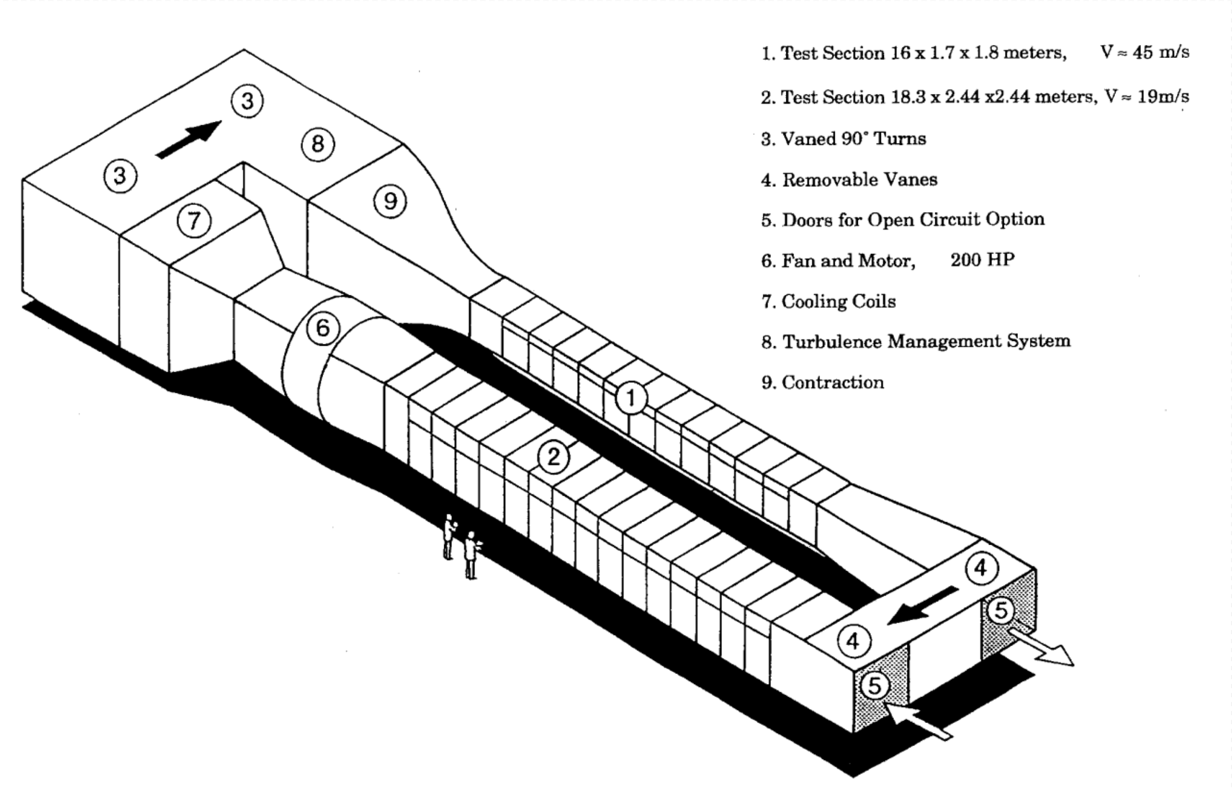
UQ, V&V, large data and Predictive Numerical Calculations

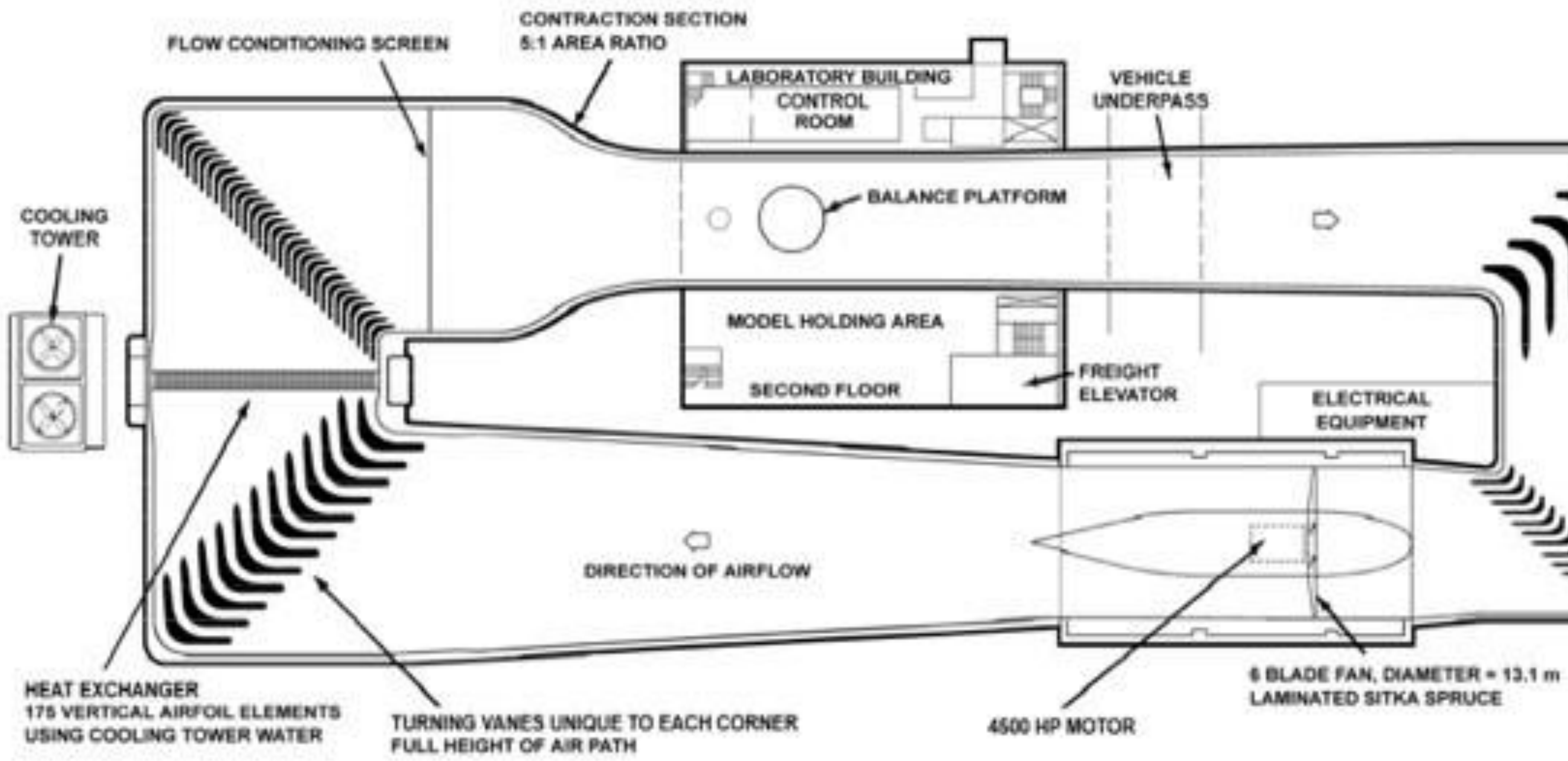
Leland Jameson
Division of Mathematical Sciences
National Science Foundation

Wind tunnel tests of airfoils

Wind tunnels not infinite but some kind of closed loop

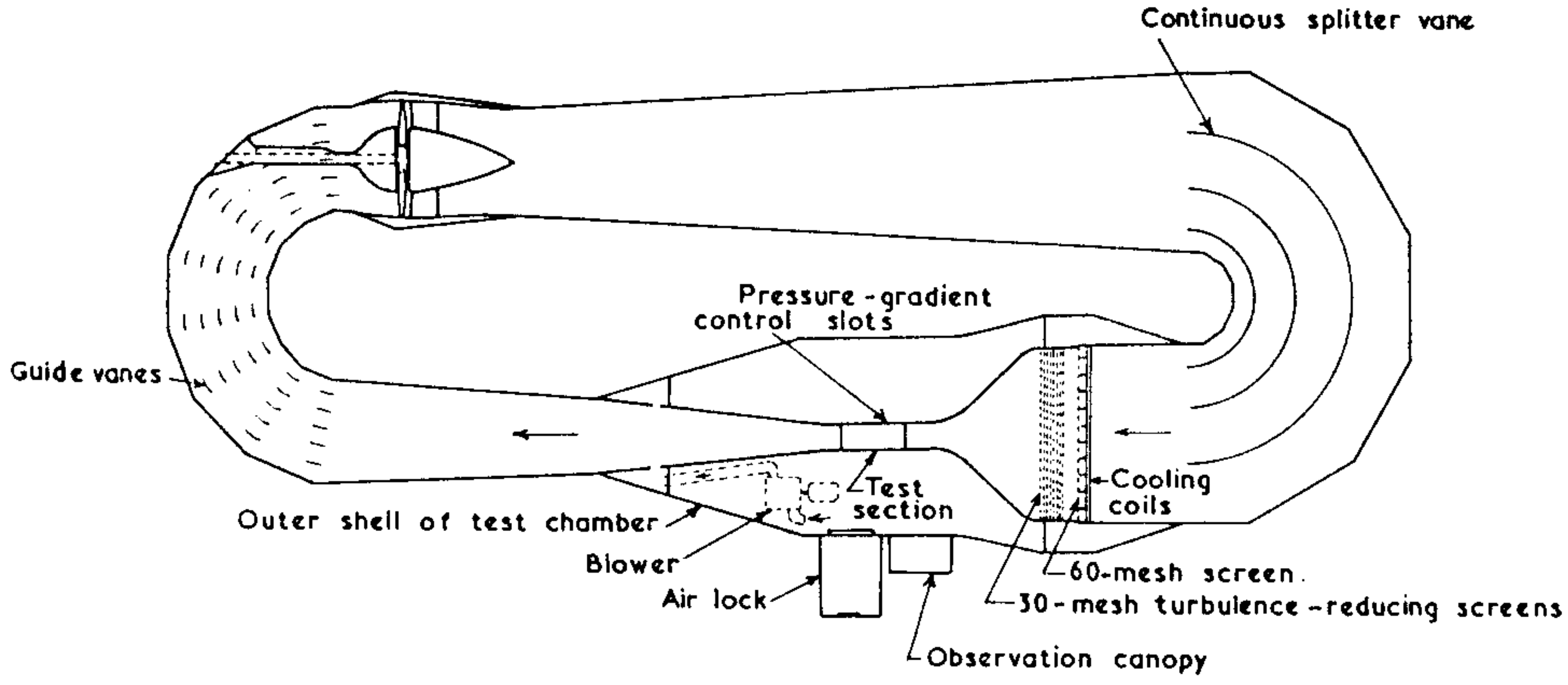


Wind tunnel



FLOW CONDITIONING SCREEN
CONTRACTION SECTION
5:1 AREA RATIO
LABORATORY BUILDING
CONTROL
ROOM
VEHICLE
UNDERPASS
COOLING
TOWER
BALANCE PLATFORM
MODEL HOLDING AREA
SECOND FLOOR
FREIGHT
ELEVATOR
ELECTRICAL
EQUIPMENT
DIRECTION OF AIRFLOW
HEAT EXCHANGER
175 VERTICAL AIRFOIL ELEMENTS
USING COOLING TOWER WATER
TURNING VANES UNIQUE TO EACH CORNER
FULL HEIGHT OF AIR PATH
4500 HP MOTOR
6 BLADE FAN, DIAMETER = 13.1 m
LAMINATED SITKA SPRUCE

Yet another wind tunnel



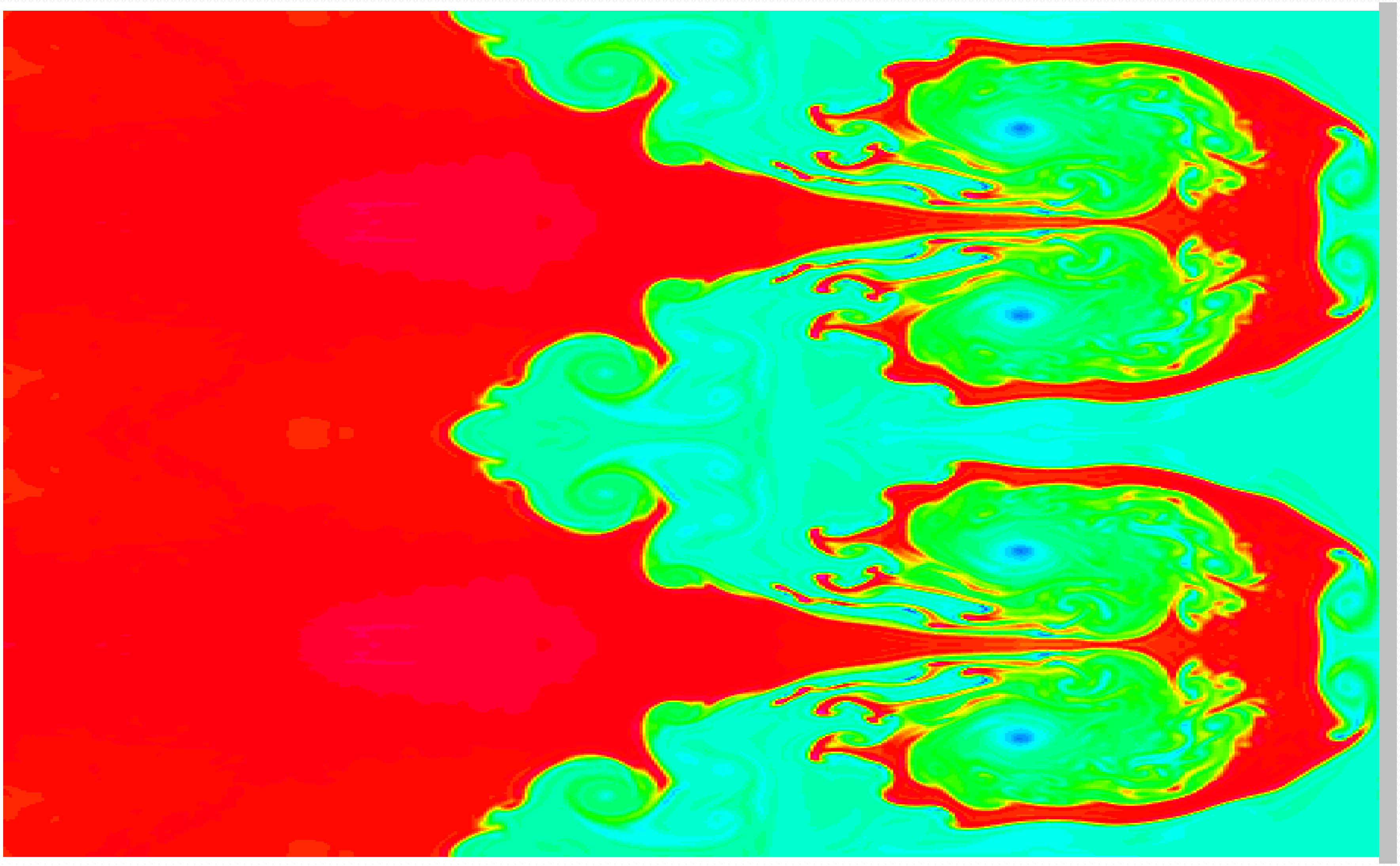
NACA Langley $7\frac{1}{2}$ ft. × 3 ft. low-turbulence pressure tunnel (1941).

The "Secondary Instability"

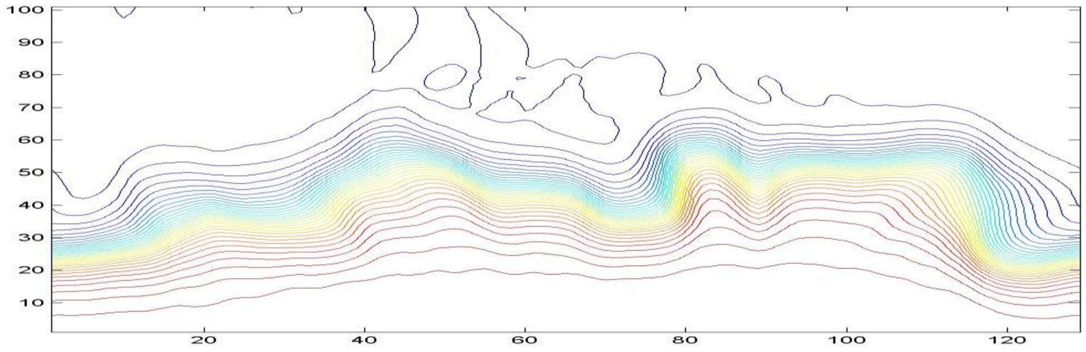
- The physical experiment showed the existence of this instability
- Numerical calculations "confirmed" the existence of this instability
- But, both were wrong.

