Spectral and High-Order Methods for Shock-Induced Mixing

Andrew W. Cook

William Cabot

Jeffrey A. Greenough

Stephen V. Weber

Lawrence Livermore National Laboratory

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High-resolution numerical simulation data are needed to augment experimental data

- Data from high-energy shock experiments are difficult to obtain and are usually in the form of integrated quantities.

- Direct numerical simulation (DNS) and large-eddy simulation (LES) can be used to obtain highly detailed data from turbulent flows (e.g., velocity, correlations, pdf's, energy budgets) which cannot be obtained from experiments.

- Our goal is to develop the capability to perform accurate, high-resolution hydrodynamic simulations for shock-induced mixing problems.

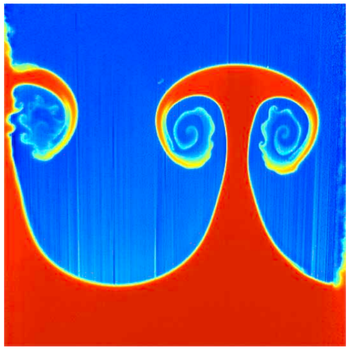
Which numerical scheme is best suited to perform high-resolution simulations of shock-induced turbulent flows?

- In astrophysical and Inertial Confinement Fusion (ICF) applications, shocks deposit vorticity at material interfaces, which subsequently evolve into turbulent mixing regions.
- Shocks and interfaces require robust numerical schemes which are typically monotonic and of low order.
- Accurate simulations of turbulent mixing requires high-resolution numerical methods to capture the large range of scales participating in the flow dynamics.

Can spectral/compact methods be made sufficiently robust to handle shocks, while maintaining their high resolution properties for turbulent mixing?

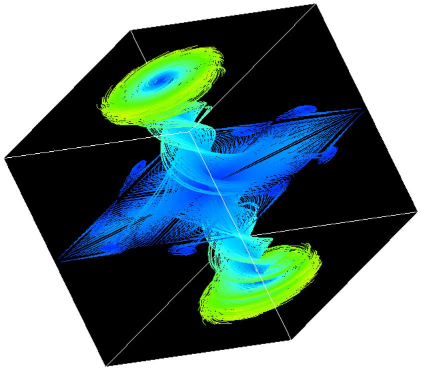
Two test problems were used for intercode comparisons

- 2D Richtmyer-Meshkov instability (RMI)
  - **vorticity deposited by a shock on a thin material interface**



(Collins & Jacobs 1999)

- 3D Taylor-Green vortex (TGV)
  - **vortex stretching; cascade to small scales**
  - **similarities to turbulence**

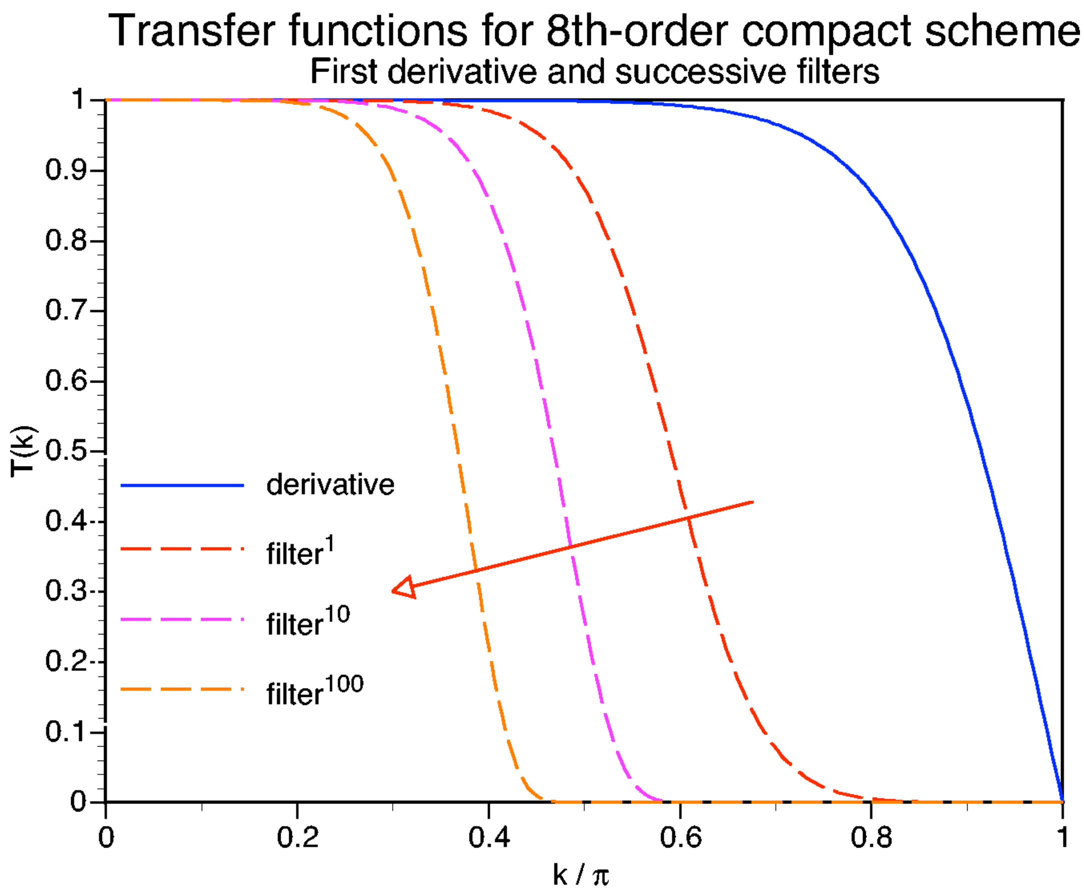


(The University of Edinburgh)

Intercode comparisons were performed with five different hydrodynamic codes/schemes

