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The Relative Effectiveness of Different Approaches to High-Resolution Methods in Simulating Compressible Mixing

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What do we mean when we say Direct Numerical Simulation DNS?

- We are resolving all the length scales in the problem.
  - Energy bearing large scales
  - Diffusive small scales
  - Requires high-order accurate numerical methods (typically)
    - E.g. spectral methods for incompressible flow
    - High-order LES methods with Sub-grid scale models that can handle shocks and un- or under-resolved gradients
- Not just solving Navier-Stokes equations.

Question: What methods are best for computing compressible (turbulent) mixing?

Assuming computation of under-resolved flows (not DNS), essentially computing weak solutions. No MILES issues addressed.

- Defining the study goals in terms of scheme accuracy, efficiency and high-resolution.
- Previous work leading to this study
- Results that support our conclusions
- The Answer (details not addressed today)

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Discontinuities are special: weak solutions have some important requirements*

- *The Lax-Wendroff theorem is one of the few rigorous theoretical results to rely upon,*
  - If the scheme is in conservation form then the solutions converge to a weak solution (not unique!),
  - and if an entropy condition is satisfied the unique solution can be found.
- Without conservation all bets are off!

***Lax & Wendroff, *Comm. Pure Appl. Math.*, 13 1960. Also see R.J. Leveque, Numerical Methods for Conservation Laws**

There is a corollary to these requirements

- *Some methods evolve internal energy or temperature (not a conservation law) in an attempt to keep a solution on the correct adiabat.*
- *BUT in the presence of shocks all bets are off is you give up conservation.*

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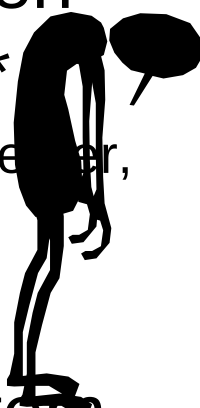
Discontinuities are special: first order accuracy is expected.

- For *coupled systems* (even linear) with *discontinuities* high-order accuracy is lost between characteristics emanating from the discontinuity*
  - Several recent works have re-confirmed this result (Osher, Carpenter, *Greenough & Rider*)
  - Can be overcome is very restrictive special cases‡



- Generally with smooth data and a nonlinear system of hyperbolic conservation laws a discontinuity (i.e., shock) will eventually form
  - *Therefore the loss of accuracy is virtually inevitable!*

***Majda & Osher, *Comm. Pure Appl. Math.*, 30 1977.**

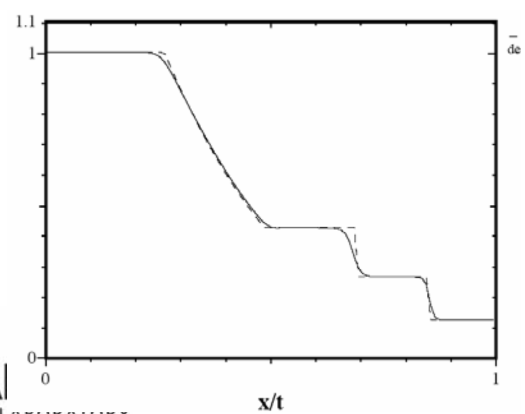
‡Siklosi & Kriess, SIAM J. Num. Anal., 41, 2003.

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

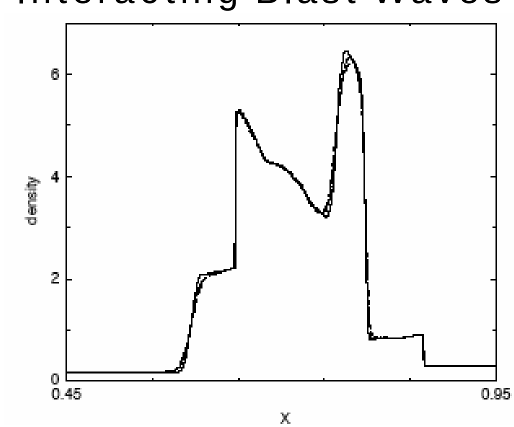
***Greenough & Rider, *J. Comp. Phys*. 196(1), 259-281, 2004.**

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

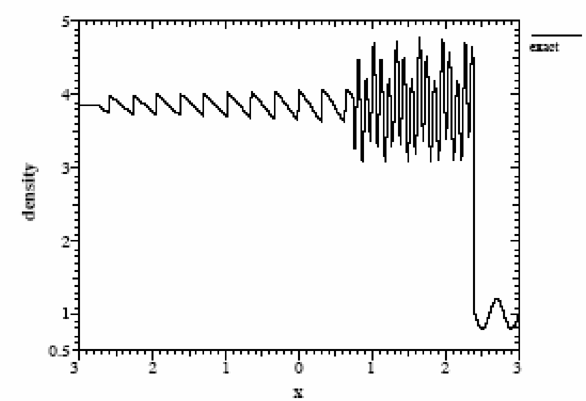
Sod's Shock Tube



Interacting Blast Waves



Shu-Osher Entropy Wave



There are several working definitions for relative efficiency

- Want to be able to ***quantitatively*** compare methods

  - *Determine the error (some norm and the “true” solution”).*

  - *Determine the cost to achieve that error (CPU time).*

How much relative effort must be expended to compute a solution of a given accuracy?

