

# Small-scale turbulence; theory, phenomenology and applications

Large-eddy simulation with stretched-vortex SGS model

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# Overview

- LES of compressible, shock-driven turbulence
  - *Extension of SGS model to compressible flow*
  - *Issues of numerical methodology*
  - *Adaptive Mesh Refinement (AMR)*
- LES of Richtmyer-Meshkov instability with re-shock
  - *Growth of mixing layer thickness*
  - *Resolved-scale turbulence statistics*
  - *Multi-scale modeling; subgrid extension of turbulence statistics*
  - *Effect of magnetic field*
  - *Cylindrical RM instability*
- Near-wall SGS modeling
  - *No large eddies near the wall*
  - *Local inner scaling and near-wall modeling*
  - *Virtual-wall model*
  - *LES of channel flow at large  $Re_{\tau}$*



# Favre-filtered Navier-Stokes equations

$$\begin{aligned}\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} &= 0 \\ \frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial (\bar{\rho} \tilde{u}_i \tilde{u}_j + \bar{p} \delta_{ij})}{\partial x_j} &= \frac{\partial \sigma_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} \\ \frac{\partial \bar{E}}{\partial t} + \frac{\partial (\bar{E} + \bar{p}) \tilde{u}_j}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( \bar{\kappa} \frac{\partial \bar{T}}{\partial x_j} \right) + \frac{\partial \sigma_{ji} \tilde{u}_i}{\partial x_j} - \frac{\partial q_j^T}{\partial x_j} \\ \frac{\partial \bar{\rho} \tilde{\psi}}{\partial t} + \frac{\partial (\bar{\rho} \tilde{\psi} \tilde{u}_j)}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( \bar{\rho} \tilde{D} \frac{\partial \tilde{\psi}}{\partial x_j} \right) - \frac{\partial q_j^\psi}{\partial x_j}\end{aligned}$$

$$\begin{aligned}\tau_{ij} &= \bar{\rho} (\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j) \\ q_j^T &= \bar{\rho} (\widetilde{c_p T u_j} - \tilde{c}_p \tilde{T} \tilde{u}_j) \\ q_j^\psi &= \bar{\rho} (\widetilde{\psi u_j} - \tilde{\psi} \tilde{u}_j)\end{aligned}$$

$$\bar{E} = \frac{\bar{p}}{(\gamma - 1)} + \frac{1}{2} \bar{\rho} (\tilde{u}_k \tilde{u}_k) + \frac{1}{2} \tau_{kk}$$

$$\bar{p} = \frac{\bar{\rho} R \tilde{T}}{\tilde{m}}$$

- Two-component Favre-filtered NS equations
- Filtering procedure strictly formal
  - *Not performed explicitly in LES*
  - *Guide to SGS modeling*
- Favre-filtered quantities identified with resolved-scale quantities in LES
  - *Modeling assumption on par with SGS modeling*
- Model subgrid flux of temperature as a passive scalar



# LES of compressible turbulence. LES and strong shocks (D. Hill).

## Hybrid WENO-TCDs algorithm:

- 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**



# SAMR and AMROC (R. Deiterding)

- Structured Adaptive Mesh Refinement (SAMR)
- Adaptive Mesh Refinement Object Oriented C++ (AMROC)
- Berger & Colella's algorithm for conservation laws of the form:

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial}{\partial x_k} \mathbf{f}^k(\mathbf{q}) = 0,$$

- Hierarchical data structure contains the solution vector and fluxes
- On each patch, a standard Cartesian fluid solver is applied to march the solution (e.g. WENO/TCD)
- Boundary conditions and synchronization between patches is accomplished by filling ghost cells with interpolated data.
  - *ghost cell interpolation is an approximation for non-linear systems of equations*

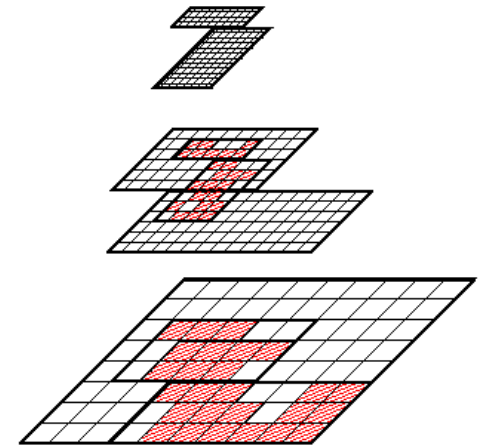
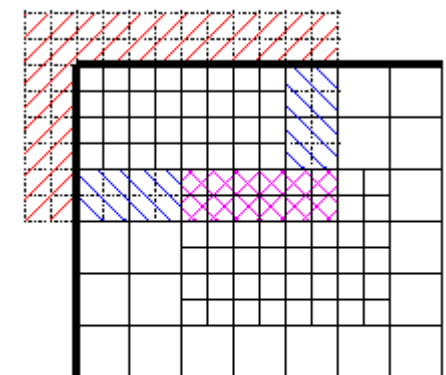
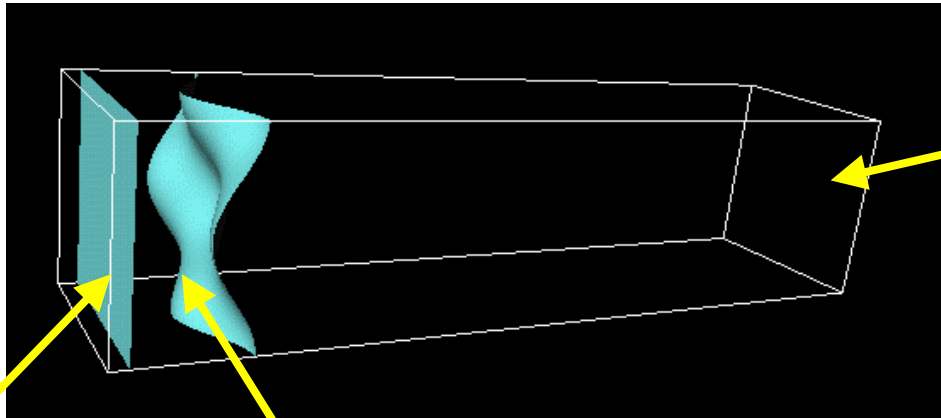


Figure 1. AMR hierarchy.



