Large-eddy simulation of Richtmyer-Meshkov instability with reshock (with multi-scale modeling)

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Outline: LES of Richtmyer-Meshkov Instability & reshock

- Physical description of the Instability and necessity for Large Eddy Simulation (LES)
- Subgrid-scale modeling issues
- Orthogonality of LES techniques and shock capturing schemes
  - *Discussion of requirements of a scheme for good LES*
    - *Modified wave number*
    - *Advance for LES without shocks or contacts: TCD*
  - *Properties of Compressible flow schemes at odds with LES*
    - *Regularizing numerical viscousity*
    - *MILES*
- Modified hybrid scheme
  - *3D simulation of RMI with k^(-5/3) spectra and subgrid activity*
  - *Model based continuation of statistical quantities into subgrid (multi-scale modeling)*
- AMR simulations (AMROC)

Richtmyer-Meshkov (R-M) Instability

- Misalignment of contact and shock

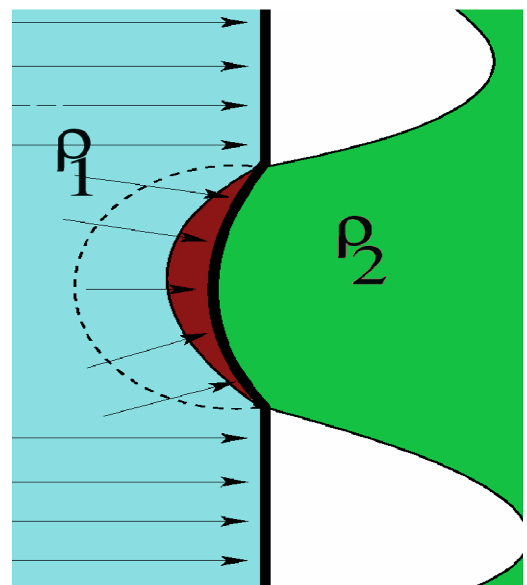
Self-stretching and Compression

Vorticity Generation

$$\frac{\partial \varpi}{\partial t} + u \bullet \nabla \varpi = \varpi \bullet \nabla u - \varpi \nabla \bullet u + \frac{1}{\rho^2} \nabla(\rho) \times \nabla(p)$$

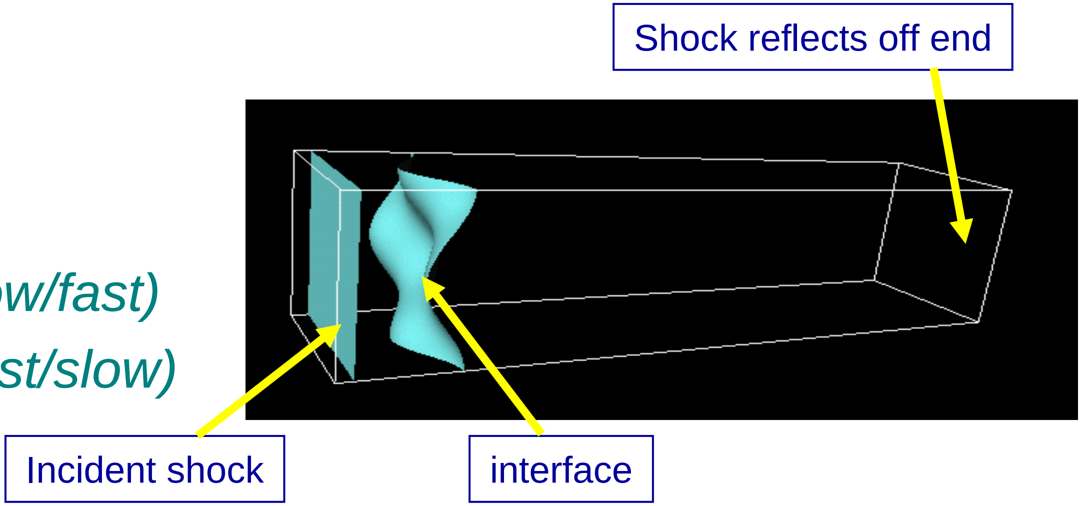
Advection

- The passage of the shock results in vorticty deposition on the interface by means of Barotropic generation.



Richtmyer-Meshkov (R-M): Target simulation

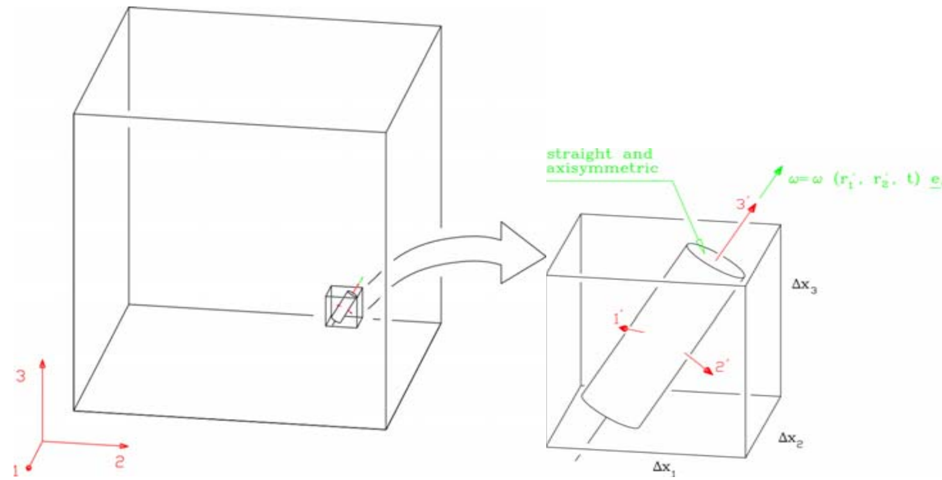
- Strong shocks
- Density ratios
  - *heavy to light (slow/fast)*
  - *Light to heavy (fast/slow)*



- LES using stretched-vortex SGS model
  - *Subgrid motion given by nearly axisymmetric vortex in each cell*
  - *Plug-in model: ease of implementation*
  - *Simple extension gives model for subgrid mixing*
- Advance in numerical methodology required (WENO/TCD)
- 2D and 3D (512×256^2 and 256×128^2) runs at M = 1.5, density ratio = 5

LES with stretched-vortex SGS model

- ***Structure-based approach***
- Subgrid motion represented by nearly axisymmetric vortex tube within each cell.
- Plug-in model: ease of implementation
- Subgrid stresses are:



$$T_{ij} = K\,(\delta_{ij} - e_i\,e_j)\,,$$

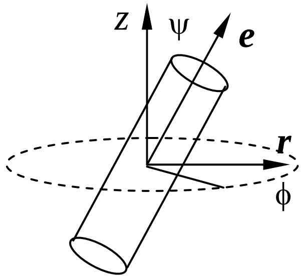
$$K = \int_{k_c}^{\infty} E(k)\,dk.$$

- Model parameters estimated locally by matching local resolved flow 2'nd-order velocity structure function to local subgrid estimate
- Subgrid strucure axes aligned with both resolved vorticity and eigenvector of principal resolved rate-of-strain
- Structures can be use to compute statistics of subgrid processes

Model parameters

- Subgrid kinetic energy (Pullin 2000, based on Lundgren spiral spectrum):

$$K \equiv \int_{k_c}^{\infty} \mathcal{K}_0\, \varepsilon^{2/3} k^{-5/3} \exp\left(-2k^2 \nu / 3 \left|S_3\right|\right) \mathrm{d}k$$



where $S_3 = \tilde{S}_{ij} e_i e_j$ (resolved strain along vortex axis)

- $\mathcal{K}_0\, \varepsilon^{2/3}$ from approximate expressions (Voekl & Pullin 2000) for the resolved second-order structure function, F_2^c (circular average in homogeneous plane)

$$\mathcal{K}_0 \varepsilon^{2/3} = \frac{\pi F_2^c(r, \mathbf{x})}{2\Delta^{2/3} \int_0^{2\pi} \int_0^{\pi} s^{-5/3} \left[1 - J_0\left(s(r/\Delta)\sqrt{1 - \sin^2\psi \cos^2\varphi}\right)\right] \mathrm{d}s\, \mathrm{d}\varphi}$$