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There are several working definitions for relative efficiency

- A function of the cost of a solution on a given grid and the relative accuracy *with same rate of convergence*

$$\eta = (\mathbf{cost})(\mathbf{RE})^{(\mathbf{d}+\mathbf{1})/\mathbf{n}}$$

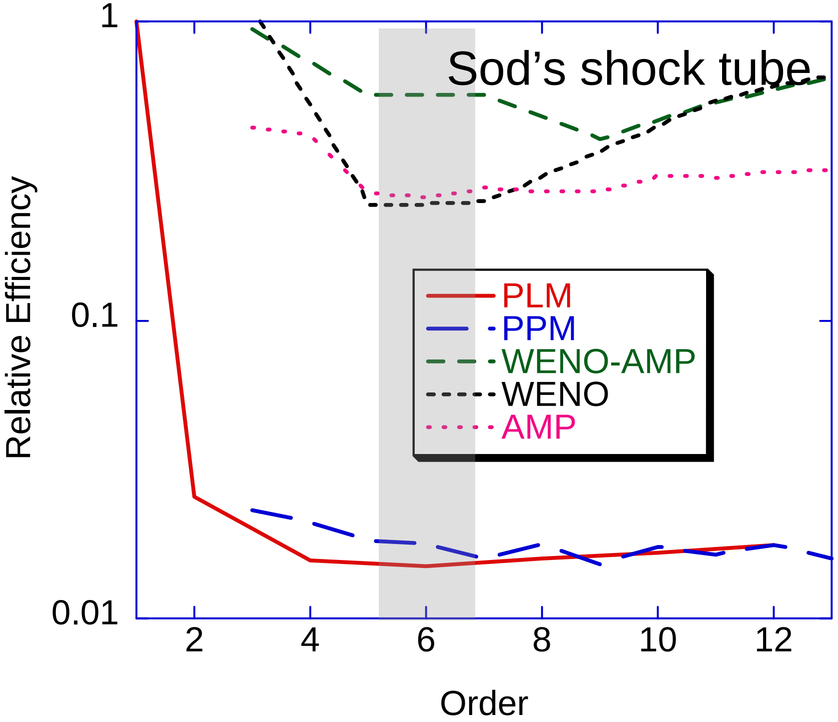
  - Where d=dimension, n=convergence rate, RE = Relative error with Error = Ah^n
  - Smaller is better

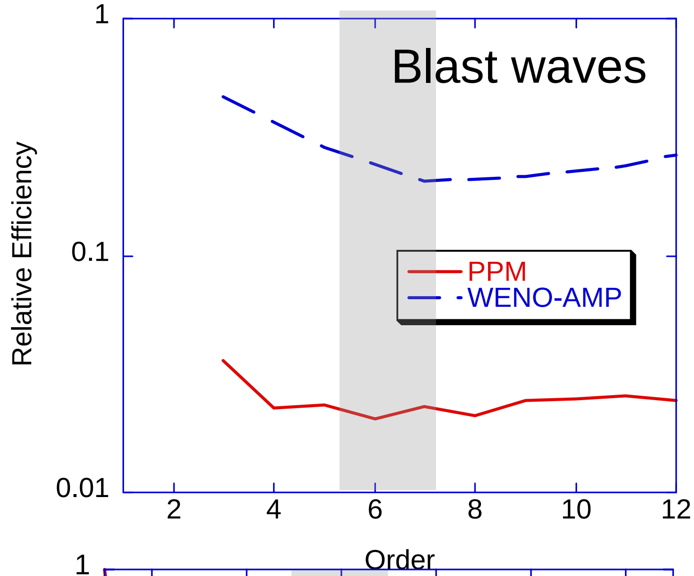
How much relative effort must be expended to compute a solution of a given accuracy?

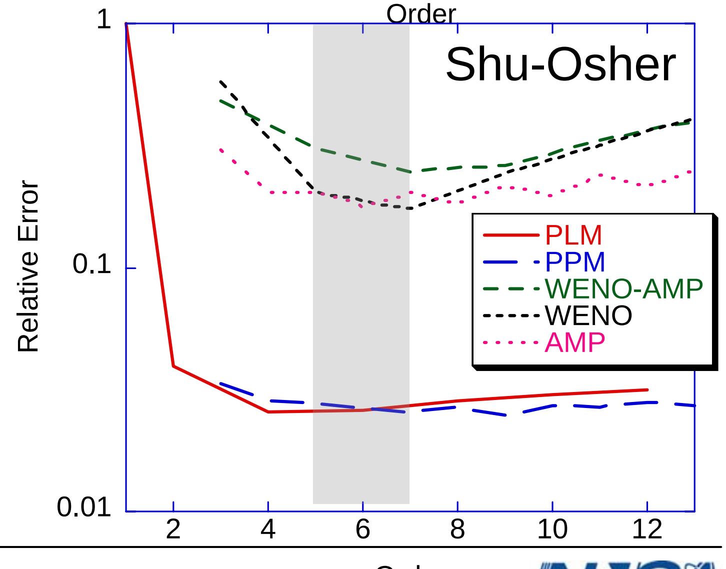
Greenough and Rider's results in terms of measured efficiency.

- Gaussian Pulse linear advection
  - WENO5 5th order accurate versus 2nd order accurate (1st order in L_∞) for PLM, WENO5 will almost always win.
- Sod's Shock Tube
  - PLM - 1.00, WENO5 - 22.8
- Interacting Blast Waves
  - PLM - 1.00, WENO5 - 8.17
- Shu-Osher shock entropy interaction
  - PLM - 1.00, WENO5 - 2.77

High-order efficiency: All problems show a saturation as order increases (5th-7th).







The shaded box shows the "sweet spot" for efficiency.

We extract the best of each type of method and attempt to construct something "better"

- The need for method nonlinearity is a consequence of Godunov's theorem:
  - A *linear* method cannot be second-order and monotone… but a *nonlinear* method can be second-order and monotone.
- *Hybridize* the nonlinear monotone/non-oscillatory methods
  - Start with a nonlinear monotone method (e.g., PLM or PPM)
  - If the solution is *not monotone locally,* then use the median of the high-order stencil, the monotone stencil, and a ENO/WENO stencil
  - We denote the new methods by "xPLM" or "xPPM", where "x" stands for "extreme"

Logically all things are created by a combination of simpler, less capable components

- Let the older high-resolution methods constitute the "*simpler, less capable*" components!

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Methods we consider in this study.