- Interpolation
- Synchronization
- Physical boundary

# Richtmyer-Meshkov (R-M) Instability



Shock reflects off end

Misalignment of contact and shock

Incident shock

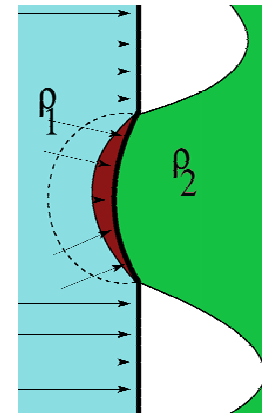
interface

Self-stretching and dilatation

Barotropic vorticity Generation

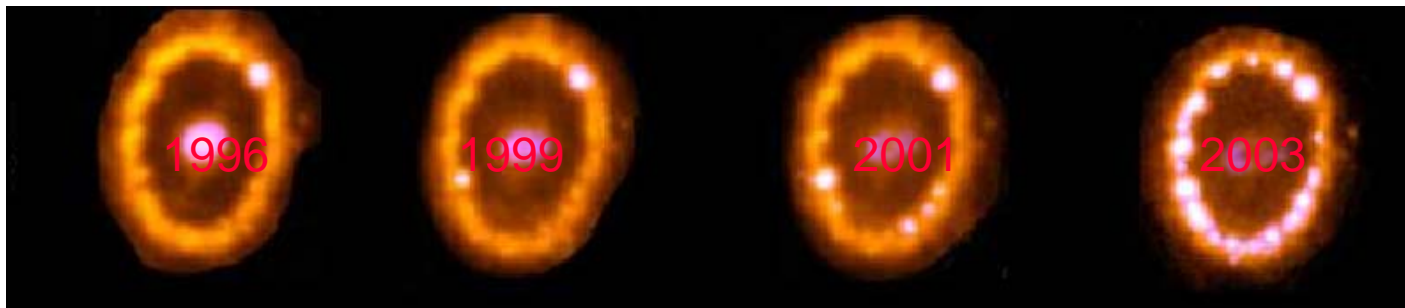
$$\frac{\partial \omega}{\partial t} + u \cdot \nabla \omega = \omega \cdot \nabla u - \omega \nabla \cdot u + \frac{1}{\rho^2} \nabla(\rho) \times \nabla(p)$$

Advection



# Richtmyer-Meshkov (R-M) Instability

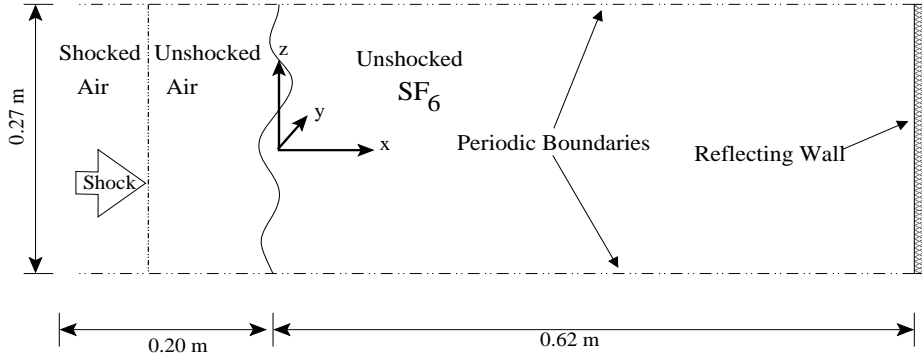
- Astrophysics: A role in the description of the explosion of supernovae (Smarr 1981, Arnett 1989.)
  - *Supernova 1987A R. McCray (JILA) Images from HST*



- A role in Inertial confinement fusion design (Lund 1997)
  - *Laser pulse drives pressure waves*
- Canonical example of shock-turbulence interaction

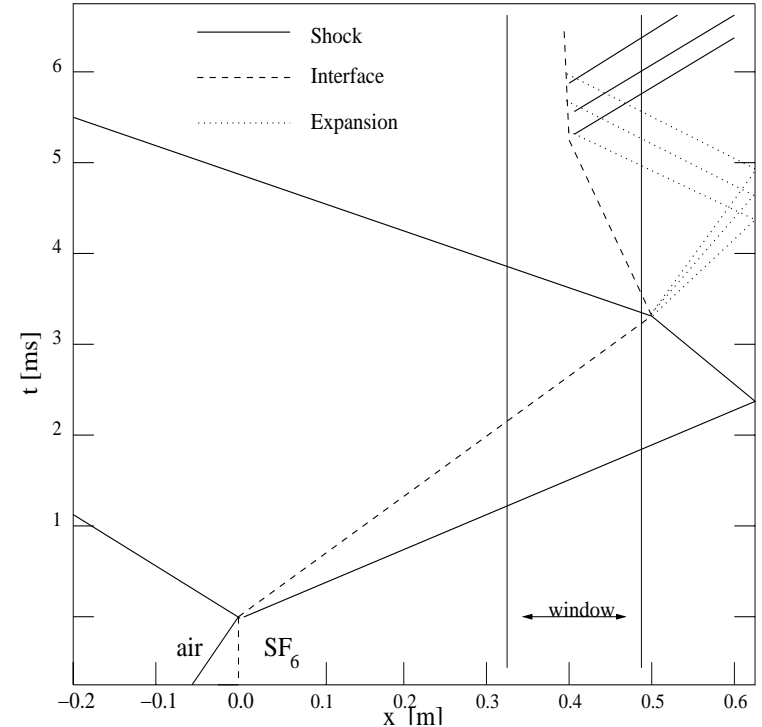


# Flow Description



	II <sup>b</sup>	VI <sup>b</sup>	VII <sup>b</sup>
Incident Mach number	1.24	1.50	1.98
Pressure (kPa)	40	23	8
Length, membrane to end wall (cm)	110	62	49
Instantaneous velocity (ms <sup>-1</sup> )	72	150	287
Shocked growth rate (ms <sup>-1</sup> )	2.1	4.2	7.5
Reshocked growth rate (ms <sup>-1</sup> )	17.0	37.2	74.4
Shocked observation times (ms)	4.7-6.7	2.2-3.2	1.7-2.5
Reshocked observation times (ms)	15.5-16.5	4.0-5.5	1.7-2.5

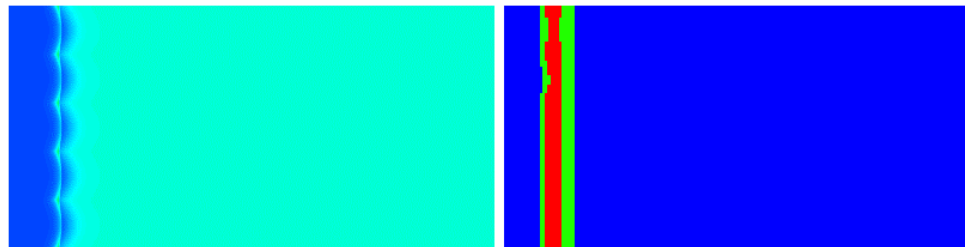
Table 1: The test conditions and growth rates of the interface thickness from Vetter & Sturtevant (1995).



