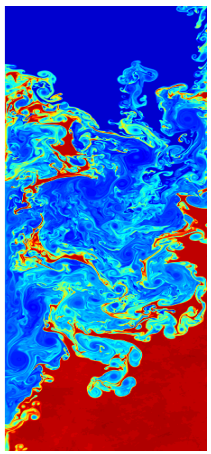
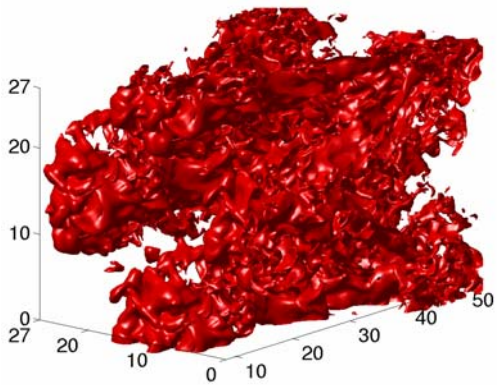
Investigation of Formally High-Order Methods for Shock-Induced Turbulent Mixing

Presented at:

The Joint Russian-American Five-Laboratory Conference on Computational Mathematics/Physics, Vienna, Austria





[1]Oleg Schilling

in collaboration with [2]Marco Latini and [3]Wai-Sun Don

[1]Lawrence Livermore National Laboratory, [2]California Institute of Technology, [3]Brown University

19-23 June 2005

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

The purpose of this research is to study the effects of order and grid resolution on flow physics in 2D and 3D Richtmyer-Meshkov instability and mixing with reshock

- Apply a high-resolution, Eulerian, shock-capturing reconstruction-evolution method to 2D and 3D single- and multi-mode Richtmyer-Meshkov instability with reshock
- Compare to experimental data (Collins-Jacobs and Vetter-Sturtevant) for validation; extend simulations/analysis to longer *t*
- Quantitatively study <u>dynamics and structure</u> of flow: time-evolution of mixing width, global mixing and flow statistics, energy spectra
- Investigate effects of order of flux reconstruction (formal order of accuracy) and grid resolution on mixing and turbulence
- Discuss implications for simulating experiments and assessing turbulent transport and mixing models

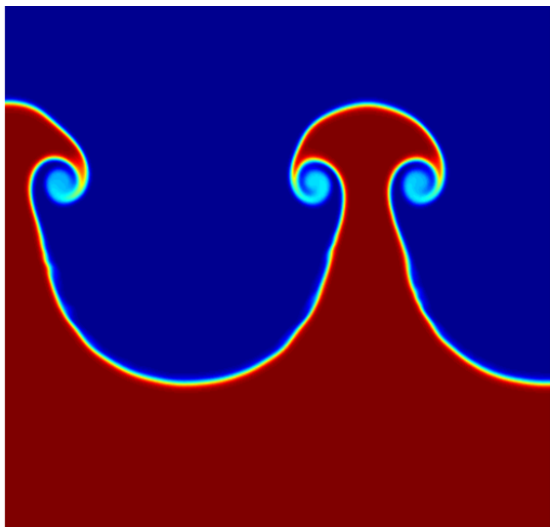
The topics of this investigation are critical to the development/validation of subgrid-scale and turbulent mixing models for shock-induced flows

2D and 3D simulations were performed using the weighted essentially non-oscillatory (WENO) method

- Euler equations solved using local Lax-Friedrichs flux-split finite-difference reconstructions
- Convex linear combination of all possible polynomial interpolations taken to achieve ENO property
  - High-order non-oscillatory solutions obtained using nonlinearly-weighted set of stencils that avoid crossing discontinuities
  - Local characteristic decomposition for flux-splitting
- 3rd-order TVD Runge-Kutta time-evolution
- 3rd-, 5th-, 7th-, 9th-, or 11th-order WENO reconstruction
- Adaptive domain method increases number of grid points dynamically
- Interface tracked by mass fraction
- Multi-resolution hybridization with high-order central-difference schemes possible (not used here)

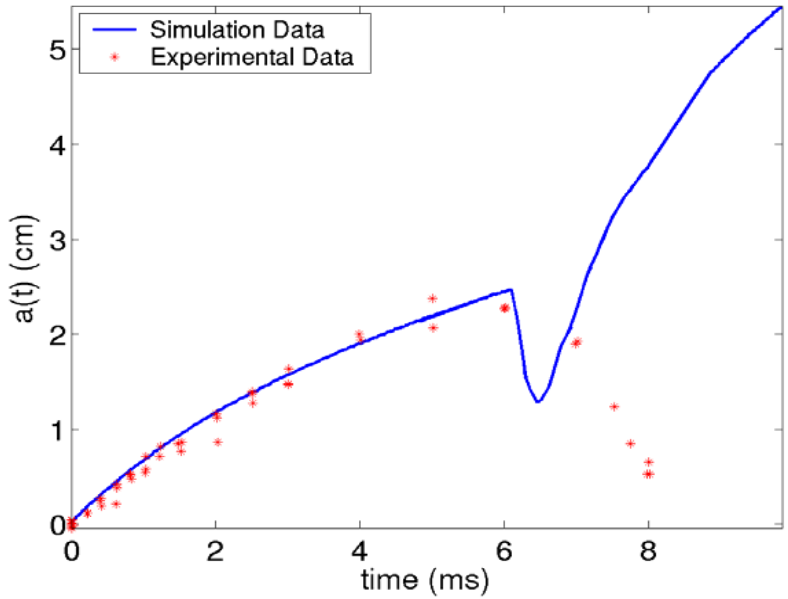
The Collins-Jacobs *Ma* = 1.21 air/SF_6(acetone) shock tube experiment was simulated using the WENO method (5th-order shown below)