- Nonlinear Monotone - High-resolution Godunov-type
  - **PLM** - Piecewise Linear MUSCL.
  - **PPM** - Piecewise Parabolic MUSCL.
- Non-Oscillatory - Does not degenerate to 1st order
  - **WENO** - Weighted Essentially Non-Oscillatory - Nth order (5th order WENO is very popular)
- Nonlinear Monotone coupled to Non-Oscillatory via accuracy, monotonicity and extrema preserving limiters (i.e. combine Godunov-type and ENO/WENO)
  - **xPLM** - Extreme Piecewise Linear Method*
  - **xPPM** - Extreme Piecewise Parabolic Method*

***It could also be "Extended".**

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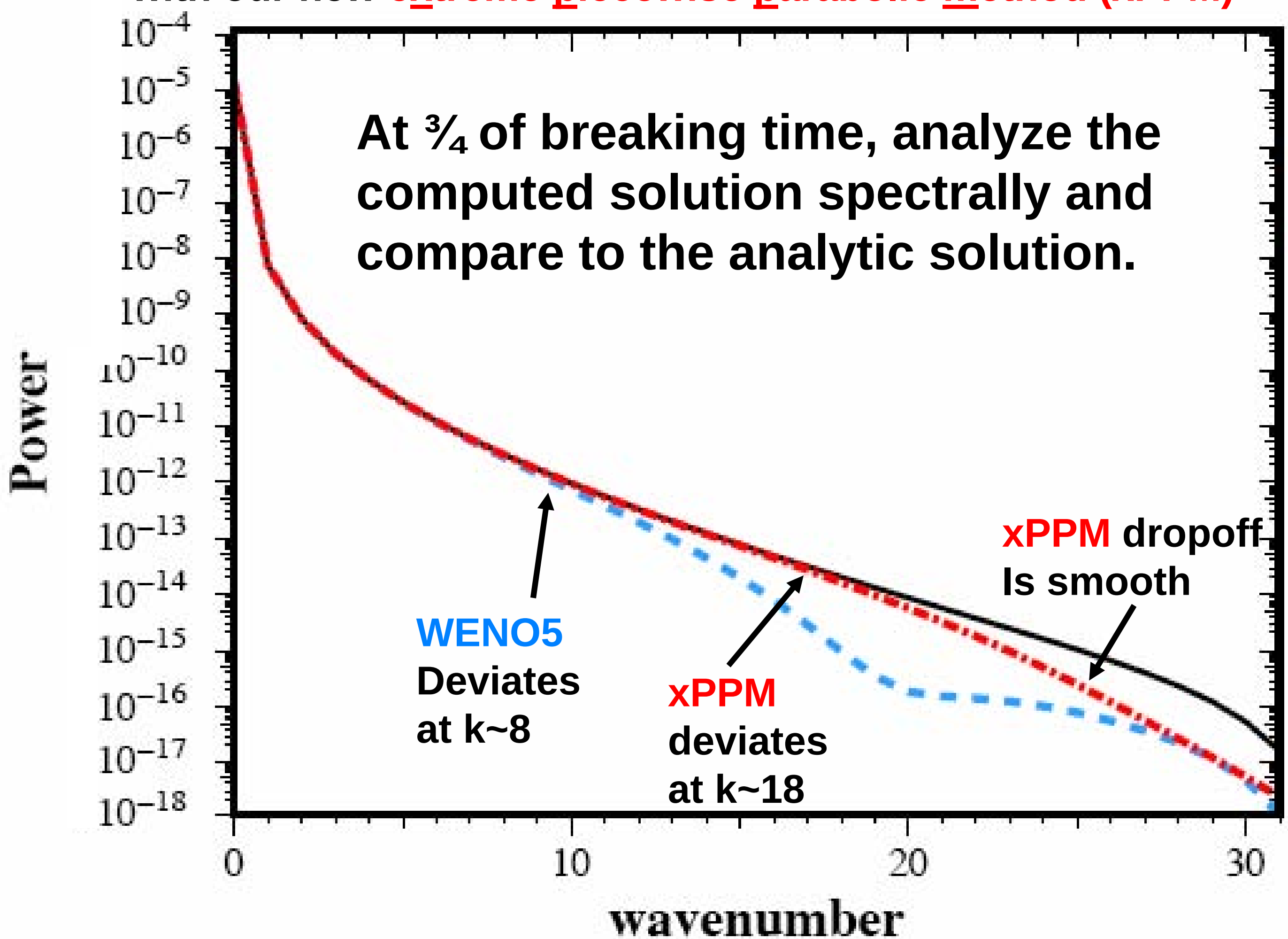
What's the impact? Look at a smooth wave-breaking problem spectrally.

Compare the 5th order weighted essentially non-oscillatory method (WENO5) with our new extreme piecewise parabolic method (xPPM)



Exact
WENO5
xPPM

The new algorithms lead to increased fidelity and better behavior where accuracy is lost. These properties equate to better efficiency and improved physical modeling.

