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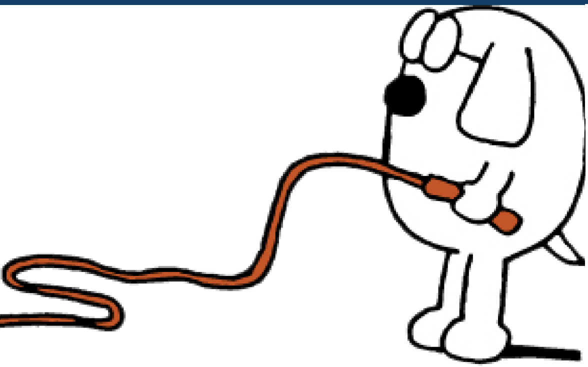

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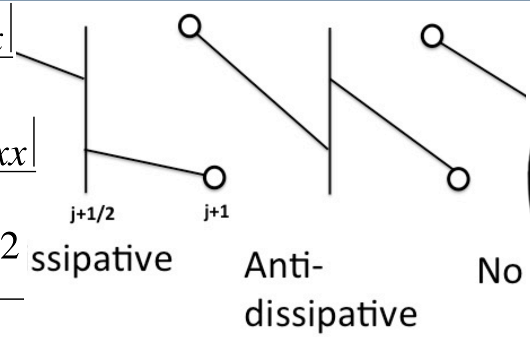

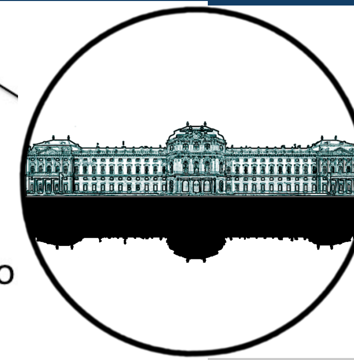

Evolution Equations for Developing Improved High-Resolution Schemes

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CCR Center for Computing Research

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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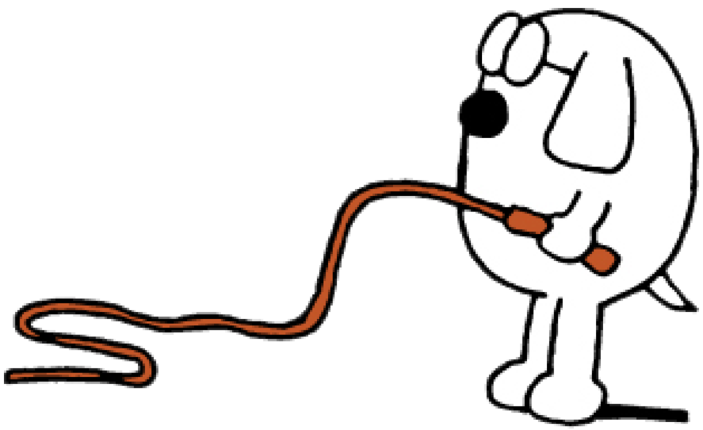
The Three Goals for this Talk

- **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 "classical" methods.



- **The Dogbert Principle: "*Logically all things are created by a combination of simpler, less capable components*"**

(see Laney in Computational Gasdynamics)

“Any sufficiently advanced technology is indistinguishable from magic.”
– Arthur C. Clarke

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. (ILES happened)
- **Reason 2:** A very robust nonlinear stability principle (that even allows linearly unstable methods to be used e.g., steepeners).
- **Reason 3:** “Huge” gains in accuracy/resolution/ fidelity over previous methods.

All these conclusions come from modified equation analysis!

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 $\quad \mathbf{U}_j = \int \mathbf{P}_j(\theta) d\theta = \mathbf{P}_0$
  - Accuracy $\quad \mathbf{U}_{j\pm1/2} = \mathbf{U}\left(x_{j\pm1/2}\right) + \mathcal{O}\left(\Delta x^n\right)$
  - Boundedness (monotonicity)