Shock tube, flow conditions (Vetter & Sturtevant 1995)  
and 1-D wave diagram

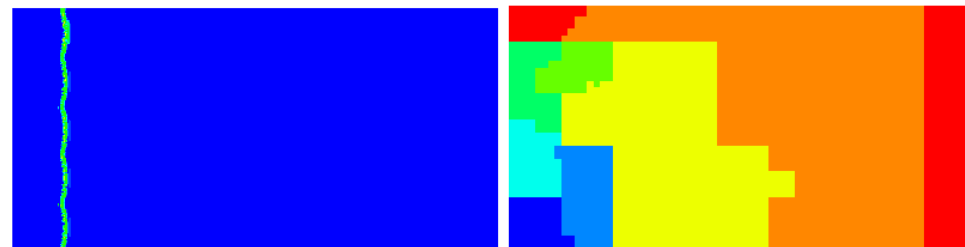


# 2D-Richtmyer-Meshkov (R-M) Instability



Density

AMR Levels



Weno Coverage

Processors



# Computational runs: unigrid

- Unigrid simulations
- QSC supercomputer (Los Alamos)

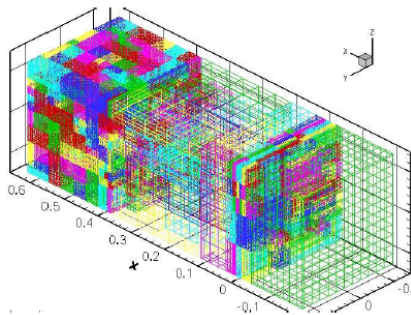
	II <sup>b</sup>	VI <sup>b</sup>	VI <sup>e</sup>	VII <sup>b</sup>
Incident Mach number	1.24	1.50	1.50	1.98
Computational grid	616x128 <sup>2</sup>	388x128 <sup>2</sup>	776x256 <sup>2</sup>	327x128 <sup>2</sup>
Computational resolution: $\Delta x$ (cm)	0.21	0.21	0.105	0.21
Simulation time (ms)	16.62	6.35	12.0	2.57
CPU hours	3,982	972	38,400	544

Table 1: The computational cost in CPU hours for each of the runs. Simulation VI<sup>e</sup> is a higher resolution version of VI<sup>b</sup> computed to about twice the experimental time.

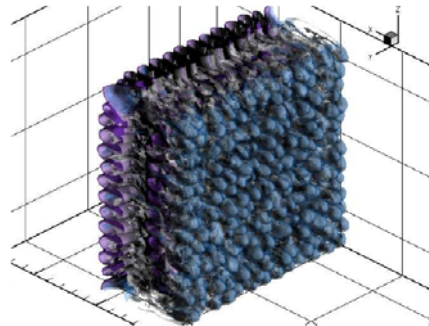


# LES of planar Richtmyer-Meshkov instability

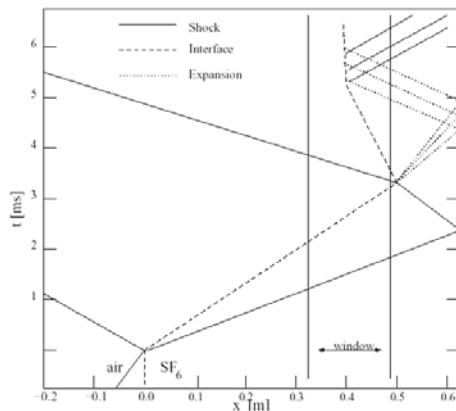
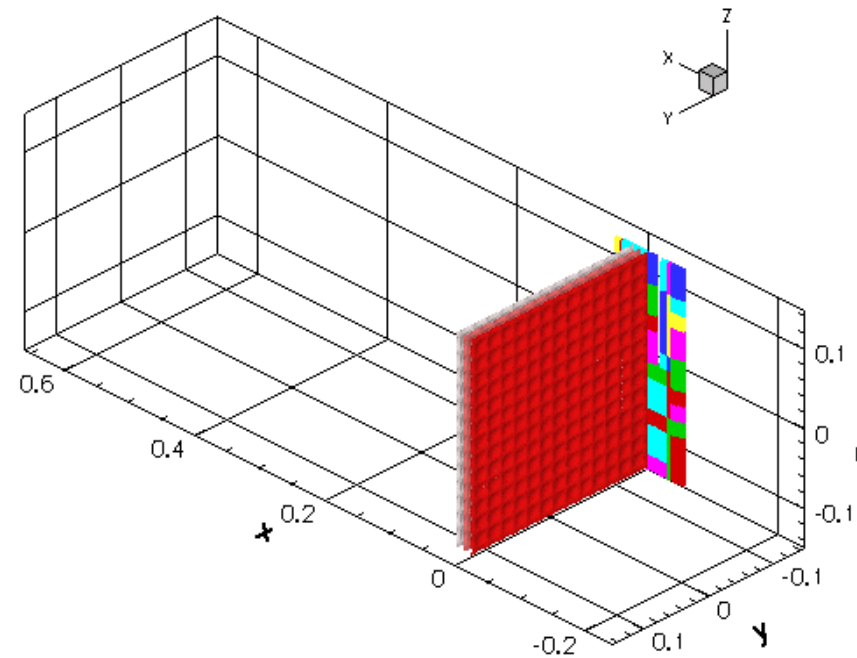
- Vetter & Sturtevant (1995) RMI with reshock off end wall
- Air/SF<sub>6</sub>, Mach=1.5
- 3 levels of refinement