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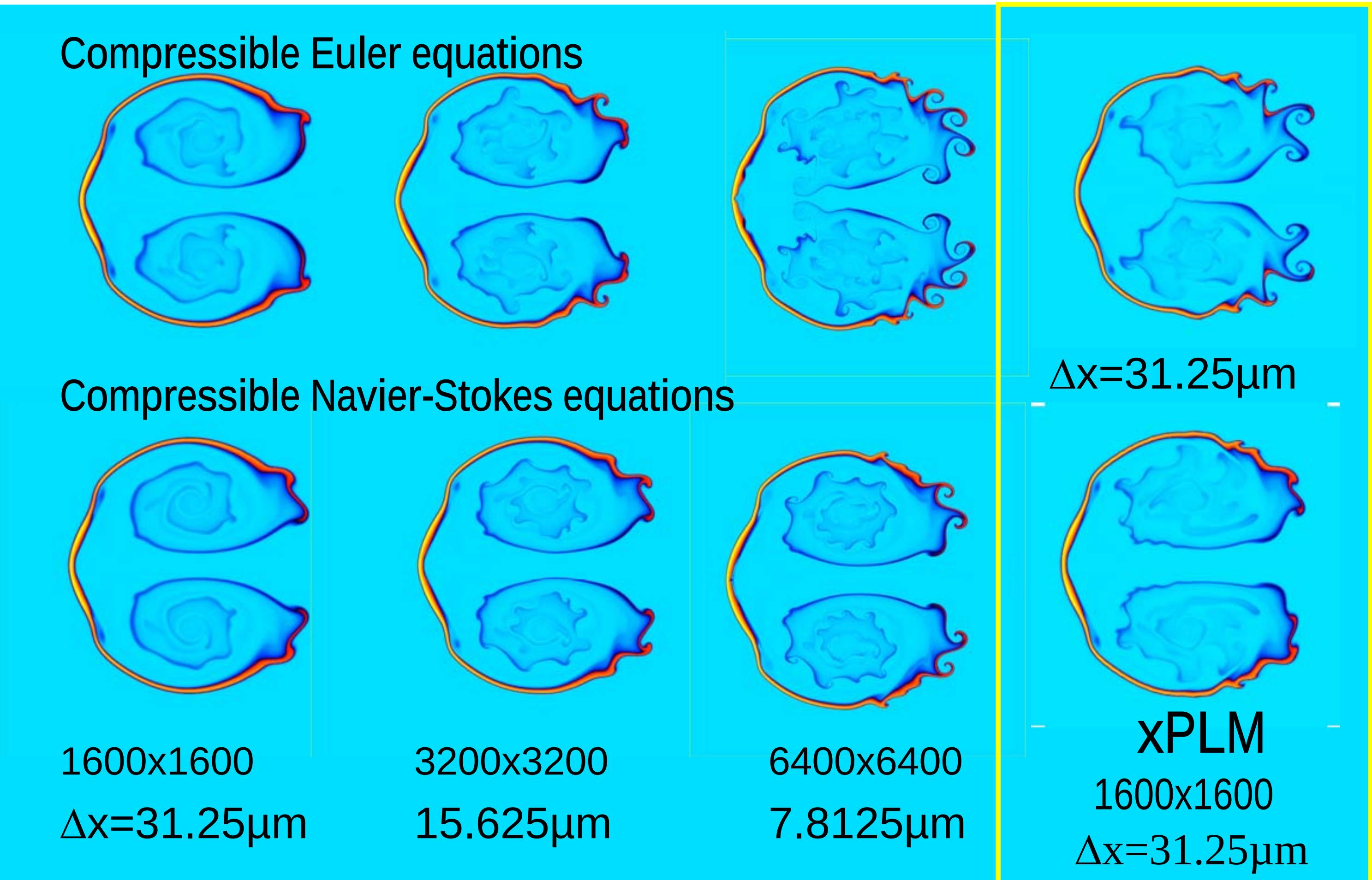
Ideal shock/cylinder problem. The new methods are approximately 30 times more efficient in 2-D.

- Our new methods improve efficiency dramatically!



(New methods are now implemented in LLNL AMR Code Raptor)

The results on the Δx=31.25μm mesh are roughly equivalent to those found on a Δx=10μm mesh with the older method.

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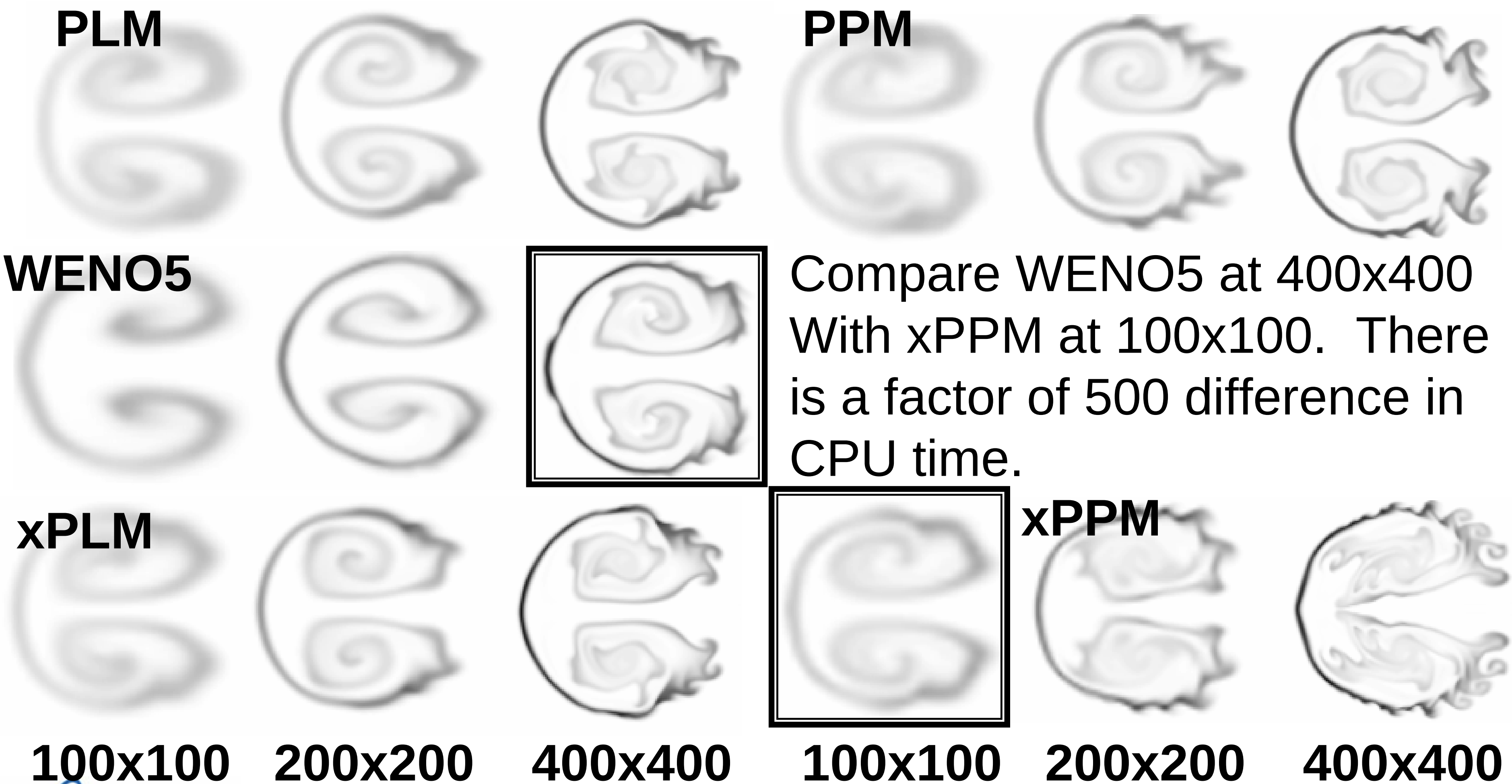
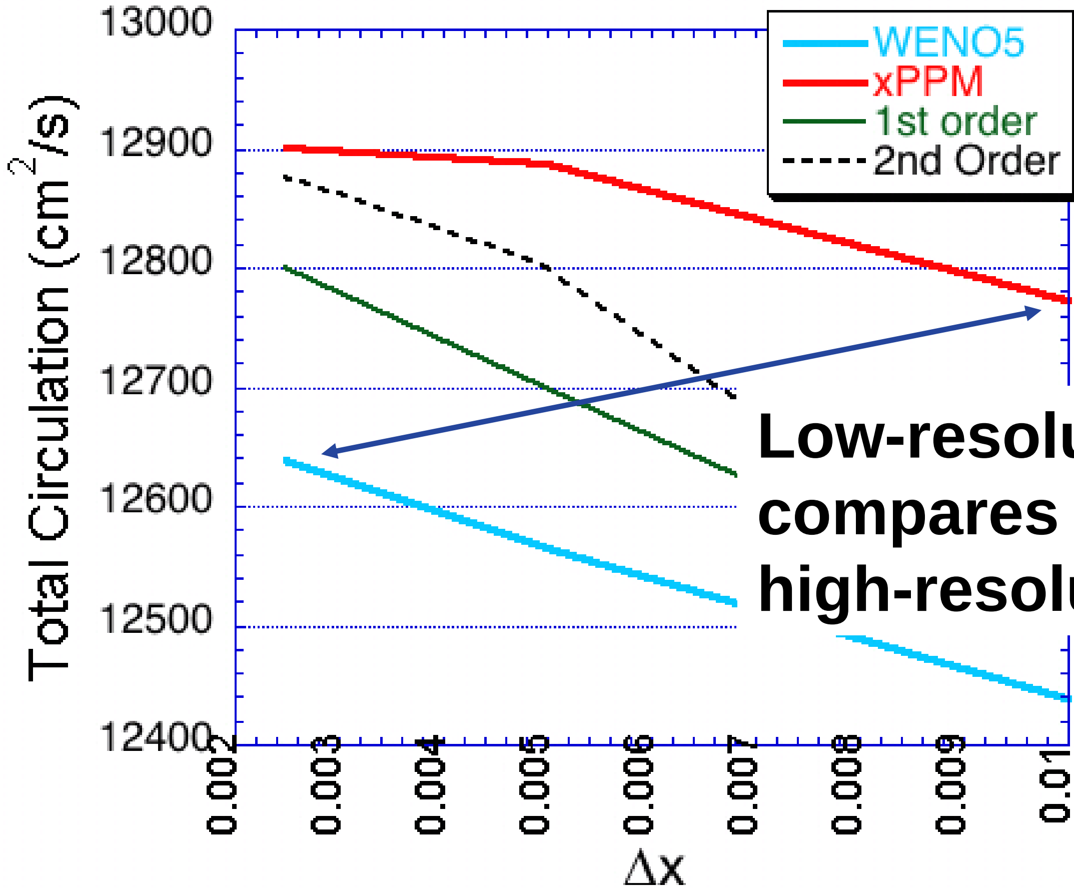
Mesh Convergence Study for all five methods. xPPM is best, WENO5 is worst.