- Initial amplitude a_0 = 0.183 cm
- Wavelength λ = 5.9 cm
- Adiabatic exponent γ = 1.24815
- Initial interface thickness 0.5 cm
- Computational domain 8.9 cm $\times$ 75 cm
- Grid resolutions 128, 256, 512 points per λ



Density at t = 5 ms

- Amplitude growth in very good agreement with experimental data before reshock
- Discrepancy following reshock due to reflected rarefaction in experiment, but not in simulation



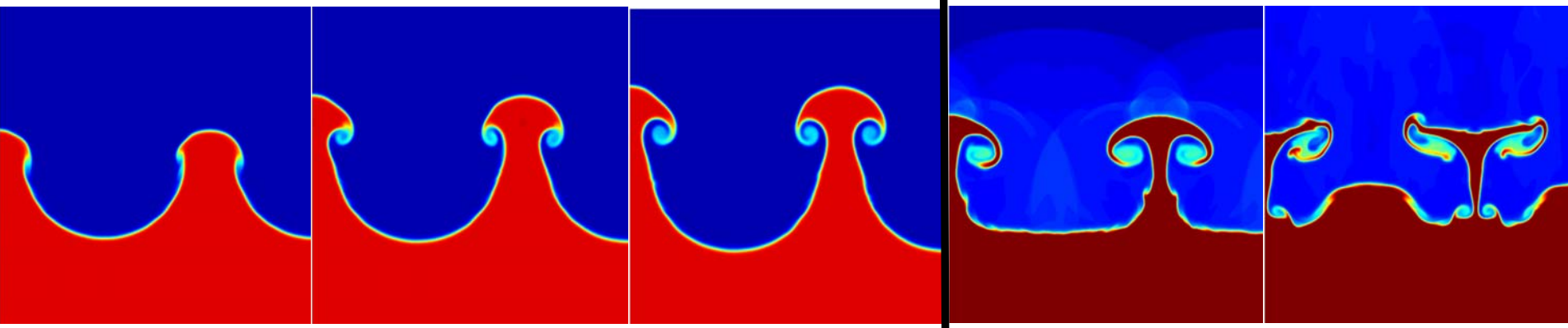
Simulation and experimental density are in good agreement initially; lack of rarefaction causes reflected shock to interact with interface ~ 1 ms sooner

PLIF images from Collins and Jacobs

after reshock

t = 2 .502 ms | *t* = 4.009 ms | *t* = 5.015 ms | *t* = 7.005 ms | *t* = 7.781 ms

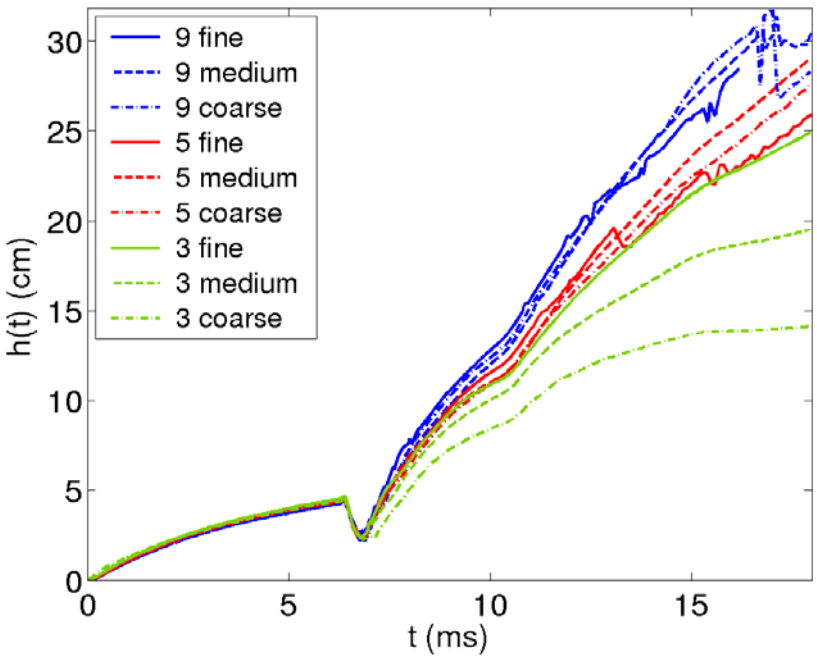
t = 2.5 ms | *t* = 4 ms | *t* = 5 ms | *t* = 6.47 ms | *t* = 6.78 ms