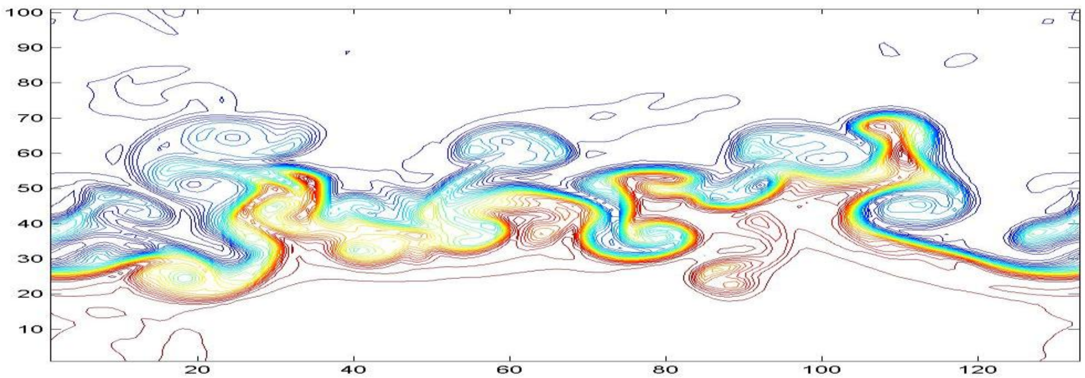
What happened with the wind tunnel test.

- In 1989 the PhD thesis of Wai Sun Don at Brown showed that wind tunnel tests of flow over a cylinder were producing an artificial "secondary instability". This instability was widely believed to exist and was confirmed by independent wind tunnel tests and low order numerical calculations. Using spectral methods and a properly formulated **outflow boundary condition** Don showed that the instability went away. Later when the length of the wind tunnel was increased the experimentally observed instability also disappeared. The instability was due to an **acoustic wave interaction with the wind tunnel wall.**



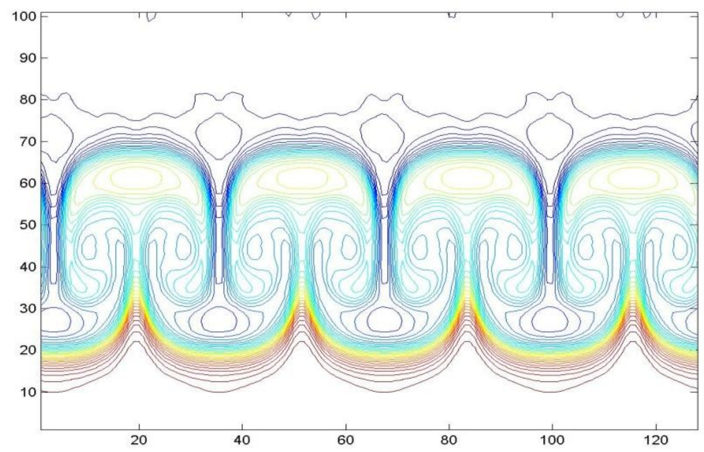
Two more pictures of the same physics in the previous slide



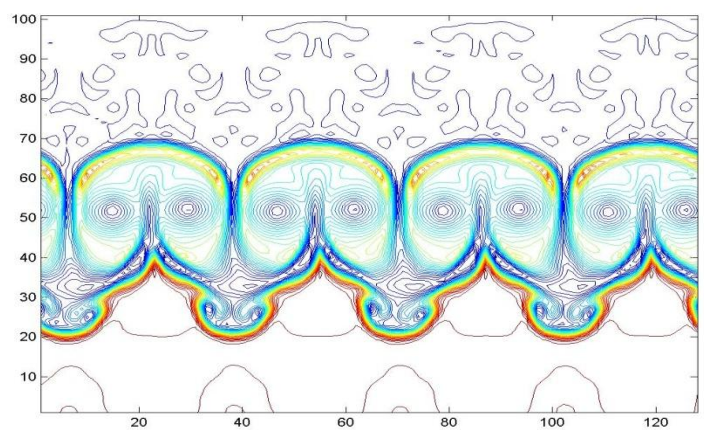


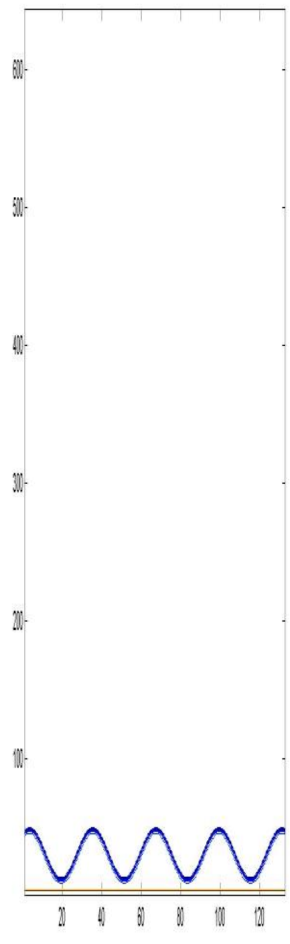
Given an Initial Condition that is symmetric, the calculation maintains the symmetry.

- 3^{rd} Order WENO

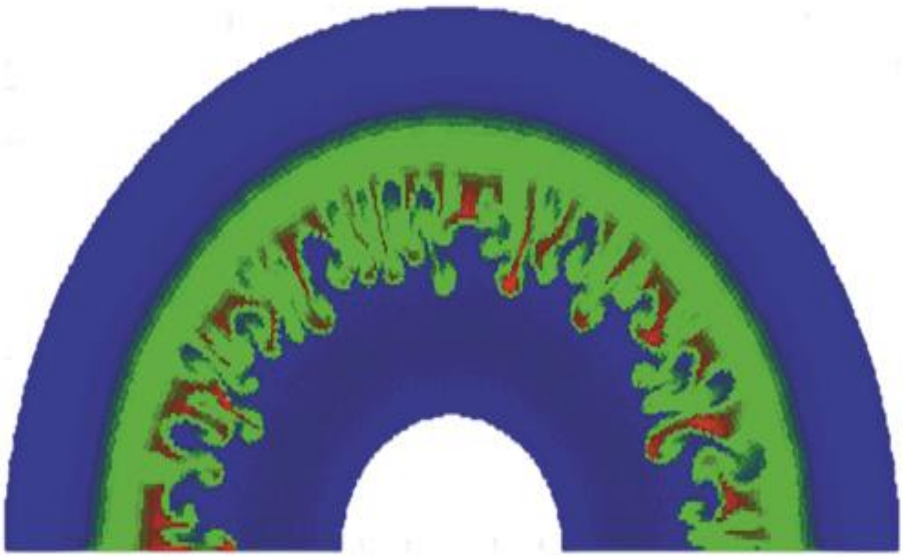


- 9^{th} Order WENO





Inertial Confinement Fusion (ICF) is a promising direction in the pursuit of a clean energy source. Accurate numerical calculation of the Richtmyer-Meshkov mixing is critical to estimating if burn is achieved.



A simulation of the the fluid motion as a function of increasing temperature, pressure, and density (a Richtmyer–Meshkov instability) in an imploding inertial confinement fusion capsule calculated with an arbitrary Lagrange–Eulerian hydrodynamics code on ASCI Blue Pacific.

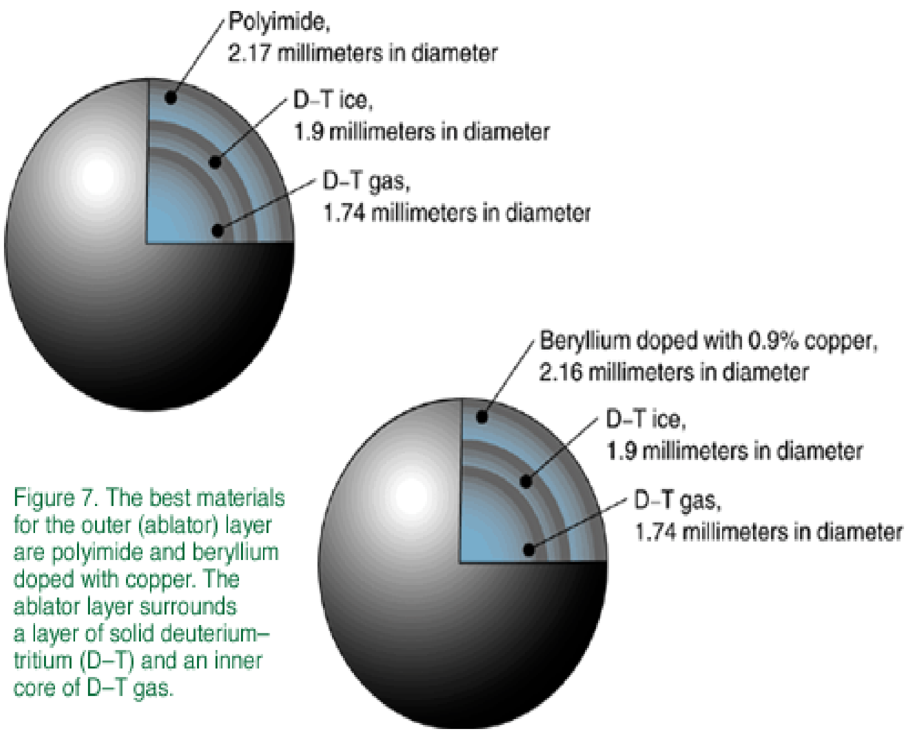
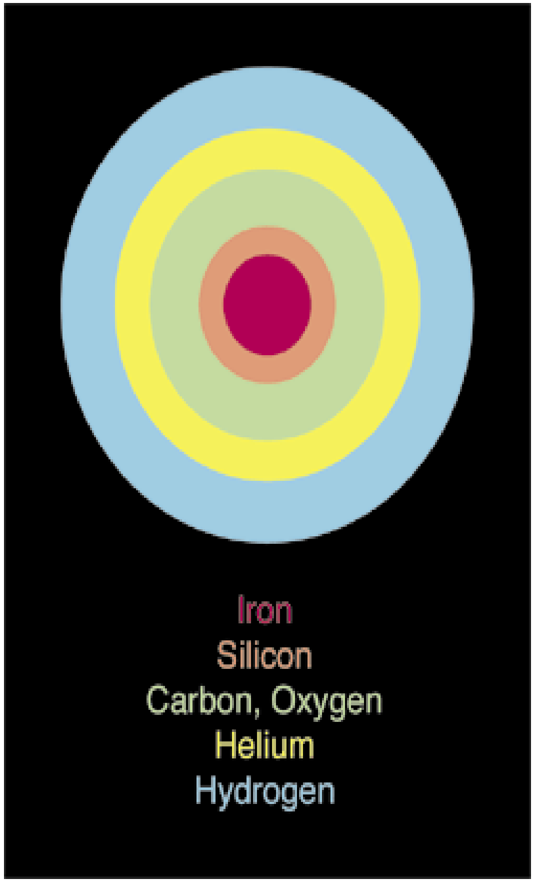
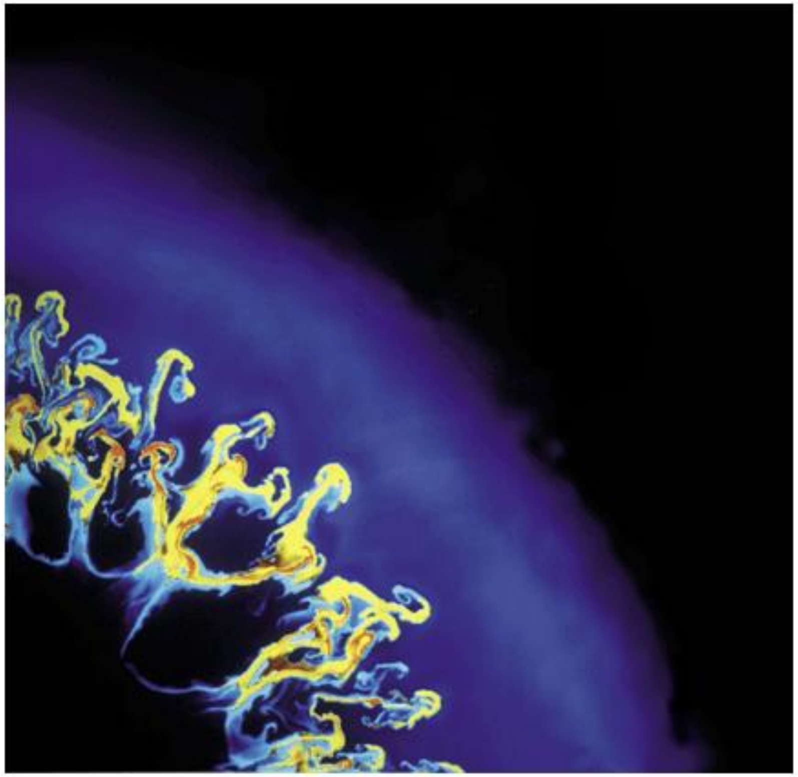


Figure 7. The best materials for the outer (ablator) layer are polyimide and beryllium doped with copper. The ablator layer surrounds a layer of solid deuterium–tritium (D–T) and an inner core of D–T gas.

Supernova, as with ICF, have a multi-layer structure. As shocks pass from layer to layer one observes shock induced mixing.

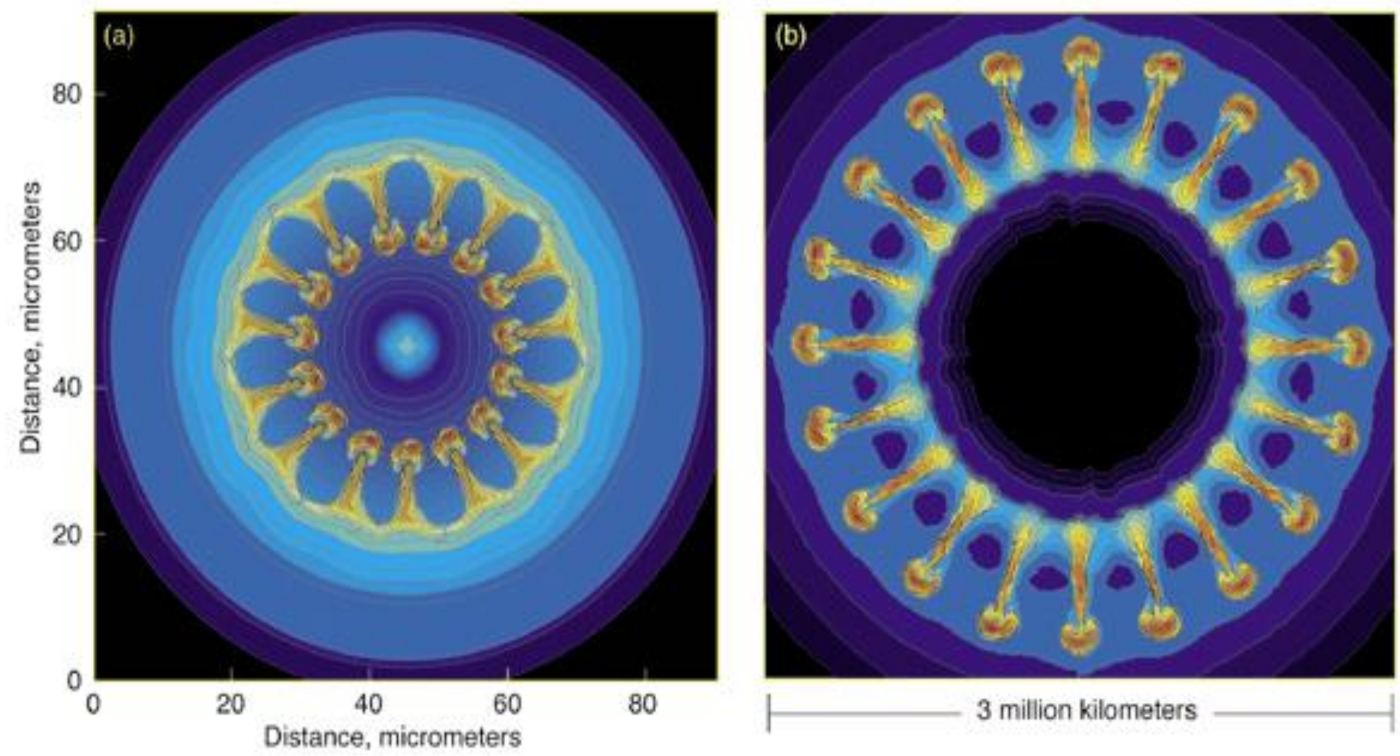


In its death throes, Supernova 1987A resembled an enormous, many-layered onion as successively heavier layers of fuel ignited and burned.



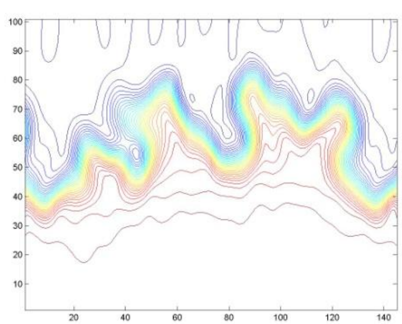
Supernova 1987A provided strong evidence of turbulence emanating from the core of the exploded star because core materials were observed well before they were predicted. The turbulence caused mixing among the layers and greatly complicated the tidy "onion" model of dying stars. [Image reproduced from Muller, Fryxell, and Arnett, Astronomy & Astrophysics 251, 505 (1991).]