Compare WENO5 at 400x400 With xPPM at 100x100. There is a factor of 500 difference in CPU time.

Calculation Verification: mesh convergence for the shocked cylinder

- Using the standard problem, idealized shock/cylinder, we ran three grids: 100^2, 200^2, 400^2, and examined integral quantities.



Low-resolution xPPM compares with high-resolution WENO

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What about 3-D? Use the Taylor-Green Vortex problem to test.

- The results are mostly the same, WENO is relatively inefficient compared with PLM/PPM.
  - WENO is about one mesh resolution less resolved than PLM/PPM,
  - And two less than xPLM and xPPM
- Shown below are entropy errors and relative CPU time.

T=2						T=10				
Grid	PLM	PPM	WENO	xPLM	xPPM	PLM	PPM	WENO	xPLM	xPPM
32^3	4.0e-04	1.5e-04	9.e-04	2.6e-04	5.0e-04	0.030	0.029	0.039	0.029	0.026
64^3	4.4e-05	1.2e-05	7.4e-05	3.7e-05	7.0e-06	0.024	0.022	0.030	0.023	0.021
CPU	1.00	0.93	17.00	1.30	1.45	15.35	14.21	261.0	19.93	22.22

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What methods are best for computing compressible (turbulent) mixing?

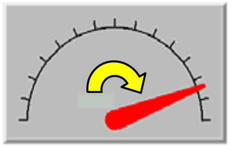
- Formal accuracy does not necessarily produce better of more efficient solutions. High-order algorithmic elements do improve algorithmic efficiency.
- Single step high-resolution Godunov methods faired best in all tests.
  - PPM outperforms PLM in terms of efficiency.
  - Accuracy and Extrema preserving limiters add additional resolution efficiently for test problems
- Weighted ENO methods based on R-K integrators do not perform well in comparison to (x)PLM or (x)PPM.

Algorithmic efficiency can significantly impact computational effort

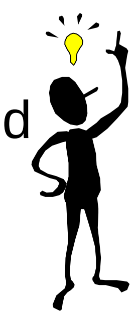
- Goal: to decrease the numerical errors by 50%
- There are basically three approaches:

You must do *all* of these!

1. Get a (significantly) bigger computer
   - For our problems, solutions are converging at ~1st order
   - Therefore, you need a factor of 2 per dimension (space and time): for time-dependent 3-D simulations this implies 16 times more total effort (~8 w/AMR) and 8 times the memory (~4 w/AMR)



2. Make the existing algorithm more efficient
   - You still have a problem, however, if the simulation will not fit in memory
   - Can we really make things an order of magnitude faster?