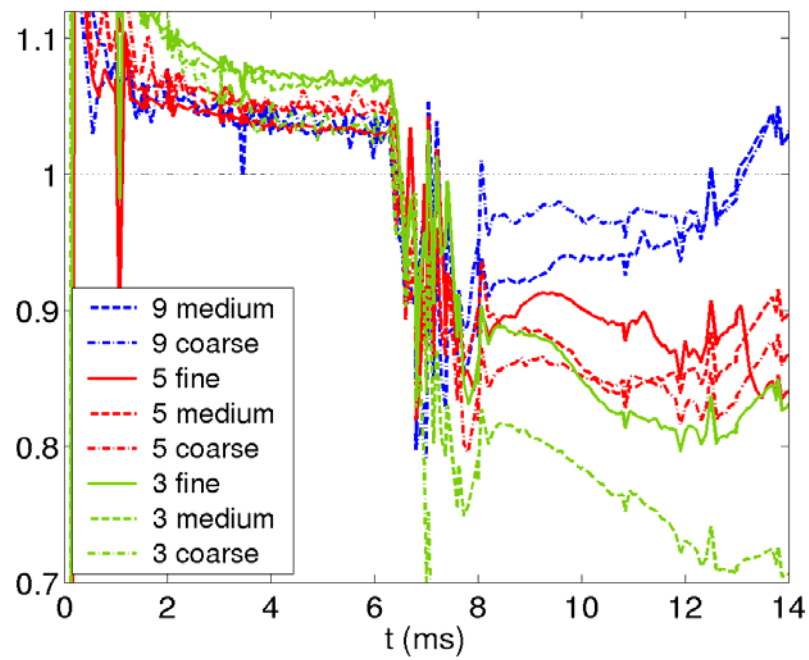
5th-order WENO simulations

Comparison of mixing layer widths obtained from 3rd-, 5th-, and 9th-order simulations on fine, medium, and coarse grids shows significant differences

Widths from 1-99% cut-off in mass fraction



Ratio of widths to 9th-order, fine grid width



- Widths generally agree before reshock, and for very short time following reshock (except for 3rd-order medium and coarse grid)
- Widths begin to diverge at later times during 'quasi-decay' phase
- The more dissipative the simulation, the smaller the width
- 9th-order results show apparent convergence

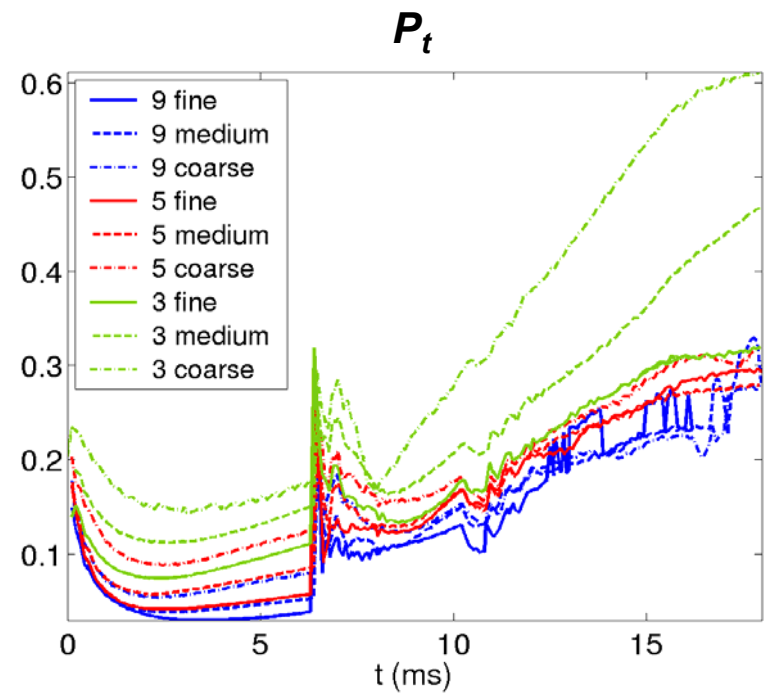
Quantities characterizing the "mixing" are also quite sensitive to the order and grid resolution

- Consider a fast kinetic reaction model in which mixing fluids are "reactants"
- In terms of the mole fraction X, amount of product produced is:
  - $X_p = X/X_s$ for $\underline{X} \leq X_s$ and
  - $X_p = (1 - X)/(1 - X_s)$ for $X > X_s$ ($X_s = ½$)
- Averaged product mole fraction $\langle X_p \rangle(x,t)$ provides information on how well mixed "reactants" are across layer
- Total "chemical product" is

$$P_t(t) = \int_{a_s}^{a_b} \langle X_p \rangle dx$$

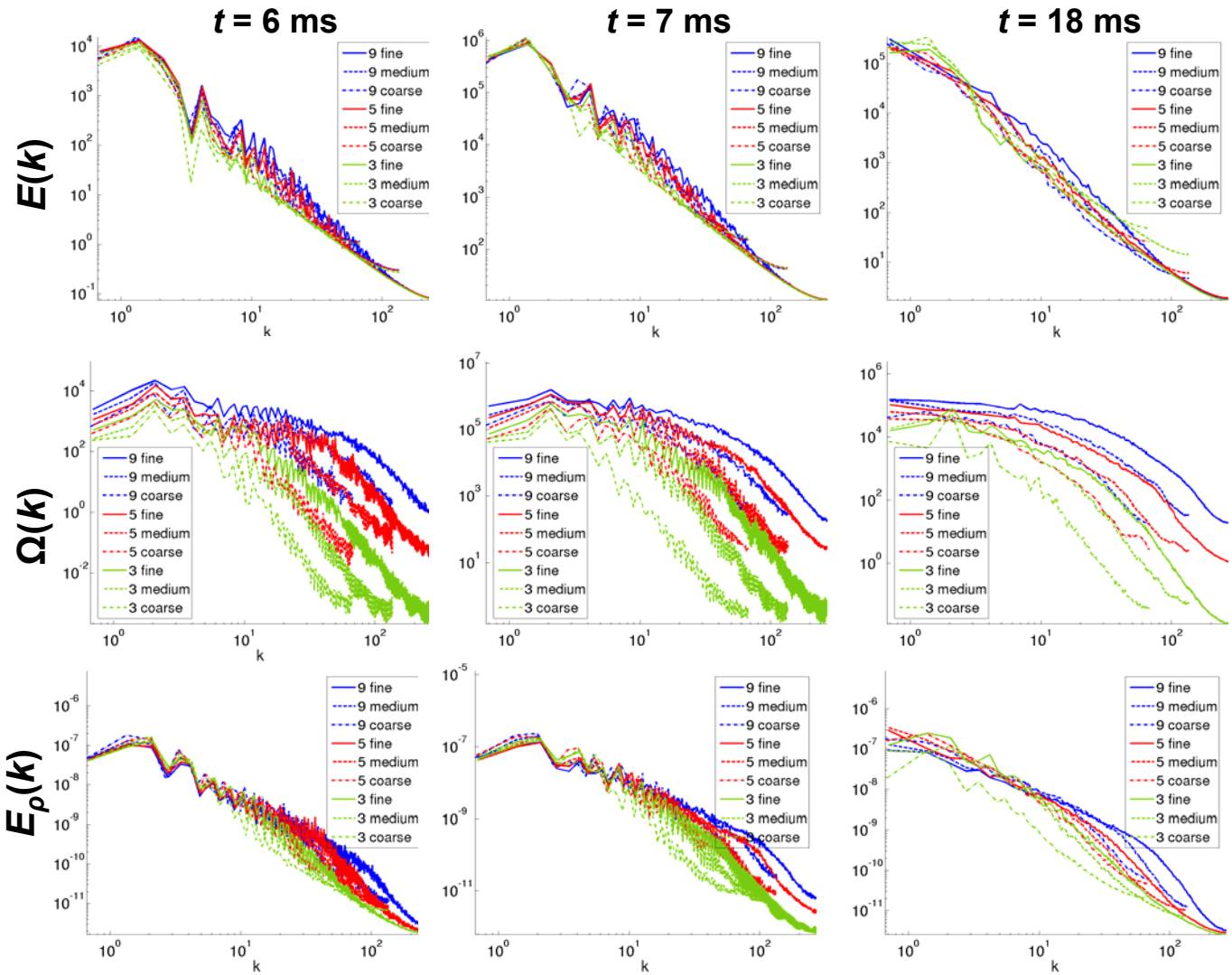
(a_b, a_s are bubble, spike amplitudes)