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

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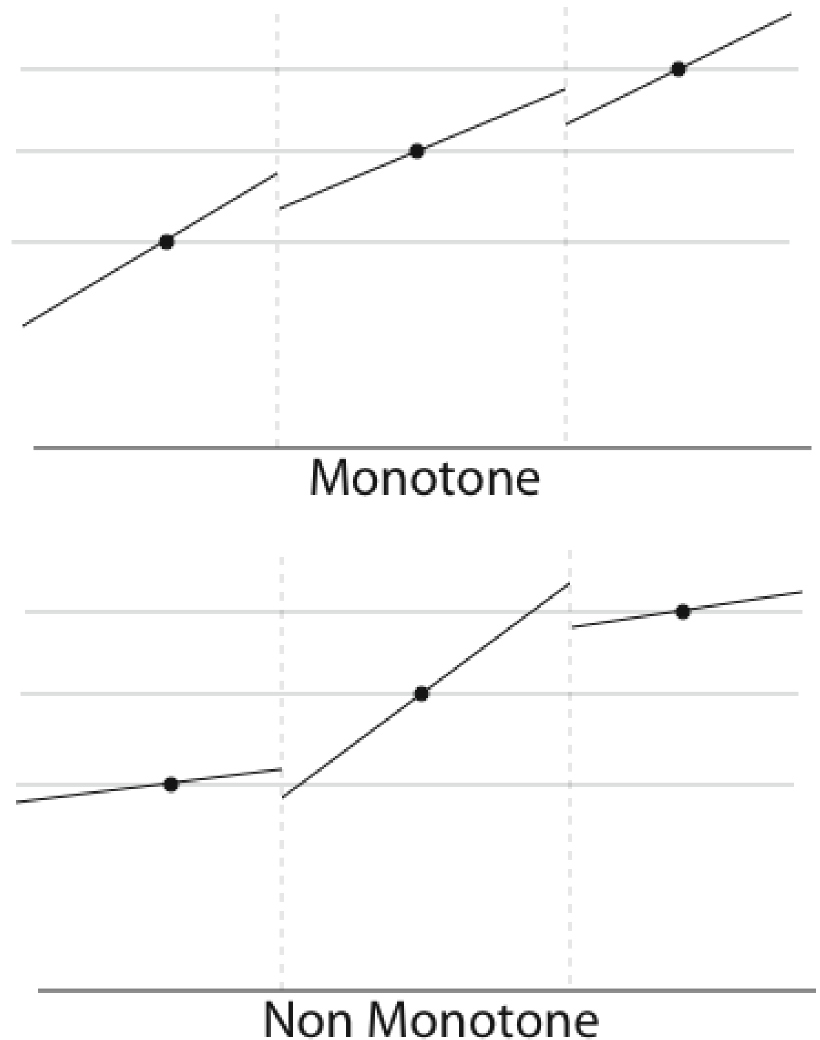
- The original statement is heuristic: the reconstruction should be bounded by the neighboring data.
- Later, time-dependence will be entertained, the time integrated edge values must be bounded.



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,

Linearity Breeds Contempt.
– Peter Lax

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 (modified equation).
  - This mode of analysis largely disappeared with the focus moving to discrete conditions providing nonlinear stability
- **Can modified equation analysis be engaged provide more benefits to modern methods?**

Vanishing viscosity and entropy satisfying schemes

- The concept of vanishing viscosity is essential

$$\partial_t u + \partial_x f(u) = \nu \partial_{xx} u \quad \nu \to 0^+$$

- Another key concept is the nature of true limiting solution – for the linear waves – entropy generation converges to a limit of zero

$$\partial_t S + \partial_x (uS) = \tfrac{\nu}{T} (\partial_x u)^2 \geq 0 \quad \nu \to 0^+, h \to 0$$

- For nonlinear waves the solutions **do not converge to a limit of zero** entropy production. The limit is finite entropy production.

$$\partial_t S + \partial_x (uS) = \tfrac{\nu}{T} (\partial_x u)^2 - Cf''(\Delta u)^3 \quad \nu \to 0^+, h \to 0$$

A fundamental limit for Euler, MHD, Burgers (and turbulence! Kolmogorov's third law) – dissipation in the absence of viscosity!

A Framework for Analysis and Understanding

- Analyze energy, a quadratic function

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

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

- Total variation- 1D

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

We will stick to linear equations for TV analysis

High Resolution Methods and their Modified Equation

- Nonlinear terms - associated with the limiters

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

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

Form for the effective artificial viscosities

- 1st order $\nu_{\text{numerical}} = ch\left|F'(U)\right|$
- 2nd order $\nu_{\text{numerical}} = ch^2\left|F'(U)\right|\left|\frac{U_{xx}}{U_x}\right|$ **A limiter will control the magnitude**

minmod

- 3rd order $\nu_{\text{numerical}} = ch^3\left|F'(U)\right|\left|\frac{U_{xxx}}{U_x}\right|$ $\nu_{\text{numerical}} = ch^3\left|F'(U)\right|\left(\frac{U_{xx}}{U_x}\right)^2$