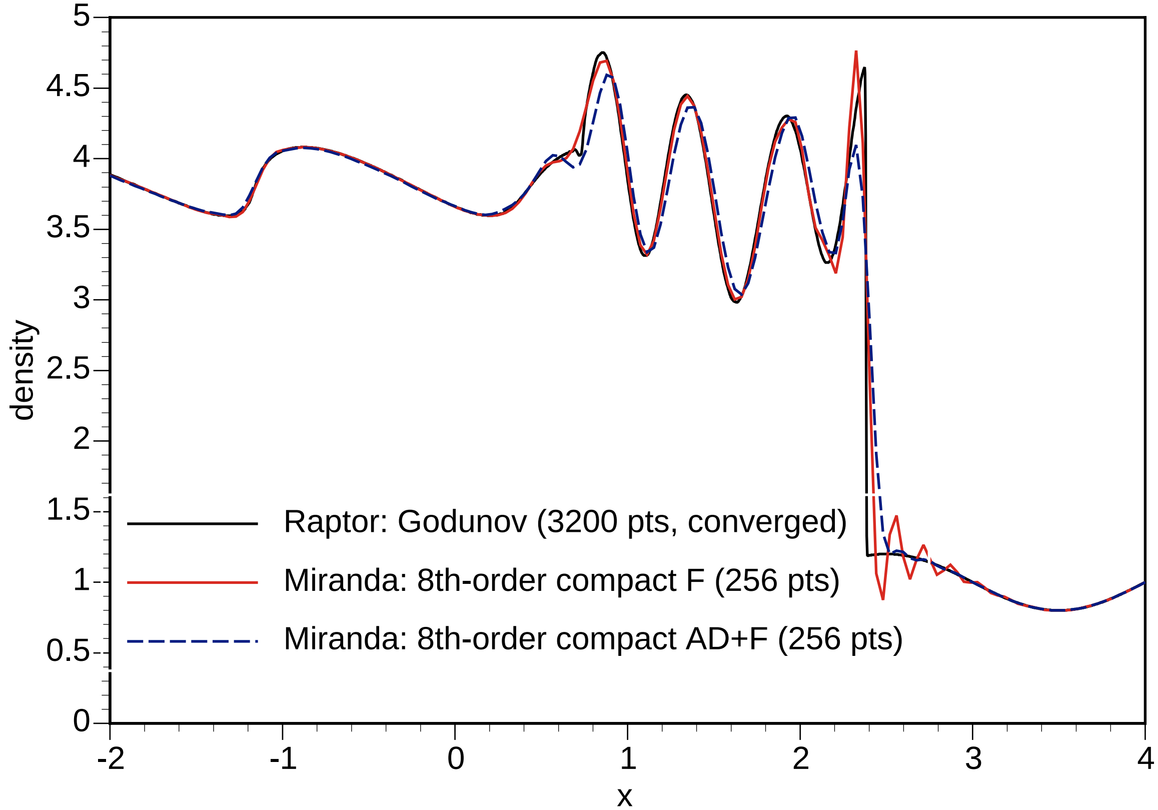
- ***Miranda* - S/C**: spectral/high-order compact scheme with modifications:
  - ♦ high-order filtering removes high frequencies **globally** for stabilization (but leaves ringing)
  - ♦ artificial viscosity/diffusivity with high-order switches smooths shocks and interfaces **locally** (removes ringing)
- ***Raptor* - HOG**: High-order Godunov scheme (formally 2nd order) in AMR framework
- ***HYDRA* - ALE**: Arbitrary Lagrangian-Eulerian scheme (2nd order) with non-standard diffuse interface treatment
- ***Miranda* - CENO**: Kurganov & Tadmor central finite difference ENO scheme (2nd order) (for RMI)
- **WENO** *(Don, Gottlieb &Shu):* weighted ENO scheme (5th-order) (for TGV)

Global filtering can degrade the resolution of the solution and generate additional ringing (Gibbs oscillations)



Local artificial diffusivity/viscosity is used in *Miranda* to remove ringing (Gibbs oscillations)

Shu-Osher 1D shock/density wave case



Compact scheme with global filtering (F) has ringing, which local artificial dissipation (AD) removes

Local Artificial Diffusion Terms in *Miranda*

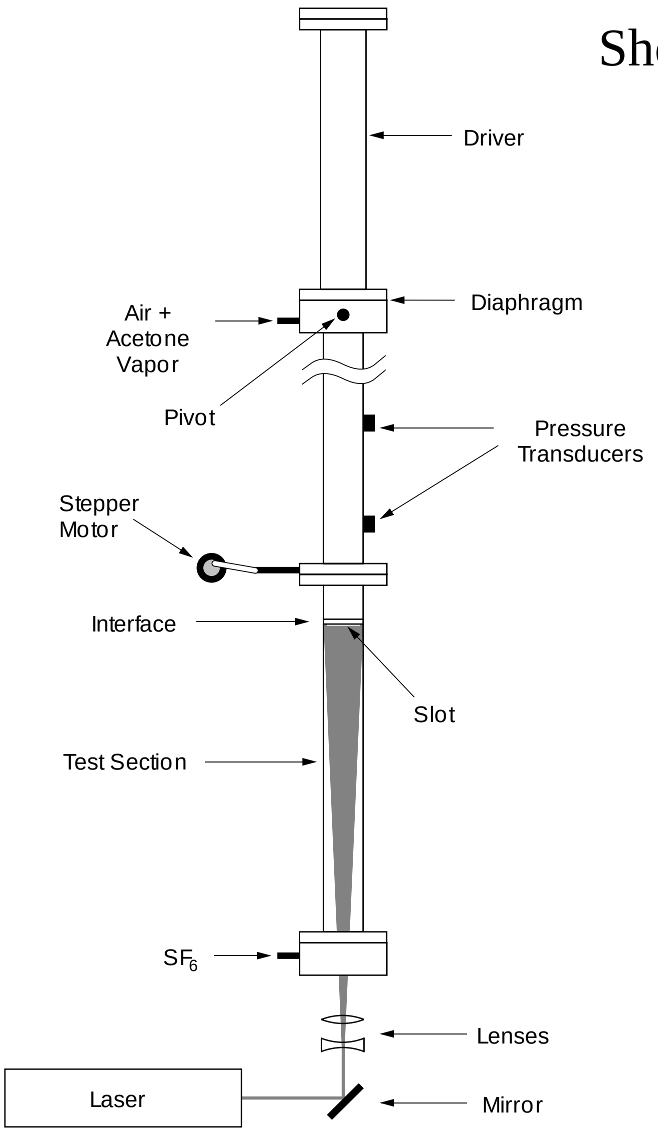
- **Artificial transport coefficients are added to the molecular transport coefficients in the Navier-Stokes equations for a multicomponent mixture of ideal gases:**