- P_t slowly increases before reshock, indicating increased "mixing", with additional "mixing" during layer compression at reshock



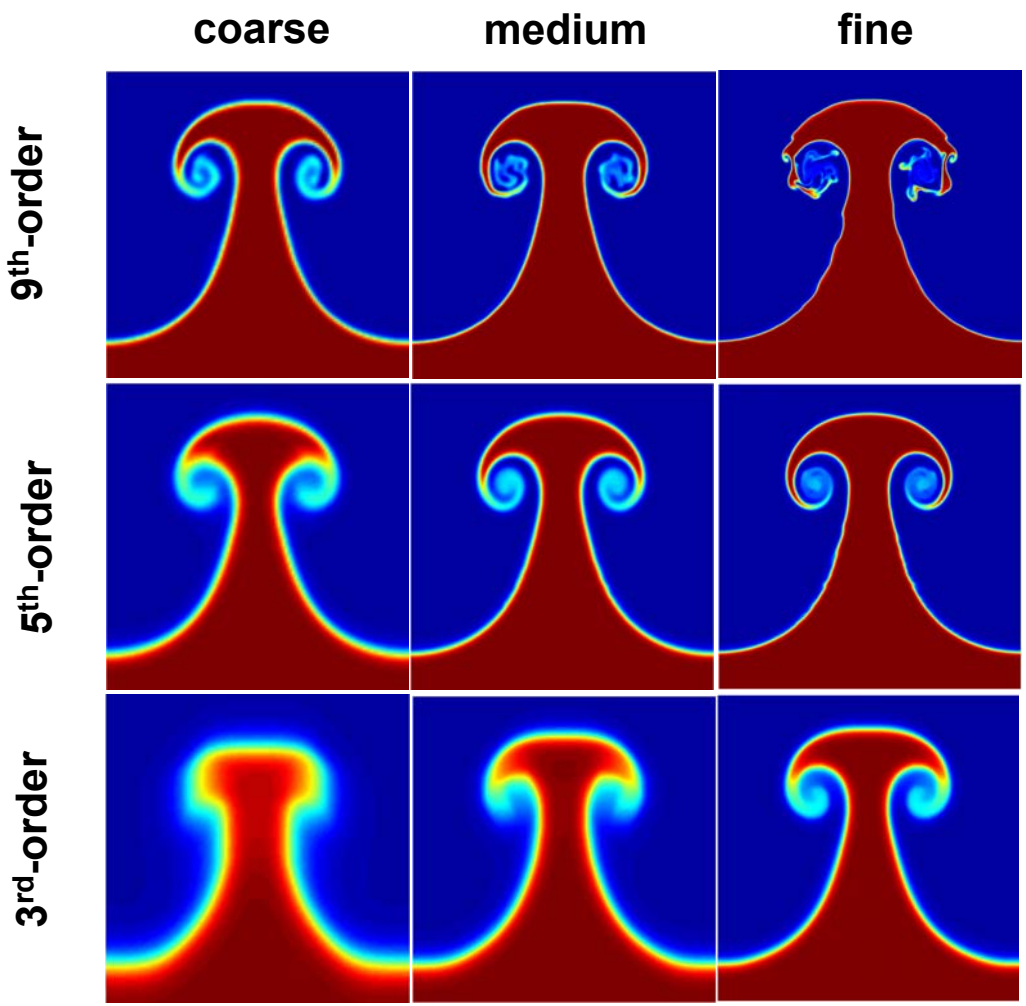
- Following reshock, P_t increases rapidly, indicated increased "mixing"
- *Algorithms with increasingly large numerical diffusion predict increasingly large "mixing"*

Turbulent energy spectra (particularly the turbulent enstrophy and density variance spectra) are quite sensitive to both order and resolution