- Subgrid vortex orientation, ***e***
  - λ *subgrid vortices fraction aligned with principal extensional eigenvector of resolved rate-of-strain tensor,* $\tilde{S}_{ij}$ *(corresponding eigenvalue,* λ_3*)*
  - (1- λ) *subgrid vortices aligned with resolved vorticity vector,* $\boldsymbol{\omega}$ *(Misra & Pullin 1997)*

$$\lambda = \frac{\lambda_3}{\lambda_3 + \left\|\boldsymbol{\omega}\right\|}$$

LES in the absence of shocks and contacts

- The nonlinear term $\frac{\partial}{\partial x_i}\left(\rho u_i u_j\right)$ is responsible primarily for the energy cascade
- The most successful methods are global
  - *Spectral*
  - *High-Order Pade*

- Good response across all (*spectral*) or most (*Pade*) of the resolved scales, I.e. modified wavenumber

$$\boldsymbol{F}(\partial/\partial x) = ik \qquad \boldsymbol{F}\left(D_x\right) = i\widehat{K}(k)$$

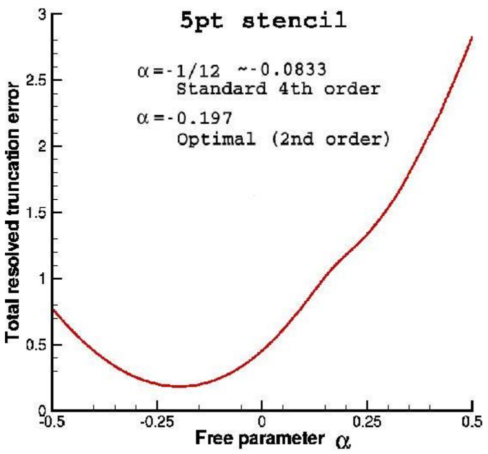
- Limitations
  - *global nature results in (fatal?) ringing at discontinuities like shocks and contacts*
  - *Limited to simple geometries*

Tuned Center-Difference Stencil (TCD)

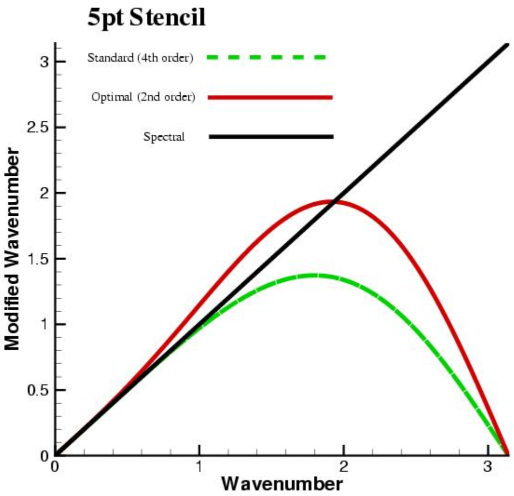
- Ghosal (JCP, 1996)
- Error in resolved-scale energy spectrum produced by one step of Navier-Stokes equations using given discretization
- Asssume –
  - *Von-Karman energy spectrum*
  - *Joint normal velocty pdf*
- $\mathcal{E}^{(\mathrm{FD})}(\kappa, \tilde{\kappa}(\kappa,\alpha))$ is spectrum of truncation error for numerical method with modified wavenumber behavior $\tilde{\kappa}(\kappa,\alpha)$
- Define total discretization error

$$\mathrm{E}_G(\alpha) = \int_0^{\frac{\pi}{\Delta x}} \mathcal{E}^{(\mathrm{FD})}(\kappa, \tilde{\kappa}(\kappa,\alpha))\,d\kappa$$

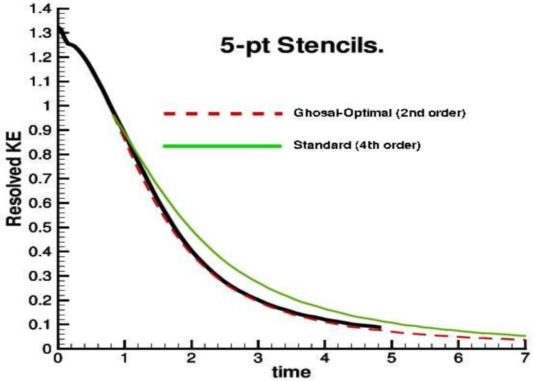
Optimized 5-point TCD stencil (second order)



Truncation error



Modified wavenumber of minimal error stencil



DNS and LES of Decaying compressible turbulence, M_t =0.488, R_lambda = 70.

Decay of total TKE. Black; 256^3 DNS (10-th order Pade)

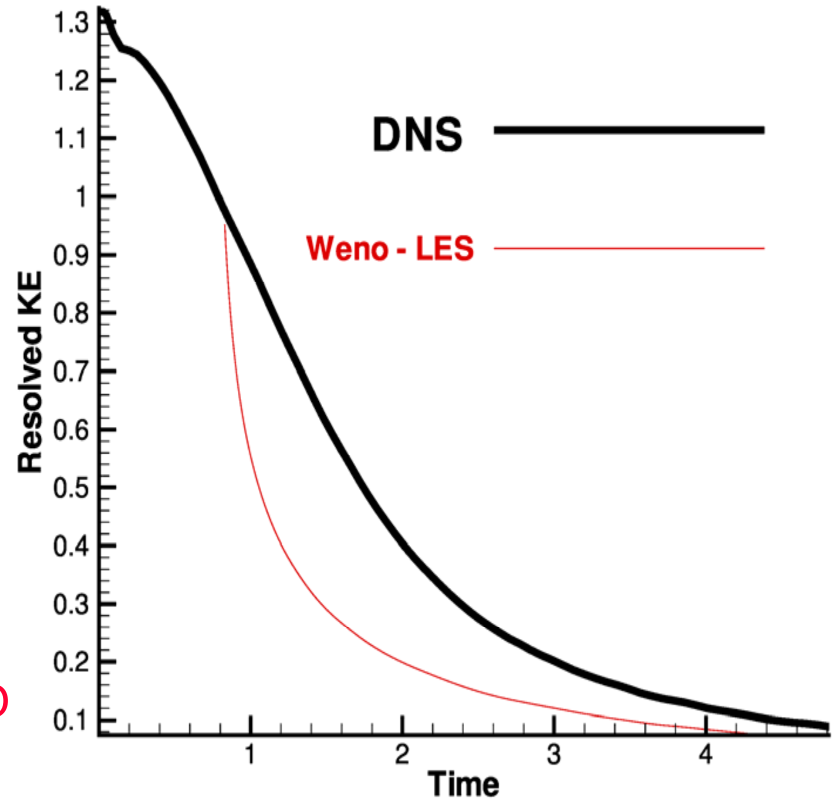
Flows with strong shocks: Shock capturing solvers

- The weak solutions of the Euler equations are regularized by the clever numerical viscosity of the methods.
- Shocks (and contacts) are 'captured', I.e. smeared across a few cells. TVD (Total Variation Diminishing) and general flux limiting schemes are popular techniques
- Drawbacks for LES
  - *Generally developed for low-order time stepping and have up-winding or other numerical dissipation for stability*
  - *Such Euler solvers have a high degree of non-uniform numerical dissipation*
  - *Dissipation active in entire flow (both at shocks and away from shocks)*

- MILES – LES with no model, relies on numerical method

Pure WENO: Numerical dissipation overwhelms simulation

WENO



DNS and LES of Decaying compressible turbulence, M_t =0.488, R_lambda = 70.

Decay of total TKE. Black; 256^3 DNS (10-th order Pade). Red; WENO.