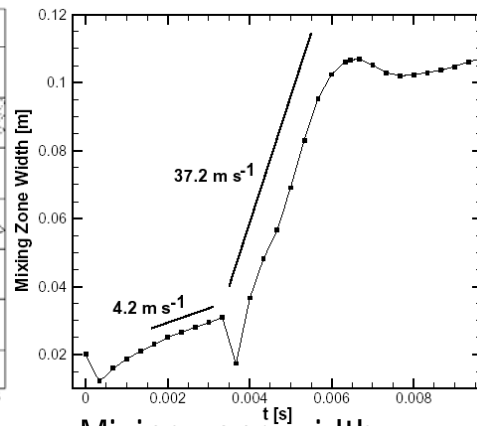
Mesh at one time



Interface at one time



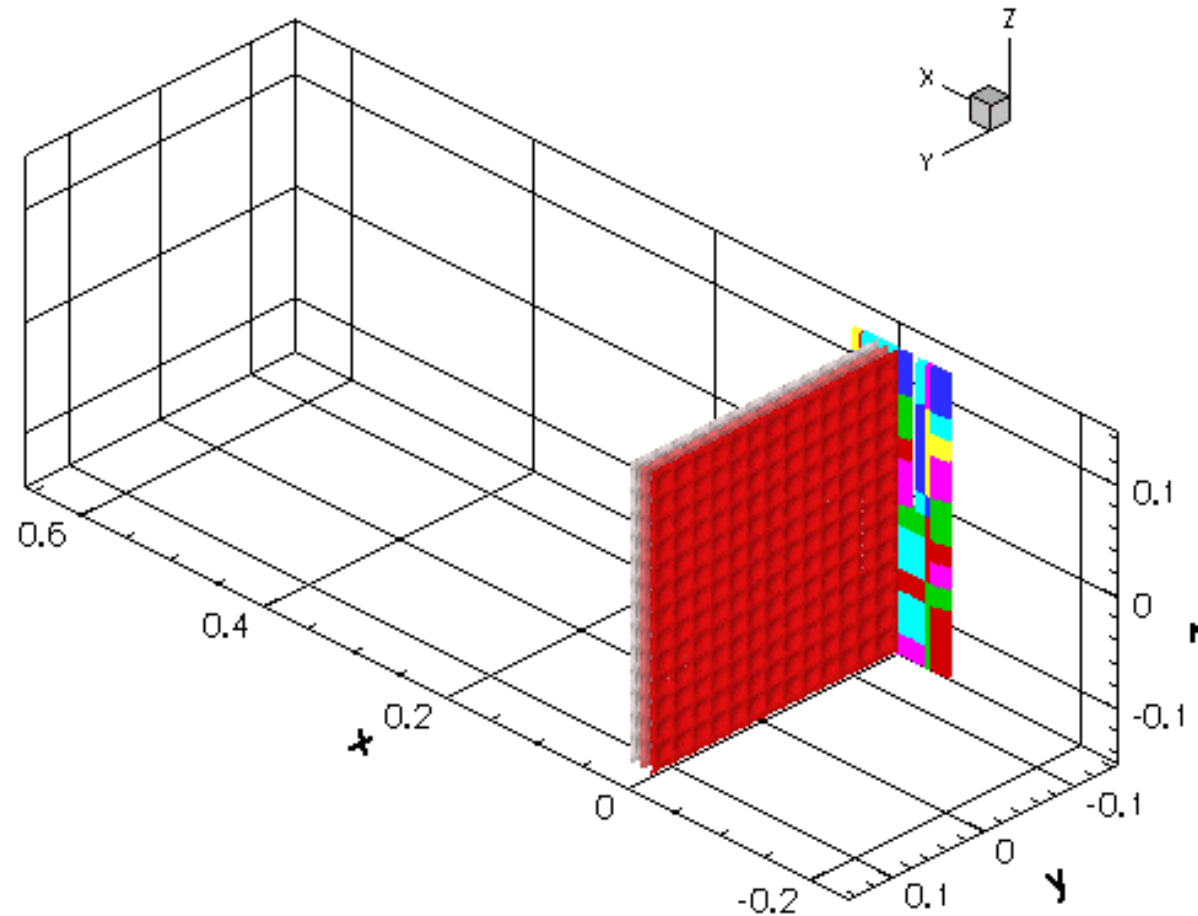
Wave diagram



Mixing zone width



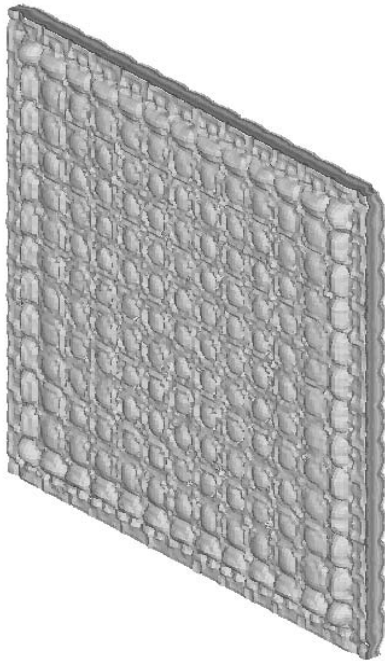
# LES of planar R-M instability;



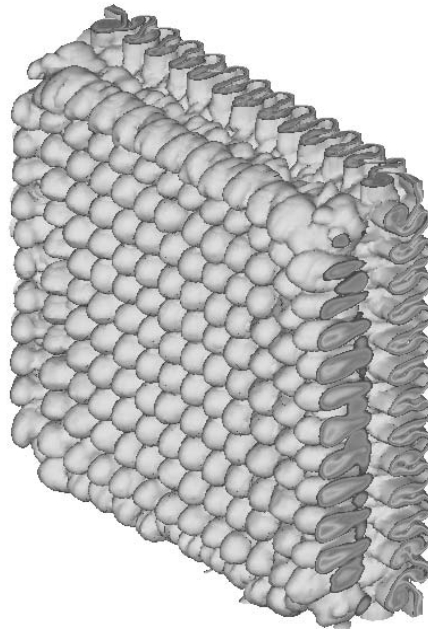
- Vetter Sturtevant (1995) RMI with reshock off end wall
- Air/SF<sub>6</sub>, Mach=1.5
- 3 levels of refinement