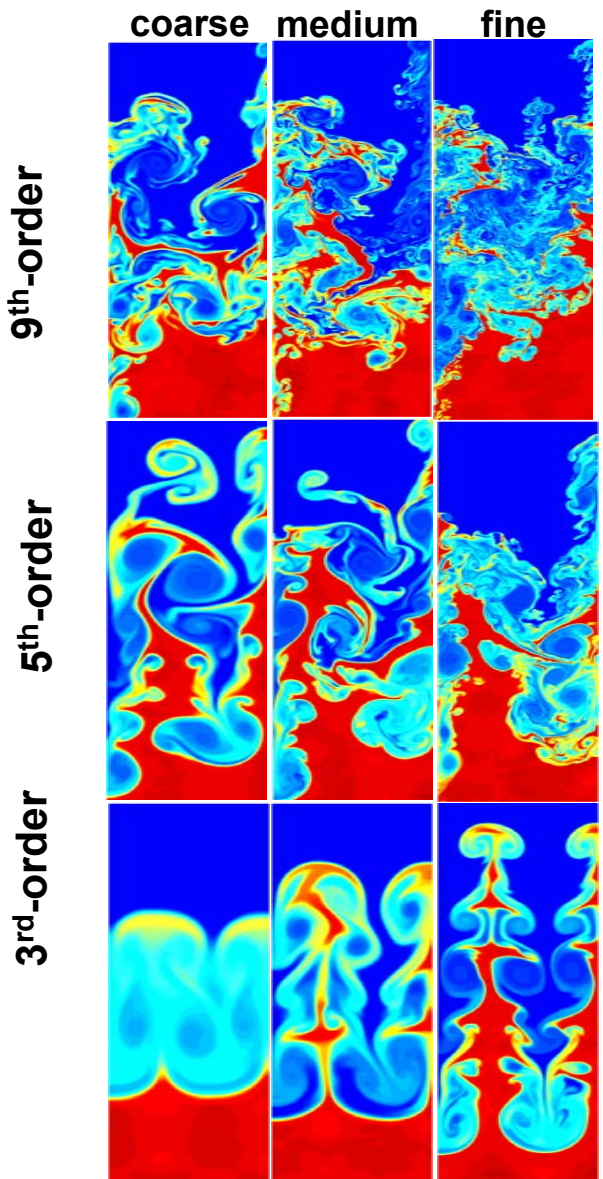
- Kinetic energy spectra differ mainly in intermediate scales
- Enstrophy spectra are highly sensitive to dissipation
- Density variance spectra extend to larger k as dissipation decreases with higher order and resolution

Significant differences are observed in the density at *t* = 6 ms (before reshock) among the different orders and resolutions



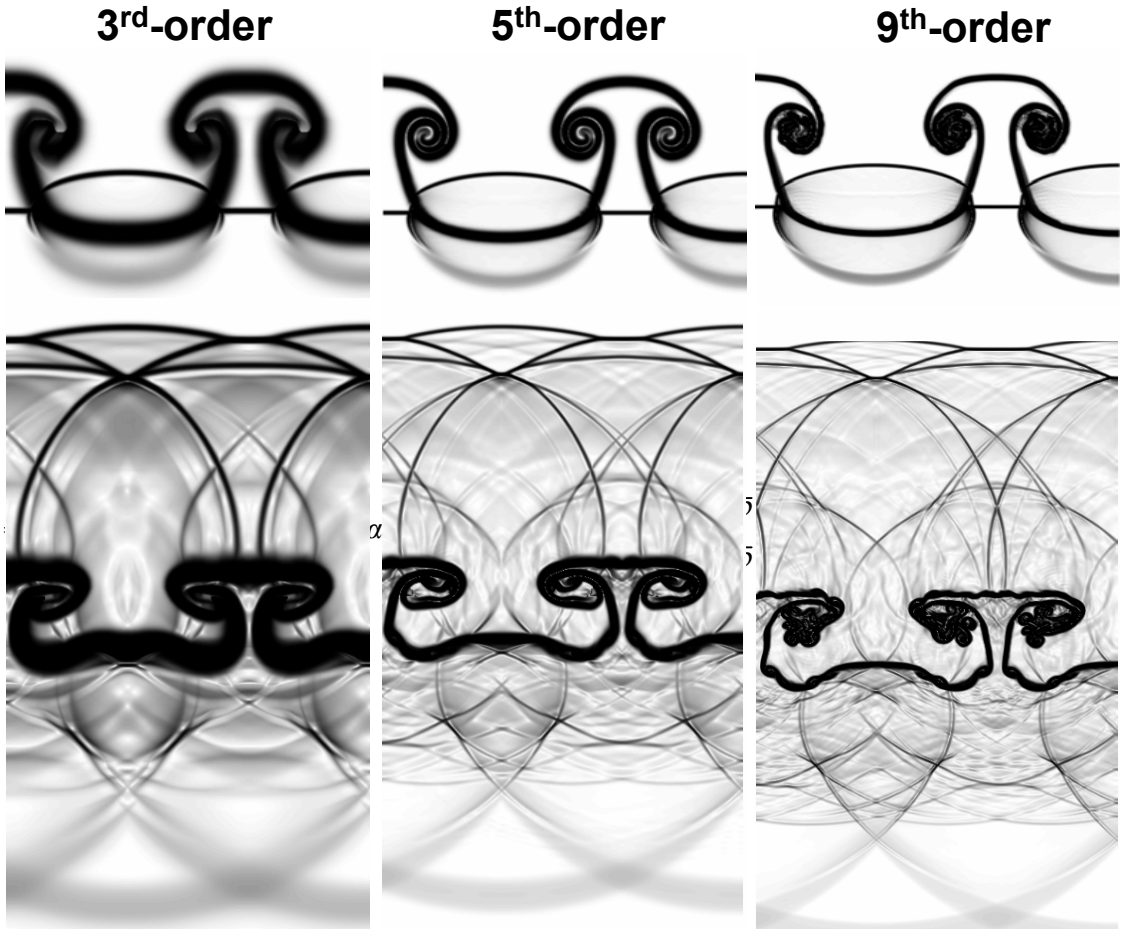
- Interface becomes much sharper with increasing order and resolution
- Very large numerical dissipation at 3rd-order inhibits roll-ups and formation of structure
- 9th-order results exhibit most small-scale structure both within roll-ups and on interface