Mixing zone observations

- Low compressibility in mixing zone: Turbulent Mach number ~0.3
- For Euler eqns, at the contact:
  - Normal velocity is continuous
  - *Pressure is continuous*

- We have resolved scale dissipation and model terms
- The contact (density) is initially smeared at vorticity deposition and at later times
  - *Resolved scale velocity parallel to the contact is continuous across the contact*
  - *Pressure and velocities are smooth enough for a centered stencil*
  - *Density is the only primitive variable that isn't –scalar 'shocks'*

Improved hybrid WENO-TCD: limit on primitives

- Approach:
  - Away from shocks exploit smoothness of (u,v,w,P)
  - At shocks (only) revert to full WENO
- Maintain conservative formulation of equations (shock speeds)
- Use a finite volume approach limiting on primitives

$$\frac{\partial \mathbf{F}(\mathbf{q}_\mathbf{i})}{\partial x} = \frac{\mathbf{F}(\mathbf{q}_{i+1/2}) - \mathbf{F}(\mathbf{q}_{i-1/2})}{\Delta x}$$

- Idea:
  - Use TCD to interpolate smooth variables
  - Use WENO to interpolate density

$$\mathbf{F}(\mathbf{q}_{\mathbf{i+1/2}}) = \mathbf{F}(\rho_{i+1/2}^{weno}, u_{i+1/2}^{tcd}, v_{i+1/2}^{tcd}, w_{i+1/2}^{tcd}, P_{i+1/2}^{tcd})$$

- Where a centered interpolation (TCD stencil split)

$$\frac{f_{i+1/2}^{tcd} - f_{i-1/2}^{tcd}}{\Delta x} = TCD(f_i) \qquad f_{i+1/2}^{weno} = \sum \varpi_k \, f_{i+1/2}^{canidates}$$

Improved hybrid WENO-TCDS algorithm: shock identification/capturing

- We only need full WENO at the shocks
- What is a captured shock?
  - *No true internal shock structure*
  - *Rankine-Hugoniot relations nearly satisfied*
  - *Increase in Entropy*

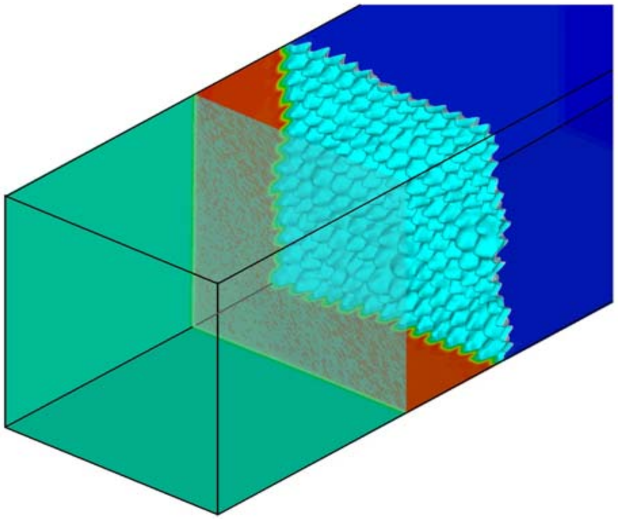
$$\mathbf{F}(\mathbf{q}) = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho u v \\ \rho u w \\ \rho u (E + P) \end{pmatrix}$$

- For numerical purposes
  - *We use correlated curvature of pressure and density:*

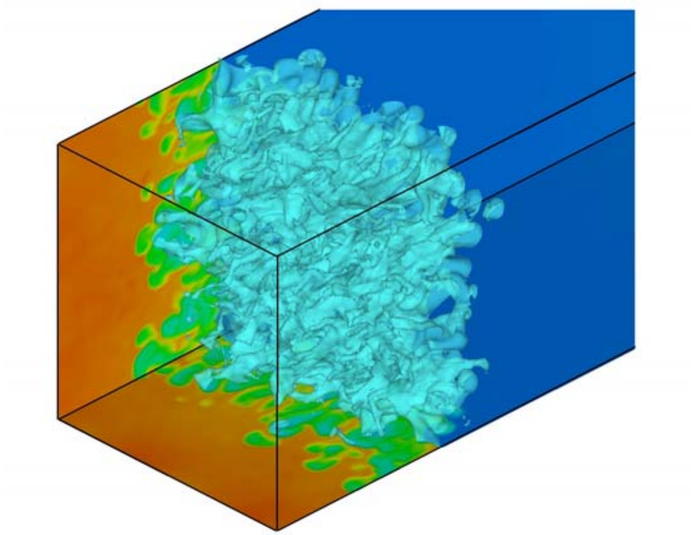
$$C(\rho) \equiv \frac{\rho_{i+1} - 2\rho_i + \rho_{i-1}}{\rho_{i+1} + 2\rho_i + \rho_{i-1}}$$