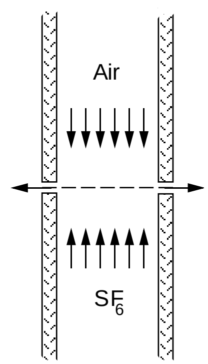
$$\begin{array}{l} \text{Momentum} \\ \text{Internal Energy} \\ \text{Mass Fraction} \end{array} \begin{Bmatrix} \mu^* / \rho \\ k^* / C_p \\ D_i^* \end{Bmatrix} = \begin{Bmatrix} \mu / \rho \\ k / C_p \\ D_i \end{Bmatrix} + \overbrace{\begin{Bmatrix} C_\mu \Delta x^2 \left|\nabla^2 u\right| / c_s \\ C_k \Delta x^2 \left|\nabla^2 T\right| / T \\ C_D \Delta x^2 \left|\nabla^2 Y_i\right| \end{Bmatrix}^n}^{\underline{\text{high-order switch}}} \Delta x^2 / \Delta t$$

- **High-order switch localizes diffusion terms to regions with ringing**

Jacobs (U of Arizona) shock tube apparatus uses no membrane and produces high-quality laser diagnostics

Shock tube configuration

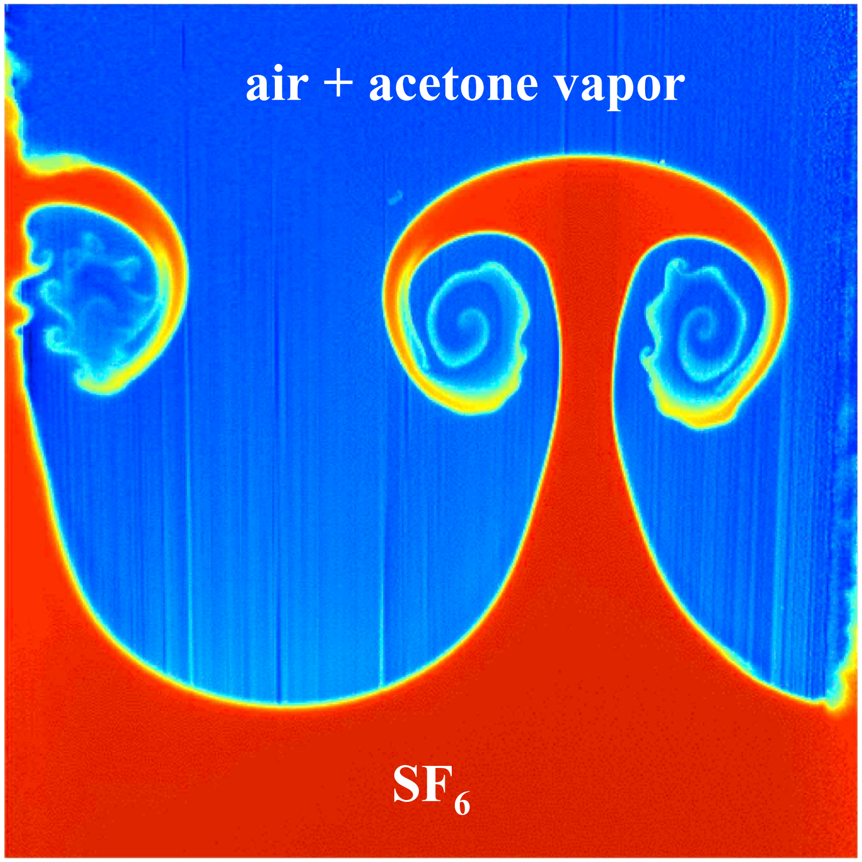




Experimental Apparatus

- **Slightly diffuse, membrane-less interface is created with a stagnation flow**
- **Single, long-wavelength perturbation is generated by a stepper motor**
- **M=1.1, 1.2, 1.3 shots**
- **PLIF laser diagnostics**

Planar Laser Induced Fluorescence (PLIF) image from Collins-Jacobs shock tube experiment (2D)



Air-acetone concentration (Collins & Jacobs 1999)

- **Richtmyer-Meshkov instability**
- **M=1.2 shock**
- **air-acetone (light) → SF_6 (heavy)**
- **single sinusoidal perturbation**
- **diffuse interface (no membrane)**

Simulation setup for Collins-Jacobs 2D test case used by all codes/methods

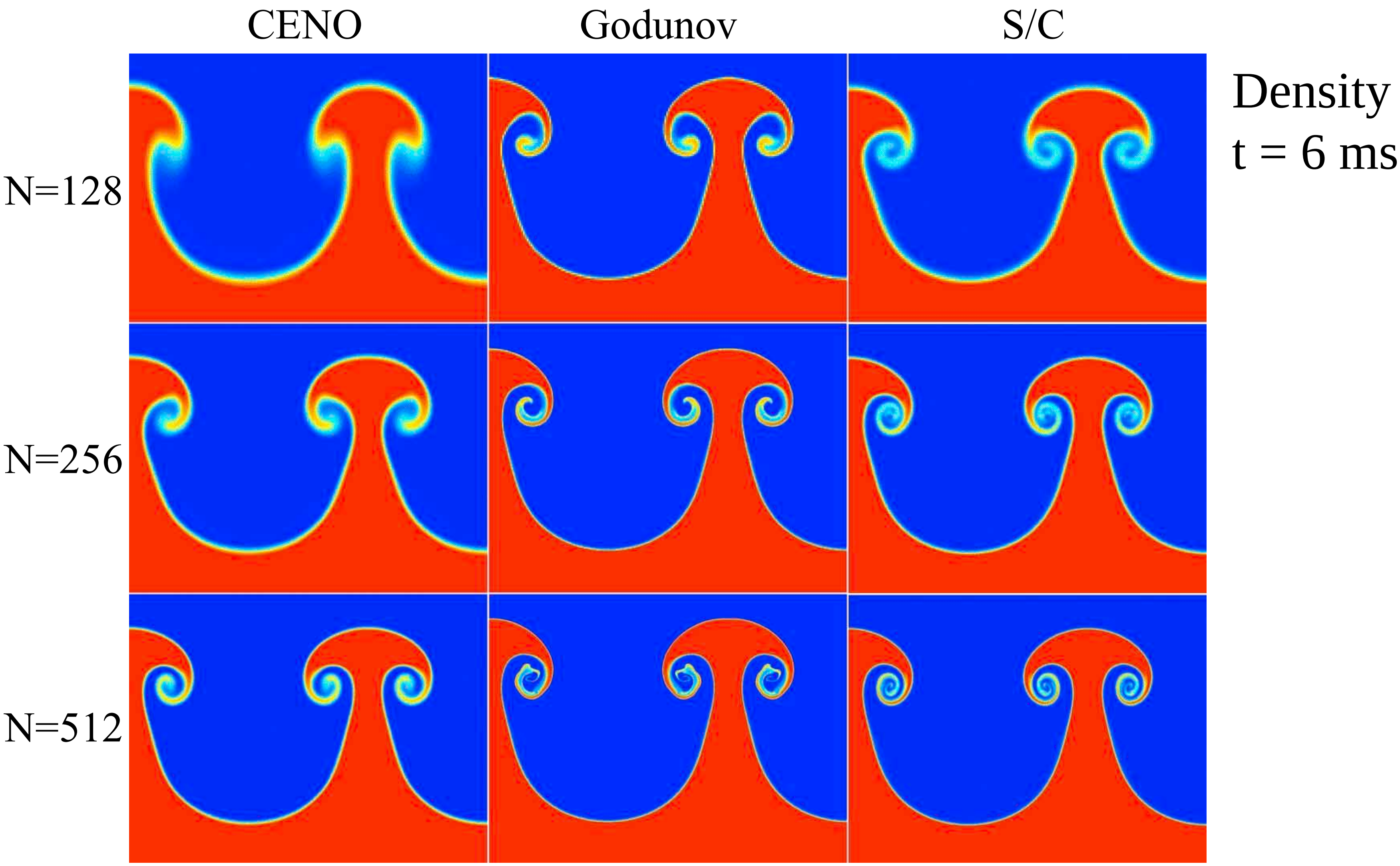
- Local domain near interface
- Periodic transverse boundary conditions