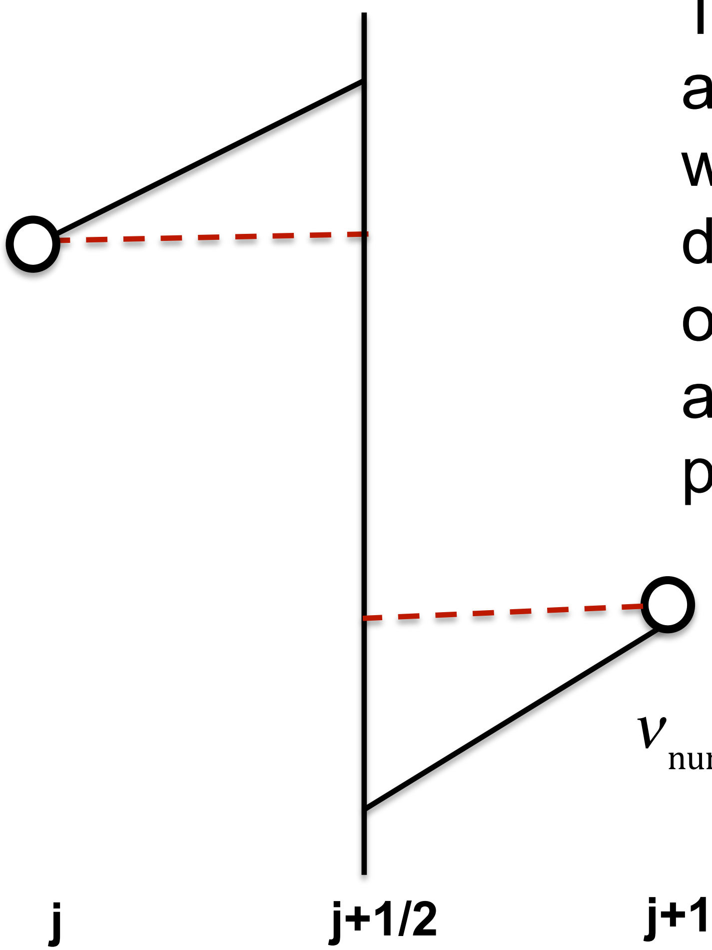
TVD or ENO

- 5th order $\nu_{\text{numerical}} = ch^5\left|F'(U)\right|\frac{\left(U_{xxx}\right)^2}{\left(U_x\right)^2}$

WENO

- 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.

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.

$$\nu_{\text{numerical}} = c_1 h^3 \left|F'(U)\right| \left|\frac{U_{xxx}}{U_x}\right| + c_2 h^3 \left|F'(U)\right| \left|\frac{U_{xxx}}{U_{xx}}\right| \frac{U_{xx}}{U_x}$$

$$c_1 = \tfrac{1}{6} > c_2 = \tfrac{1}{12} \text{ or } \tfrac{1}{24}$$

A consequence of no bounds on the "viscosity" coefficient!

Energy Analysis

$O(\Delta x)^2$

- Stick with 1-D for simplicity's sake

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

This is the "control volume" term

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

For convex fluxes this term produces appropriate entropy production congruent with important physical laws. (SS-LES)

Margolin, Len G., and William J. Rider. "A rationale for implicit turbulence modelling." *International Journal for Numerical Methods in Fluids* 39, no. 9 (2002): 821-841.

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

The dispersion term conserves energy

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

Analysis results - Variation

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

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

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

What about TV results for high resolution schemes?

- Upwind – variation diminishing term

$$-\lambda(\Delta x)\operatorname{sign}'(V)(V_x)^2$$

- Minmod

$$\lambda(\Delta x)^2\left(\operatorname{sign}'(V)\tfrac{1}{12}V_xV_{xx}-\tfrac{1}{4}\operatorname{sign}'(V_x)(V_{xx})^2\right)$$

- Third-order ENO

$$-\lambda(\Delta x)^3\operatorname{sign}'(V_{xx})(V_{xxx})^2\left[\tfrac{1}{12}\left(1+\operatorname{sign}(V)\operatorname{sign}(V_x)\right)+\tfrac{1}{24}\left(1+\operatorname{sign}(V_x)\operatorname{sign}(V_{xx})\right)\right]$$

- Third-order ENO-like scheme (uses the "comparison" principle described later)

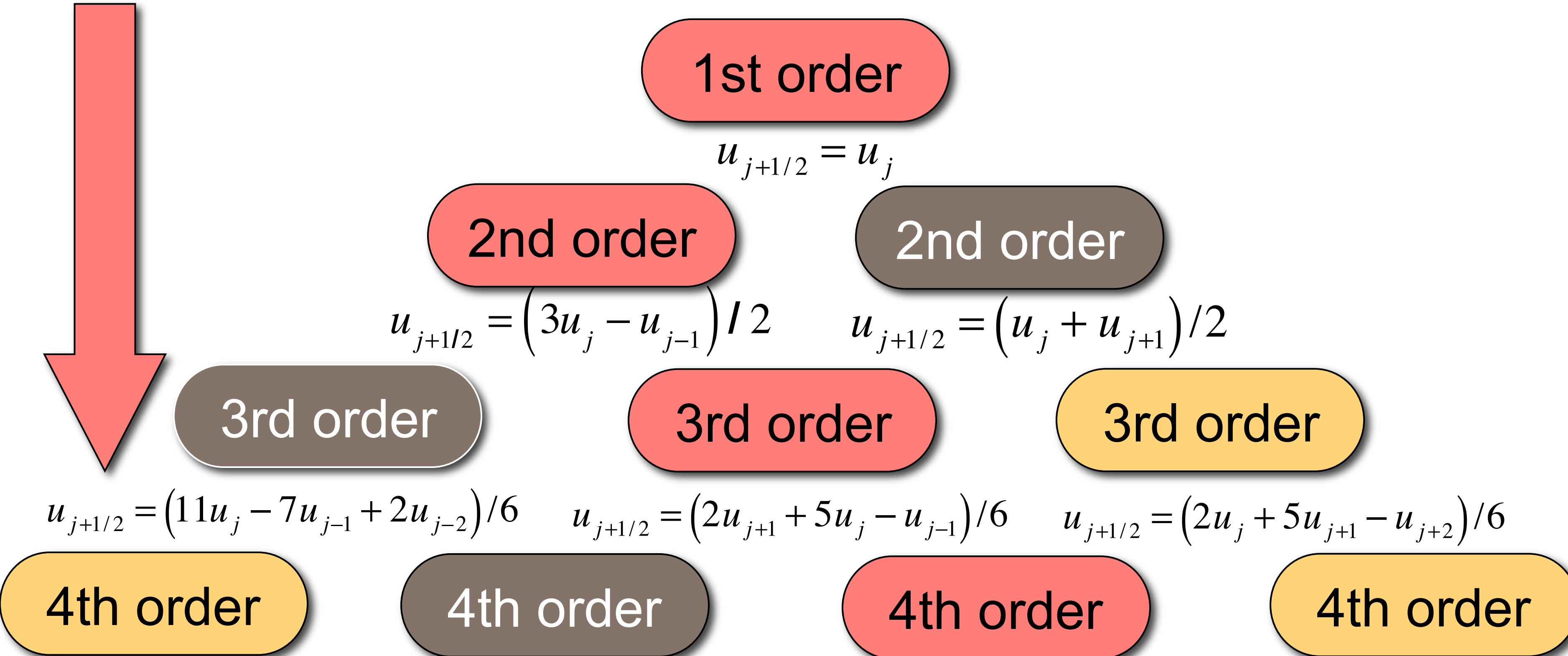
$$-\lambda\tfrac{1}{12}(\Delta x)^3\operatorname{sign}'(V_{xx})(V_{xxx})^2$$