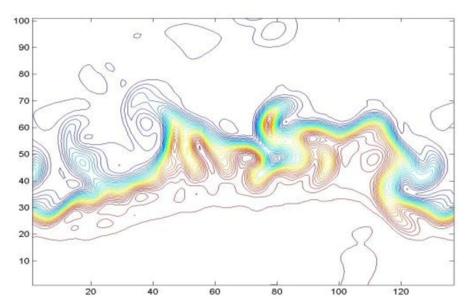
Numerical errors accumulate with increasing time and can eventually dominate a calculation especially for long-time integration of ICF, Super-novas, climate models, etc.

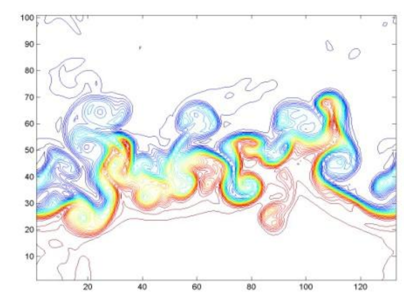


The numerical error can produce drastically different "physics".

- The following three frames show the final time mixing region for a Richtmyer-Meshkov calculation. The three frames show mixing regions with varying amounts of small scale structure. The only difference between the frame is that the numerical error (dissipation in this case) decreases as one progresses right

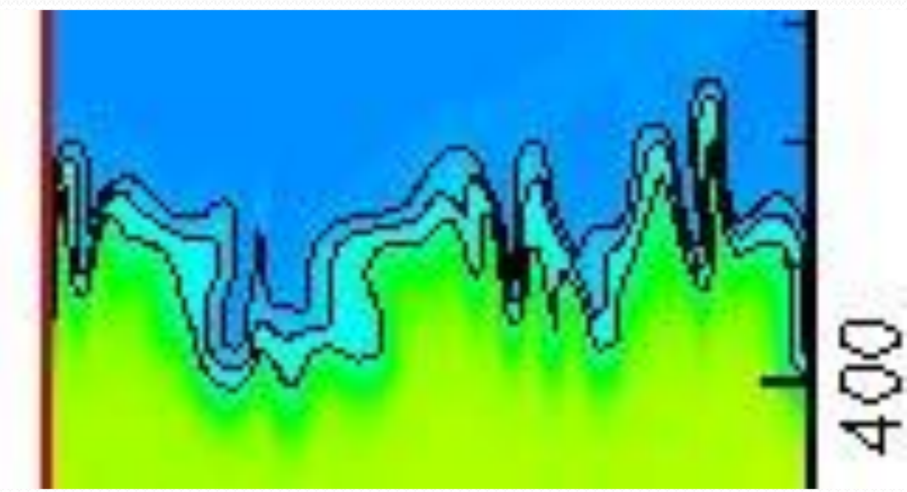




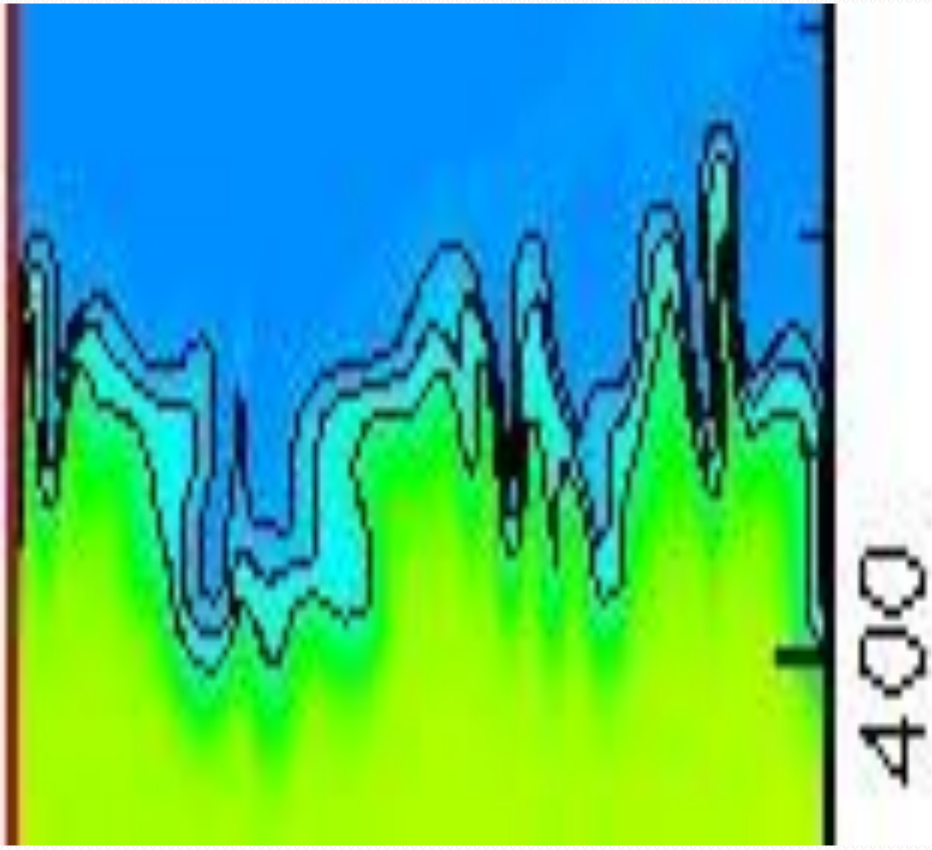


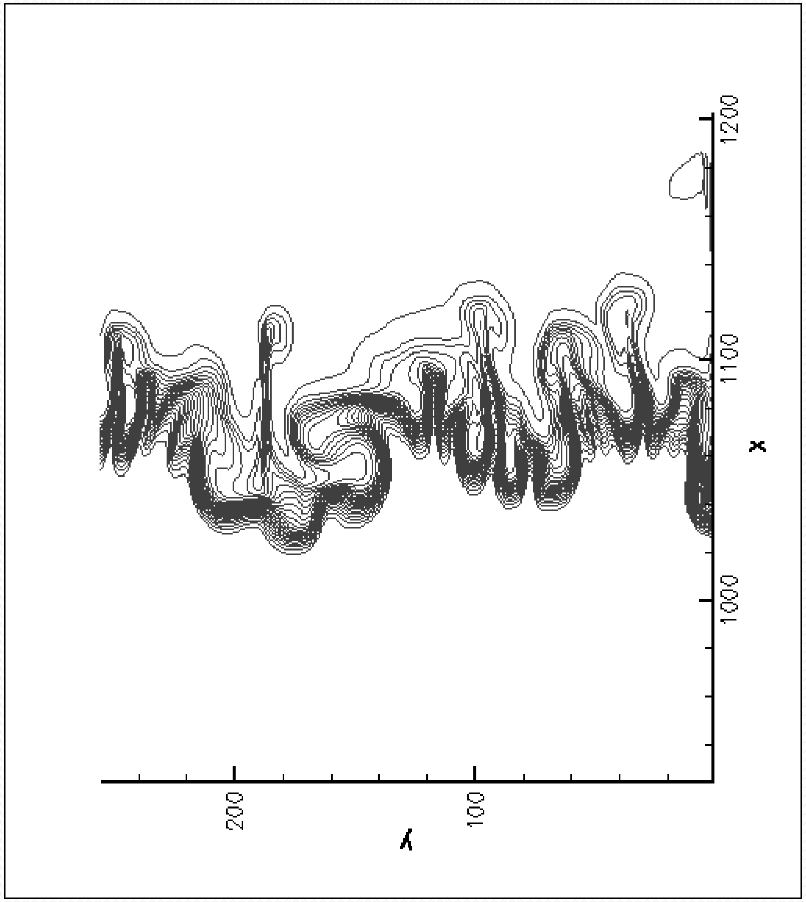
Here we visually examine the mix zone of an 11th order WENO and a 2nd order Godunov method.

- One can see visually the 11th order WENO supports much more structure for a given grid.
- Our goal as stated is to get away from eyeball norms.

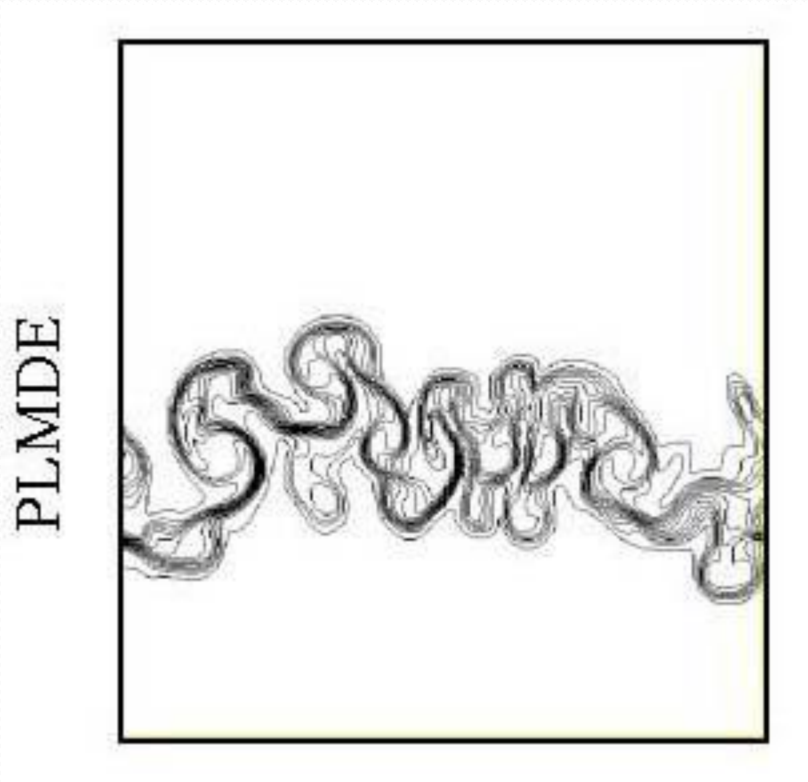


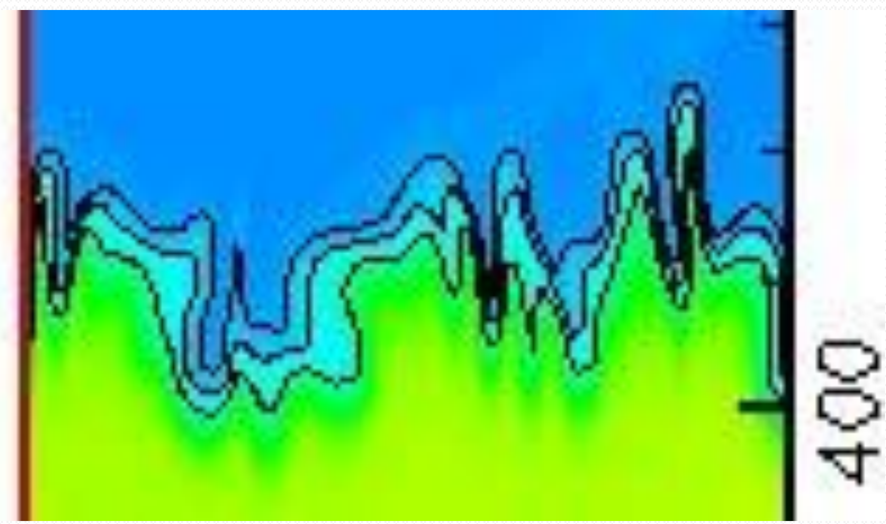
2nd Order Godunov at 128x640 and 256x1280.





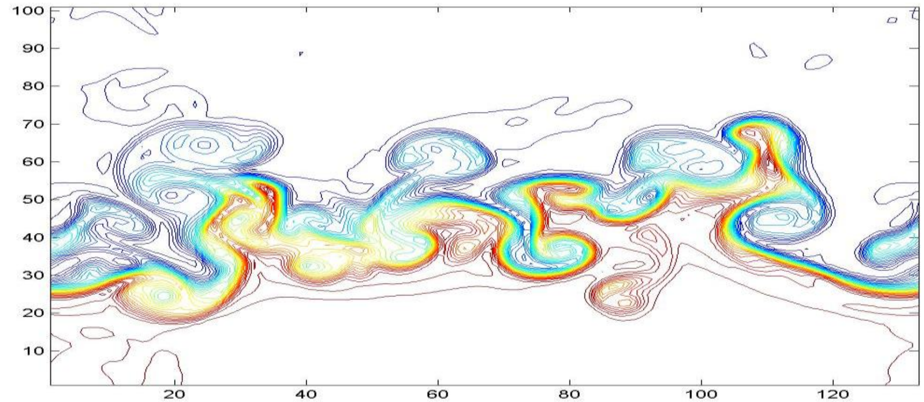
understand exactly why two different 2^{nd} order Godunov schemes give very different results.



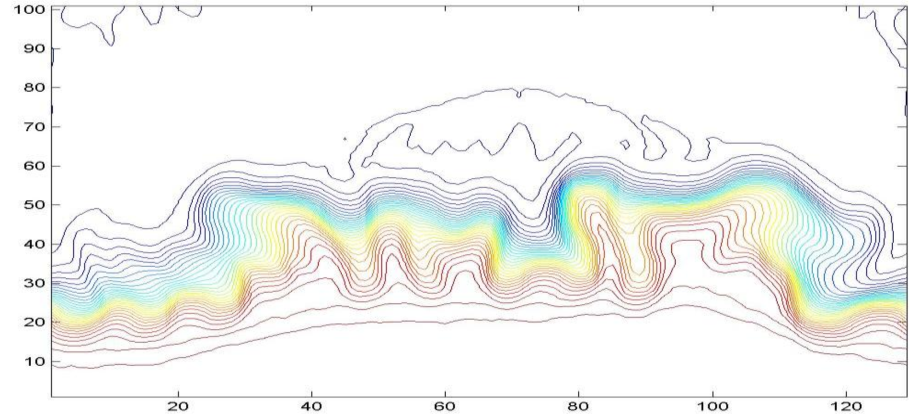


WENO to the 3rd order on a grid of 128 by 640 one can visually see much more structure.

- 9th Order WENO

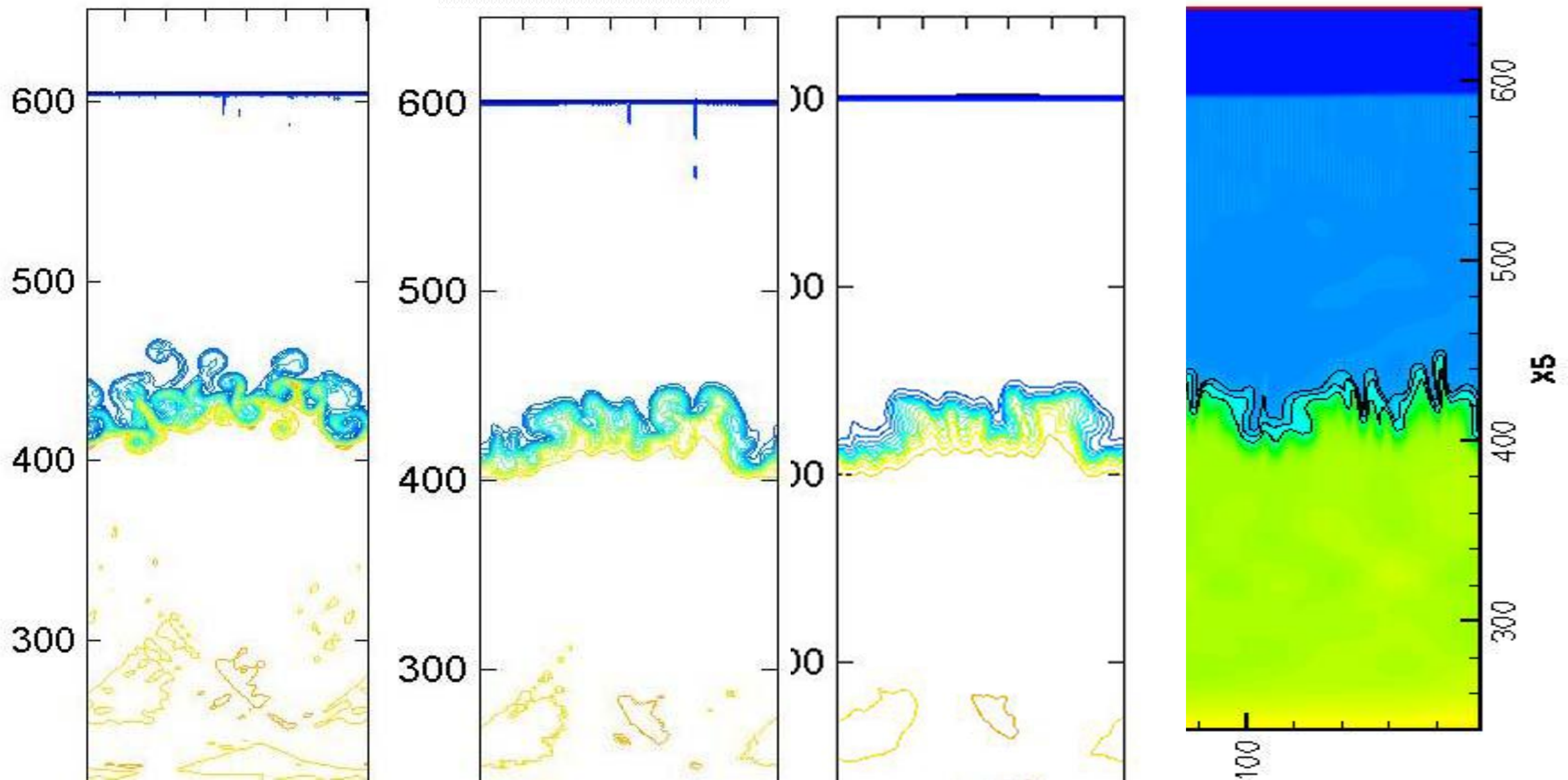


- 3rd Order WENO



conjecture that 2^{nd} order Godunov is "more or less" equal to 3^{rd} order WENO. M5, 140microseconds.