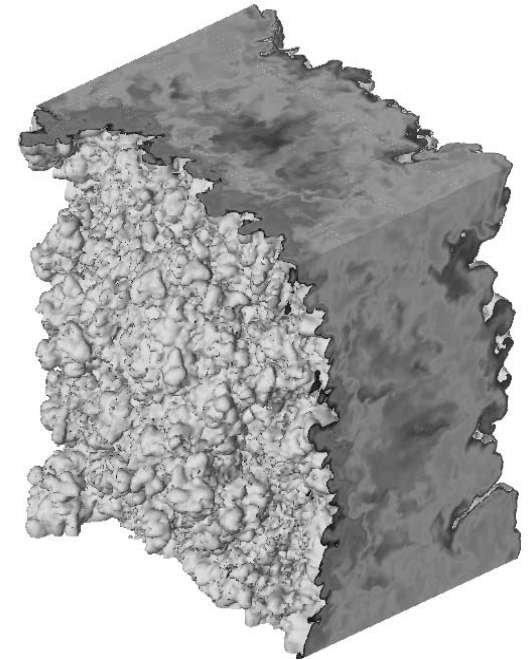
# Growth of turbulent mixing zone



$T = 0. \text{ ms}$



$T = 3.6 \text{ ms}$



$T = 10.0 \text{ ms}$

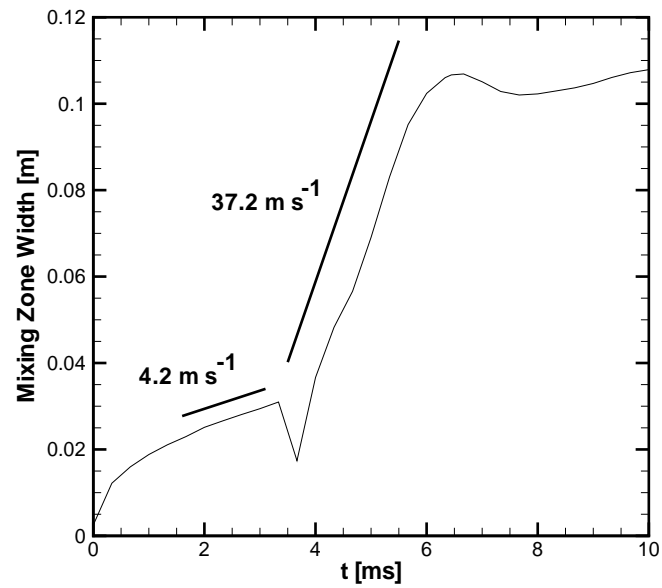
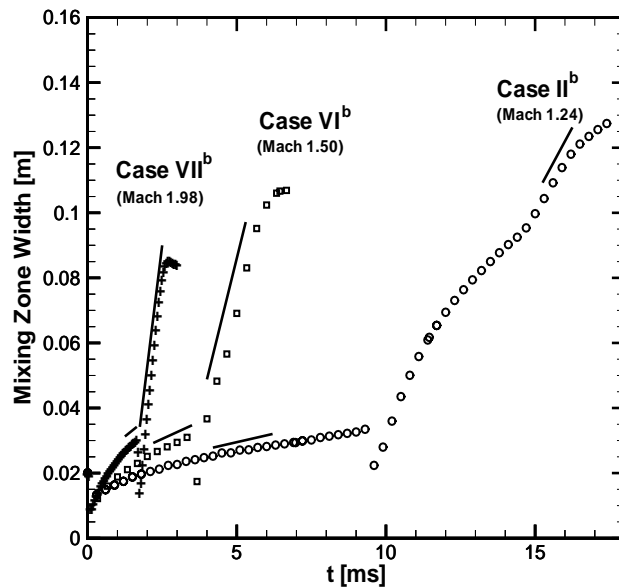
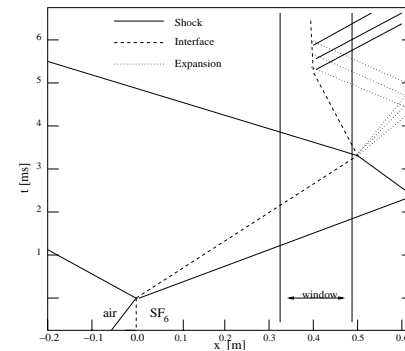


# Growth of turbulent mixing zone

y-z plane-averaged mixing-layer width  
compared with Vetter & Sturtevant (1995)

$$\langle f(x, t) \rangle = \frac{1}{A} \int \int f(x, y, z, t) dy dz$$

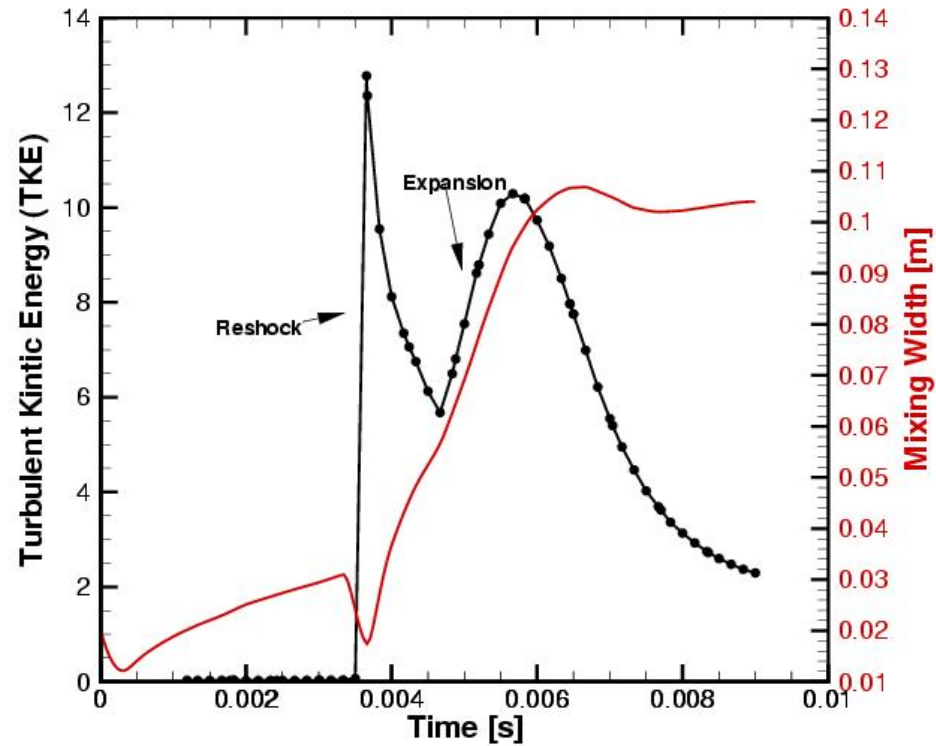
$$\delta_{MZ}(t) = 4 \int_{\text{tube}} (1 - \langle \psi \rangle) \langle \psi \rangle dx$$



Case VIe; 776x256x256



# Kinetic energy in mixing layer



# Resolved-scale radial spectra in y-z plane

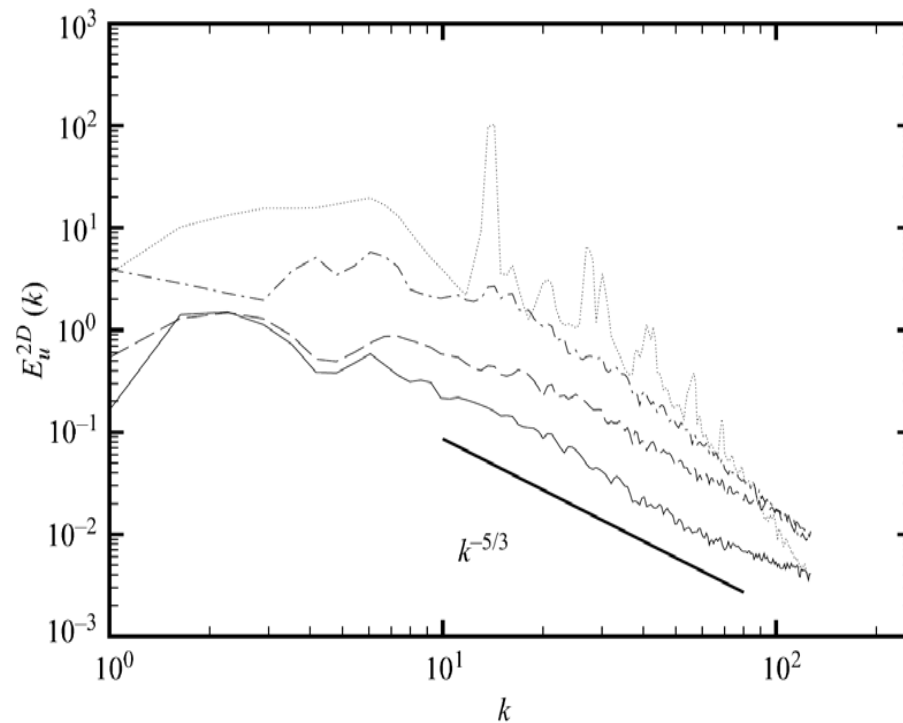
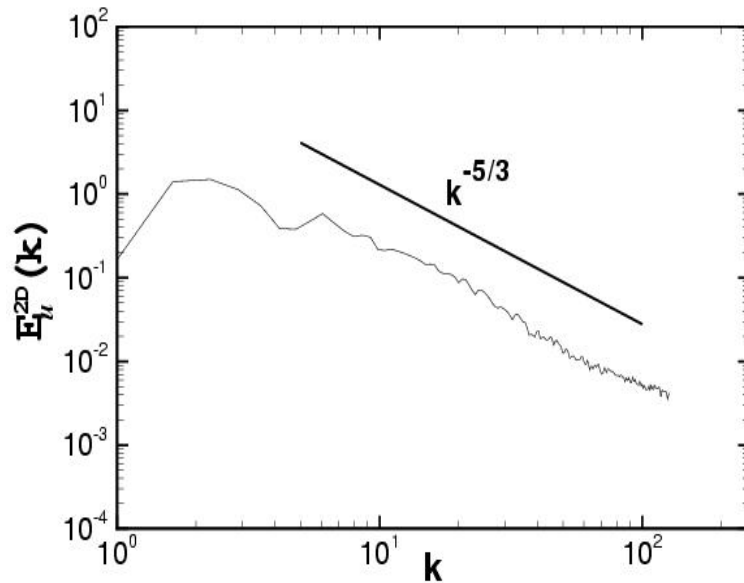