3. Design a more accurate algorithm
   - Verification can help guide such algorithm development and measure its impact

***"As machines become more powerful, the efficiency of algorithms grows more important, not less"* - Nick Trefethen**

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BEGIN BACKUP SLIDES

Examples of show how factors in algorithms and solutions effect the efficiency

- Take n=2, d=3, R.E. = 1/2, cost = 2
  - η=1/2
- Take n=1, d=3, R.E. = 1/2 , cost = 2
  - η =1/8
- Take n=1/2, d=3, R.E. = 1/2 , cost = 2
  - η =1/128
- Take n=1/2, d=1, R.E. = 1/2 , cost = 2
  - η =1/8

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An advantage of PPM: It asymptotically preserves limit solutions

- If one looks at solutions where there is asymptotic structure, the truncation error can inhibit convergence, unless the small scale structure is resolved. PLM does this! WENO5 does this!
  - PPM: Continuous edge values as $\Delta \mathbf{t} \rightarrow 0$
- Example 1 - Reaction system with a diffusive limit

$$\partial_t \mathbf{u} + \partial_x \mathbf{v} = 0; \partial_t \mathbf{v} + \frac{1}{\varepsilon^2} \partial_x \mathbf{u} = -\frac{1}{\varepsilon^2} \mathbf{v} \Rightarrow \partial_t \mathbf{u}^{(0)} - \partial_x^2 \mathbf{u}^{(0)} = 0$$

- Example 2 - Acoustics in the zero(low)-Mach limit

$$\partial_t \mathbf{u} + \partial_x \mathbf{v} = 0; \partial_t \mathbf{v} + \frac{1}{\varepsilon^2} \partial_x \mathbf{u} = \mathbf{0}; \lambda = \pm \frac{1}{\varepsilon}$$

- This may explain different structural character of PPM solutions

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There is a handful of basic elements of dethod design

Weighted ENO Method

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

High-Order Godunov

- Riemann solver
- Characteristic Projection
- High-order differencing
- Limiter
- Time-centering

Weighted ENO methods can have very high formal order of accuracy.

- A nonlinear convex combination of schemes - 3-3rd order to a 5th order, 4-4th order to a 7th order…
- Nonlinearity with smoothness detectors

$$f(u) = f^{-}(u) + f^{+}(u), f^{\pm}(u) = \tfrac{1}{2}\left(f(u) \pm \alpha u\right)$$

$$u^{(1)} = u^{n} + \Delta t L\left(u^{n}\right)$$

$$u^{(2)} = \frac{3}{4}u^{n} + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L\left(u^{(1)}\right)$$

$$u^{n+1} = \frac{1}{3}u^{n} + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L\left(u^{(2)}\right)$$

$$L = -\frac{1}{h}\left(f_{j+1/2} - f_{j-1/2}\right)$$

$$\omega_k = \frac{w_k}{\sum_m w_m} \qquad w_k = \frac{C_k}{(IS_k + \varepsilon)^p}$$

$$f_{j+1/2} = \sum_m \omega_m f^{m}_{j+1/2,m}$$

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5th Order WENO is the most commonly used form of this method.

- Start with smoothness measures

$$IS_k = \sum_{l=1}^{r-1} \int_{x_{j-1/2}}^{x_{j+1/2}} h^{2l-1} \left(q_k^{(l)}\right)^2 dx$$

$$IS_1 = \tfrac{13}{12}\left(f_{j-2} - 2 f_{j-1} + f_j\right)^2 + \tfrac{1}{4}\left(f_{j-2} - 4 f_{j-1} + 3 f_j\right)^2$$

- 3rd Order fluxes

$$f_{j+1/2,1} = \frac{1}{3} f_{j-2} - \frac{7}{6} f_{j-1} + \frac{11}{6} f_j$$

$$f_{j+1/2,2} = -\frac{1}{6} f_{j-1} + \frac{5}{6} f_j + \frac{1}{3} f_{j+1}$$

$$f_{j+1/2,3} = \frac{1}{3} f_j + \frac{5}{6} f_{j+1} - \frac{1}{6} f_{j+2}$$

- Constants to give 5th order

$$C_1 = 1, C_2 = 6, C_3 = 3$$

$$f_{j+1/2,\mathrm{HO}} = \frac{1}{30} f_{j-2} - \frac{13}{60} f_{j-1} + \frac{47}{60} f_j + \frac{9}{20} f_{j+1} - \frac{1}{20} f_{j+2}$$

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The PPM method is based on polynomial interpolation.

- We find a parabolic interpolant

$$\mathbf{w}(x) = p(\theta) = p_0 + p_1\theta + p_2\theta^2; \theta = \left(x - x_j\right)/\Delta x$$

- Where

$$p_0 = \tfrac{3}{2}\mathbf{w}_j - \tfrac{1}{4}\left(\mathbf{w}_{j-1/2} + \mathbf{w}_{j+1/2}\right)$$

$$p_1 = \mathbf{w}_{j+1/2} - \mathbf{w}_{j-1/2}$$

$$p_2 = 3\left(\mathbf{w}_{j-1/2} + \mathbf{w}_{j+1/2}\right) - 6\mathbf{w}_j$$

In the original PPM the edges were found by a fourth-order formula

- The edges simplify to the following

$$\mathbf{w}_{j+1/2} = \frac{7\left(\mathbf{w}_{j} + \mathbf{w}_{j+1}\right) - \left(\mathbf{w}_{j-1} + \mathbf{w}_{j+2}\right)}{12}$$

Other high-order edge values can be used.

- First compute the edge values: Sixth-order centered

$$\mathbf{w}_{j+1/2} = \frac{37\left(\mathbf{w}_j + \mathbf{w}_{j+1}\right) - 8\left(\mathbf{w}_{j-1} + \mathbf{w}_{j+2}\right) + \left(\mathbf{w}_{j-2} + \mathbf{w}_{j+3}\right)}{60}$$

- Seventh-order upwind

$$\mathbf{w}_{j+1/2} = \frac{-3\mathbf{w}_{j-3} + 25\mathbf{w}_{j-2} - 101\mathbf{w}_{j-1} + 319\mathbf{w}_j + 214\mathbf{w}_{j+1} - 38\mathbf{w}_{j+2} + 4\mathbf{w}_{j+3}}{420}$$

- Seventh-order parabolic

$$\mathbf{w}_{j+1/2} = \frac{-111\mathbf{w}_{j-3} + 849\mathbf{w}_{j-2} - 3010\mathbf{w}_{j-1} + 8510\mathbf{w}_j + 6645\mathbf{w}_{j+1} - 1349\mathbf{w}_{j+2} + 148\mathbf{w}_{j+3}}{11520}$$

- Six-point optimal stencil [0,3π/4]

$$\mathbf{w}_{j+1/2} = a\left(\mathbf{w}_j + \mathbf{w}_{j+1}\right) + b\left(\mathbf{w}_{j-1} + \mathbf{w}_{j+2}\right) + c\left(\mathbf{w}_{j-2} + \mathbf{w}_{j+3}\right)$$

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

In the original PPM the edges tested for their production of a monotone interpolant.