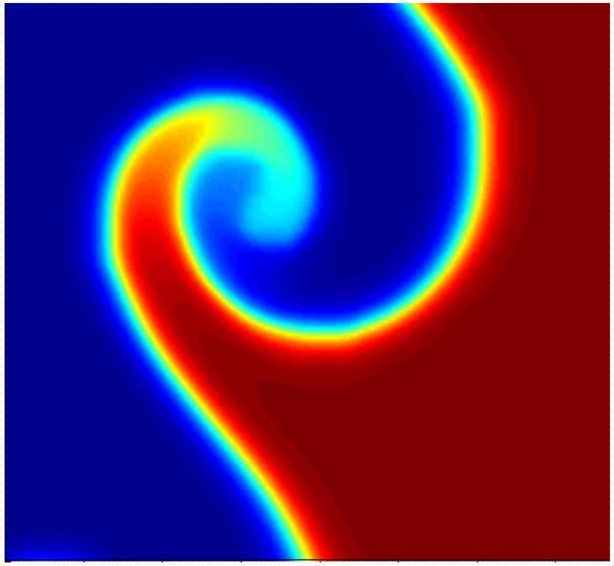
- 11^{th} WENO 5^{th} WENO 3^{rd} WENO 2^{nd} Godunov

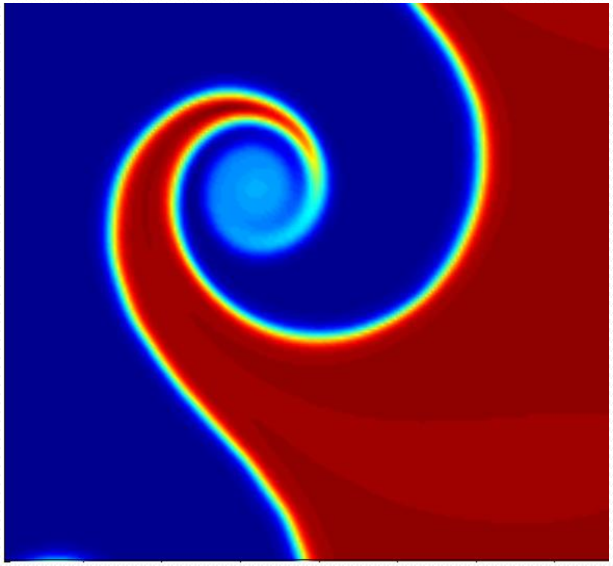


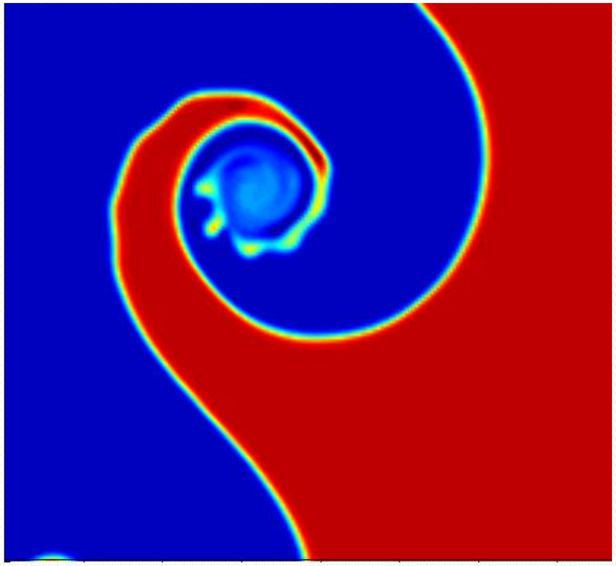
–3rd order WENO

–5th order WENO

–9th order WENO



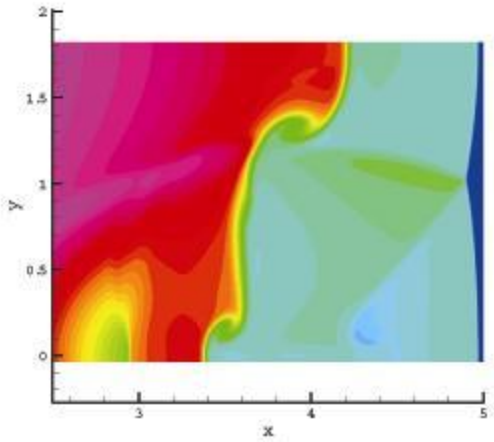




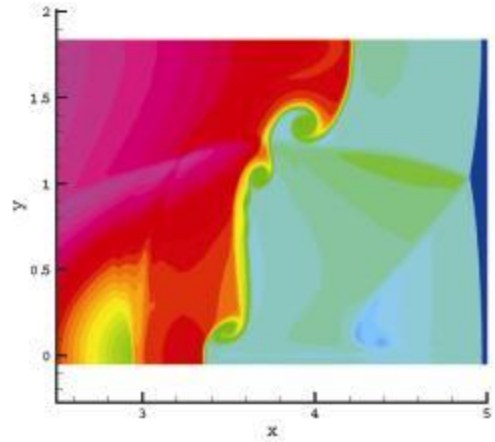
Richtmyer-Meshkov Instability

Convergence Study $(M = 4.46, \delta = 0.2\ cm, t = 50\ \mu s)$ **: Density**

WENO 3rd



WENO 5th

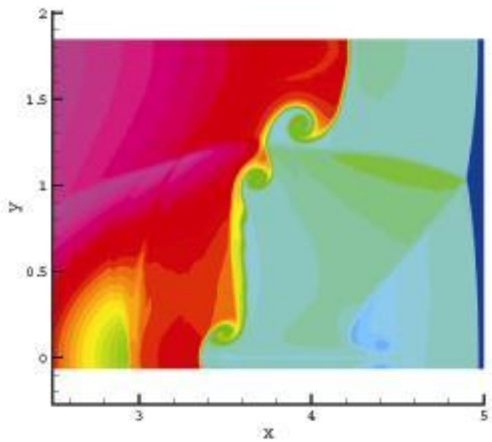


- Grid size for the Spectral and WENO schemes are 1024x256 in Full Domain.

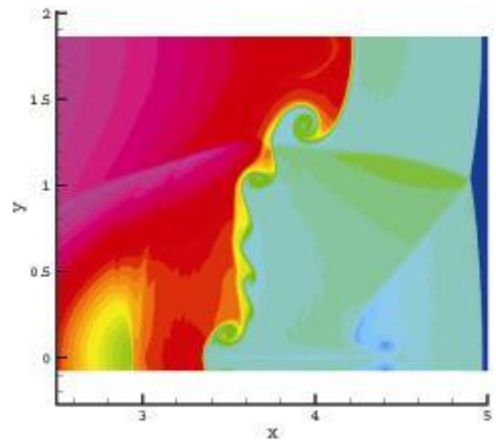
Richtmyer-Meshkov Instability (Cont.)

Convergence Study $(M = 4.46, \delta = 0.2\ cm, t = 50\ \mu s)$ **: Density**

WENO 7rd



WENO 9th

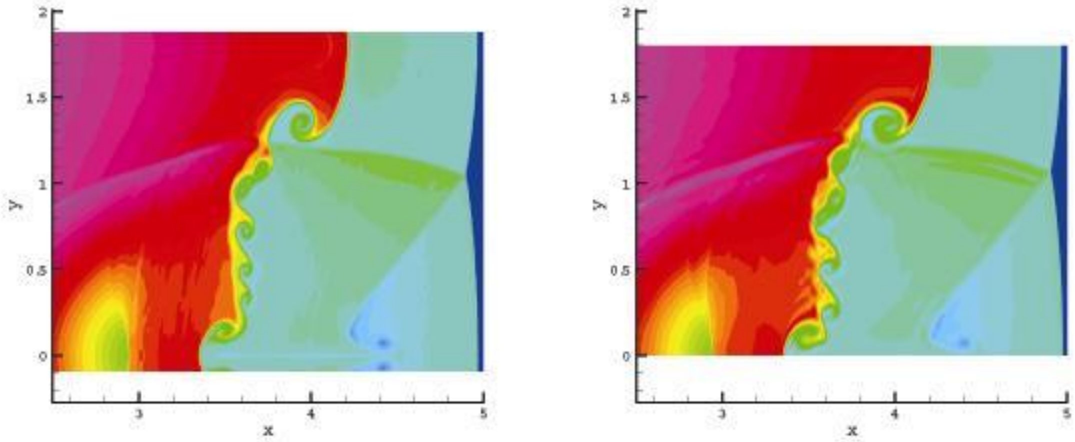


- Grid size for the Spectral and WENO schemes are 1024x256 in Full Domain.

Richtmyer-Meshkov Instability (Cont.)

Convergence Study ($M = 4.46, \delta = 0.2\ cm, t = 50\ \mu s$) **: Density**

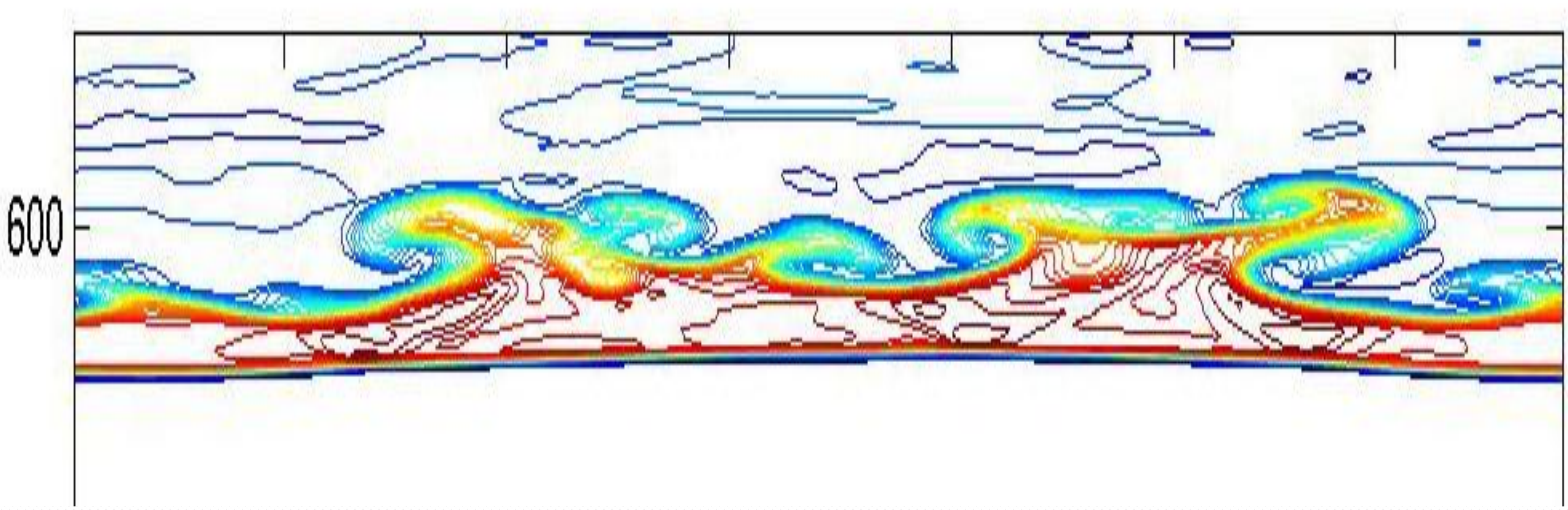
WENO 11st **Spectral**



- Grid size for the Spectral and WENO schemes are 1024x256 in Full Domain.

Let's challenge the code with a Mach 100 shock followed by a reshock using the 5th order option.

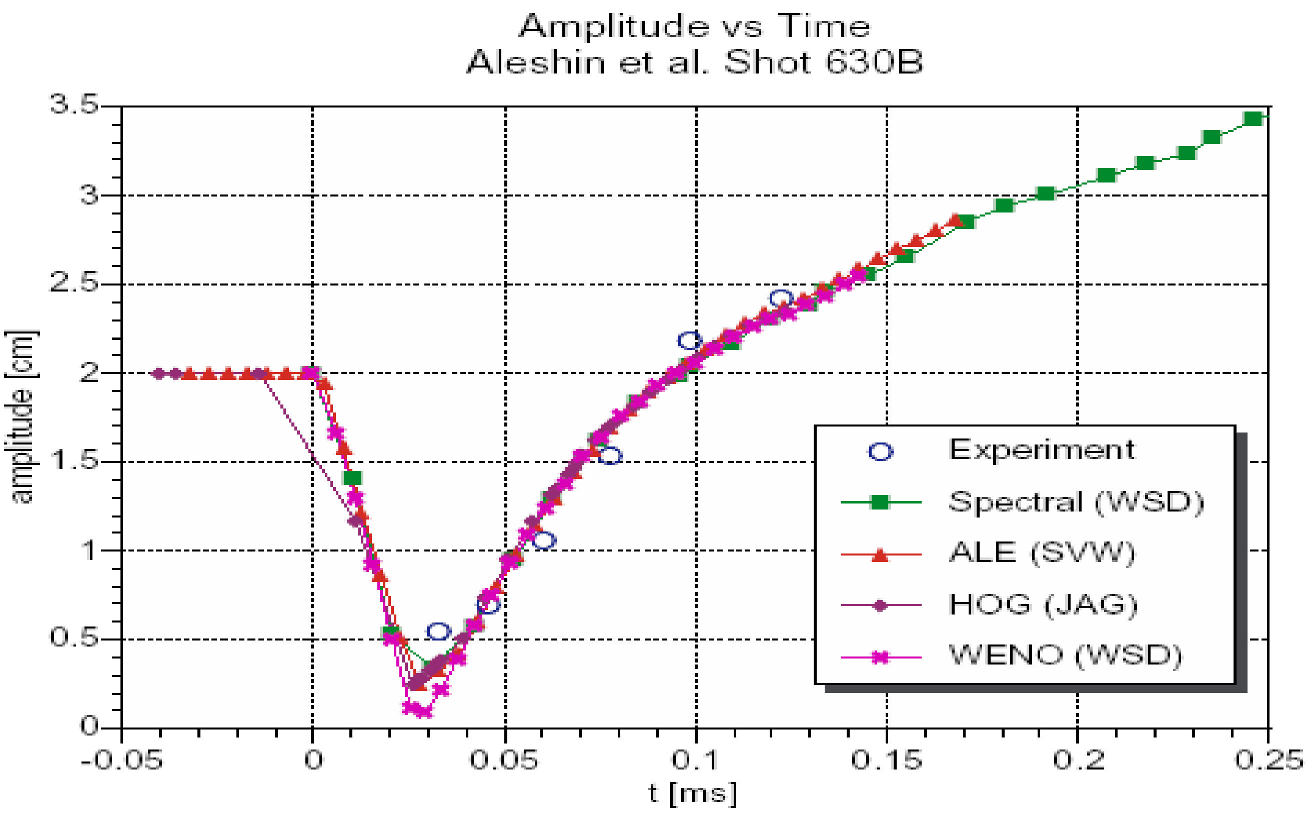
- Here we simply we want to demonstrate that with even a mach 100 shock on the notch interface followed by a reshock that the code runs. Below we see the mixing zone



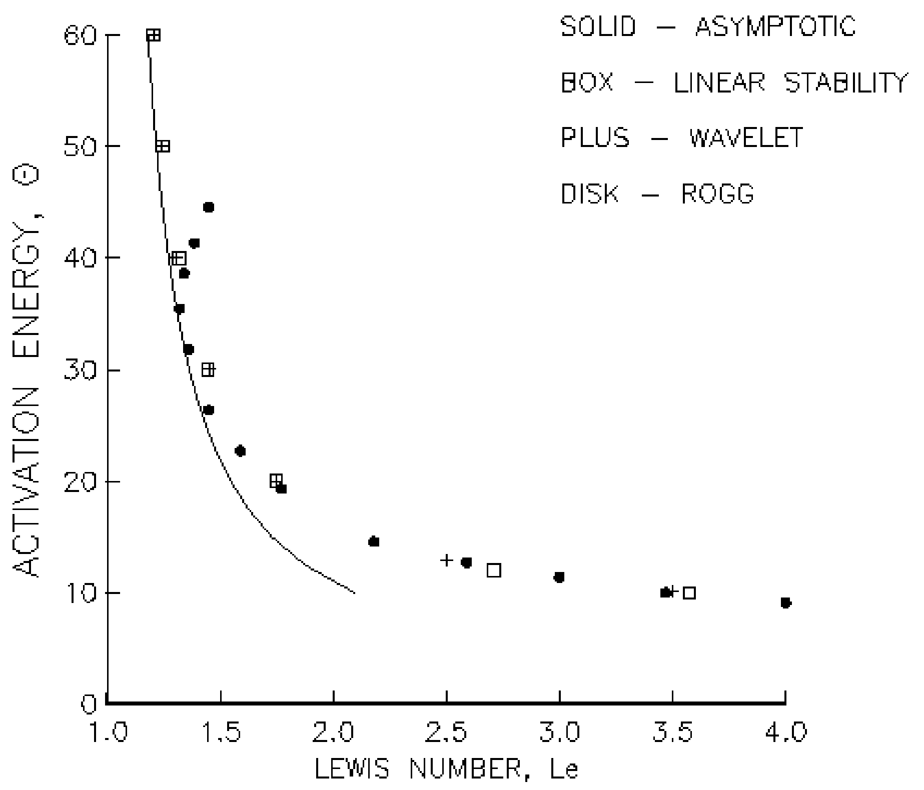
How much error and what kind of error is acceptable?