- Two perfect gases (Atwood number = 0.6)
  - ♦ air+acetone vapor (γ =1.27)
  - ♦ sulfur hexafluoride (γ =1.09)

- M=1.186 to match displacement speed

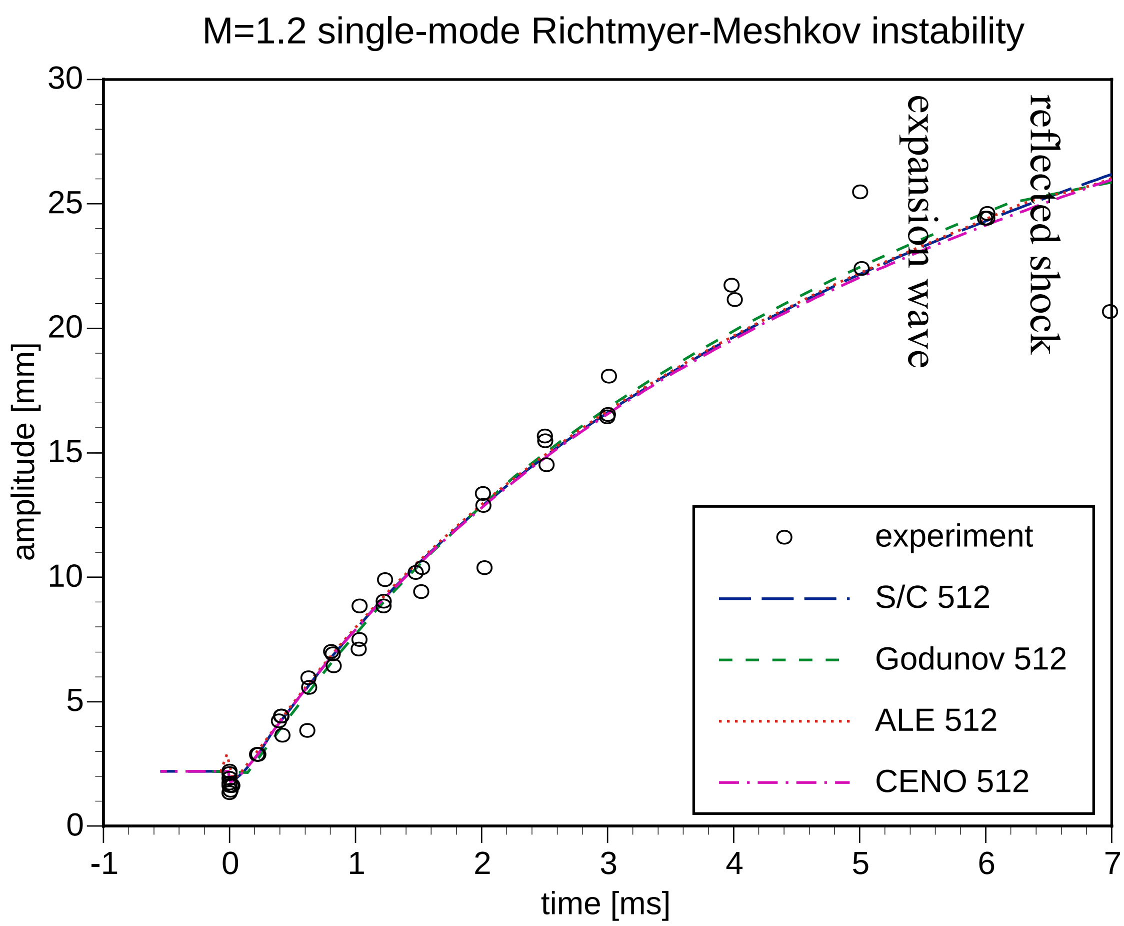
- Initial interface (ka_0 = 0.2)
  - ♦ thickness δ_0 = 5 mm
  - ♦ amplitude a_0 = 2.2 mm
  - ♦ wavelength λ_0 = 59 mm

Results from all simulations show similar large-scale growth, but different small-scale phenomena