- Fifth-order WENO

$$-\lambda(\Delta x)^5\operatorname{sign}'(V)\left(\frac{1}{60}V_{xxxxx}-\frac{1}{20}\frac{(V_x)^2(V_{xx})^2}{V^2}+\frac{1}{10}\frac{V_xV_{xx}V_{xxx}}{|V|}\right)$$

“The trick to forgetting the big picture is to look at everything close up.”
— Chuck Palahniuk

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

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

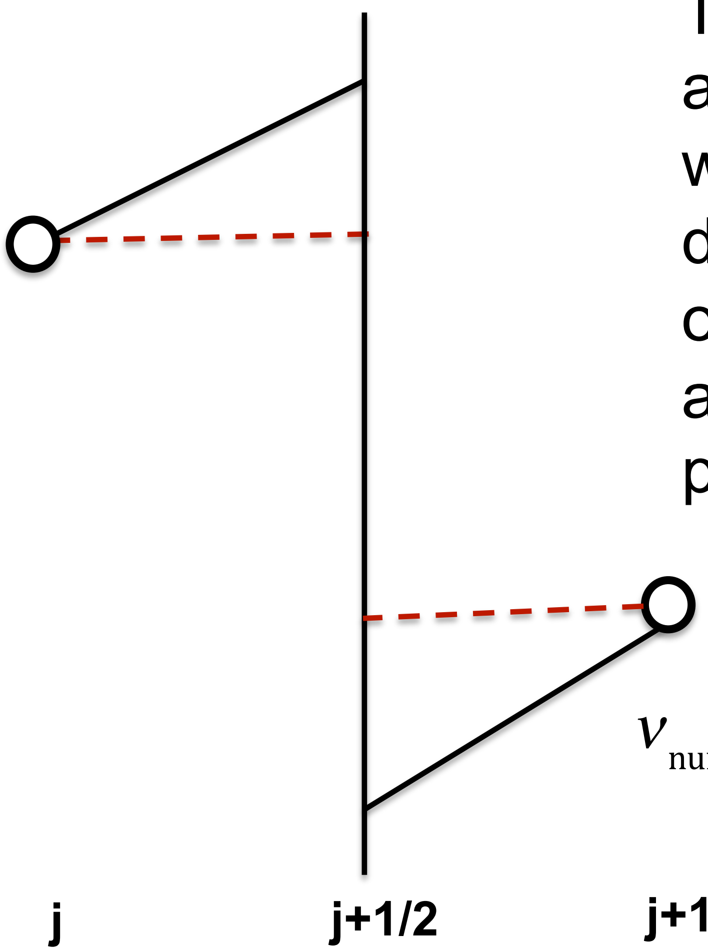
4th order | 4th order | 4th order | 4th order

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

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 (not always!) 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.

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.