- Transport of large-scale (low wave number) features can be done with almost any scheme and one will obtain an acceptable result.
- Mixing at a fine scale requires a great deal of attention to magnitude of the error and type
  - Dissipation: clearly increased dissipation damps high wave numbers and smooths the flow
  - Dispersion: waves travel at different speeds. Does this increase or decrease mixing or neither?

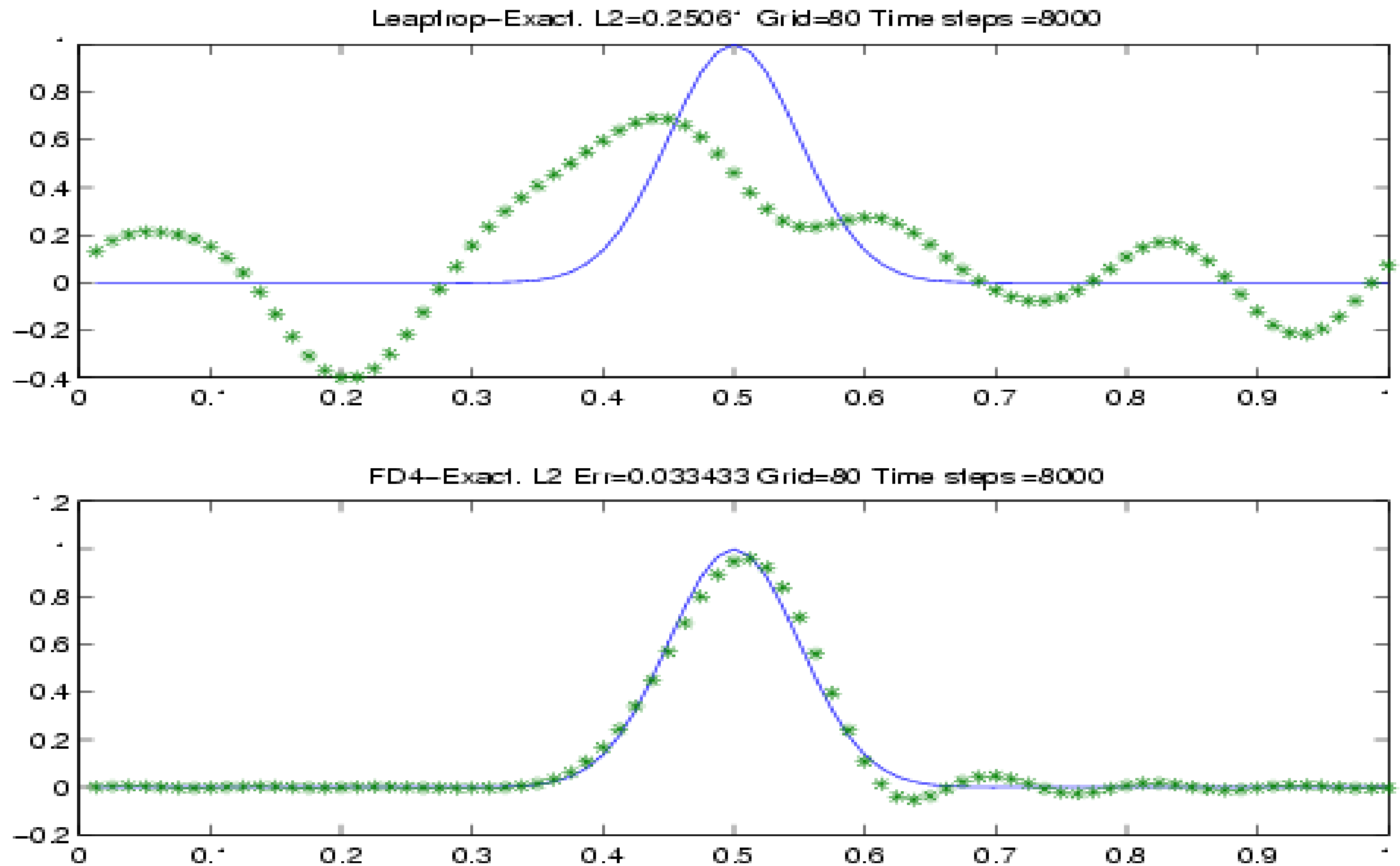
High order methods affect most the small scale structures in a flow and large scale features such as location of peaks and valleys are calculated equally well with low order schemes.



Correctness of Numerical Calculations (with T. Jackson and G. Leseign 1994 and 1999)



Electromagnetics: For the Simple Convection Equation Error is Dispersive

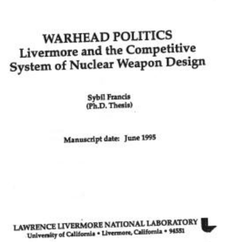


Computational Mathematics 2007 Dear Colleague Letter on Long-Time Behavior of Numerical Methods

- The number of degrees of freedom, in particular the number of time steps, for solving partial differential equations grows as computational resources grow. **Errors or numerical artifacts that may be insignificant when the number of time steps to solution is relatively small can dominate a calculation as this number reaches the tens or hundreds of thousands. Such non-physical artifacts can come in a variety of forms, from the accumulation of numerical truncation error, round-off error, uncertainty in physical parameter values, model uncertainty,** etc. Theoretical error estimates containing constants that grow exponentially with time are not adequate to address these effects. Further, as computational platforms grow in size with increasing numbers of CPUs, the advent of commodity multi-core processors, and the increasing heterogeneity of computing environments, increasing care must be paid to designing algorithms that are conducive to such architectures. The trend in computational hardware is to have tens or hundreds of thousands of processors with limited memory associated with each processor and nodes that contain clusters of processors. It is critical that proposed numerical approaches take into account various latencies and load balancing issues that will certainly be encountered on such architectures. Such large calculations produce very large data sets. Algorithms for the efficient analysis and visualization of very large data sets on such modern architectures in order to uncover hidden correlations and structures are also of interest. Above all, the physical correctness of the calculation is the most important issue. Arriving at a physically relevant answer requires careful attention to the above issues as well as others.

Large 3D code efforts should have at least 2 totally independent implementations

- Physics: For complex systems, e.g., turbulence, not everyone will agree on the physical model such as closure models.
- Numerics: For complex systems in 3 dimensions with various complexities such as topological structure change, not everyone will agree if one should use ALE, 2nd Order FD, WENO, ENO, 2nd Order Godunov, spectral methods, compact schemes, …
- Software: For large supercomputers, in my experience pilers are not bug free for at least 2 years.


WARHEAD POLITICS
Livermore and the Competitive System of Nuclear Weapon Design

Sybil Francis
(Ph.D. Thesis)

Manuscript date: June 1995

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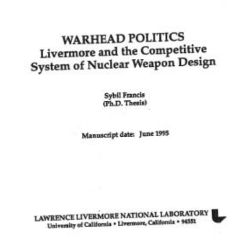
ect Management should also be independent.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Summary: How many ways can we get the wrong answer?

- "Incorrect" physics, e.g., turbulence model
- Incorrect implementation
- Excessive dispersion with studying moving phenomenon
- Excessive dissipation when studying small scale features
- Immature compilers (less than 2 years old)
- Staff with the wrong training
- Compiler options…
- Etc.

Estimating Reliability of Numerical Results:
It is Critical to know…

- Dissipation:
  - Alters the magnitude of the Fourier modes but not the phase. Therefore, events will occur at the "right" time but the magnitude of the event will be reduced.
  - "Mix" or Turbulent mix will be reduced since small scale information is lost due to reduced high frequency Fourier Coefficients.

- Dispersion
  - Alters Fourier phase but not magnitude. So, events occur with the right magnitude but not at the right time.
  - "Mix" is not significantly altered since Fourier modal is unchanged.

Large 3D code efforts should have at least 2 totally independent implementations

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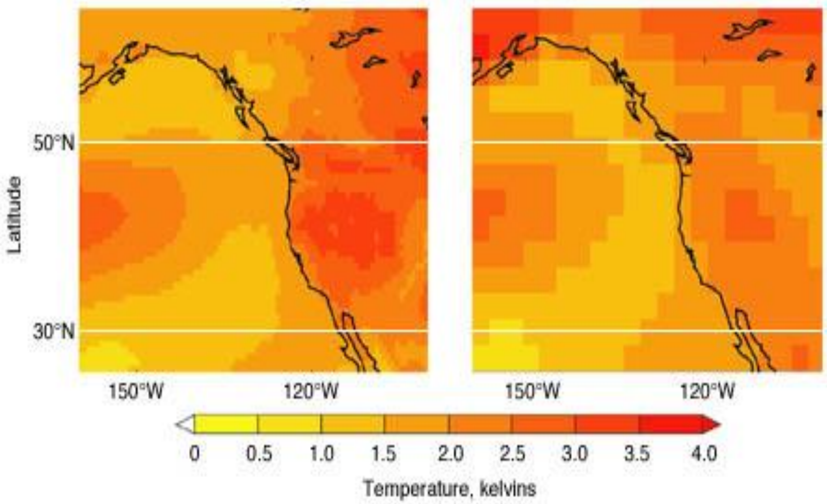
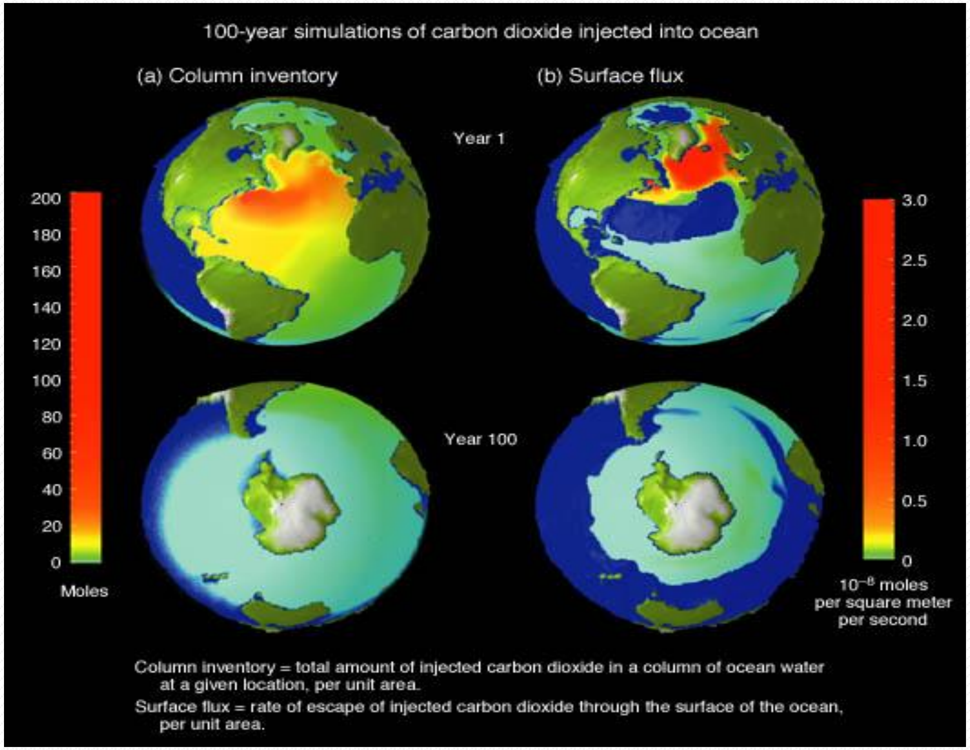
numerical calculations do not agree it is not always the numerical calculation that is incorrect.

- In 1989 the PhD thesis of Wai Sun Don at Brown showed that wind tunnel tests of flow over a cylinder were producing an artificial "secondary instability". This instability was widely believed to exist and was confirmed by independent wind tunnel tests and low order numerical calculations. Using spectral methods and a properly formulated outflow boundary condition Don showed that the instability went away. Later when the length of the wind tunnel was increased the experimentally observed instability also disappeared. The instability was due to an acoustic wave interaction with the wind tunnel wall.

Numerical Simulations of the human impact on global climate change require calculations lasting for months on the worlds largest computers. How reliable are the results?





Direct Numerical Simulation is the notion that one can compute exactly all the modes in a computational domain as long as one has enough grid points, etc.

- Scale resolution has a one-to-one correspondence with grid point density only for Fourier spectral operators and one can expect the spatial differentiation to be exact for N/2 modes on a grid of N points.
- For non-spectral operators the issue is completely different. Non-spectral numerical schemes are low-order polynomial approximations of sine modes and fundamentally one is asking how well a given Fourier mode is approximated after a given time.
- Even for spectral methods no calculation is ever exact even in a domain that is completely resolved. This is due to time advancement which is, as above, a polynomial approximation of Fourier modes.

Estimating Reliability of Numerical Results:
It is Critical to know…

- Dissipation:
  - Alters the magnitude of the Fourier modes but not the phase. Therefore, events will occur at the “right” time but the magnitude of the event will be reduced.
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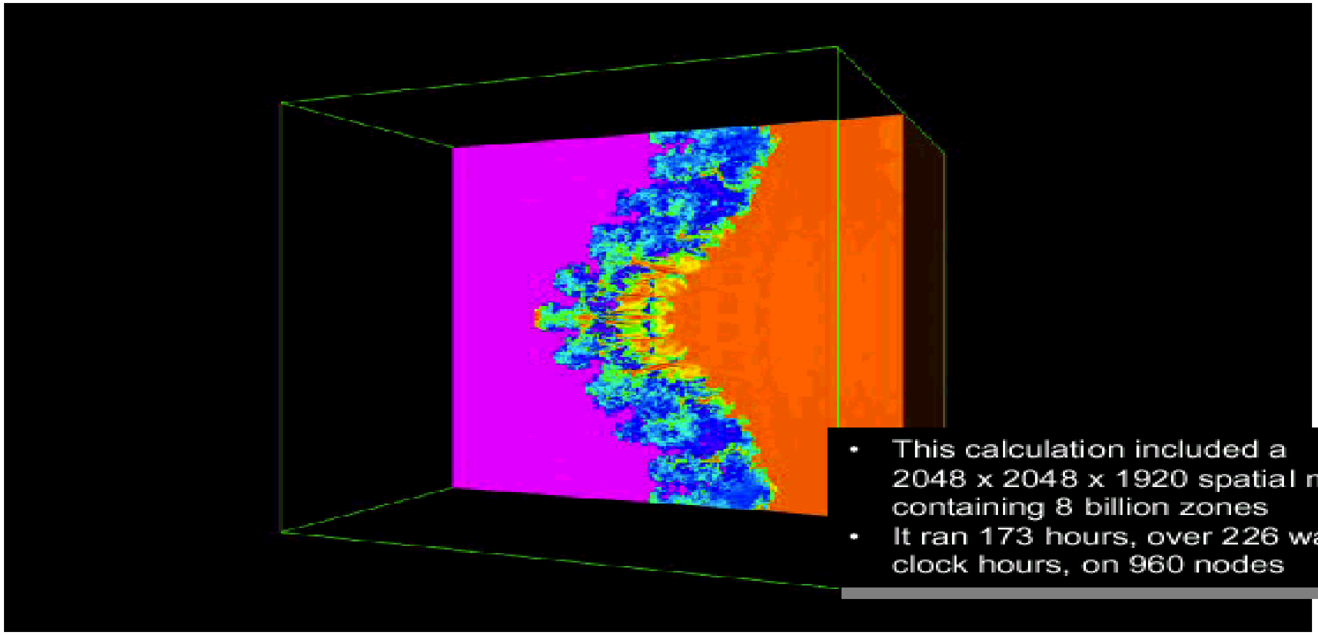
- Dispersion
  - Alters Fourier phase but not magnitude. So, events occur with the right magnitude but not at the right time.
  - “Mix” is not significantly altered since Fourier modal is unchanged.