Significant differences are also observed in the density at *t* = 18 ms (quasi-decay phase) among the different orders and resolutions



- 3rd-order results highly diffused to late times, with high degree of symmetry
- Much finer scale structure appears in 9th-order results across all resolutions
- 5th- and 9th-order results exhibit disorder
  - Reshock breaks symmetry
  - Very small numerical dissipation in 9th-order simulations allows small numerical instabilities to grow
- Structure observed in 9th-order, fine grid density most reminiscent of structure in PLIF images from shock tube experiments

Simulated density Schlierens show that much more wave structure is captured at 9th-order following reshock, with a sharper interface



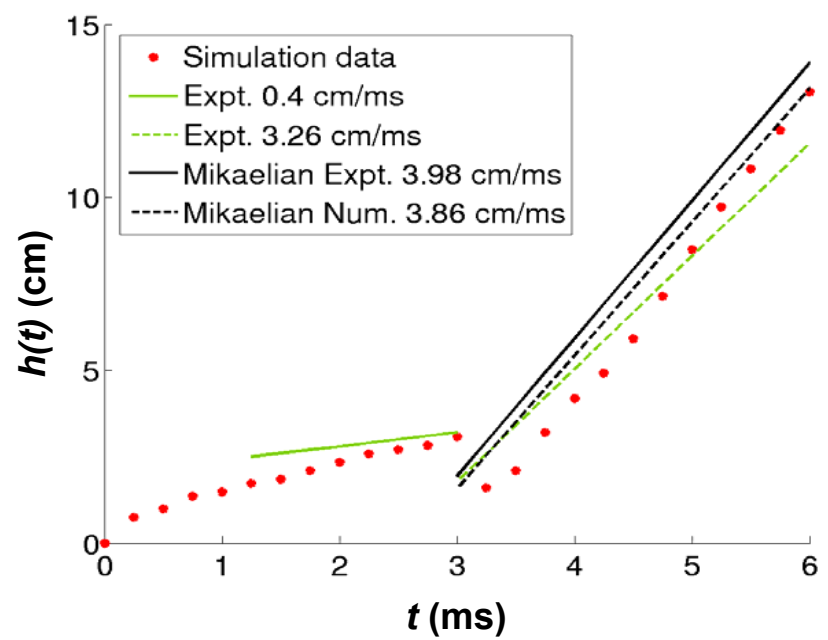
- Smaller difference between 5th- and 9th-order results compared to 3rd- and 5th-order results
- Numerical dissipation tends to thicken waves
- Slight differences in wave patterns due to small difference in times (± 0.01 ms)

$$\Phi(x,y) = \exp\left[-\alpha(m_{SF_6})\frac{|\nabla\rho|}{\max|\nabla\rho|}\right] \quad , \quad \alpha(m_{SF_6}) = \begin{cases} 20 & \text{if } m_{SF_6} > 0.25 \\ 100 & \text{if } m_{SF_6} < 0.25 \end{cases}$$

The *Ma* = 1.5 air/SF_6 Vetter Sturtevant experiment with wire mesh and membrane is modeled using a two-mode initial perturbation

Initial perturbation model:

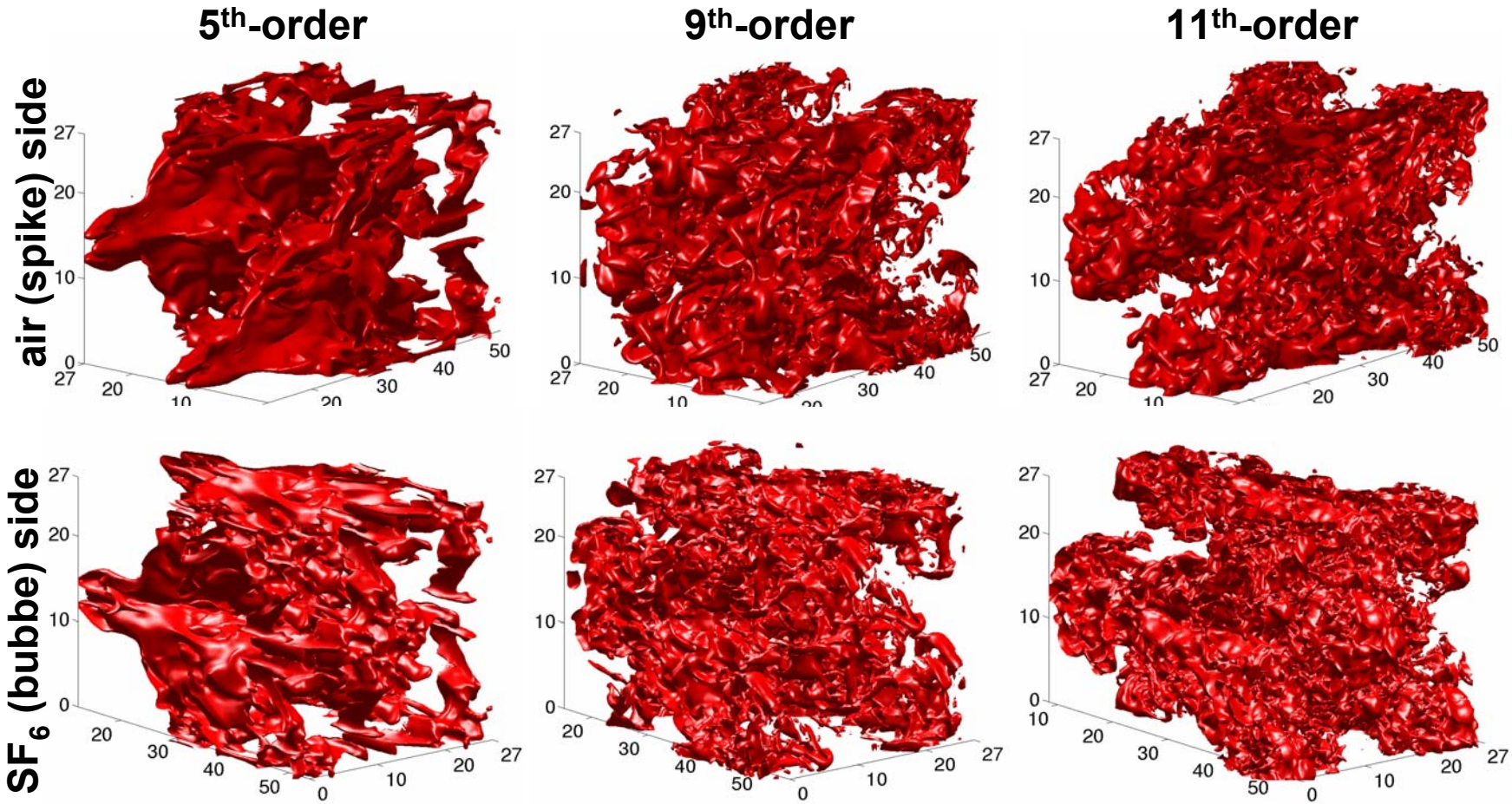
$$\eta(y,z)=0.27\left[\underbrace{\left|\sin\left(\frac{10\pi}{27}y\right)\right|\left|\sin\left(\frac{10\pi}{27}z\right)\right|}_{\text{Models membrane pushed through mesh}}-\underbrace{\cos\left(\frac{2\pi}{27}y\right)\cos\left(\frac{2\pi}{27}z\right)}_{\text{Models mesh distortion}}\right]$$



- Adiabatic exponent γ = 1.24815
- Initial interface thickness 0.5 cm
- Computational domain (test section) 27^2 cm $\times$ 61 cm
- Grid resolution 129^2 x 257
- Orders: 5th, 9th, 11th

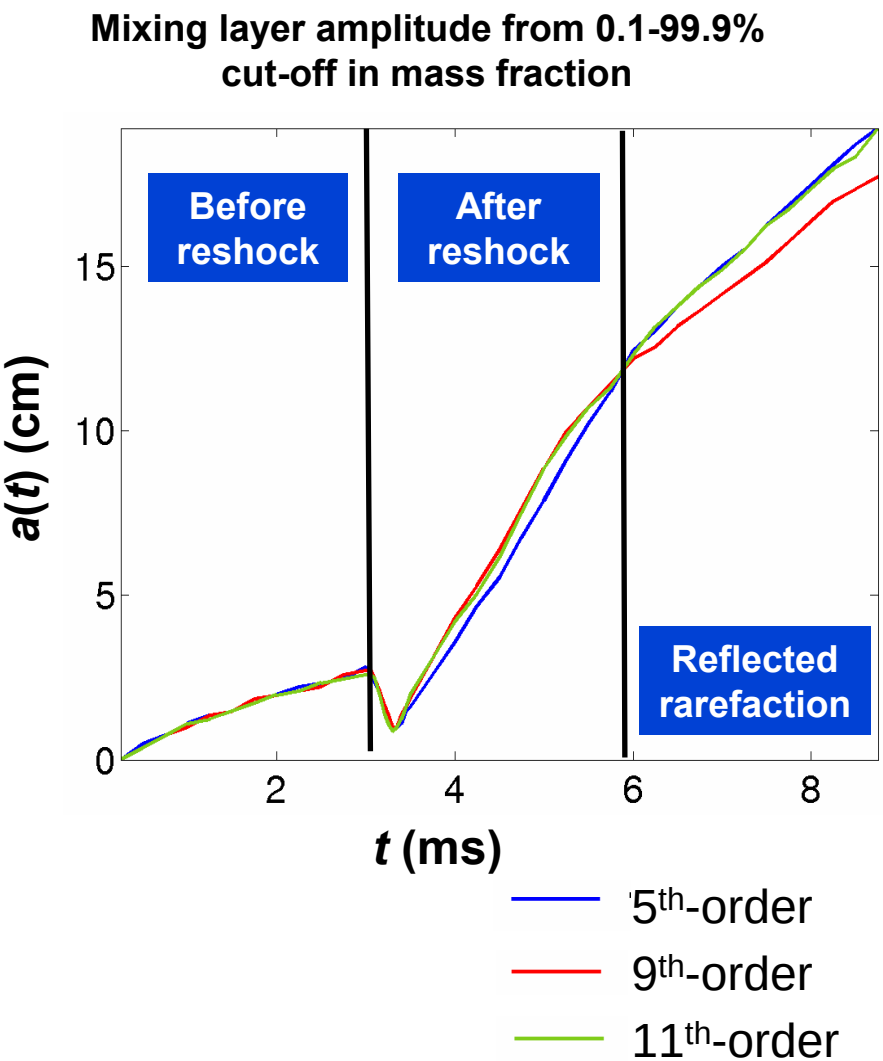
- Mixing layer growth in very good agreement with experimental data following reshock (5th-order shown)
- Amplitude growth also in generally good agreement with Mikaelian reshock model $h(t) = 0.28\, A^+\, \Delta u\, t$