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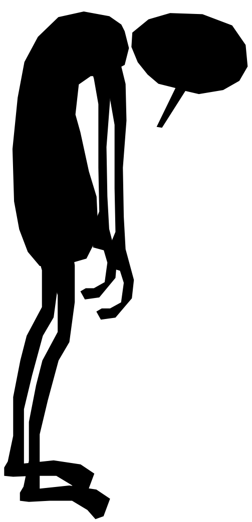
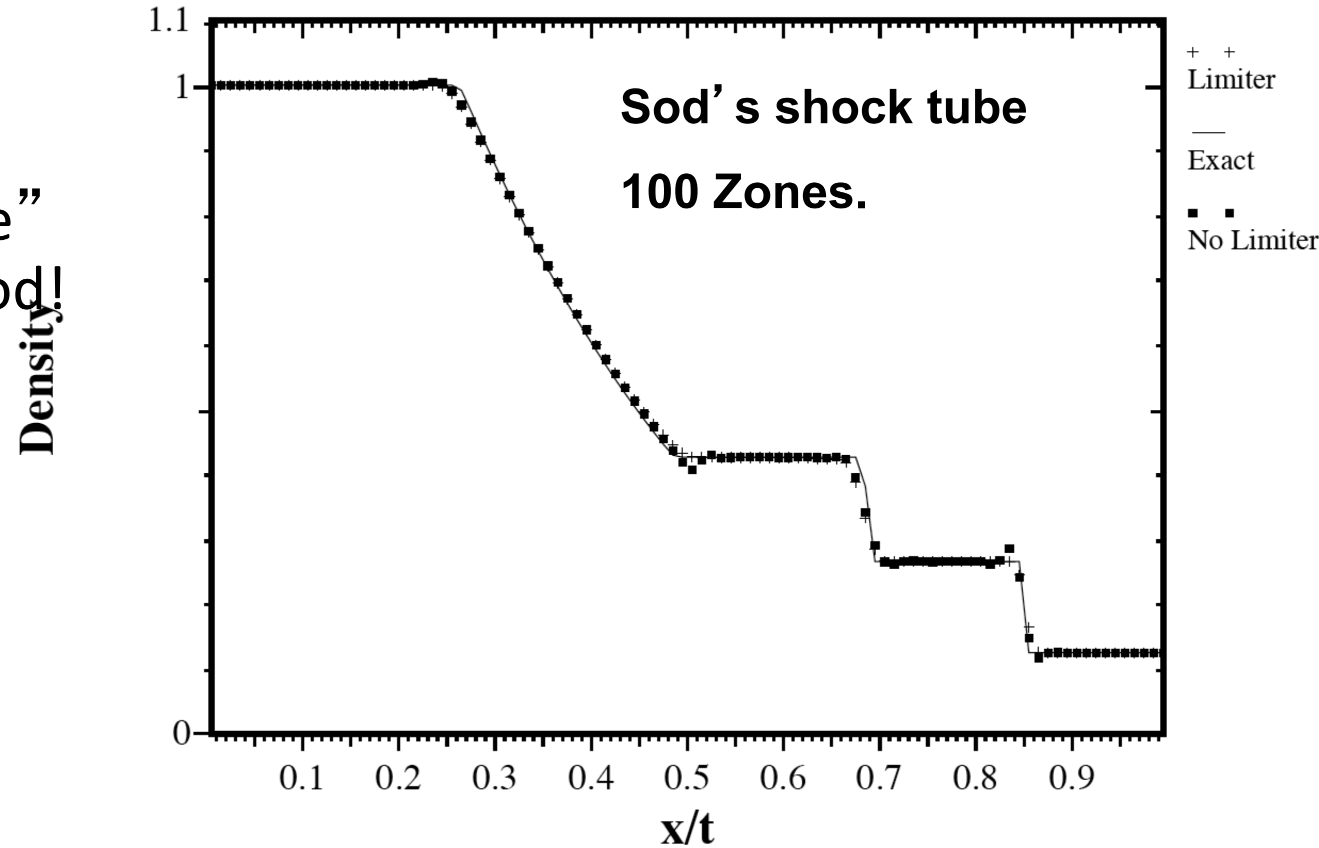
$c_1 = \frac{1}{6} > c_2 = \frac{1}{12}$ or $\frac{1}{24}$

A consequence of no bounds on the "viscosity" coefficient!

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!





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
  - Loss of second-order might be as detrimental too because of the value of the control volume term
- **Reason 3:** Use of much weaker nonlinear stability mechanisms and new potential instability mechanisms

“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.

An “ENO” method based on a TVD Comparison Principle

- The current ENO (and WENO) algorithms are based on the adaptive stencil approach that *recursively* finds the “smoothest” stencil.
- Use a different principle than the smoothest stencil - **Using a comparison with a TVD scheme to choose the high-order stencil.**
- 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 well-defined sense.
- Similar idea in principle to work by Suresh & Huynh, Rider Greenough & Kamm, and Colella & Sekora – all extrema preserving methods

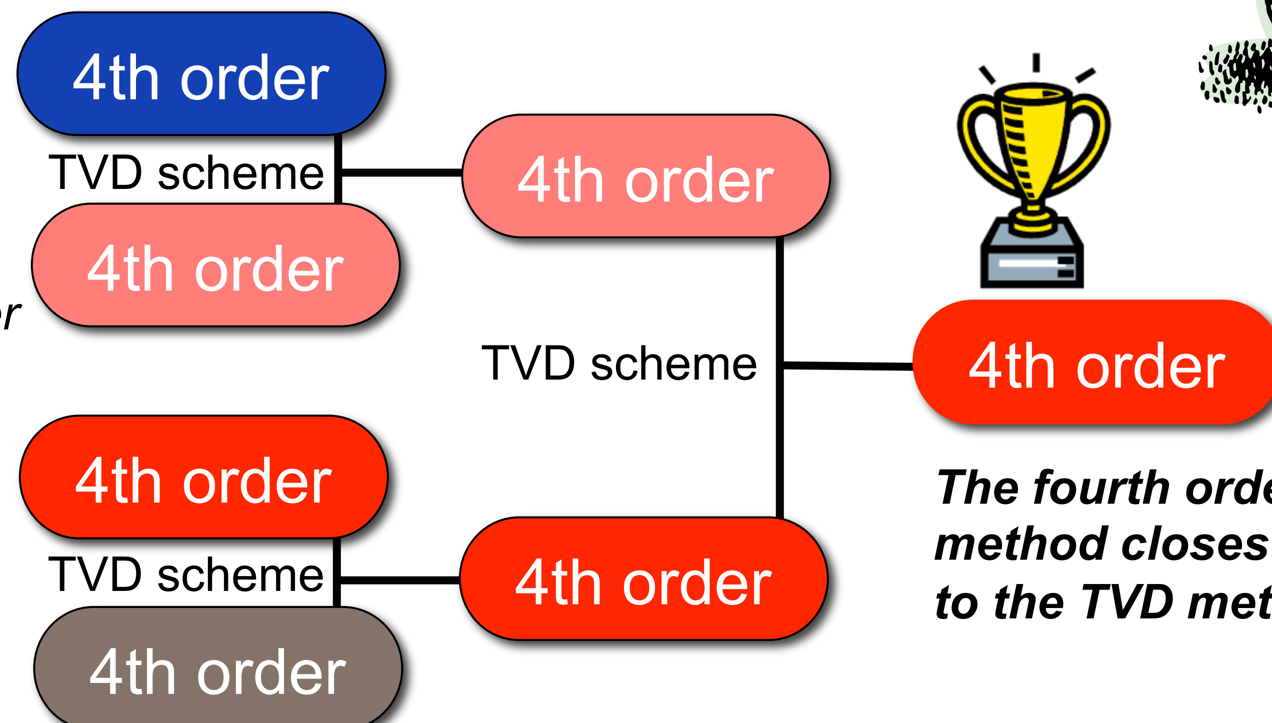
The TVD comparison algorithm can be arranged like a tournament