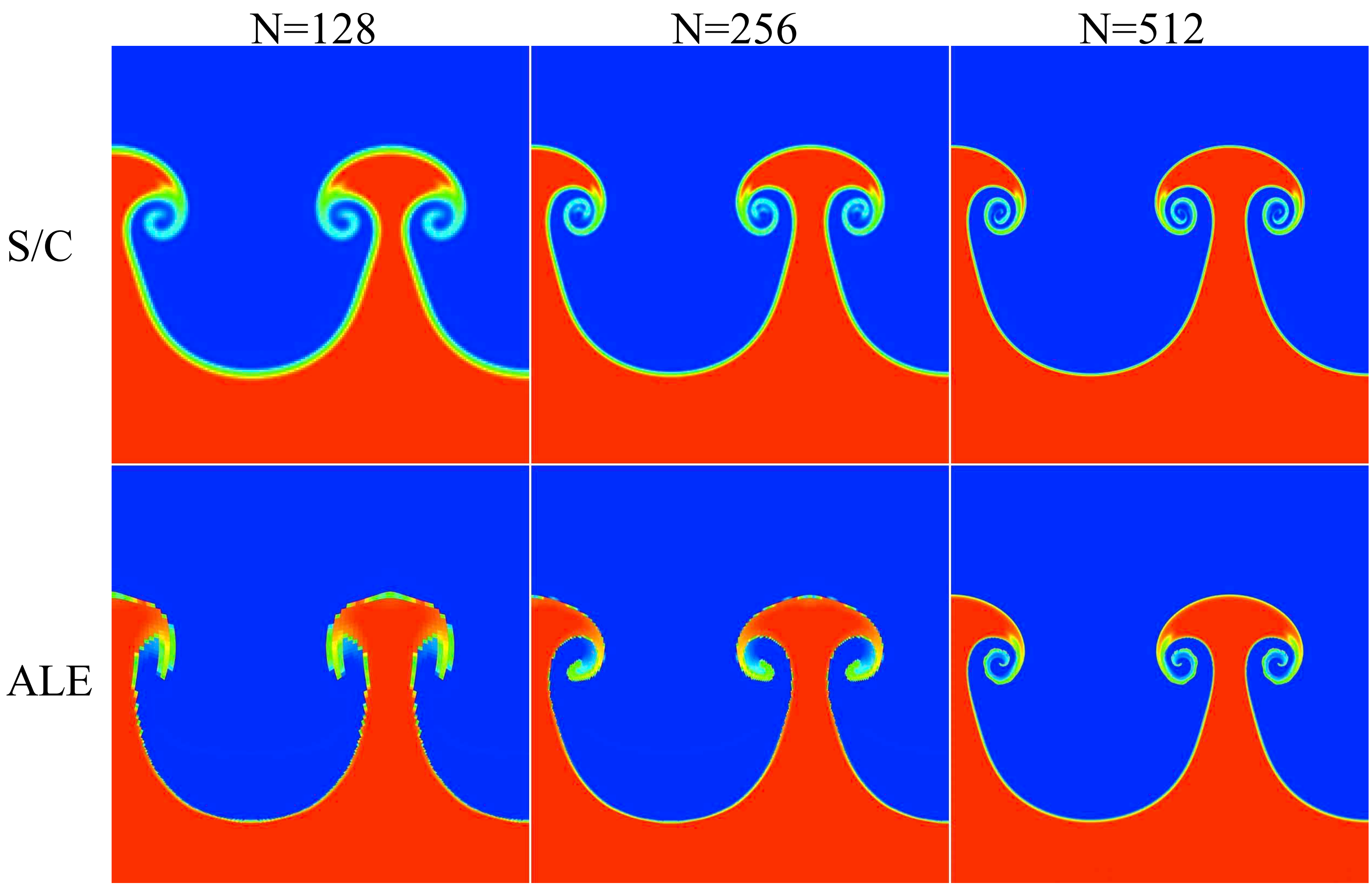


Large-scale structure and amplitude growth are *insensitive* to the numerical scheme and resolution

Jacobs-Collins Shock Tube: Amplitude

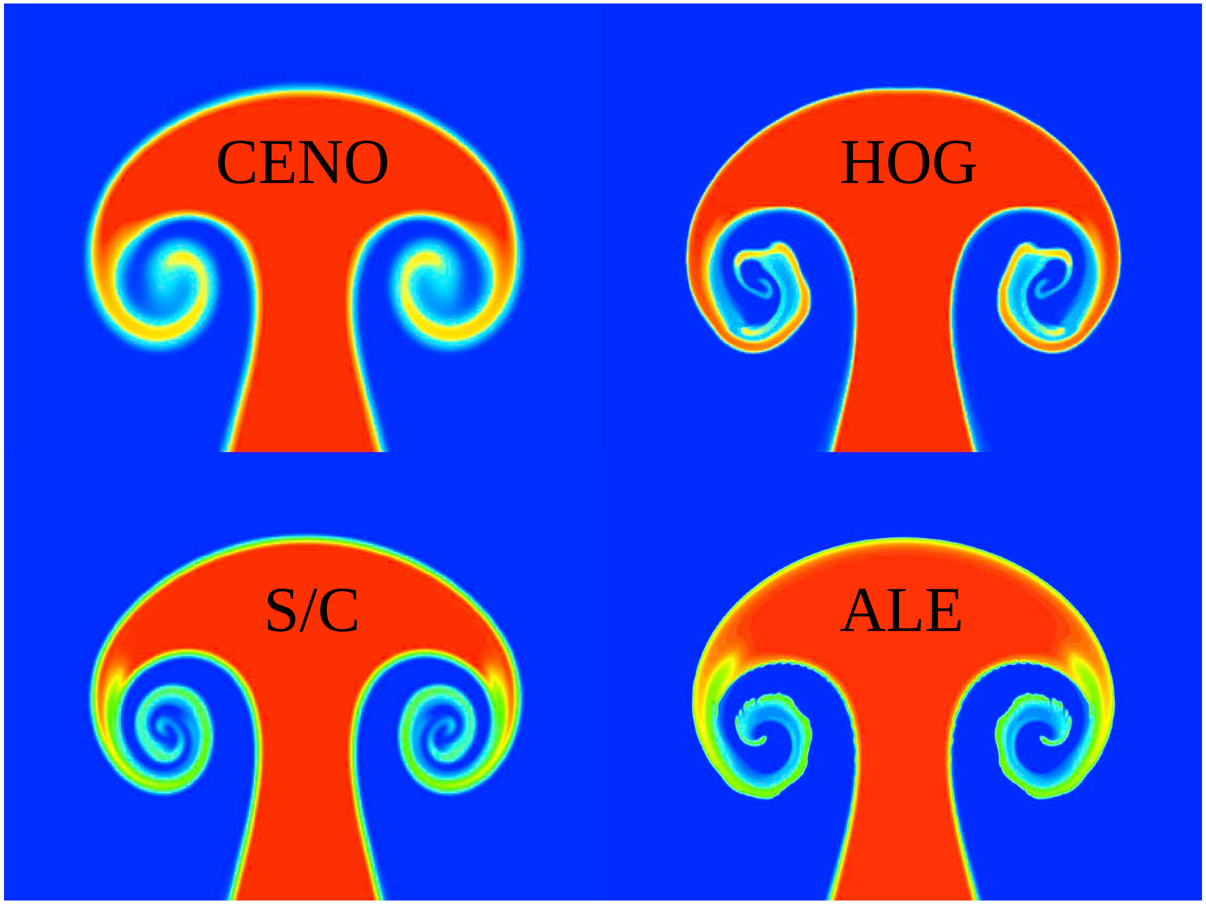


Greater differences are evident between numerical schemes at low resolution than at high resolution