- One follows this step with checking monotonicity
  - Make sure that $w_{j+1/2}$ is between w_j and w_{j+1}
  - Next make sure the polynomial is monotone, the original expression is not clear, but this amounts to making sure that $w_{j+1/2}$ is between w_j and $3w_j - 2w_{j-1/2}$
- Our new method uses a bounding function, median(a,b,c) that returns the middle argument
  - The one that is bounded by the other two
  - If two arguments are $O(h^n)$ the median is too!

Monotonicity

- Standard montonticity can be implemented with two steps at each edge,

$$\mathbf{w}_{j\pm1/2} := \mathbf{median}\left(\mathbf{w}_j, \mathbf{w}_{j\pm1/2}, \mathbf{w}_{j\pm1}\right)$$

$$\mathbf{w}^M_{j\pm1/2} = \mathbf{w}_{j\pm1/2} := \mathbf{median}\left(\mathbf{w}_j, \mathbf{w}_{j\pm1/2}, 3\mathbf{w}_j - 2\mathbf{w}_{j\mp1/2}\right)$$

ENO or WENO values could just as easily be used.

- Stencils are precomputed (like WENO) and selected hierarchically using the differences in between stencils to select the smoothest (first 2nd order, then 3rd, then 4th, ...)

$$\mathbf{w}^{2nd}_{j+1/2} = \frac{\left(\mathbf{w}_j + \mathbf{w}_{j+1}\right)}{2}; \frac{\left(3\mathbf{w}_j - \mathbf{w}_{j-1}\right)}{2}$$

$$\mathbf{w}^{3rd}_{j+1/2} = \frac{\left(2\mathbf{w}_{j-2} - 7\mathbf{w}_{j-1} + 11\mathbf{w}_j\right)}{6}; \frac{\left(-\mathbf{w}_{j-1} + 5\mathbf{w}_j + 2\mathbf{w}_{j+1}\right)}{6};$$

$$\frac{\left(2\mathbf{w}_j + 5\mathbf{w}_{j+1} - \mathbf{w}_{j+2}\right)}{6}$$

- WENO is like that in the literature, but not on fluxes.

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Time-Centering

- This is done using a time-integral form

$$\mathbf{w}_{j+1/2}^{n+1/2} = \frac{1}{\nu} \int_{1/2}^{1/2-\nu} p(\theta) d\theta$$

$$\mathbf{w}_{j-1/2}^{n+1/2} = \frac{1}{-\nu} \int_{-1/2}^{-1/2-\nu} p(\theta) d\theta$$

- Specifically it evaluates to

$$\mathbf{w}_{j+1/2}^{n+1/2} = p(1/2) - \tfrac{\nu}{2} p_1 + \left(-\tfrac{\nu}{2} + \tfrac{\nu^2}{3}\right) p_2$$

$$\mathbf{w}_{j-1/2}^{n+1/2} = p(-1/2) - \tfrac{\nu}{2} p_1 + \left(\tfrac{\nu}{2} + \tfrac{\nu^2}{3}\right) p_2$$

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Finishing Up

- Solve the Riemann problem to get single valued solutions and fluxes

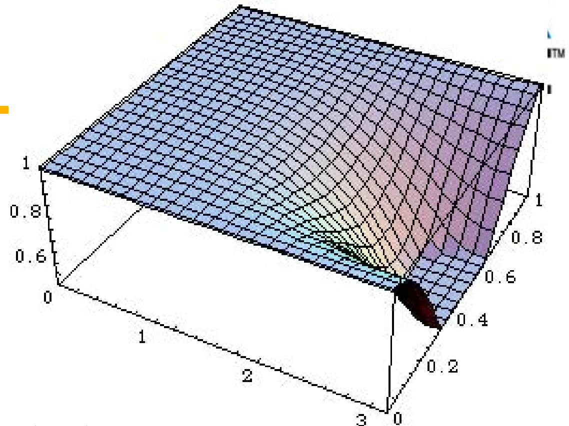
$$\mathbf{U}_{j+1/2}^{n+1/2} = \mathbf{riemann}\left(\mathbf{U}_{j+1/2;-}^{n+1/2}, \mathbf{U}_{j+1/2;+}^{n+1/2}\right)$$

- Update the conserved variables

$$\mathbf{U}_{j}^{n+1} = \mathbf{U}_{j}^{n} - \tfrac{\Delta t}{\Delta x}\left(\mathbf{F}\left(\mathbf{U}_{j+1/2}^{n+1/2}\right) - \mathbf{F}\left(\mathbf{U}_{j-1/2}^{n+1/2}\right)\right)$$

Scheme Stability & Truncation Error is exceptional

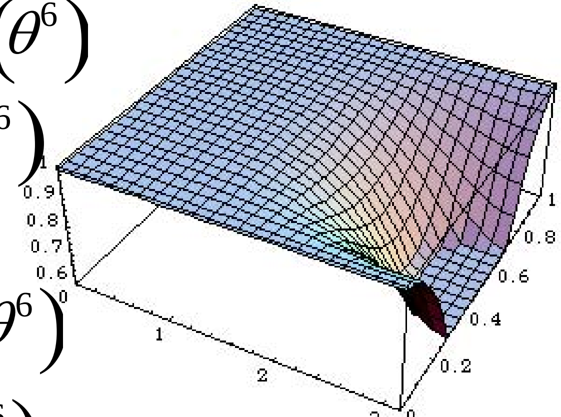
- Using Fourier analysis:
  - All stable to CFL=1