The TVD scheme chosen for comparison is used to test the "fitness" of each high-order method. The method's "fitness" is determined by its "closeness" to the TVD method.

One of these 4th order methods Is upstream-centered

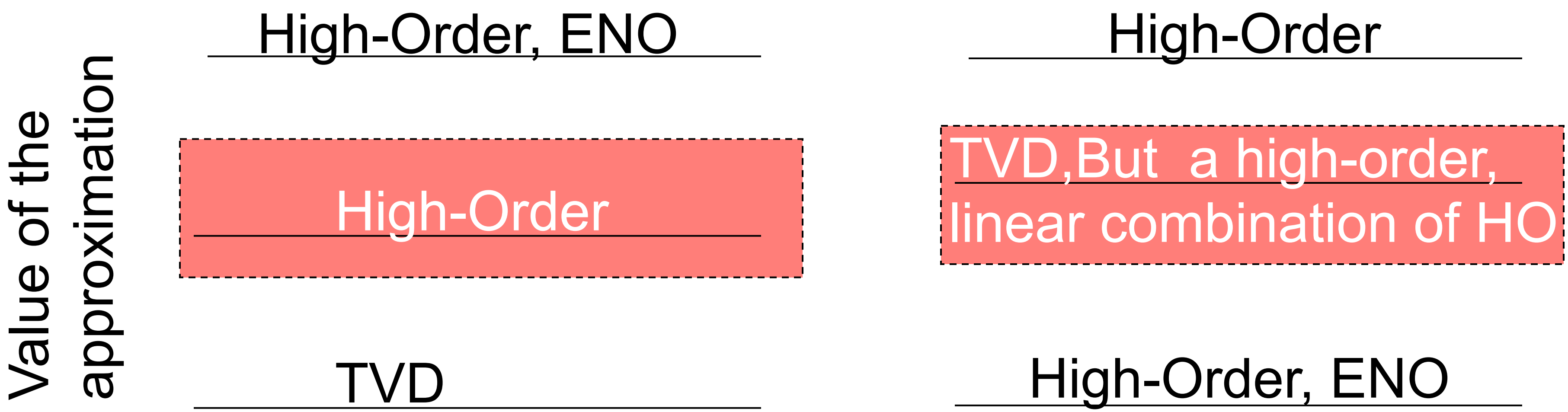
The same or another 4th order method would be the same as the ENO flux

We have <u>accuracy</u>, <u>linear</u> & <u>nonlinear</u> stability



The fourth order method closest to the TVD method

The median function bounds the different approximations.