Density at t = 6 ms

Fine-scale features of the vortex cores are very sensitive to the numerical scheme and resolution of the thin interface

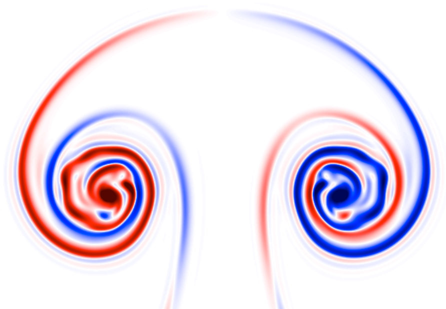


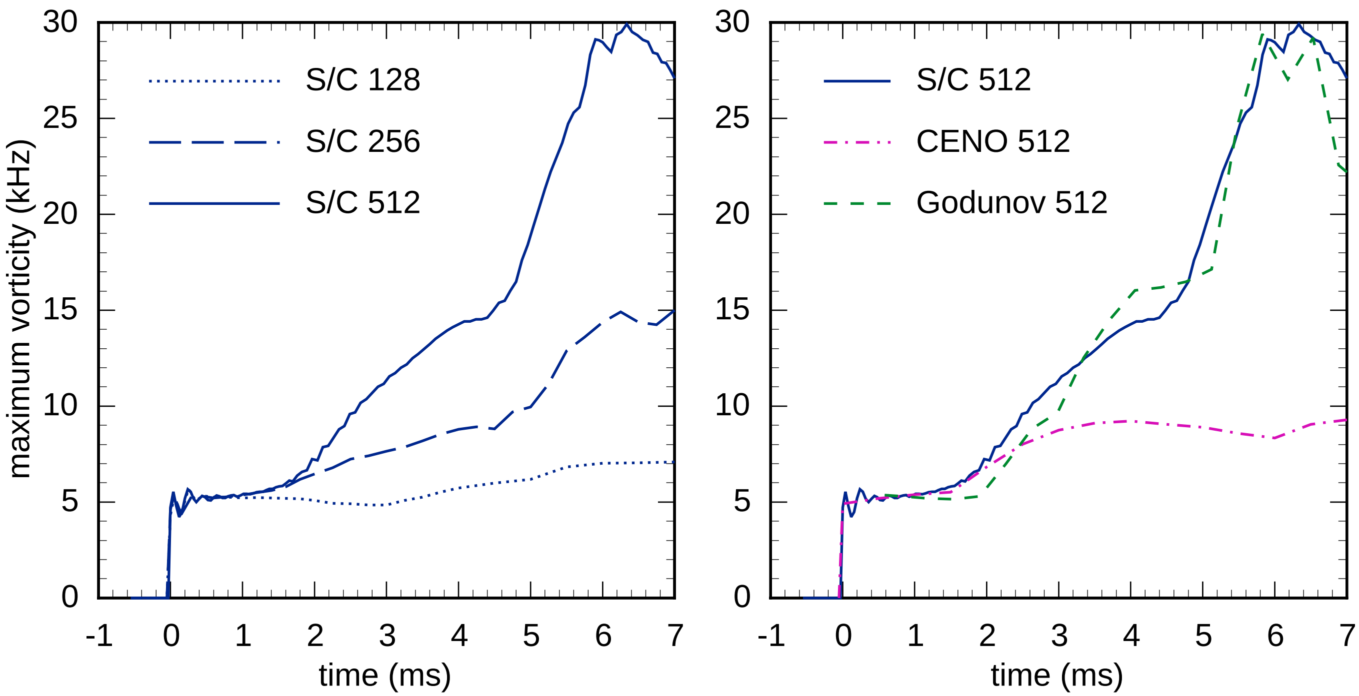
Density
N = 512
t = 6 ms

The S/C interface with artificial diffusion is about 6 points thick, retarding vortex breakdown and allowing more rollup.