- Fourth-order edges
  - Amplitude
  - Phase

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

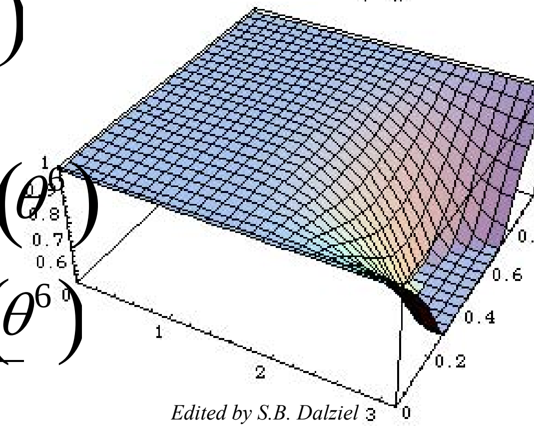
$$P \approx 1 + \left(-\frac{1}{30} + \frac{\nu}{12} - \frac{\nu^3}{12} + \frac{\nu^4}{30}\right)\theta^4 + O\left(\theta^6\right)$$



- Sixth-order edges
  - Amplitude
  - Phase

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

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



- Seventh-order edges
  - Amplitude
  - Phase

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

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

Los Alamos NATIONAL LABORATORY EST. 1943

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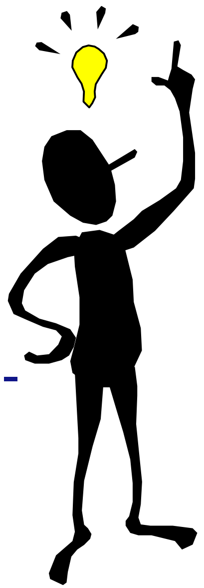
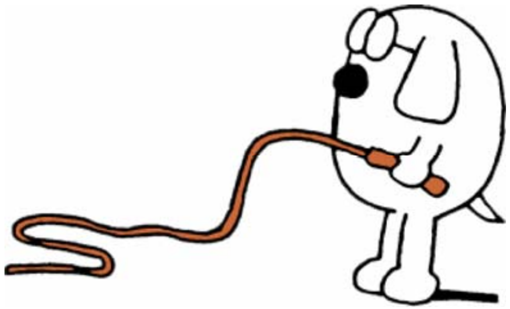
New algorithm development was motivated by the Greenough-Rider results.

- *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)



***Similar to Huynh, *SIAM J. Num. Anal.,* 32 1995,
Suresh & Huynh, *J. Comp. Phys.,* 136 1997,
Daru & Tenaud, *J. Comp. Phys*., 193, 2004**

Again quoting Dogbert:



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

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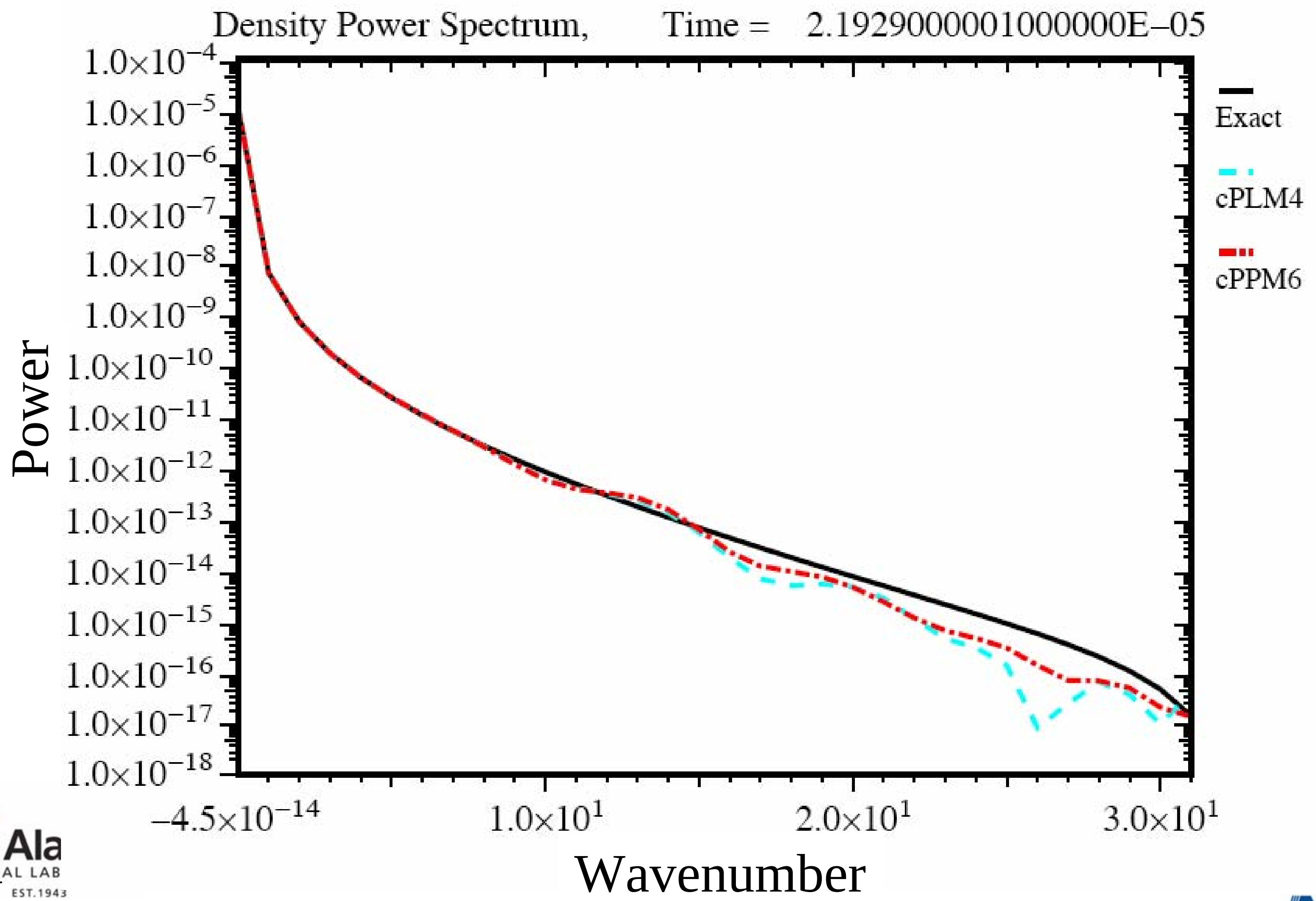
What's the impact? Look at a smooth wave-breaking problem spectrally



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