The mass fraction isosurface exhibits the differences in small- and larger-scale structure obtained from simulations using different orders of reconstruction



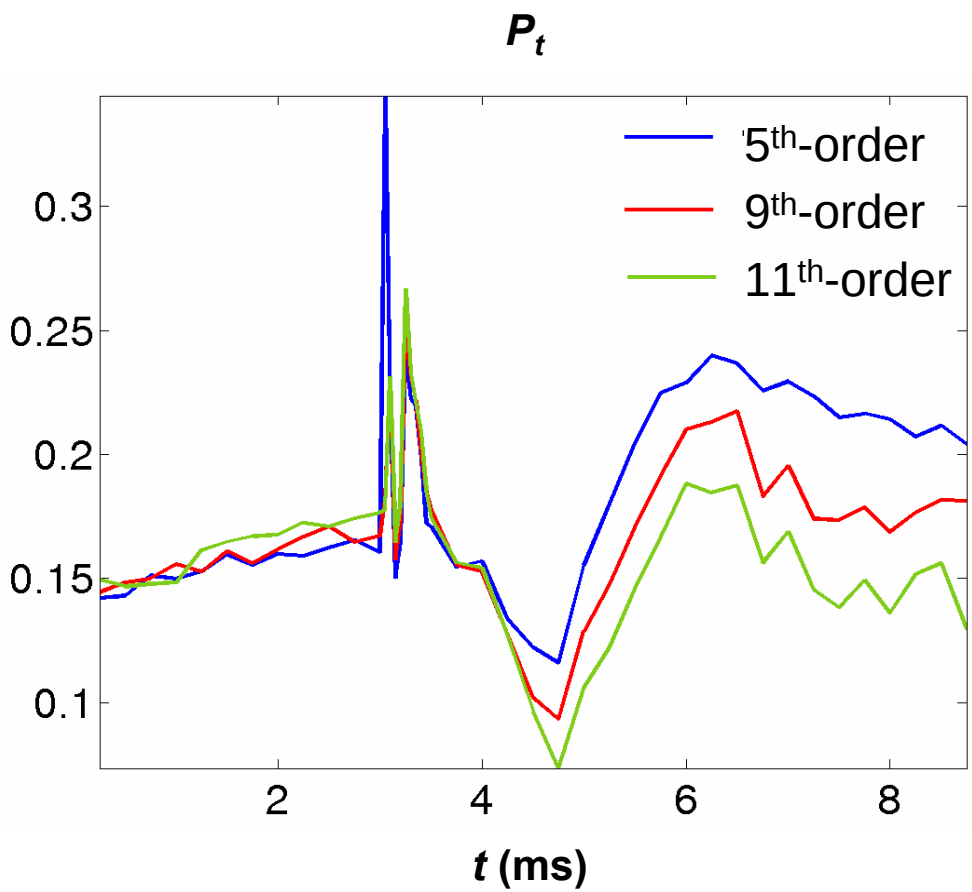
- *Both large- and small-scale structure different*
- 9th- and 11th-order simulations exhibit smaller scale structures than present in 5th-order data
- Even smaller scale structures exist in 11th-order simulation than in 9th-order simulation

Comparison of mixing layer amplitudes obtained from 5th-, 9th-, and 11th-order simulations also shows differences after reshock and at late times



- Amplitudes agree before reshock
- Between reshock and arrival of reflected rarefaction at $t \sim 6$ ms, 5th-order amplitude is smaller than 9th- and 11th-order amplitudes
- Difference in $a(t)$ after $t \sim 6$ ms is due to reflected rarefaction
  - As order increases, reflected rarefaction is stronger, "pulling back" interface more, resulting in a larger $a(t)$ (9th- and 11th-order)
  - If reflected rarefaction is weakened, interface is not "pulled back" and growth following reshock continues to be rapid (5th-order)
- At $t \sim 9$ ms, layer reaches end wall of shock tube

Quantities characterizing the global "mixing" due to numerical diffusion are also quite sensitive to the order and grid resolution



- Before reshock, P_t is similar among three cases
- After reshock, P_t differs among all cases
- Higher numerical diffusion results in larger "mixing", as in 2D

Quantities at all spatial scales characterizing "mixing" and turbulence in reshocked, Richtmyer-Meshkov instability exhibit a significant dependence on order and resolution

- As shown in 2D, independent of $O(1)$ error from shock, late-time flow in quasi-decay regime is especially sensitive to numerical algorithm
- 3rd- and 5th-order WENO are excessively dissipative
- 9th-order WENO shows evidence for numerical convergence of quantities dominated by large scales, at resolutions considered in 2D
- As expected, quantities determined by gradients (e.g., enstrophy spectrum) are most sensitive
- Qualitatively and quantitatively, approximately doubling order gives results similar to doubling resolution in 2D
- Study was systematic and self-consistent, using same algorithm and initial/boundary conditions, but with different order and resolution
- Further comparisons among 3D results in progress

The numerical evidence presented here suggests that formally high-order methods are desirable for simulating turbulent transport and mixing with or without explicit models for unresolved physics