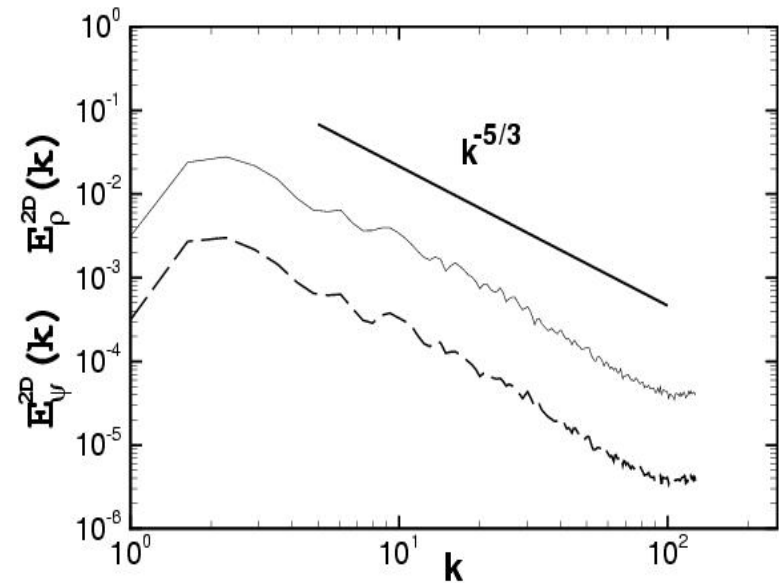
FIGURE 12. Radial power spectra of velocity  $E_u^{2D}(k)$  computed in the centre plane of the TMZ at four different times:  $t = 4.5$  ms (dotted line),  $t = 6.5$  ms (dashed-dot line),  $t = 7.6$  ms (dashed line) and  $t = 10$  ms (solid line). All computed wavenumbers shown and  $k_{max} = 128$ .



# Resolved-scale radial spectra in y-z plane



*Radial spectrum of x-velocity,  
center of mixing layer*

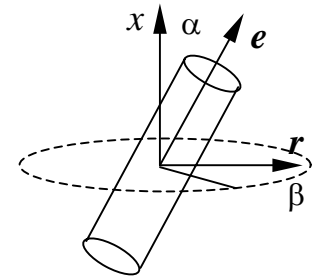


*Radial spectrum of density  
(solid) and mixture fraction,  
center of mixing layer*



# Subgrid continuation

- Stretched-spiral vortex SGS model used for subgrid continuation
  - Contains description of local anisotropy
  - Computation of local and plane-averaged Kolmogorov scale  $\eta$
  - Parameters computed from LES (structure functions)



$$E(k) = \mathcal{K}_0 \epsilon^{2/3} k^{-5/3} \exp[-2k^2 \nu / (3|\tilde{a}|)]$$

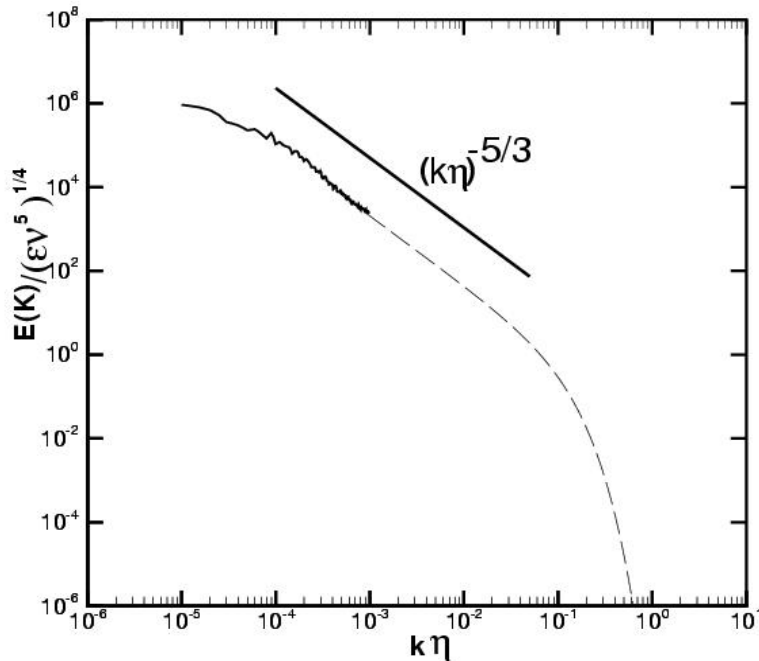
$$\tilde{a} = \tilde{S}_{ij} e_i^v e_j^v, \quad \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)$$

$$E_{qq}^{2D}(k_r, \alpha_0) = \frac{2k_r}{\pi} \int_{k_r}^{|k_r / \cos \alpha_o|} \frac{E(\kappa)}{(\kappa^2 - k_r^2)^{1/2} (k_r^2 - \kappa^2 \cos^2 \alpha_o)^{1/2}} d\kappa.$$

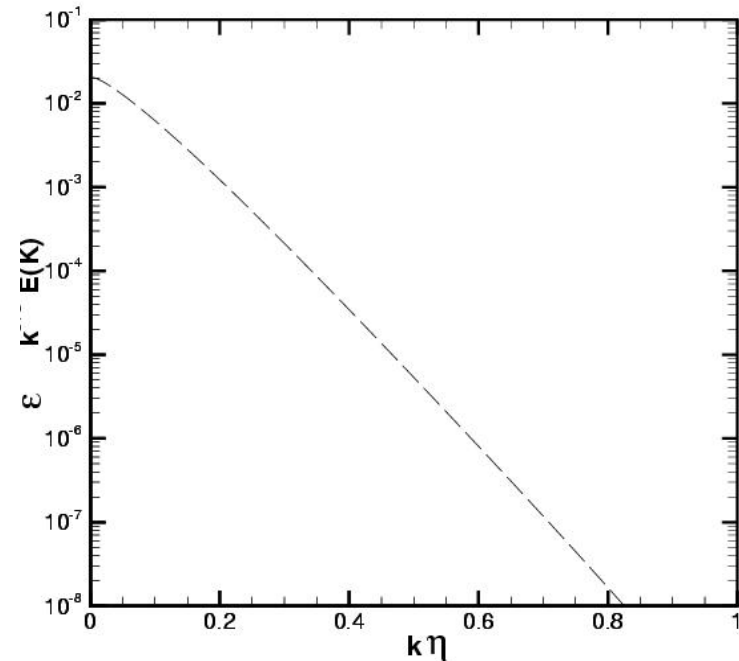
$$E_{33}^{2D}(k_r, \alpha_0) = \frac{2k_r}{\pi} \int_{k_r}^{|k_r / \cos \alpha_o|} \frac{(k_r^2 - \kappa^2 \cos^2 \alpha_o)^{1/2} E(\kappa)}{\kappa^2 (\kappa^2 - k_r^2)^{1/2}} d\kappa.$$