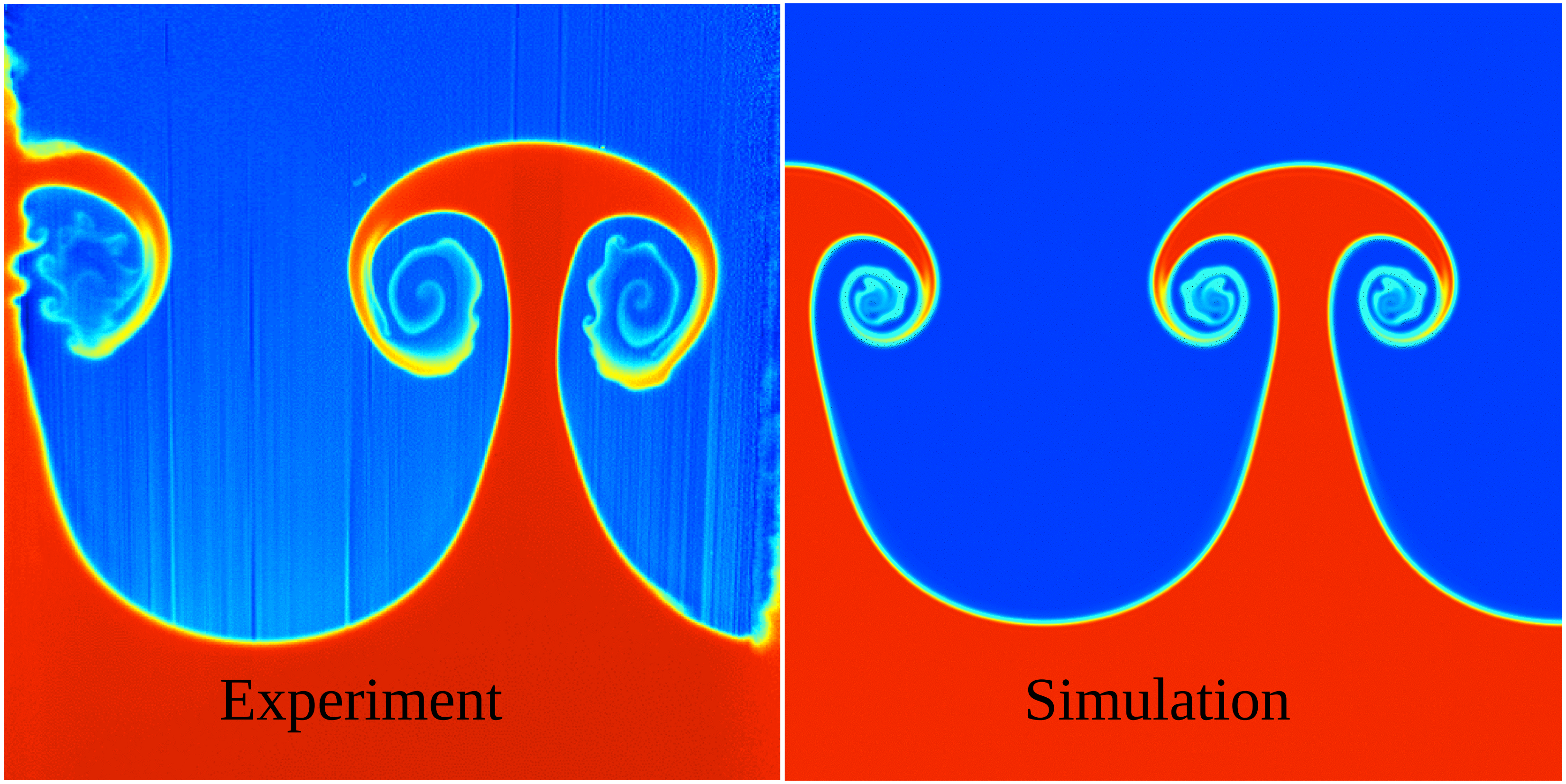
The maximum vorticity in the interface/vortex core is sensitive to the effective resolution

Jacobs-Collins M=1.2 Shock Tube: Vorticity





Despite intercode agreement for large-scale features, there is lack of agreement between simulation and experiment



Differences in the setup of initial, boundary, and/or physical conditions between simulation and experiment may account for this.

Features neglected in the simulations that may lead to the observed discrepancies:

- **Boundary conditions**
  - ❑ side slots
  - ❑ no-slip walls
  - ❑ reflected expansion from top wall

- **Initial conditions**
  - ❑ subharmonics in forcing
  - ❑ non-uniform interface thickness

- **Physical conditions**
  - ❑ gravity
  - ❑ materials
  - ❑ 3D
  - ❑ DNS resolution

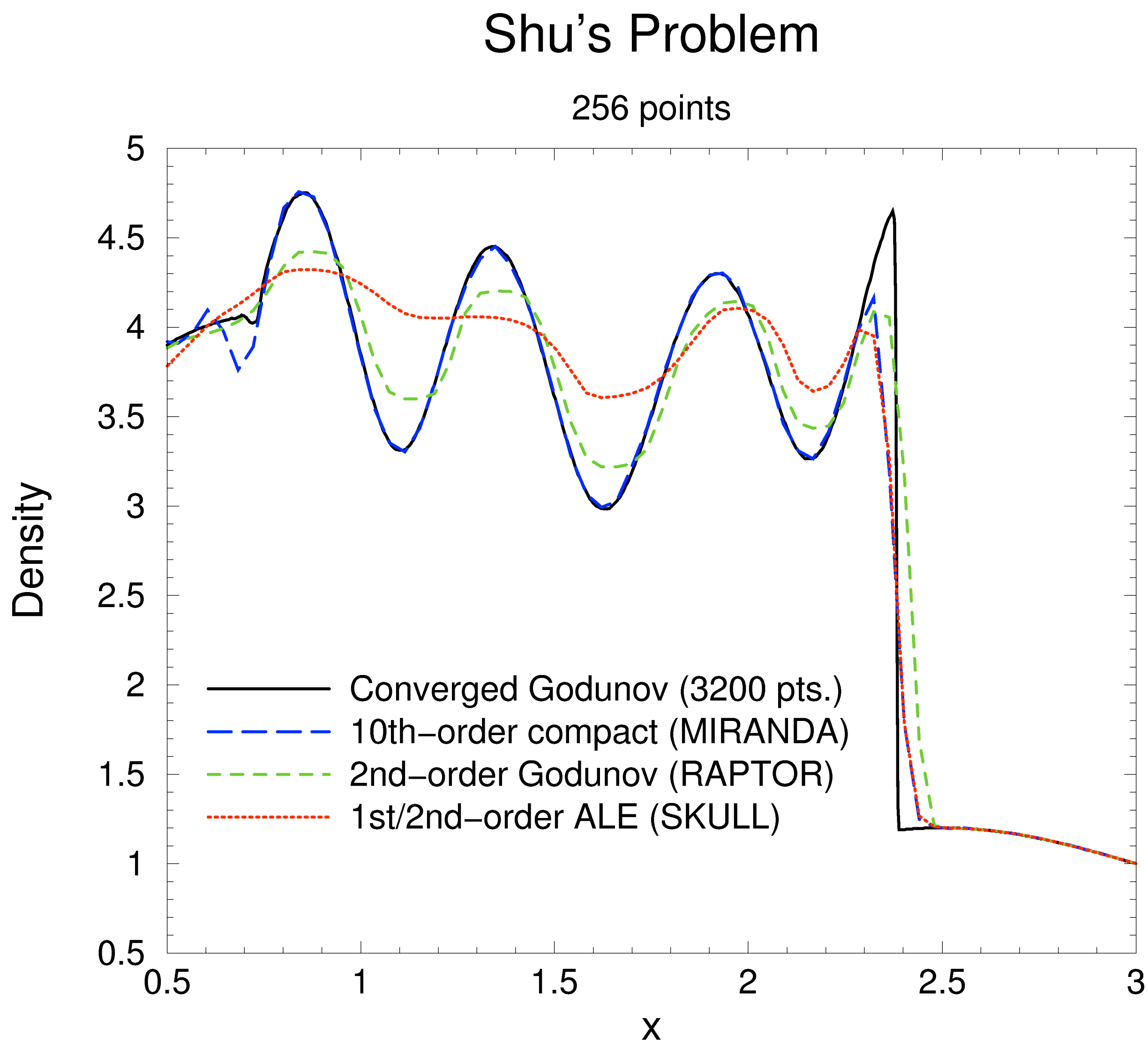
New tests use no global filtering to improve resolving power

- High-order simulations of the previous 2D RMI case used both local artificial dissipation and global filtering.