$$C(\rho)C(P) > 0, \quad C(\rho), C(P) > thrs\Delta x$$

LES of 3-D R-M instability: 256 processors on QSC

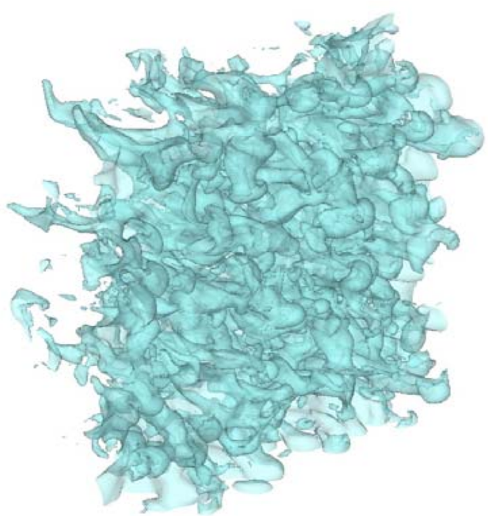


Post-shock interface/shock



Post-re-shock flow

Post re shock



Simulation parameters

Mach 1.5 shock

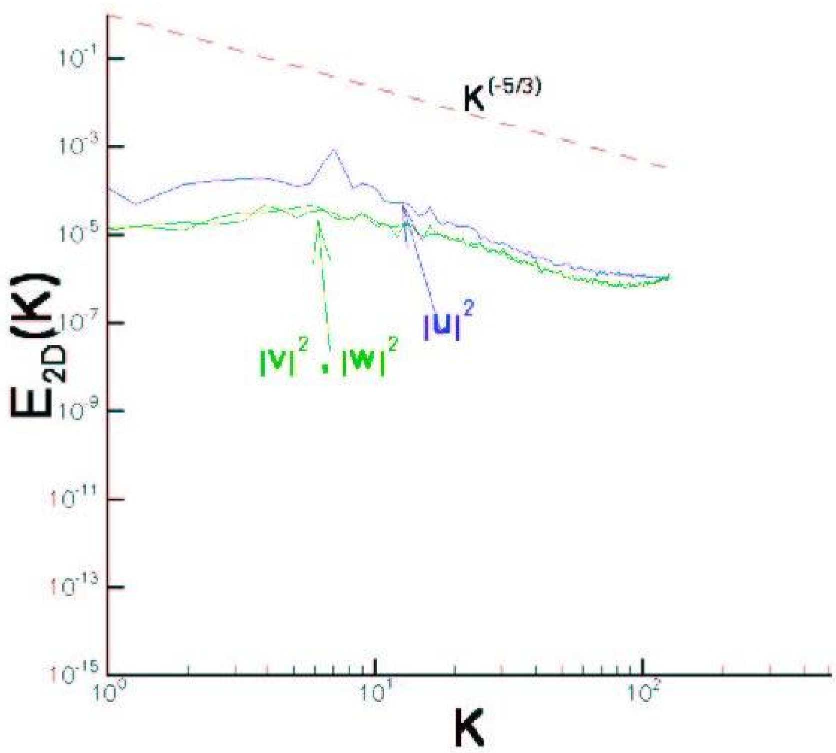
Density ratio 1:5

512x256x256

Hybrid WENO-TCD

Stretched-vortex SGS/LES model

Spectra: Comparison with –5/3 decay



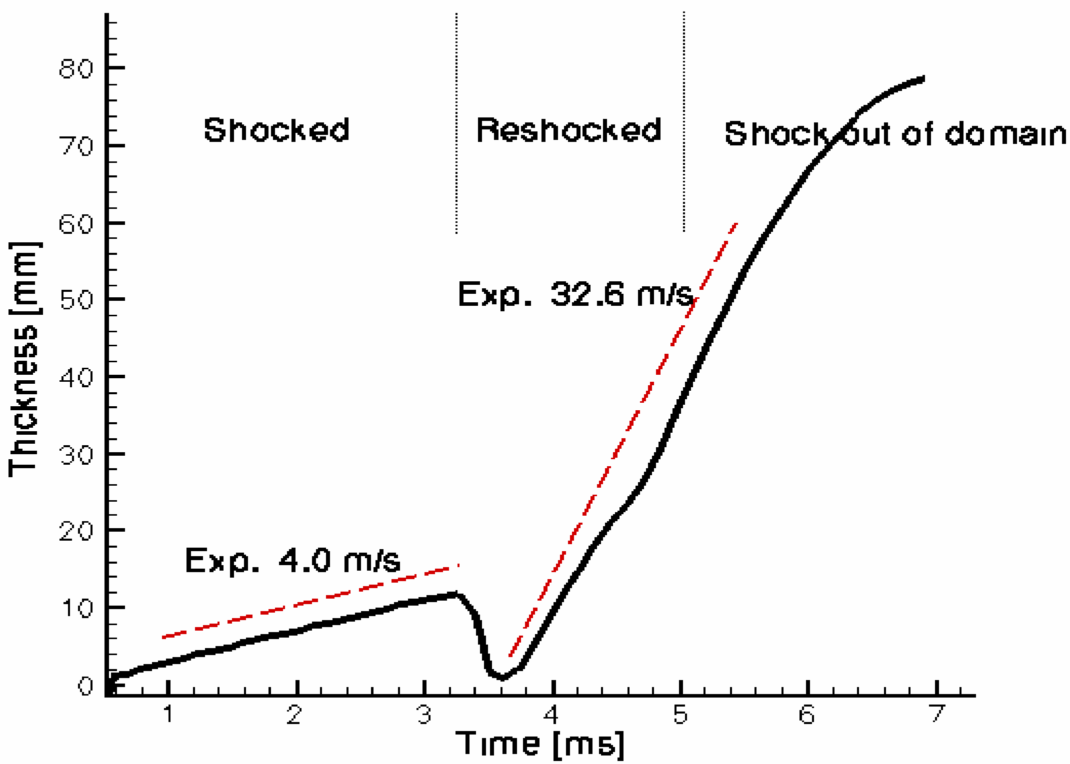
Velocity spectra from plane centered in mixing zone after reshock: 512x256x256 simulation. Lack of dealiasing evident in last computed wavenumbers

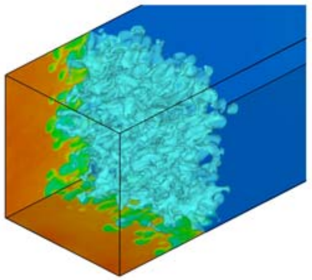
R-M Instability: Turbulent Mixing Zone (TMZ)

- The small perturbations grow rapidly into non-linear regime – For our problem this occurs by 0.7ms (Vetter and Sturtevant 1995)
- Analytic estimate (Mikaelian 1989) for thickness of non-linearly staturated zone: $\delta = 0.28[u]A't$
- In experiments, spark-schlieren photography and high-speed video are used to measure this thickness
- In our simulation, we use a passive scalar: $-1 \le \varphi(x,y,z,t) \le 1$
- The interface is taken to defined to be the zero surface of the scalar
- The width of the TMZ is calculated from the plane average of the scalar

$$-0.99 < \frac{1}{L^2}\iint \varphi(x,y,z,t)\,dydz < 0.99$$

Mixing width vs. time





- The width of the TMZ is calculated from the plane average of a scalar

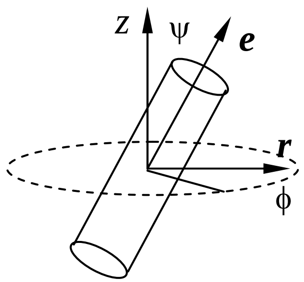
$$-0.99 < \frac{1}{L^2}\iint \varphi(x,y,z,t)\,dydz < 0.99$$

Experiment: Vetter & Sturtevant(1995)

Re_h =50,000-100,000: 512x256x256

Multi-Scale Modeling

- True multi-scale modeling: *matching of 'inner' and 'outer'*
- No free parameters employed in matching
- Use stretched model to compute subgrid statistics



Example – Continuation of the spectra

From the definition of the two-point correlation, a form for the 2D-spectral contribution from each cell may be derived

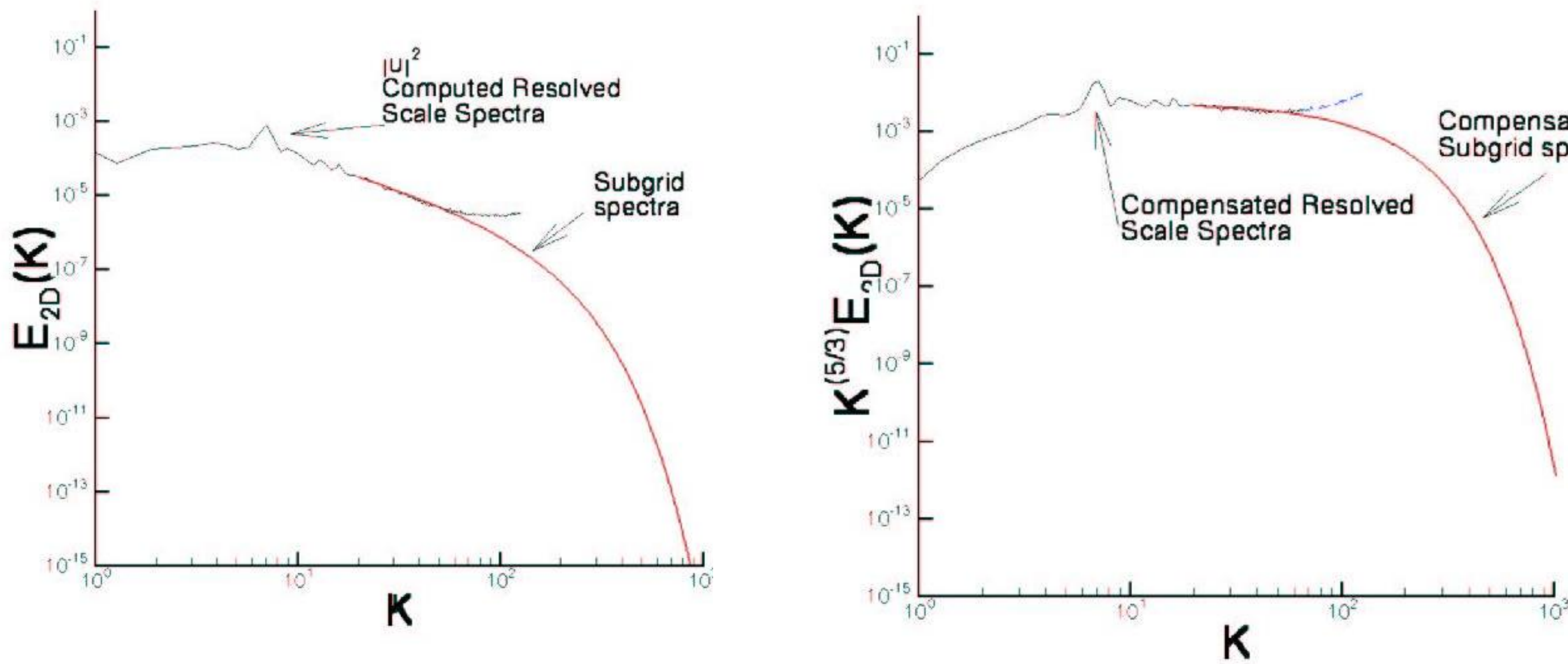
$$E_{2D}(K) = K\,\frac{2}{\pi}\int_{K}^{\left|\frac{K}{\cos\alpha}\right|} \frac{E(\kappa)}{(\kappa^2-K^2)^{1/2}(K^2-\kappa^2\cos^2\alpha)^{1/2}}\,d\kappa$$

Using the stretched vortex model the contribution from each cell becomes

$$E_{2D}(K) = \frac{2}{\pi}K_o\epsilon^{2/3}K^{-5/3}e^{-\nu K^2/4|a|}\int_{1}^{\left|\frac{1}{\cos\alpha}\right|} \frac{u^{-5/3}e^{-\nu K^2(u^2-1)/4|a|}}{(u^2-1)^{1/2}(1-u^2\cos^2\alpha)^{1/2}}\,du$$