# Subgrid continuation of radial velocity spectra



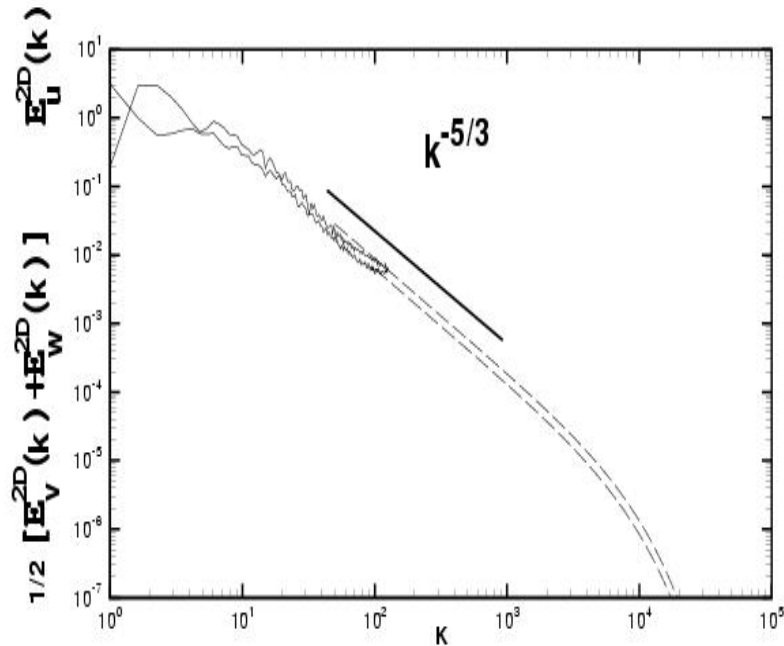
- Radial (in k-space) velocity spectrum on center plane of mixing layer
  - Resolved-scale spectrum (solid)
  - Subgrid continuation (dashed)
  - Parameters computed from LES (structure functions)



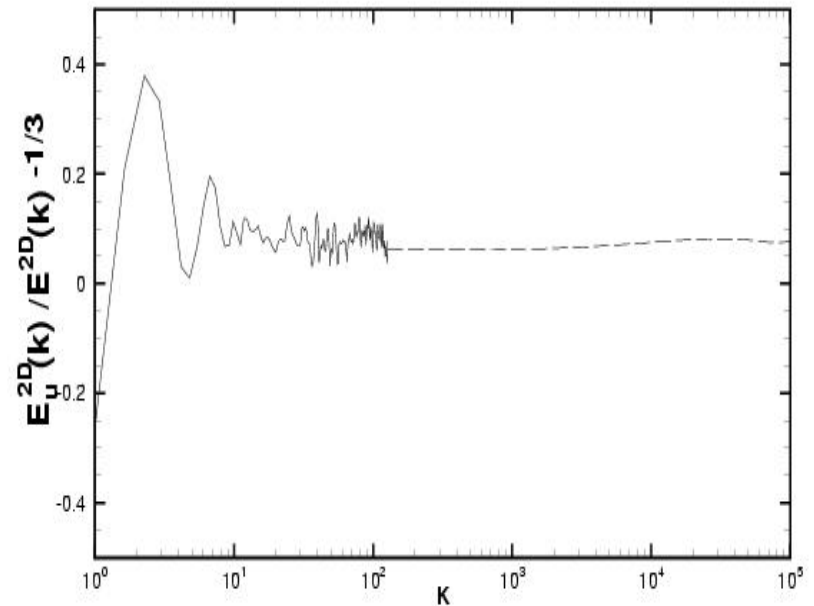
- Subgrid velocity spectrum in dissipation range
  - Log-linear scale
  - Note exponential roll-off



# Subgrid continuation of radial velocity spectra. Anisotropy of in-plane and normal velocity spectra



- Radial spectrum of  $u$  (top) and  $u+w$  (below)
  - Resolved-scale spectrum (solid)
  - Subgrid continuation (dashed)



- Measure of anisotropy for radial velocity spectra
  - Resolved-scale spectrum (solid)
  - Subgrid continuation (dashed)



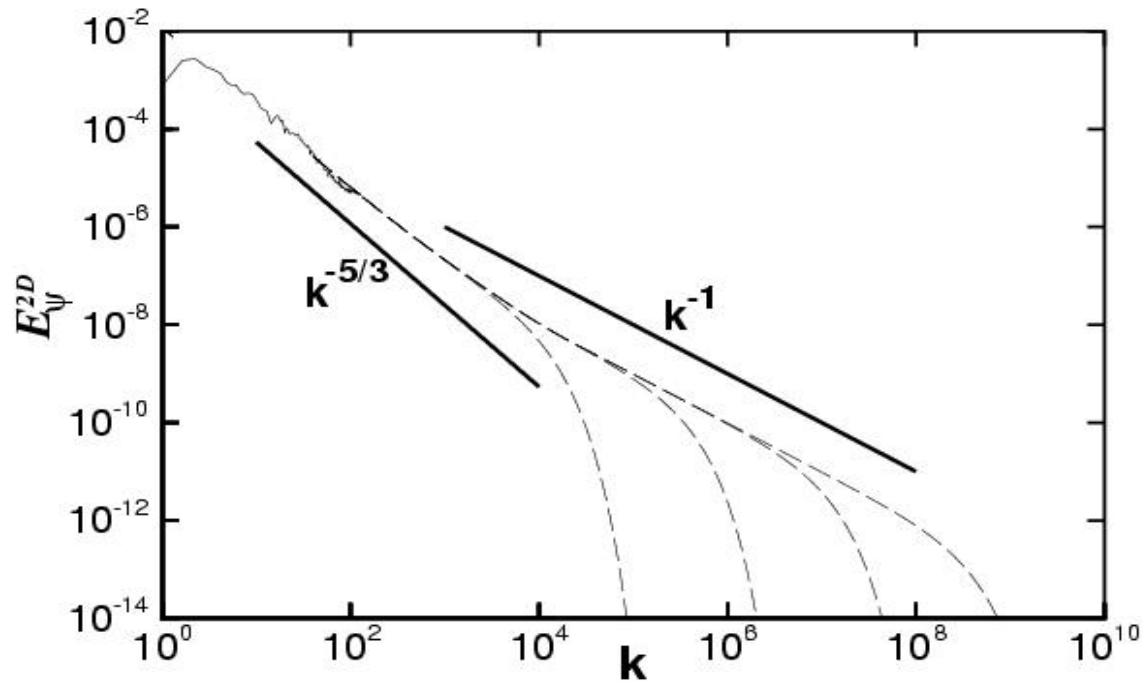
# Subgrid continuation of scalar spectrum in y-z plane