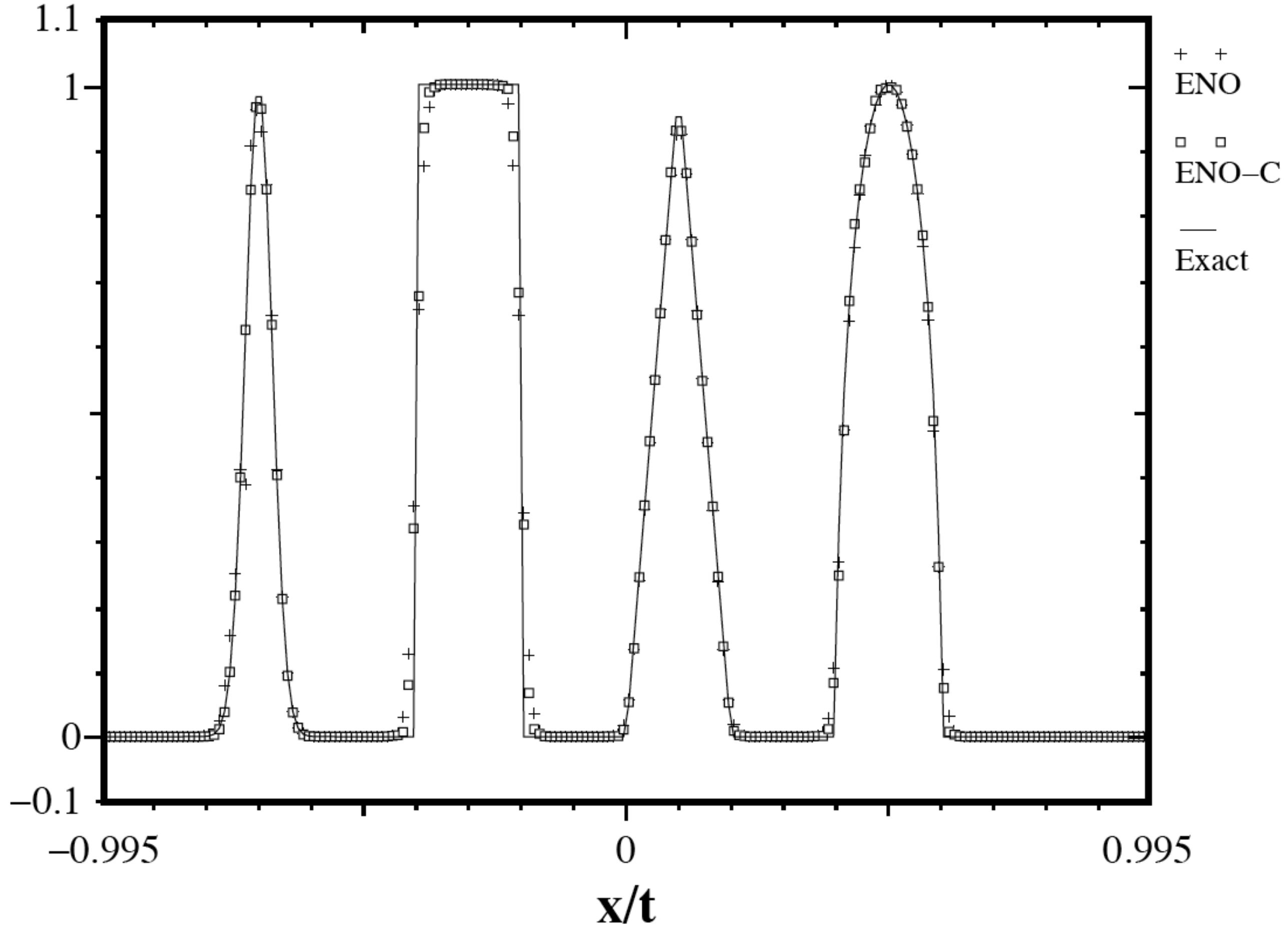
The median(a,b,c) returns the value bounded by the other two values. Preserves the accuracy given by at least two arguments.

Conjecture: If two arguments produce a linearly stable method, the **median** will as well.

Results: Accuracy on Scalar Waves

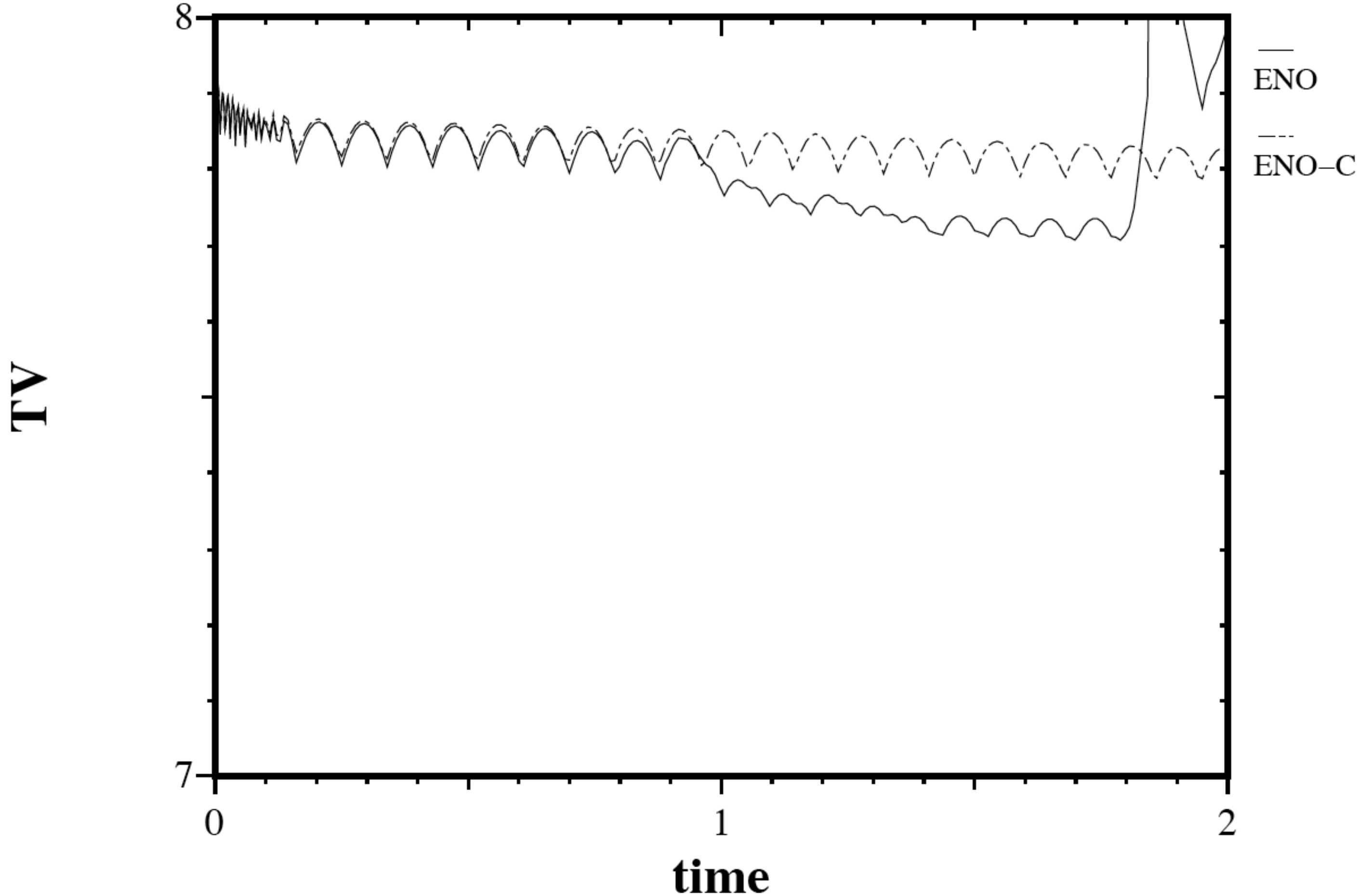
- Compare usual ENO with a comparison ENO