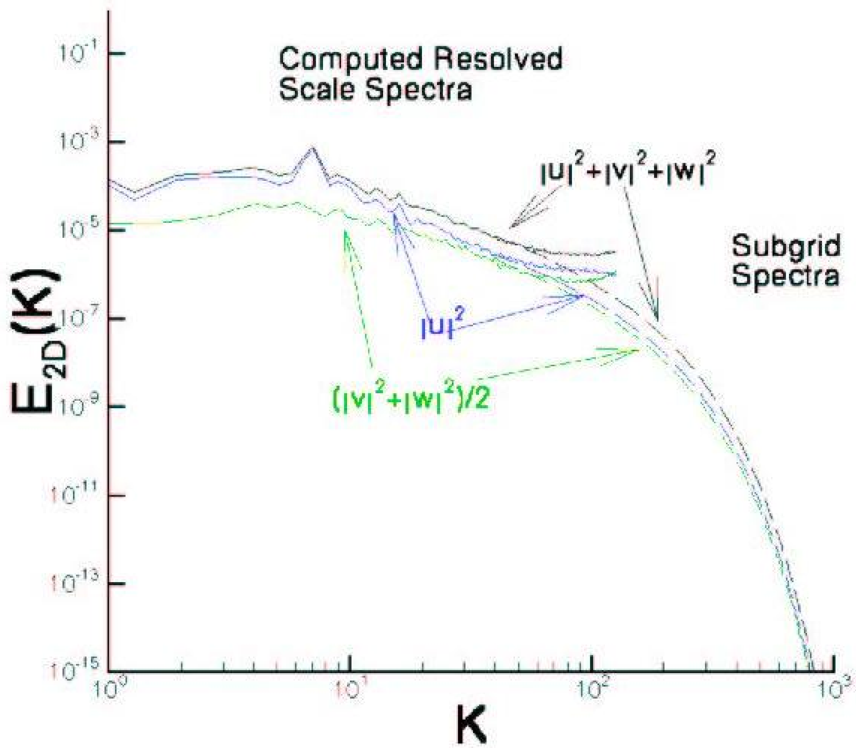
Where the alpha is the orientation of the vortex relative to the 2D-plane in which the spectra is computed

Multi-Scale Modeling: Spectra



Velocity spectra from plane centered in mixing zone after reshock: 512x256x256 simulation. Lack of dealiasing evident in last computed wavenumbers

Multi-Scale Modeling: Anisotropy

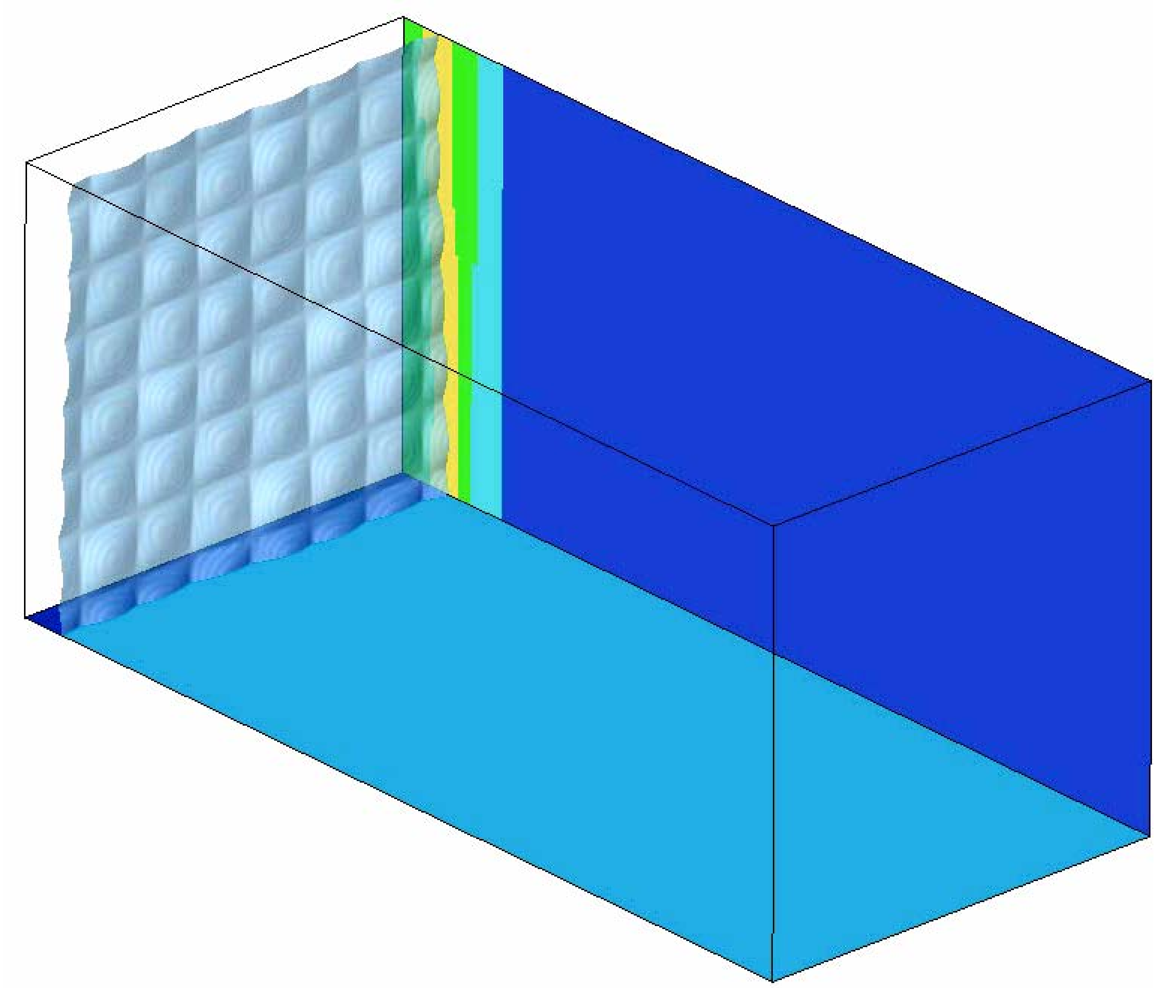


Velocity spectra from plane centered in mixing zone after reshock: 512x256x256 simulation. Lack of dealiasing evident in last computed wavenumbers

3D RM instability with AMROC (R.Deiterding)

- AMROC – Adaptive Mesh Refinement engine
- 3D Richtmyer-Meshkov instability with reshock in rectangular geometry
- Modeled on Vetter and Sturtevant (1995)
- M = 1.5, density ratio =1:5
- 5-point WENO-TCD algorithm
- Base resolution = 120x30x30 with 3 levels of refinement
- Effective resolution of 960x240x240
- No subgrid-scale model (under-resolved Euler)
- Initial density interface ; sin^2 perturbation in each direction
- 83 hours on 48 nodes of ASAP cluster
- Animation shows shock and zero isosurface of density (mean density level)
- Horizontal plane shows density
- Vertical plane shows the refinement level information

RM Instability using adaptive mesh refinement



Simulation parameters

Mach 1.5 shock

Density ratio 1:5

512x256x256

Hybrid WENO-TCD

Euler simulation

Parameters chosen to match Vetter & Sturtevant (1995)