- There appeared to be no great benefit in using high-order schemes for the 2D RMI case rather than some lower-order schemes.

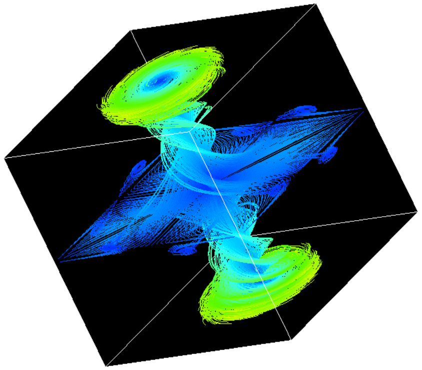
- More recent tests are being conducted without global filtering to reduce ringing and degradation of resolution, using only local artificial dissipation with an exponential switch.

Compact scheme with no global filtering gives most accurate result in 1D test case



Shock passing through density wave

3D Test Case: Taylor-Green Vortex
(inviscid, mildly compressible)


(The University of Edinburgh)

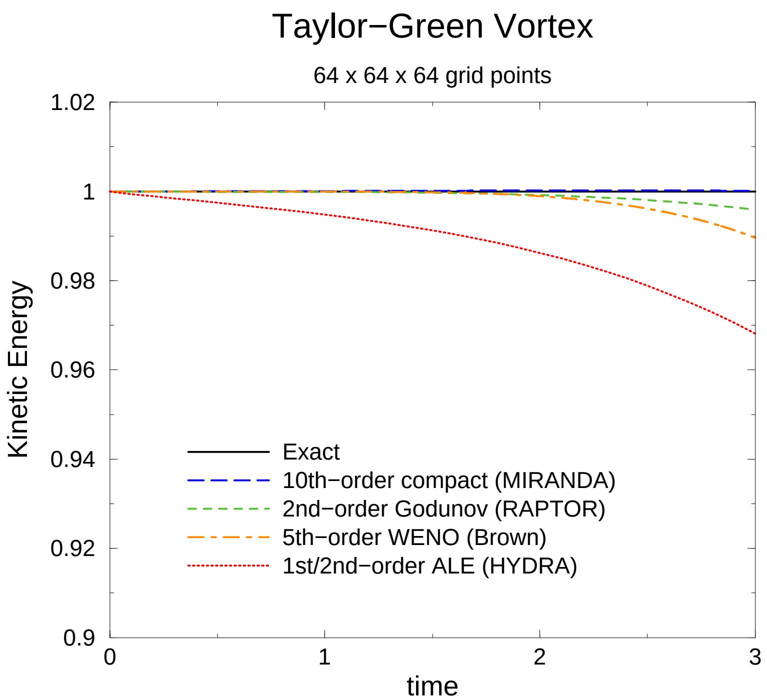
Initial conditions on $2\pi^3$ domain:

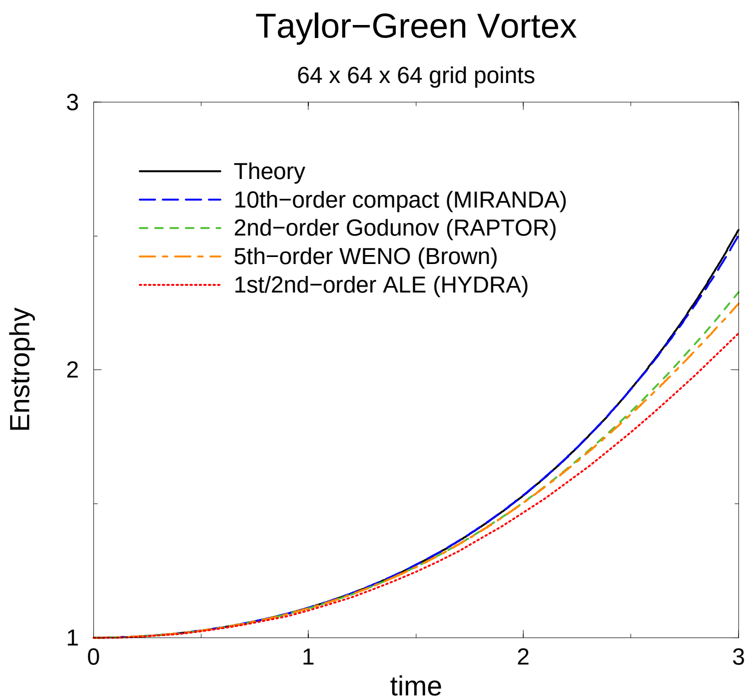
$$u = \sin(x)\cos(y)\cos(z)$$
$$v = -\cos(x)\sin(y)\cos(z)$$
$$w = 0$$
$$\rho = 1$$
$$p = 100 + (\rho/16)\{[\cos(2z) + 2][\cos(2x) + \cos(2y)] - 2\}$$

Features

- Vortex stretching, cascade to small scales (similar to turbulence)
- Exact incompressible solution for $t < 3.5$
- Inviscid solution becomes singular at $t \approx 5$
- For 64^3 grids, small scales become unresolved for $t \geq 3$

Compact scheme with no global filtering gives the most accurate results in 3D TGV case





Conclusions

- Spectral/compact methods can be made sufficiently robust to capture shocks and contact discontinuities.

- The benefits of higher-order differencing are readily apparent in certain cases (Shu, TGV), but less so in cases dominated solely by shocks and interfaces (2D RMI).

- Shear flow cases and fully turbulent test cases (late-time RMI, reshock) still need to be examined to assess whether high-order or low-order methods are more effective for shock-induced turbulence.