If a Calculation does NOT blow up, is the Final Result always Correct?

- The answer to this question is, of course, a resounding no.

Modeling of turbulent mixing, using the sPPM code, will help validate subgrid-scale models



- This calculation included a 2048 x 2048 x 1920 spatial mesh containing 8 billion zones
- It ran 173 hours, over 226 wall clock hours, on 960 nodes

2/18/00

D. Post-IDA

Numerical errors are generally poorly understood and often not carefully considered.

- The simulation that produced the previous slide was with a second order numerical scheme applied to the Euler equations, thus the leading order truncation error is dispersive with the second order truncation error is dissipative.
- The small scale vortical structure is produced by "viscosity" that is introduced solely by the numerical scheme. In other words, the "turbulence" is an artifact of the errors.

away from ad hoc turbulence models and one needs precise estimates of final time errors.

- The final result of numerical simulations of fluids related problems almost always depend heavily on somewhat ad hoc modeling of small scale features.
- Numerical simulations that do not explicitly incorporate random noise are deterministic processes and one can thus find error bounds on the final answer. With such error bounds one can know exactly how reliable the simulation is and make decisions accordingly.

The proposed work would have a very broad impact.

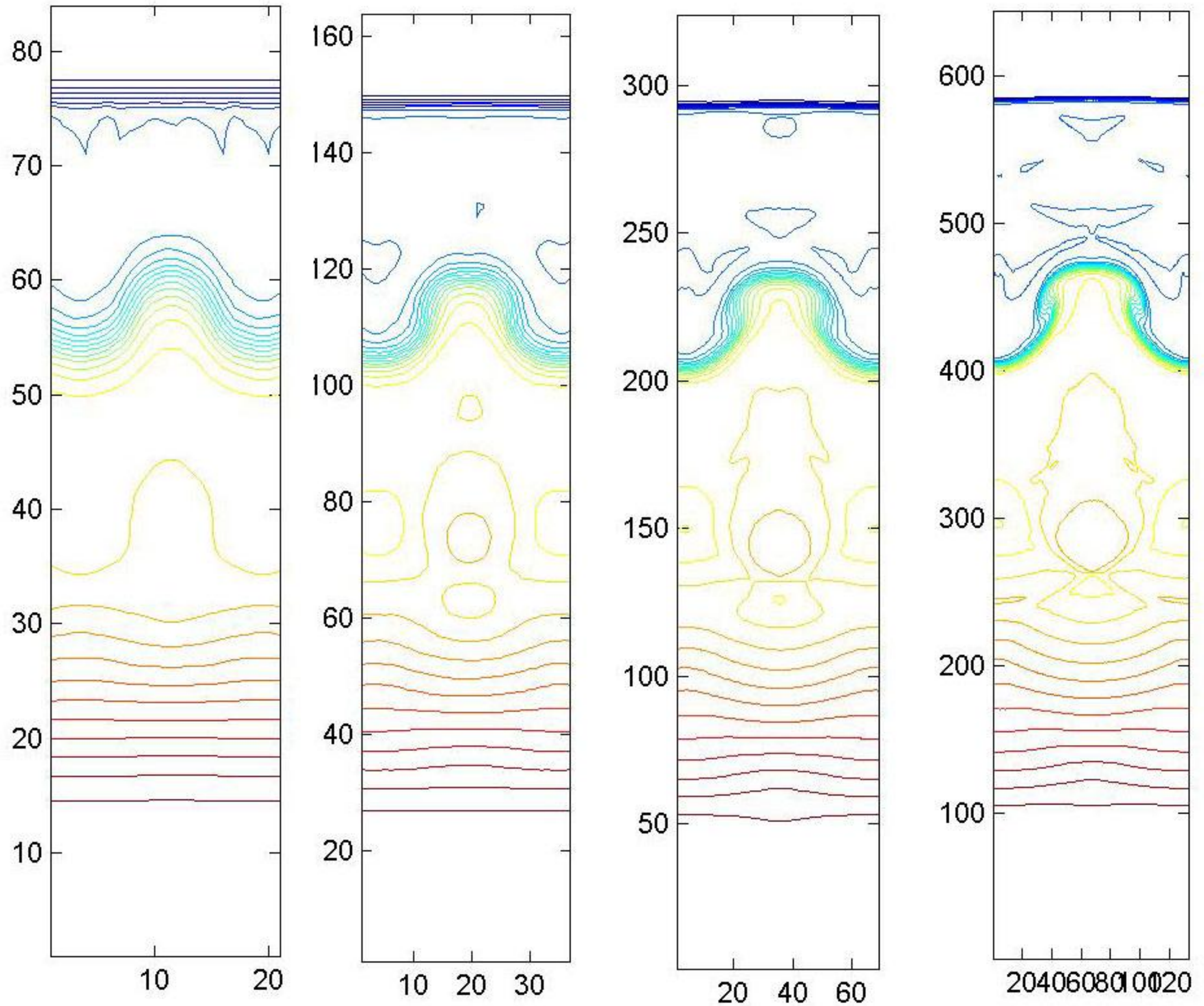
- Climate and weather simulations depend heavily on the turbulence model. One can obtain completely different climate patterns by changing arbitrary parameter values in the turbulence model. Improved weather prediction can positively impact battlefield planning.
- Likewise, ocean models can give drastically different results depending on the turbulence model. Improved ocean modeling can impact the guiding of submarines.

estimates of the final time errors for Euler and Navier-Stokes calculations.

- First, one impact of obtaining such estimates is that one can finally have an estimate on how reliable the final solution to a numerical calculation is.
- Second, there are numerous examples of calculations that can not be correct given the number of time steps taken or the nature of the numerical error.

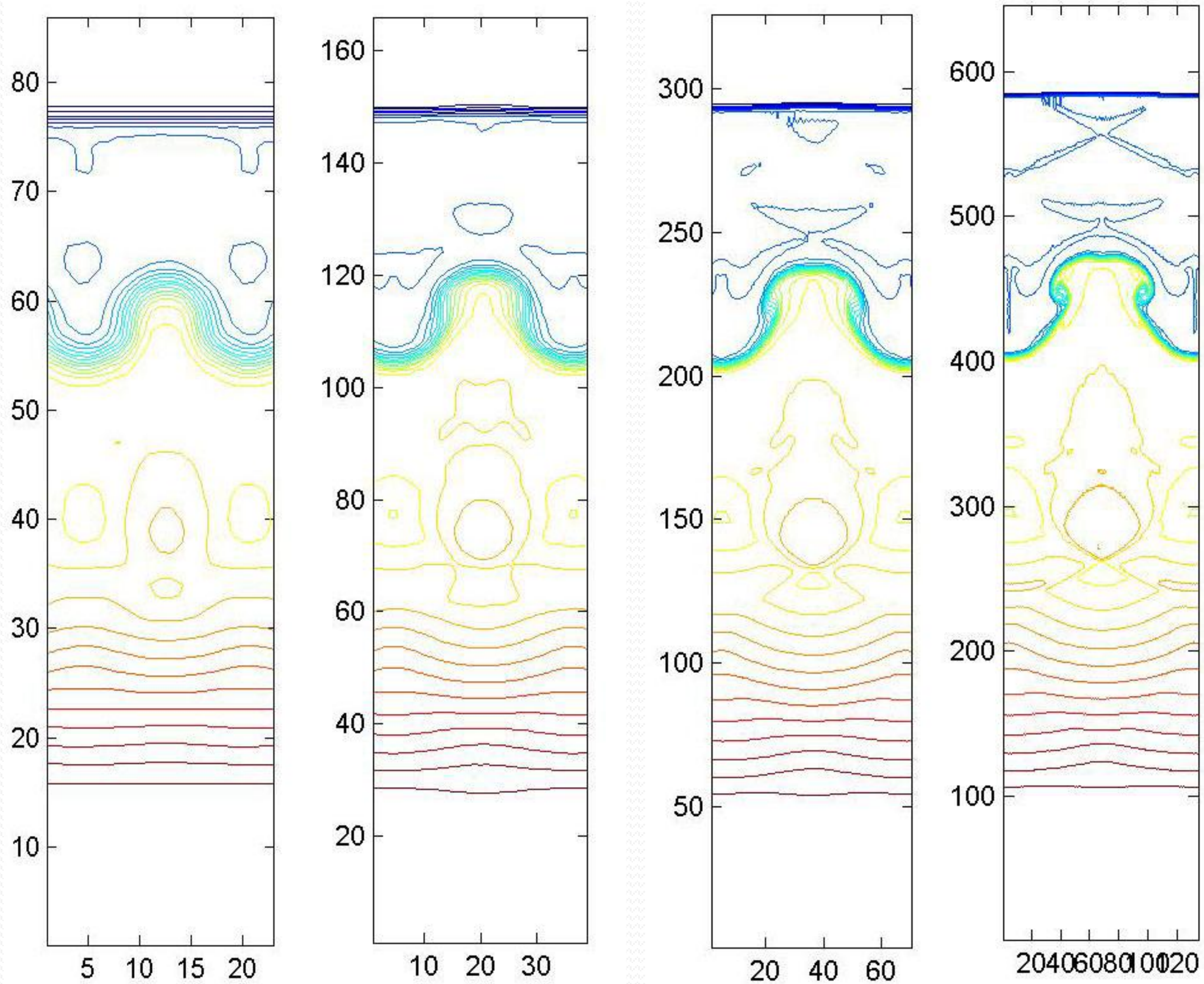
Here we compare 3rd order WENO at four levels of grid refinement run on 16cpus of ASCI Blue.

From left to right we have contour plots at increasing grid point resolution,
16x80 RT=9s
32x160 RT = 28s
64x320 RT = 2m,14s
128x640 RT = 12m,55s
of the density at the final time.

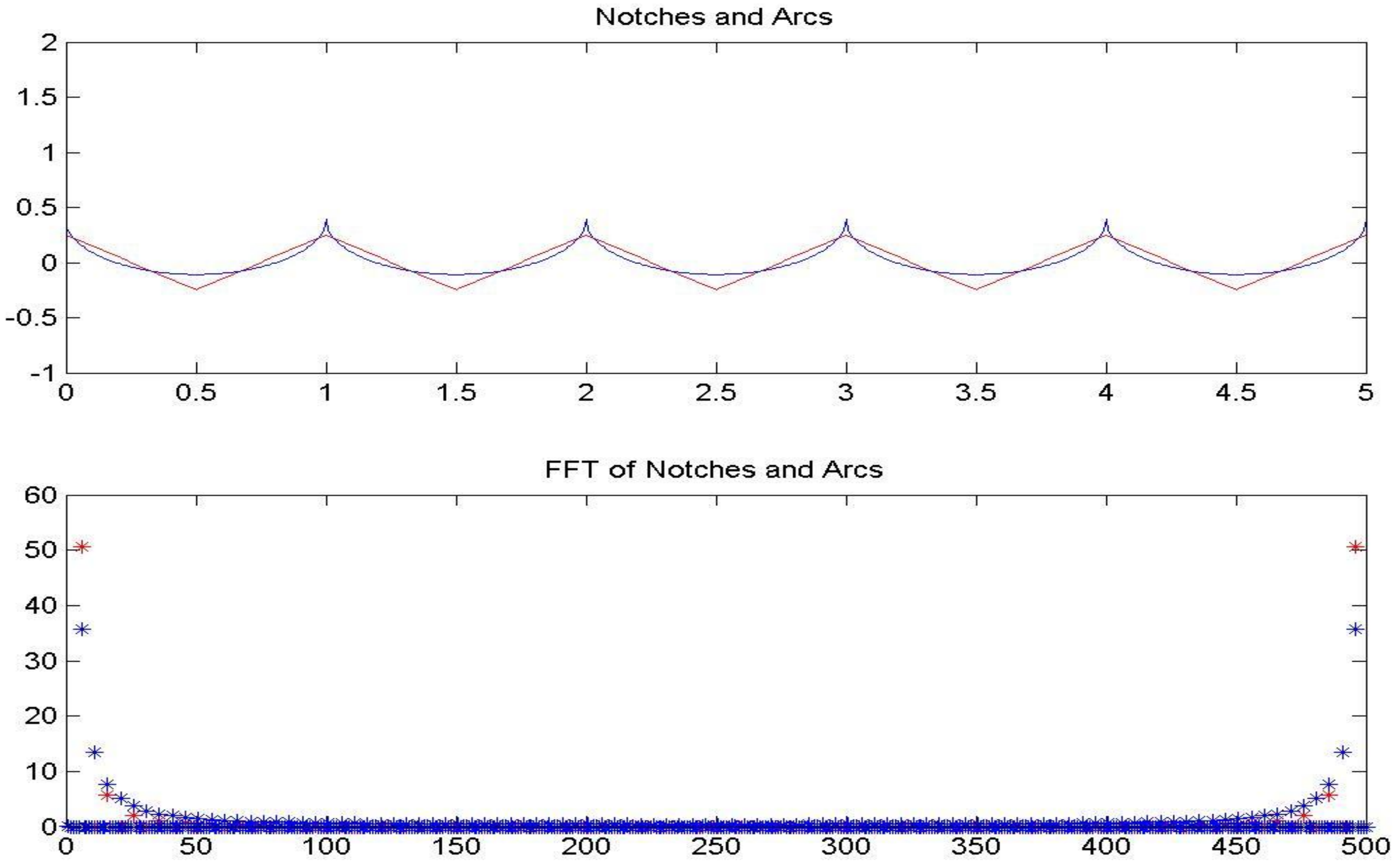


Here we compare 5th order WENO at four levels of grid refinement run on 16cpus of ASCI Blue.

From left to right we have contour plots at increasing grid point resolution,
16x80 RT = 12s
32x160 RT = 36s
64x320 RT = 2m,47s
128x640 RT = 17m,0s
of the density at the final time.

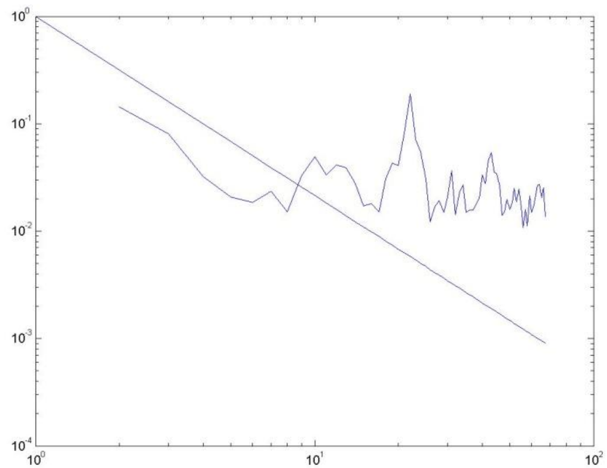


interface conditions where the Fourier amplitudes and phases have a specific relationship.

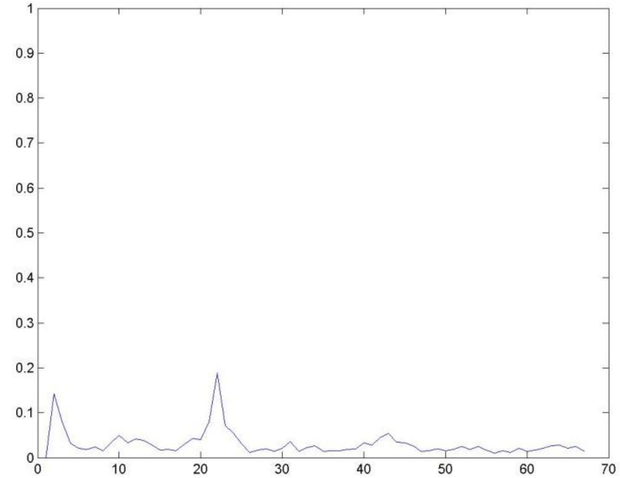


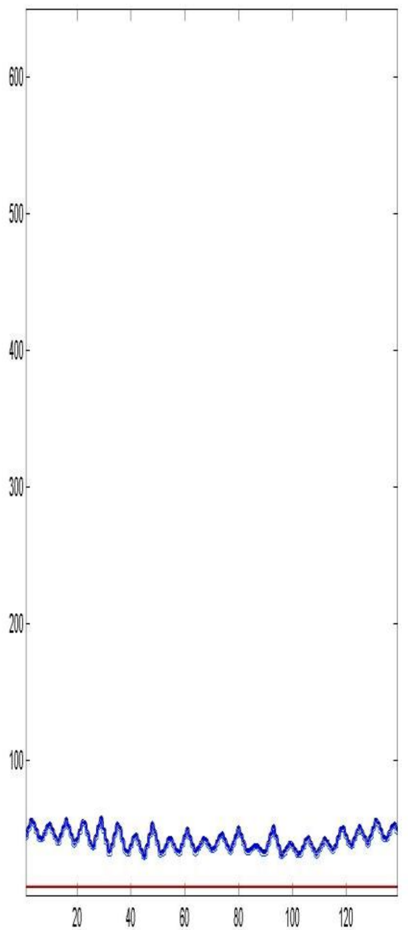
Initial interface should have a broad spectrum.