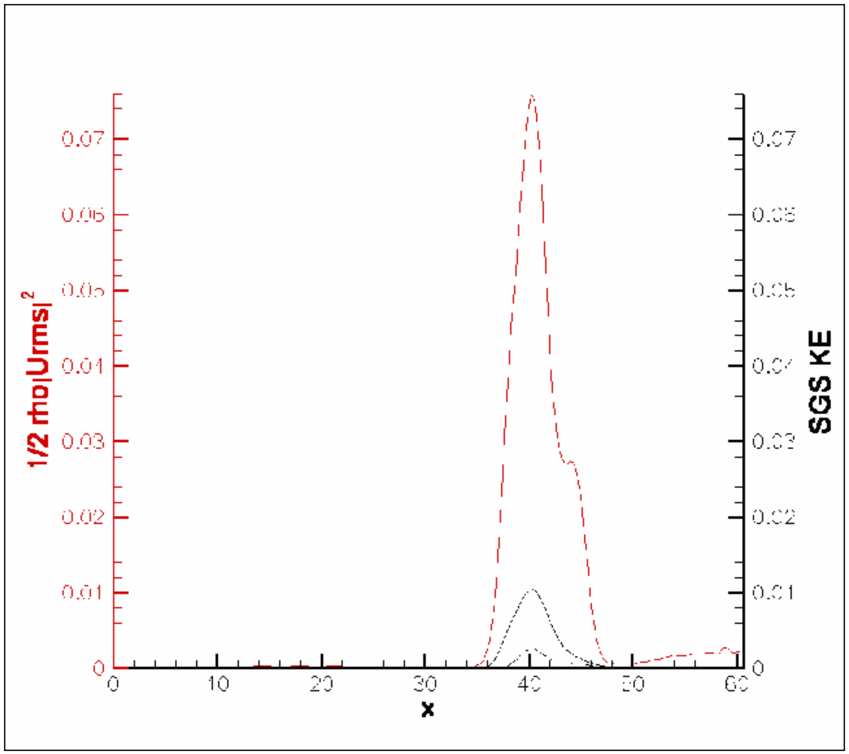
Re_h = 50,000-100,000

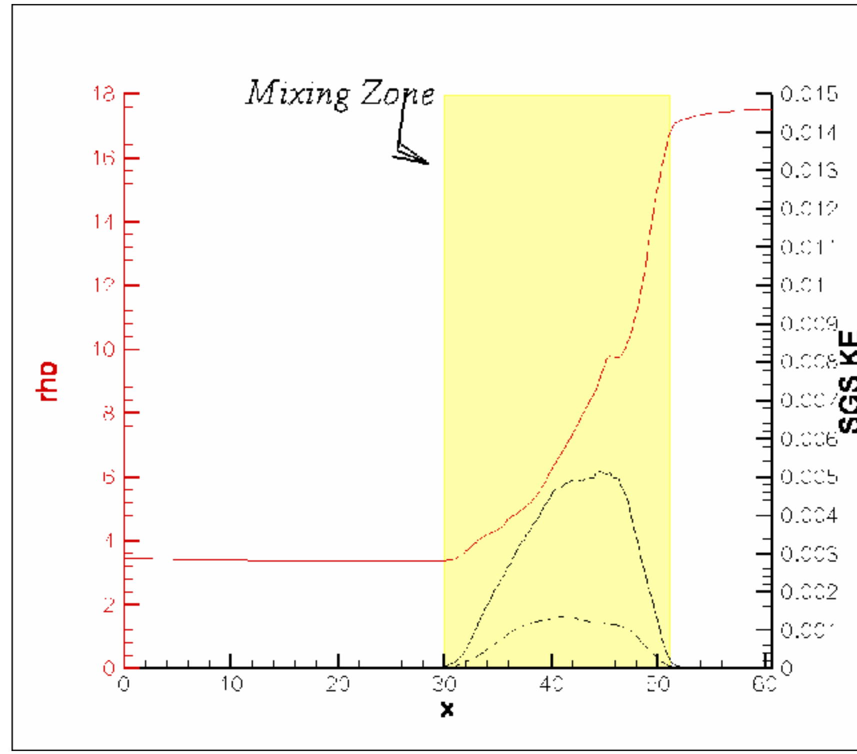
Movie shows shock and density interfaces. Note transition to turbulence of interface after reshock

Concluding comments

- Hybrid TCD-WENO for shock driven turbulence to with mixing
  - *Uses conservative formulation*
  - *Full WENO at shocks*
  - *TCD/WENO in mixing region*
  - *Uses Stretched vortex sub-grid model*
- 3D RM Instability simulation
  - *LES of shock and reshock phase*
  - *Mixing zone is slightly compressible*
  - *Very large density gradient*
- Structure Based SGS model allows multi-scale modeling
  - *Extends spectra into the viscous dissipation range*
  - *Good matching with resolved scale spectra*
  - *Distinguish between homogeneous and nonhomogeneous directions (anisotropy)*
- AMR (AMROC)
  - *Extending the WENO-TCD and multi-scale modeling to the AMROC framework*

Comparisons of subgrid energy

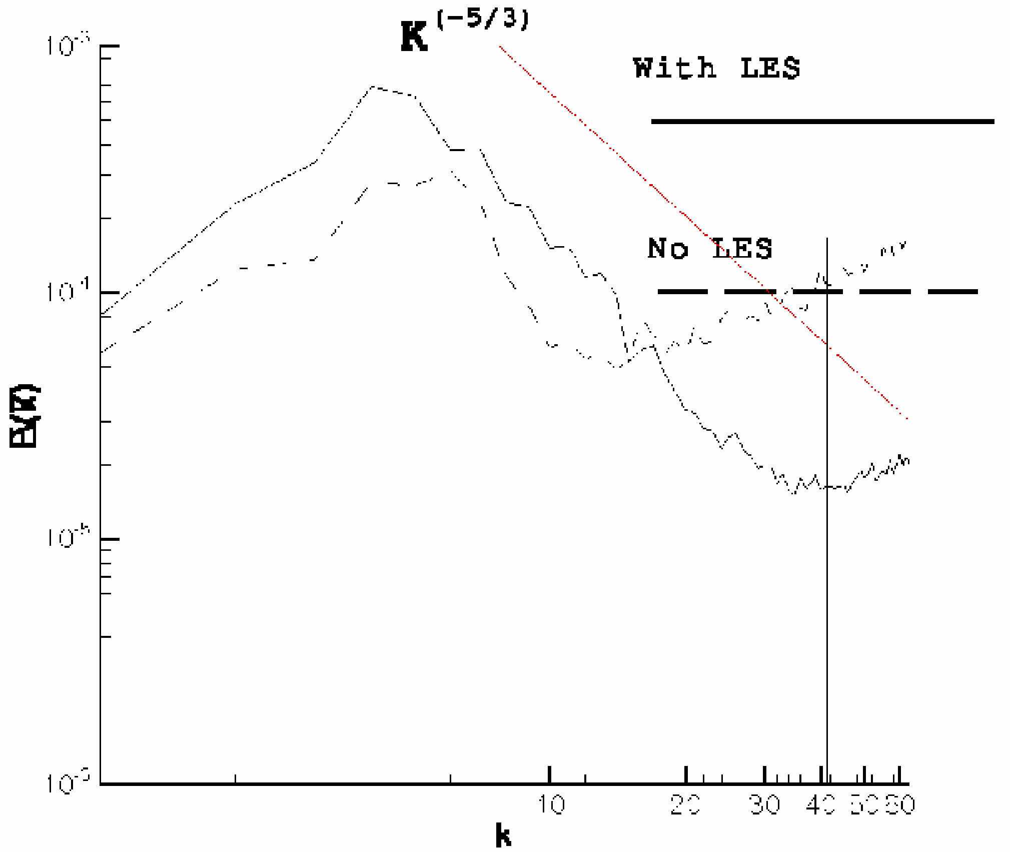




Subgrid Kinetic Energy (SGS KE) (*from new method and old*) compared against resolved scale energy fluctuation.

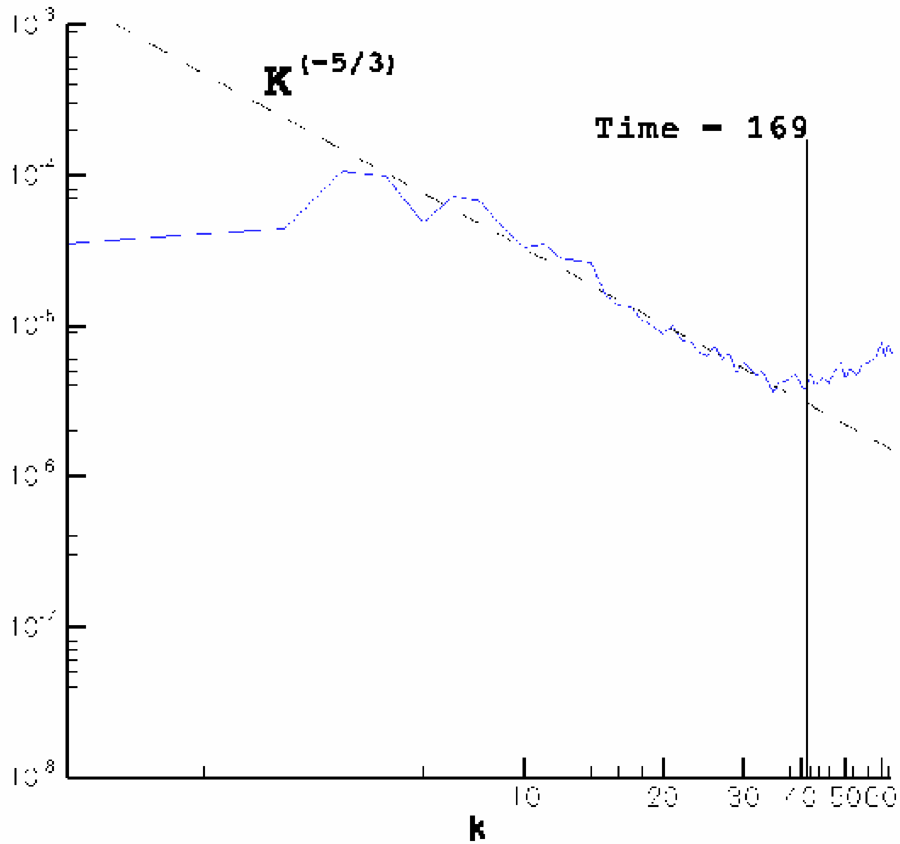
Subgrid Kinetic Energy (SGS KE) (*from new method and old*). From Mach 1.5 run. Grid 256x128x128

