.



Accuracy for Coupled Systems

- Look at Sod's Shock tube again w/11th order WENO-C (comparison scheme) - about the same as the regular WENO, and with about 25% lower CPU cost.



What would a proof of the ENO property look like?

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- Base this on the TVD schemes proof

$$\frac{\partial u}{\partial t} = -C_{j-1/2}\left(u_j - u_{j-1}\right) - C_{j+1/2}\left(u_{j+1} - u_j\right); C_{j\pm1/2} \geq 0$$

- Use an upwind method as the comparison method,

$$\frac{\partial u}{\partial t} = -C_{j-1/2}\left(u_j - u_{j-1}\right); C_{j-1/2} = \frac{1}{\Delta x}; C_{j+1/2} = 0$$

- Express the high-order method as follows,

$$\frac{\partial u}{\partial t} = -\frac{1}{\Delta x}\left(u_{j+1/2} - u_{j-1/2}\right); u_{j+1/2} = u_j + Q\left(u_{j+1/2} - u_j\right)$$

- Now rewrite the scheme as 1st order plus a correction

$$\frac{\partial u}{\partial t} = -\frac{1}{\Delta x}\left(u_j - u_{j-1}\right) + \frac{1}{\Delta x}\left(Q_{j+1/2} - Q_{j-1/2}\right)$$

Just like the TVD proof so far!

What would a proof of the ENO property look like?

- Now it comes down to proving the properties of the "Q" function. Note that the truncation error of the first order method is well defined in terms of the total variation.
- The scheme can definitely be high-order and deviations in total variation will be proportional to the high-order truncation error, $O(h^r)$
- Q: What should the "Q" function look like?
  - A: the minmod function, just as TVD methods.
- Putting this together with the original method returns us to **the median function** as serving the necessary role.
- Note: The second-order version of this method is TVD. A proof based on a 2nd order TVD comparison method follows the same path. Same for WENO version.

The current endpoint for the proof is the following conjecture.

- If the comparison scheme is TVD and the analytic result is a constant variation, the difference is proportional to the truncation error.
- *The any deviation in variation will be proportional to the leading order truncation error difference with the high-order method*
- Thus, the coefficient will be potentially negative to the following degree, $C_{j-1/2} \geq -O\left(h^r\right)$
- This <u>may</u> lead to the desired inequality (not complete).

xWENO scheme

- Again start with a high-order edge(flux) f_{HO}
- Check monotonicity $f_M = \mathrm{median}\left(f_{\mathrm{HO}}, f_j, f^*\right)$
  - If monotone, return high-order
  - If not then construct the regular WENO value f_{WENO}
- Check the high-order flux against the monotone and WENO one $f^* := \mathrm{median}\left(f_{\mathrm{j}}, f_{\mathrm{WENO}}, f^*\right)$

$$f = \mathrm{median}\left(f_{\mathrm{HO}}, f_{\mathrm{WENO}}, f^*\right)$$

How does this method do as compared with the regular WENO scheme?

Relative Errors and Efficiency for the New Enhanced Methods

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Relative Errors

Method	Sod's	Blast	Shu-Osher	CPU Cost	Efficiency 1-D
cPLM6	0.62	0.53	0.73	1.30	0.40
xPLM6	0.61	0.52	0.58	1.28	0.31
cPPM6	0.56	0.44	0.41	1.25	0.19
xPPM6	0.54	0.35	0.33	1.34	**0.14**
WENO3	2.13	1.55	2.03	3.76	18.8
WENO5	1.43	0.78	0.72	5.37	**5.06**

Smaller is Better

$$\eta_{1\mathrm{D}} = \mathrm{cost}(\mathrm{R.E.})^{5/2}; \eta_{2\mathrm{D}} \mathrm{cost}(\mathrm{R.E.})^{15/4}; \eta_{3\mathrm{D}} = \mathrm{cost}(\mathrm{R.E.})^{5}$$

Closing Thoughts

- Occam's Razor, "*It is vain to do with more what can be done with less,*" simplicity is a virtue
- Simulations are ultimately discrete - *discrete/nonlinear stability is an asset*
- **Modified equation analysis forms a systematic bridge between the discrete and continuous.**
  - **It has been underutilized*!***
- Modeling and numerics is notoriously hard (if not impossible) to separate, but development of each is typically independent - this is a problem

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