- Log Fourier
- Spectrum of
- Initial interface



- Fourier spectrum
- Of initial interface



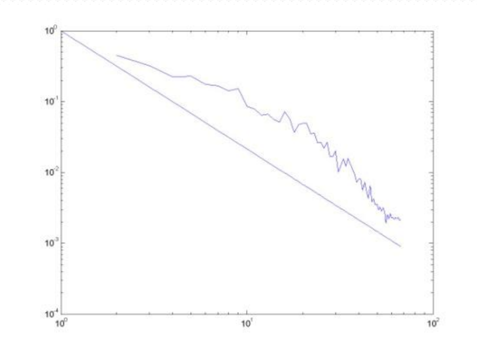


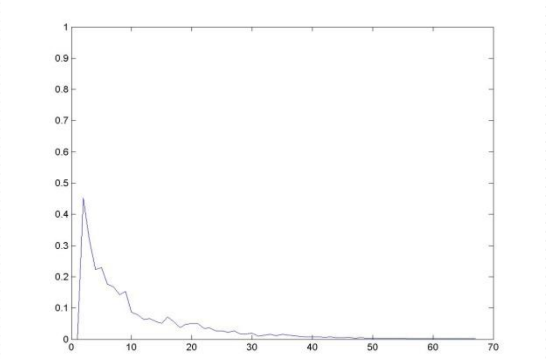
I chose a Richtmyer-Meshkov setup that is of interest to us with and without reshock.

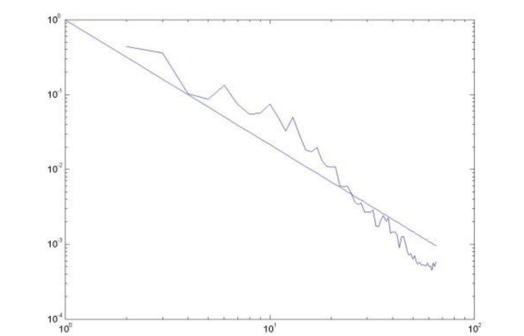
- First, a relatively strong Mach 10 shock is chosen for all calculations in order to get into the regime of ICF.
- The domain size and run time, 70ms, were chosen so that I could run the same setup with and without a reshock.
- The grid point density was chosen in order to keep the runtimes short, less than 20min, at the highest grid point density.
- The multimode interface was chosen with very high modal content in order to help distinguish between the lower and higher order implementations of WENO.

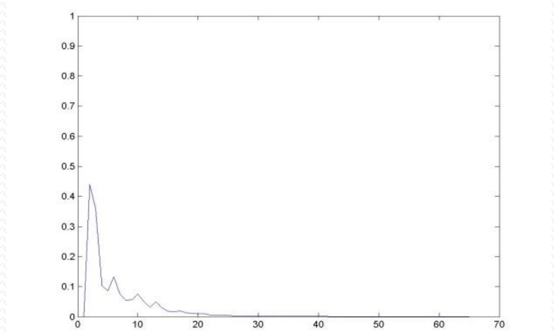
One needs a "measure" of success other than the eyeball norm and we choose the language of Fourier analysis since it is commonly used in the field of turbulence. 640 by 128.

- Fourier spectrum
- For 9th order
- Integral = 6.02





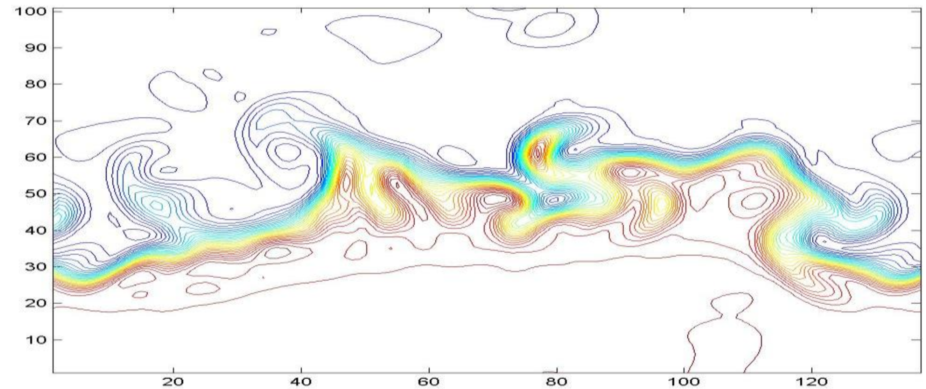




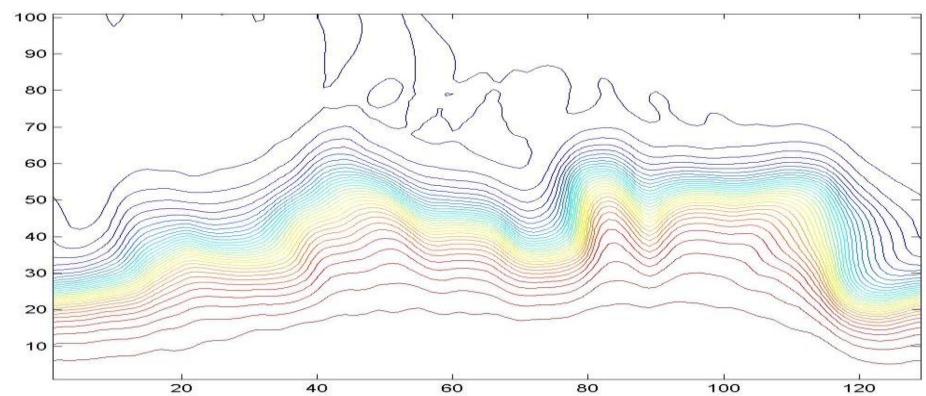
- Fourier spectrum
- For 3rd order
- Integral = 3.42

# of 64 by 320 one can “see” the additional structure the 9^{th} order propagates.

- 9^{th} Order WENO

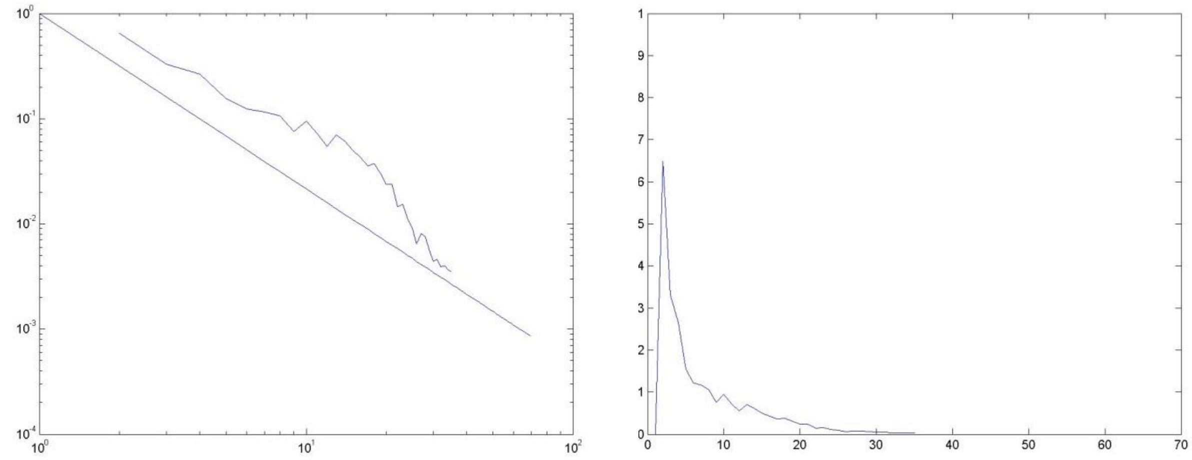


- 3^{rd} Order WENO

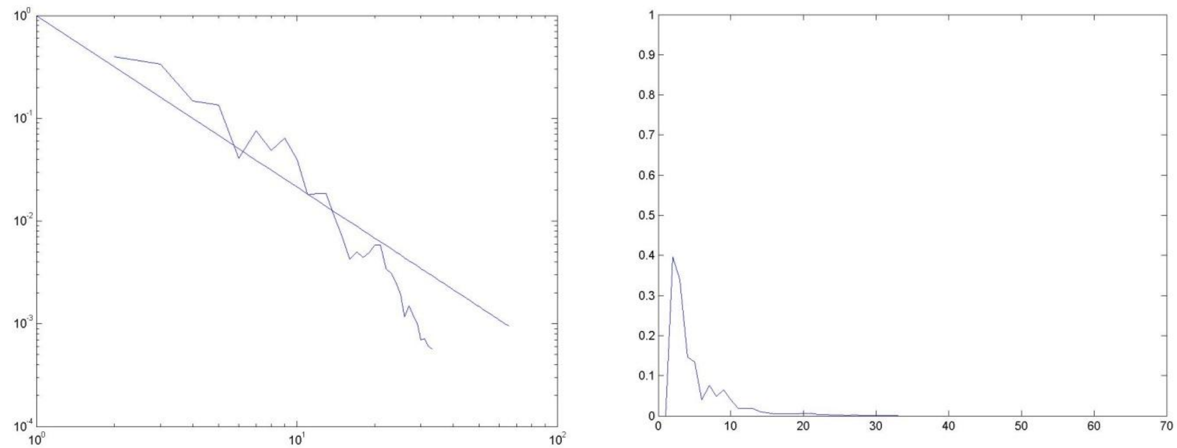


for 9^{th} order WENO compared to 3^{rd} order WENO on a grid of 64 by 320.

- Fourier spec
- For 9^{th} order
- Integral = 5.20

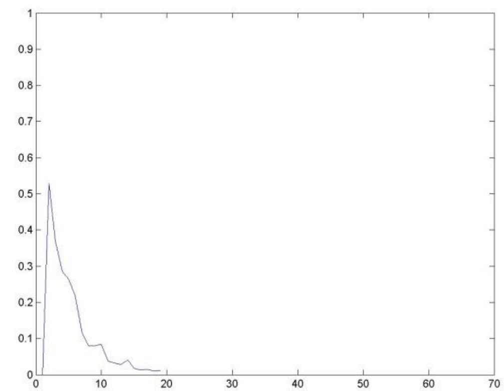


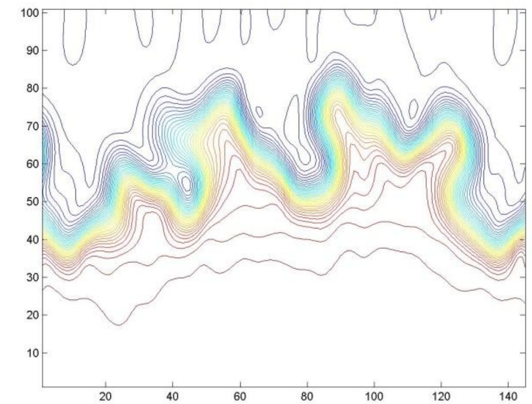
- Fourier spec
- For 3^{rd} order
- Integral = 2.81



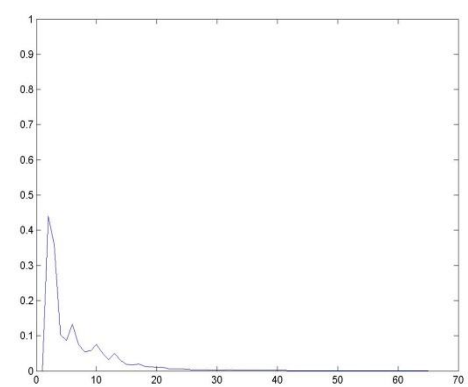
Visually and Quantitatively, when is 9^{th} order WENO most similar to 3^{rd} order WENO

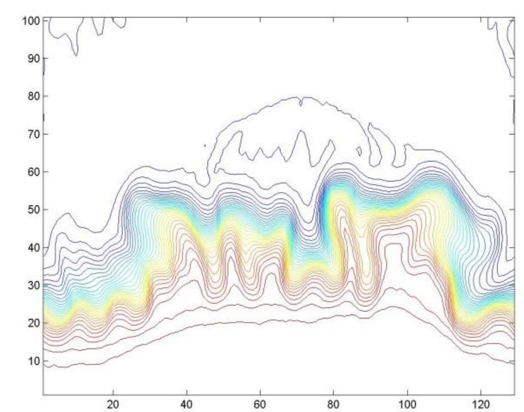
- 9^{th} Order WENO on a
- Grid of 32 by 160
- Integral = 4.84





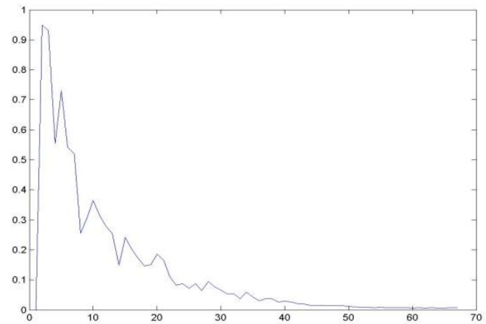
- 3^{rd} Order WENO on a
- Grid of 128 by 640
- Integral = 3.42

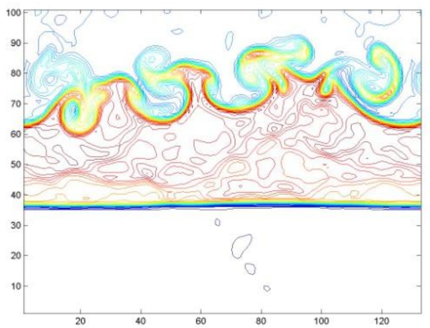




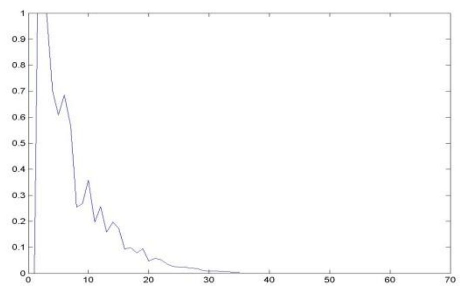
Studying RM reshock with high order WENO.

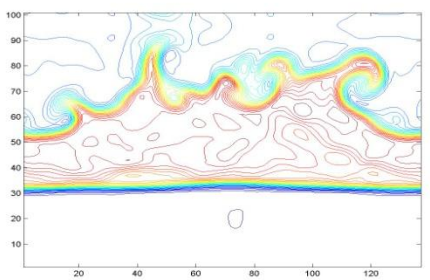
- 9^{th} order WENO
- Grid 128 by 384
- Integral 17.73



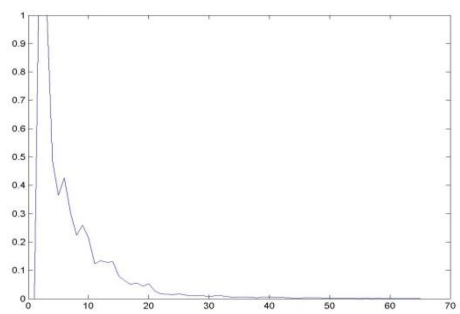


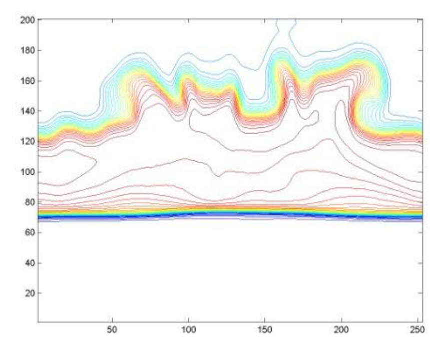
- 9^{th} order WENO
- Grid 64 by 192
- Integral 16.16