Spectra: Affect of model on energy cascade



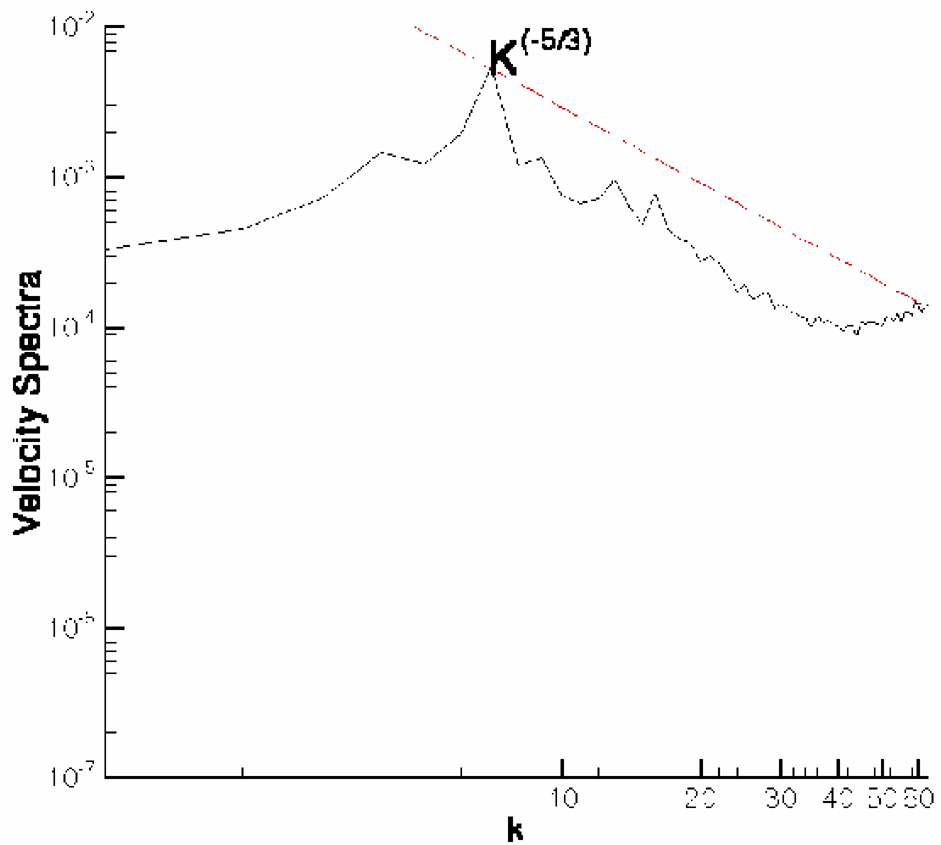
Comparison of spectra after reshock: With and without subgrid model
Mach 1.5 shock, 256x128x128 grid points

Spectra: 256x128x128



Velocity spectra from plane center plane in mixing zone after reshock: 256x128x128 simulation. Lack of dealiasing seen in upper 3rd

Spectra: Mach 5



Velocity spectra from plane center plane in mixing zone after reshock: 256x128x128 simulation. Lack of dealiasing seen in upper wavenumbers

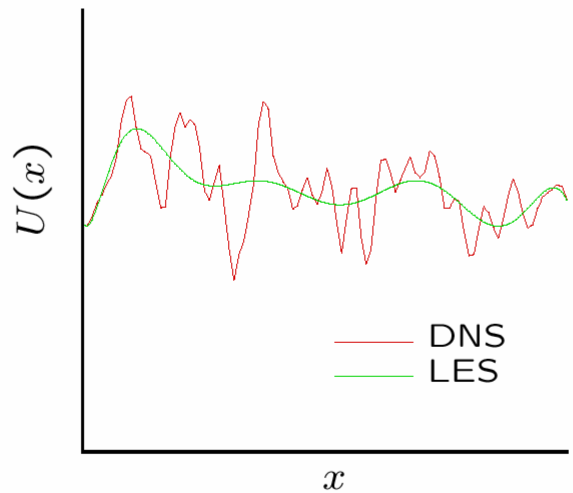
Stretched-vortex SGS vortex model II

- Lundgren form assumed for subgrid energy spectrum:

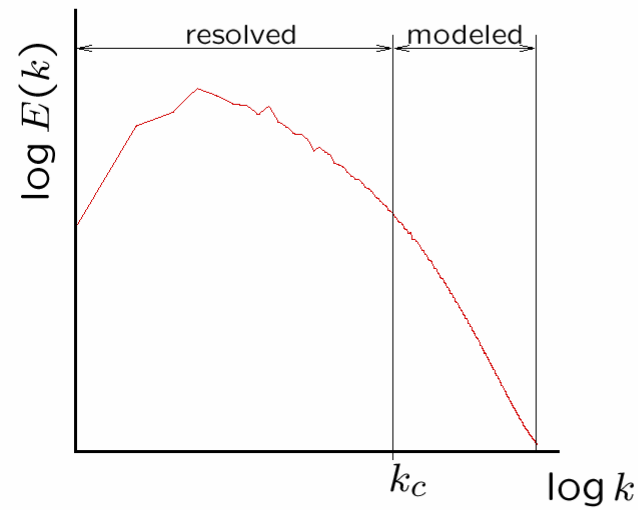
$$K_0 \varepsilon^{2/3} k^{-5/3} \exp(-2k^2 \nu / 3 |S_3^{'}|)$$

- Model parameters estimated locally by matching local resolved flow 2'nd-order velocity structure function to local subgrid estimate
- Stretched-vortex model is *not* an eddy-viscosity model
- Elements of subgrid stress tensor and subgrid energy calculated directly
  - *Important for scalar and other subgrid quantities*

Large-eddy simulation (LES)



physical space: fine-scale fluctuations not resolved, their influence is modeled.



spectral space: resolved range, $k < k_c$ (cutoff wavenumber k_c), subgrid range $k > k_c$.

Favre-filtered Navier-Stokes equations

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\widetilde{u}_i}{\partial x_i} = 0, \qquad \widetilde{q} = \bar{\rho} q/\bar{q}$$

$$\frac{\partial \bar{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial (\bar{\rho}\widetilde{u}_i\widetilde{u}_j + \bar{p}/\gamma M^2 \delta_{ij})}{\partial x_j} = Re^{-1}\left(\frac{\partial \widetilde{\sigma}_{ij}}{\partial x_j}\right) - \frac{\partial T_{ij}}{\partial x_j}, \qquad T_{ij} = \bar{\rho}(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j) \equiv \bar{\rho}\,\tau_{ij}$$

$$\frac{\partial \bar{E}}{\partial t} + \frac{\partial (\bar{E} + \bar{p}/\gamma M^2)\widetilde{u}_i}{\partial x_i} = \frac{1}{Pr Re(\gamma - 1)M^2}\frac{\partial}{\partial x_i}\left(k\frac{\partial \widetilde{T}}{\partial x_i}\right) + Re^{-1}\frac{\partial(\widetilde{\sigma}_{ij}\widetilde{u}_j)}{\partial x_i}$$

$$- \frac{1}{(\gamma - 1)M^2}\frac{\partial(\bar{\rho} q_i)}{\partial x_i} - \frac{1}{2}\frac{\partial[\bar{\rho}(\widetilde{u_j u_j u_i} - \widetilde{u_j u_j}\widetilde{u}_i)]}{\partial x_i} + Re^{-1}\frac{\partial(\widetilde{\sigma_{ij} u_j} - \widetilde{\sigma}_{ij}\widetilde{u}_j)}{\partial x_i}$$

$$\bar{E} = \frac{\bar{p}}{(\gamma - 1)\gamma M^2} + \frac{1}{2}\bar{\rho}(\widetilde{u}_j\widetilde{u}_j) + \frac{1}{2}T_{jj}, \qquad q_i = \widetilde{T u_i} - \widetilde{T}\widetilde{u}_i, \qquad \bar{p} = \bar{\rho}\widetilde{T}$$