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



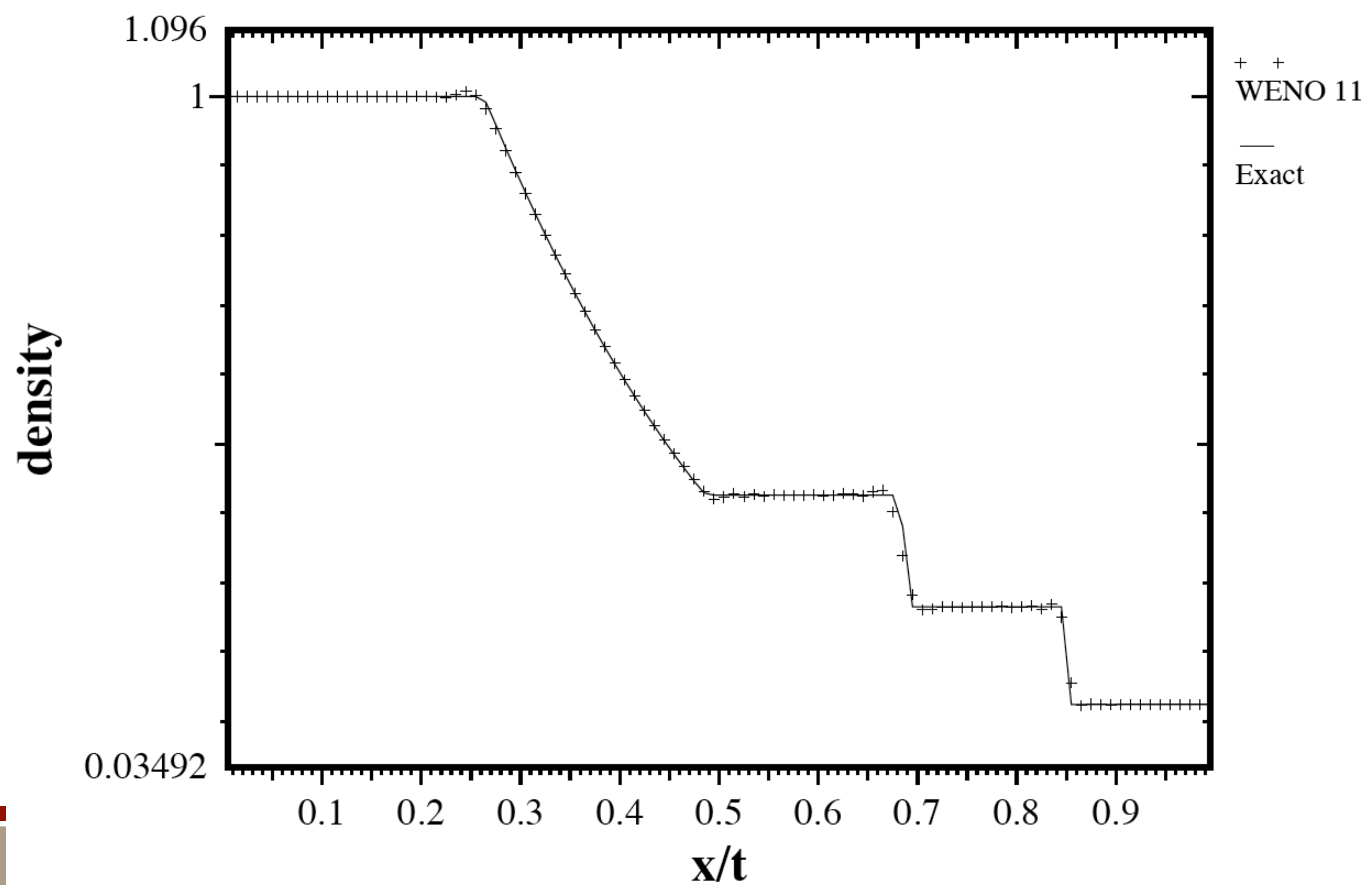
Results: Total Variation Behavior

- 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.



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

“Some people see the glass half full. Others see it half empty. I see a glass that's twice as big as it needs to be.”

— George Carlin

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