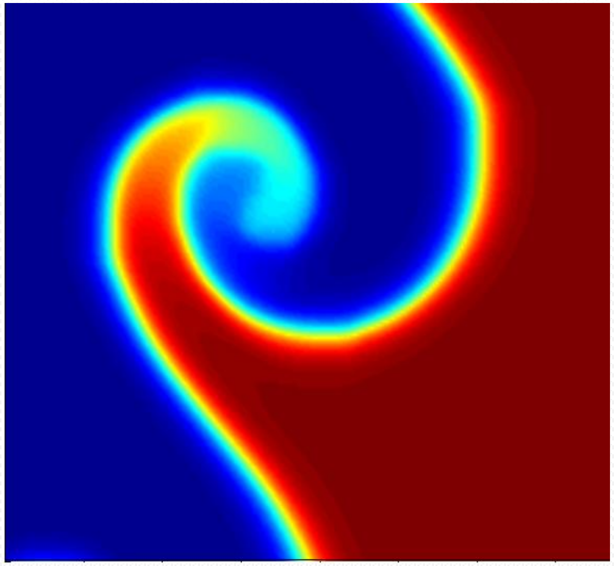


- 3^{rd} order WENO
- Grid 128 by 384
- Integral 11.82

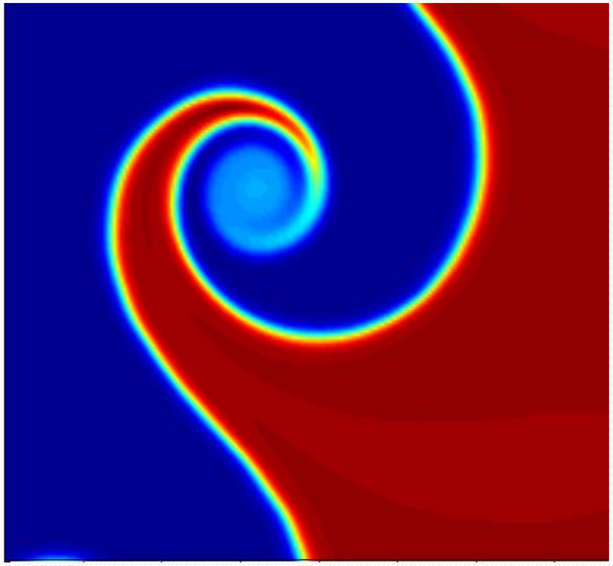




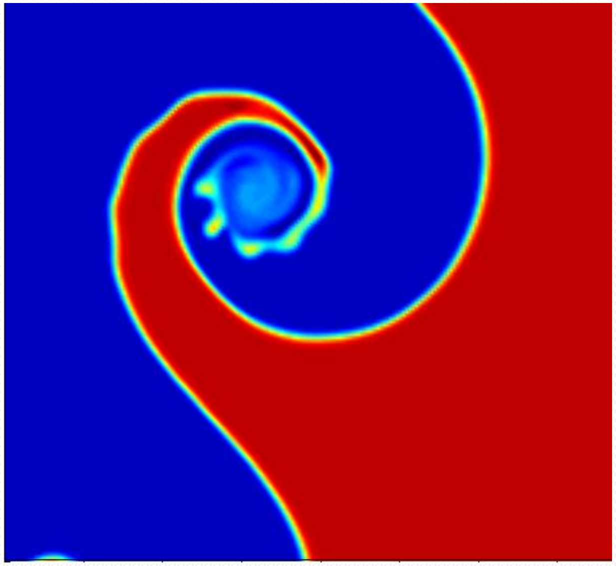
–3rd order WENO



–5th order WENO



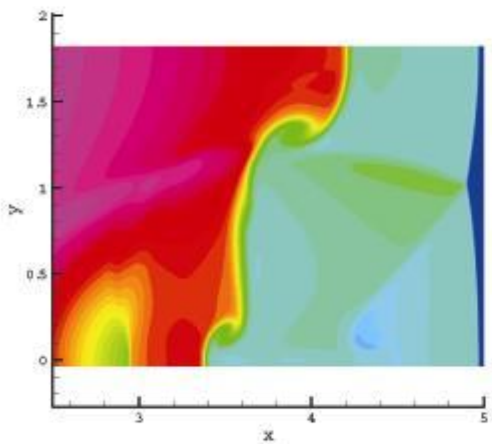
–9th order WENO



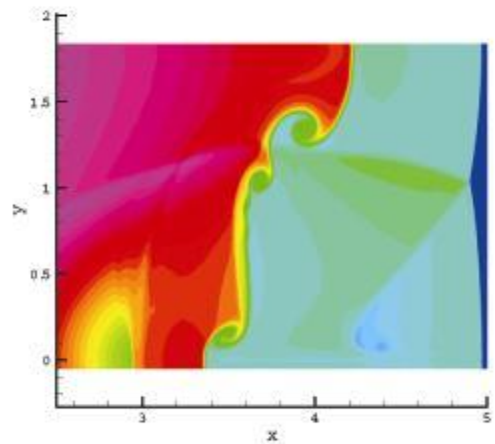
Richtmyer-Meshkov Instability

Convergence Study $(M = 4.46, \delta = 0.2\ cm, t = 50\ \mu s)$ **: Density**

WENO 3rd



WENO 5th

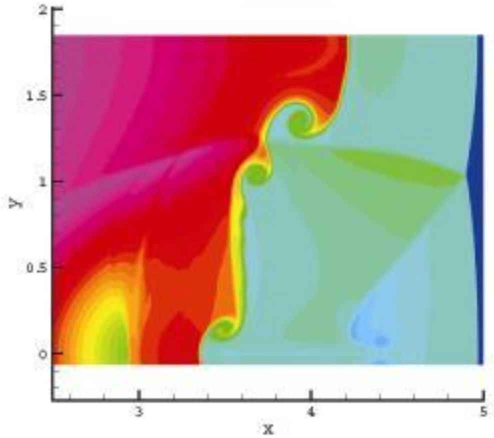


- Grid size for the Spectral and WENO schemes are 1024x256 in Full Domain.

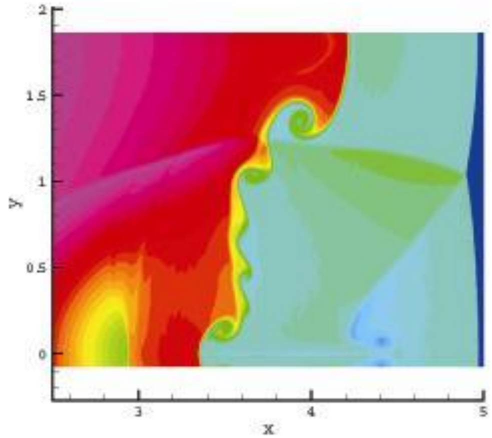
Richtmyer-Meshkov Instability (Cont.)

Convergence Study $(M = 4.46, \delta = 0.2\ cm, t = 50\ \mu s)$ **: Density**

WENO 7rd



WENO 9th

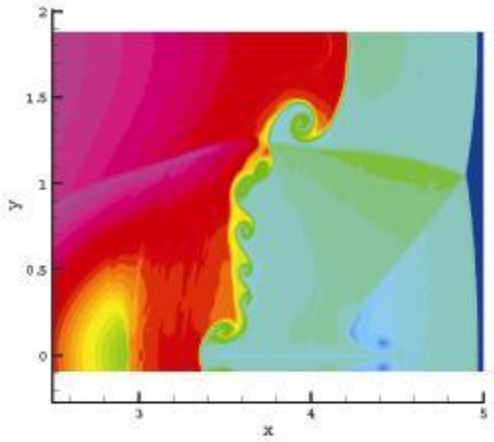


- Grid size for the Spectral and WENO schemes are 1024x256 in Full Domain.

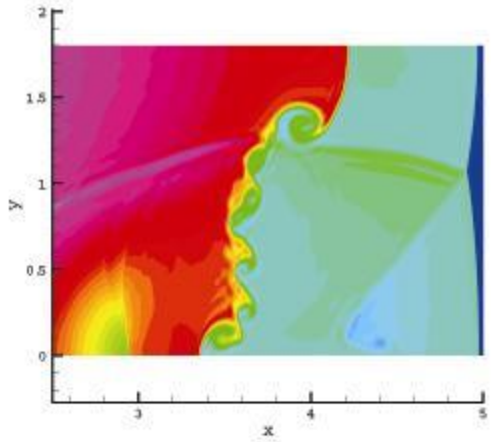
Richtmyer-Meshkov Instability (Cont.)

Convergence Study ($M = 4.46, \delta = 0.2\ cm, t = 50\ \mu s$) **: Density**

WENO 11st



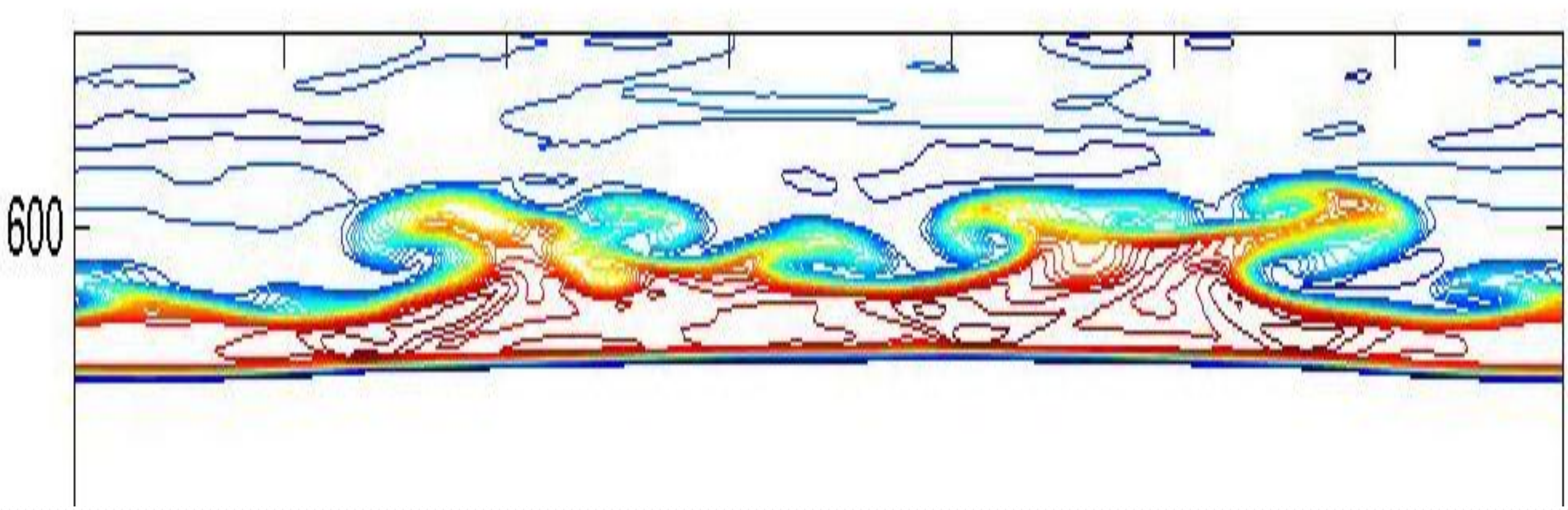
Spectral



- Grid size for the Spectral and WENO schemes are 1024x256 in Full Domain.

Let's challenge the code with a Mach 100 shock followed by a reshock using the 5th order option.

- Here we simply we want to demonstrate that with even a mach 100 shock on the notch interface followed by a reshock that the code runs. Below we see the mixing zone



passes does the high order information persist or is it destroyed?

- Signal processing, in general, allows one to "see" information that is otherwise obfuscated by some source of noise (such as seeing chips in cutting tools).
- The question is, if one cares only about pointwise convergence can the first order error introduced downstream from a shock be processed out so that the underlying high order signal can be observed?
- For a general set of nonlinear set of nonlinear equations this can be demonstrated but not proved.

# of a 2nd order Godunov method with 9th or 11th order show the following:

- On a given grid, the Godunov method is between 2 and 4 times as fast but with far more dissipation.
- The Godunov method requires about 4 times as many grid points in each direction in order to obtain roughly the same result at the final time.
- Recall that floating point operations for hyperbolic equations go as flops = C * N^(d+1)
- Thus in 2D we have an improvement of between (4*N)^(3)/2= 32 and (4*N)^(3)/4 = 16
- In 3D the improvement is between (4*N)^(4)/2 = 128 and (4*N)^(4)/4 = 64.

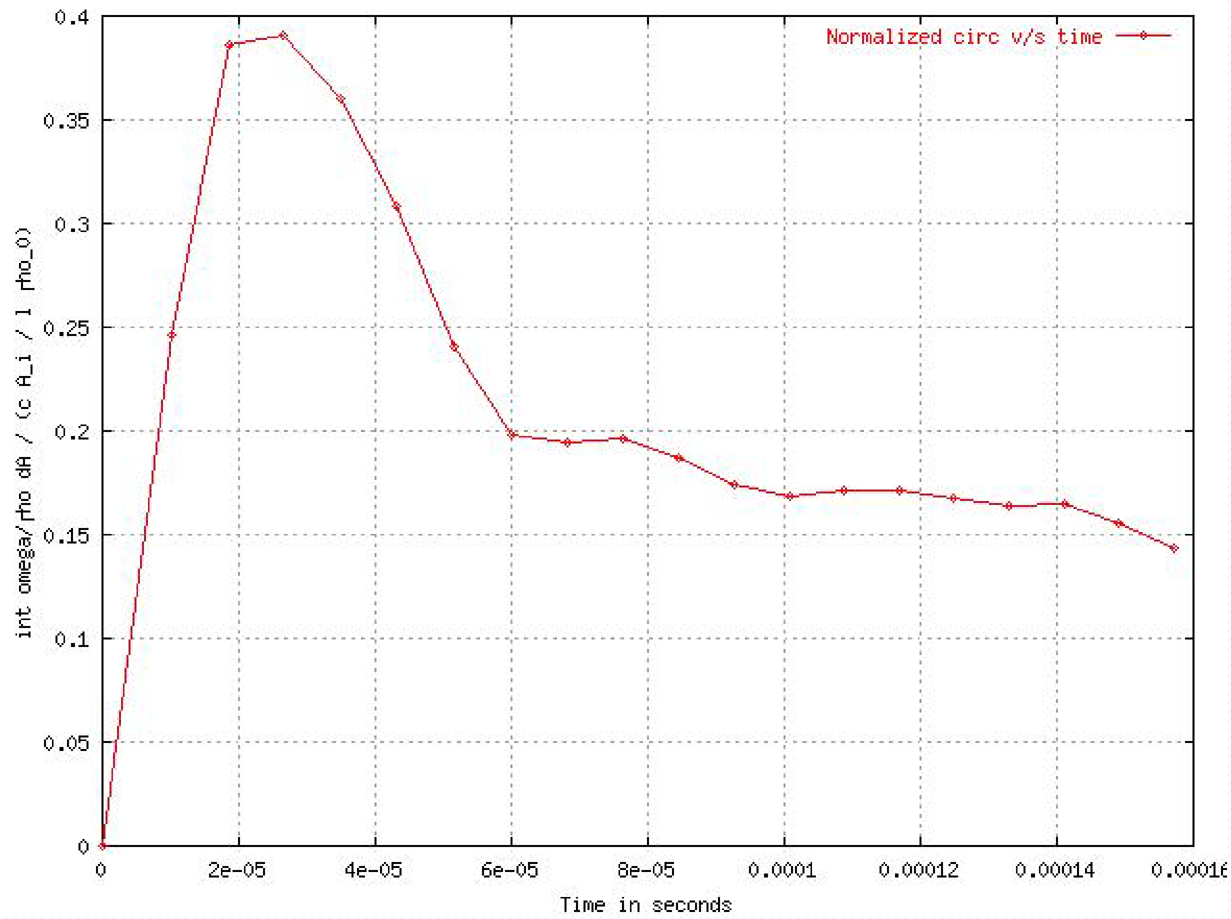
times, but by problem size. We have at most (2000)^(3) points available.

- There is always an upper bound on available machine and we don't want to be in a situation where we have to wait 1 year for a run to complete.
- Thus, we can not always just double or quadruple the grid in each direction without quickly hitting the upper bound on available computational resources.

affect on the flow field depending on if the error is dissipative or dispersive.

- For the Euler equations (first derivatives) the leading term in the truncation error is of the form (dx)^(p)f^(p+1)(x) where p is the order.
- Substitute f(x) = e^(ikx) we see that for even order schemes the dominant error is dispersive in nature.
- The problem with the leading error being dispersive is that it does not occur in NS as does a dissipative error.
- NS = Euler + (effective dissipation)

As another way to quantify the numerical dissipation, one might look at the “mass-weighted” circulation which is the integral of the vorticity divided by density.



tool for establishing the numerical dissipation of a scheme away from a discontinuity.

- Ut = (UU)x Burgers equation is used to verify that one's scheme can keep its formal order of accuracy even in the presence of a discontinuity. This is to insure that when Euler or NS are calculated (with shocks) that the numerical dissipation is the same as when the scheme is applied to a smooth problem.

It is important to keep in mind the fundamental reasons why high order methods are advocated.

- First of all, one MUST have high Fourier mode content in order to distinguish between the low order and high order methods.
- Second, the advantage of high order increases with increasing computational time.
- Thus, if one examines only the single mode RM one will never see convincing evidence for why high order is advocated.

methods for studying shock induced mixing is not new. Let's review what is known.

- For spectral methods, the first order error introduced by the shock can be post-processed out, or removed via a Gegenbauer projection method. Proofs exist for the linear case and computationally it has been shown for the Euler equations.
- It has been shown recently that the same result holds for WENO and the results will be available soon.
- Most importantly, one generally does not bother with the post-processing because the first order error does has no impact on flow features of interest such as mixing.

When is it appropriate to choose high order methods?

- High order methods are suitable only if the computational fields develop high order information, such as the vortices where mixing occurs.

- If ones computational fields are essentially piecewise low-order then one should choose low-order operators.

- In other words, choose numerical differentiation operators that have an order no greater than the order of the data, which can be measured by ether wavelet or Fourier analysis.

Correctness of Numerical Simulations

- Above all, numerical calculations need to produce answers that are physically correct.
  - No two ocean models give the same answer
  - No two coupled ocean-atmosphere models give the same answer
  - No two Inertial Confinement Fusion codes give the same answer