Idea: Improve K(k) for center-difference

- Finite-difference operator

$$\mathbf{D}f(x) = \frac{1}{\Delta x}\sum_{j=-3}^{j=3} d_j\,[f(x+j\,\Delta x) - f(x-j\,\Delta x)]$$

$$d_1 = \frac{2}{3}, \quad d_2 = -\frac{1}{12}, \quad d_3 = 0, \qquad \rightarrow 5-pt,\ 4^{th}\text{order}$$

$$d_1 = \frac{3}{4}, \quad d_2 = -\frac{1}{10}, \quad d_3 = -1/2, \rightarrow 7-pt,\ 6^{th}\text{order}$$

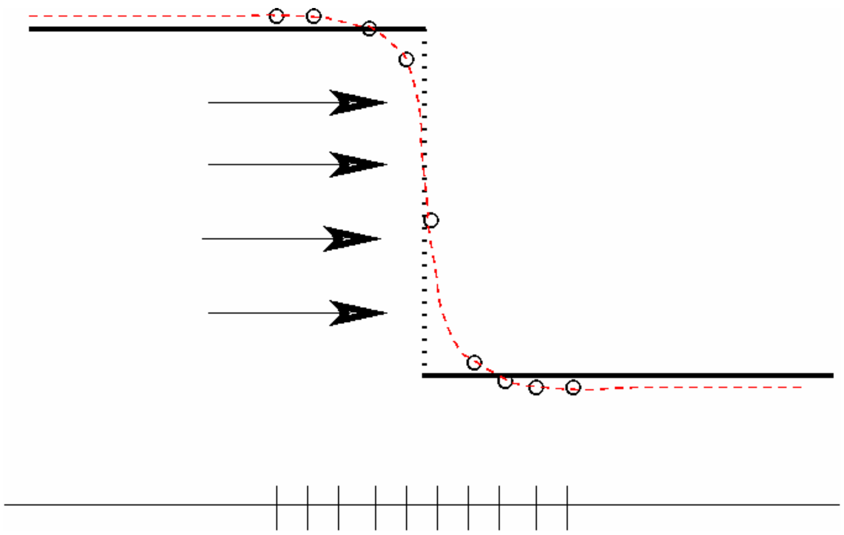
- Tuned 5-point with parameter α

$$d_1 = \frac{1}{2} - 2\,\alpha, \quad d_2 = \alpha, \qquad d_3 = 0, \rightarrow 5-pt,\ 2^{nd}\text{ order}$$

- Tuned 7-point with parameter α

$$d_1 = \frac{2}{3} + \alpha, \quad d_2 = -\frac{1}{12} - 4\,\alpha, \quad d_3 = \alpha, \rightarrow 7-pt,\ 4^{th}\text{ order}$$

Flows with strong shocks: Shock capturing solvers



- True shocks have a thickness on the mean free path order
- The shocks are not resolved: Euler equations are solved in conservative form
- Euler solver shocks are 'captured', I.e. smeared across a few cells – first-order accurate at shocks

$$\frac{d\mathbf{q}}{dt} + \frac{\partial \mathbf{F}(\mathbf{q})}{\partial x} + \frac{\partial \mathbf{G}(\mathbf{q})}{\partial y} + \frac{\partial \mathbf{H}(\mathbf{q})}{\partial z} = 0$$

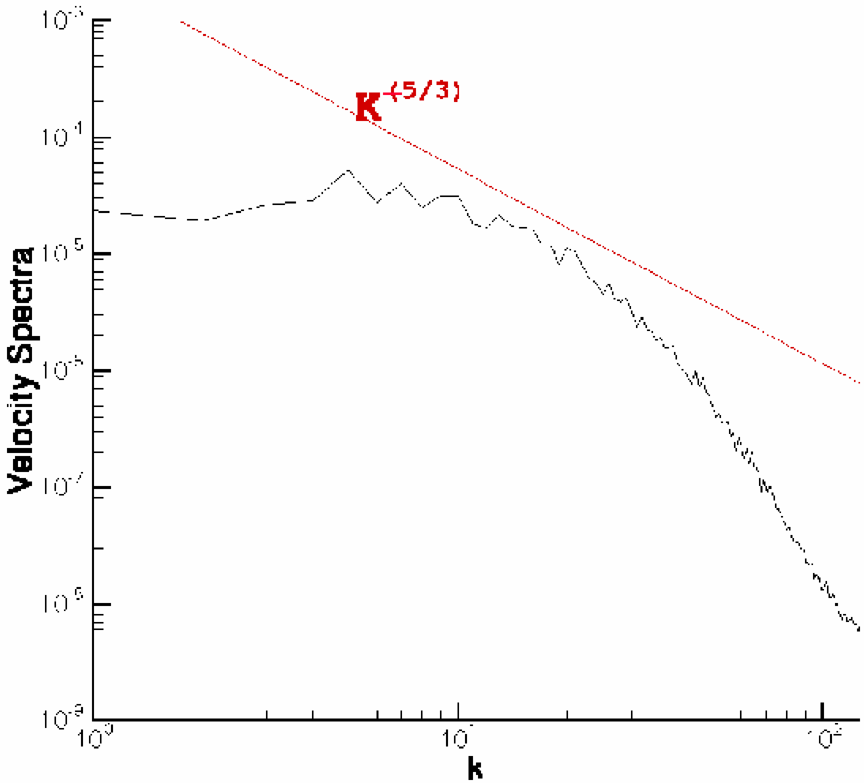
$$\mathbf{q} = \left(\rho, \rho u, \rho v, \rho w, E\right)^T$$

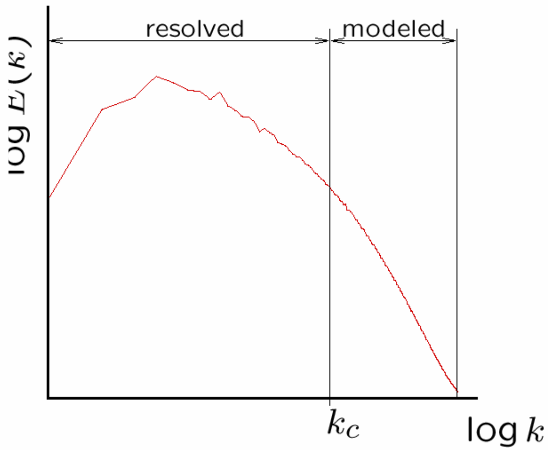
$$\mathbf{F}(\mathbf{q}) = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ \rho uw \\ \rho u(E+P) \end{pmatrix}$$

Hybrid WENO-TCDS algorithm: LES and strong shocks

- Numerical methods for shock-capturing and LES `orthogonal'.
- Our solution: hybrid technique: blending Weighted Essentially Non-Oscillatory (WENO) scheme with Tuned Centered-Difference (TCD) stencil.
- WENO in regions of very-large density ratio (Shocks)
  - *But WENO is not suitable for LES in smooth regions away from shocks.*
  - *Upwinding strategy is too dissipative*
- TCD stencil in smooth regions away from shocks
  - *Low numerical dissipation (centered method)*
  - *optimized for minimum resolved-scale discretization error in LES (Ghosal, 1996)*
  - *5- or 7-point stencil trades off formal order of accuracy for small dispersion errors*
- Target WENO stencil = TCD stencil
- In practice, target TCD stencil not always achieved; switch is used based on acceptable WENO smoothness measure
- Hybrid method designed for LES in presence of strong shocks

Spectra: The bad news





spectral space: resolved range, $k < k_c$ (cutoff wavenumber k_c), subgrid range $k > k_c$.

Velocity spectra from plane center plane in mixing zone after reshock: exhibits too much roll-off