Scalar spectrum for  
stretched-spiral  
vortex

Pullin & Lundgren  
(2000)

$$E_\psi(k) = \mathcal{K}_\psi \left( k^{-5/3} \exp\left(-\frac{(4\nu + 2D)k^2}{3\tilde{a}}\right) + \frac{8}{5\pi} \left(\frac{2\Gamma}{\tilde{a}}\right)^{1/3} k^{-1} \exp\left(-\frac{2Dk^2}{3\tilde{a}}\right) \right)$$

$$\tilde{\mathcal{F}}_2^\psi(\Delta) = 4\mathcal{K}_\psi \Delta^{2/3} \int_0^\pi \left( s^{-5/3} + \frac{8}{5\pi} \left(\frac{2\Gamma}{\tilde{a}\Delta^2}\right)^{1/3} s^{-1} \right) \left(1 - \frac{\sin s}{s}\right) ds$$



Resolved-scale and continued scalar spectrum in center y-z  
plane,  $t = 10\text{ms}$ . Left to right,  $Sc = 1, 1000, 1000,000$



# P.D.F. of mixture fraction with subgrid correction

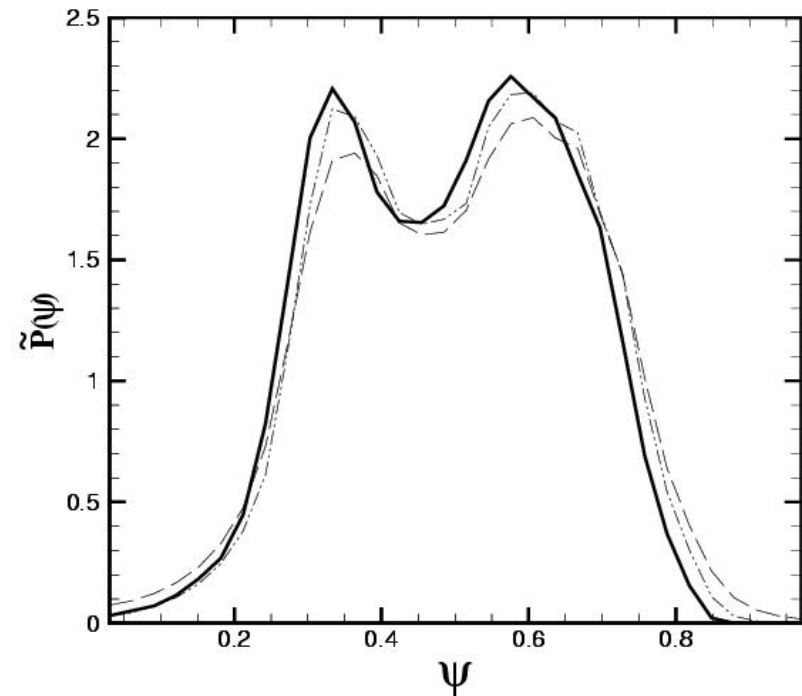
$$\tilde{\mathcal{P}}_{sgs}(\psi, \tilde{\psi}, \sigma_{\tilde{\psi}}^2; \mathbf{x}, t) = \tilde{\mathcal{P}}_{sgs}(\psi | \tilde{\psi}, \sigma_{\tilde{\psi}}^2) \tilde{\mathcal{P}}_{sgs}(\tilde{\psi}, \sigma_{\tilde{\psi}}^2; \mathbf{x}, t)$$

$$\tilde{\mathcal{P}}_{sgs}(\psi; \mathbf{x}, t) = \int \int \tilde{\mathcal{P}}_{sgs}(\psi | \tilde{\psi}, \sigma_{\tilde{\psi}}^2) \tilde{\mathcal{P}}_{sgs}(\tilde{\psi}, \sigma_{\tilde{\psi}}^2; \mathbf{x}, t) d\tilde{\psi} d\sigma_{\tilde{\psi}}^2$$

$$\tilde{P}(\psi; \mathbf{x}, t) \simeq \frac{\langle \bar{\rho} \tilde{\mathcal{P}}_{sgs}(\psi; \mathbf{x}, t) \rangle}{\langle \bar{\rho}(\mathbf{x}, t) \rangle}$$

$$\tilde{\mathcal{P}}_{sgs}(\psi; \mathbf{x}, t) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \psi^{a-1} (1-\psi)^{b-1}$$

$$a = \tilde{\psi}[\tilde{\psi}(1-\tilde{\psi})\sigma_{\tilde{\psi}}^{-2} - 1], \quad b = a(\tilde{\psi}^{-1} - 1)$$



*P.D.F of mixture fraction in center y-z plane,  $t = 10\text{ms}$ . Resolved-scale and  $Sc = 1, 1000,000$*



# Suppression of RM instability by Magnetic Field

(V. Wheatley, R. Samtaney)

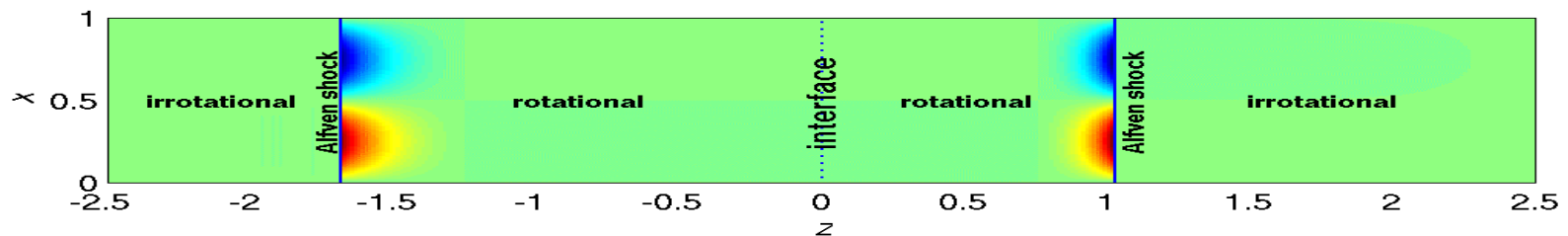
- Suppression due to change in shock refraction process at interface when  $B \neq 0$  (Wheatley, Pullin & Samtaney, JFM 2004)
- Linear initial-value problem for impulsive acceleration of interface in presence of magnetic field solved exactly



Vorticity (top) and  $\rho$  (bottom) at  $t=1.8$ ,  $B=0$ , interface unstable



Vorticity (top) and  $\rho$  (bottom) at  $t=1.8$ ,  $B \neq 0$ , instability suppressed



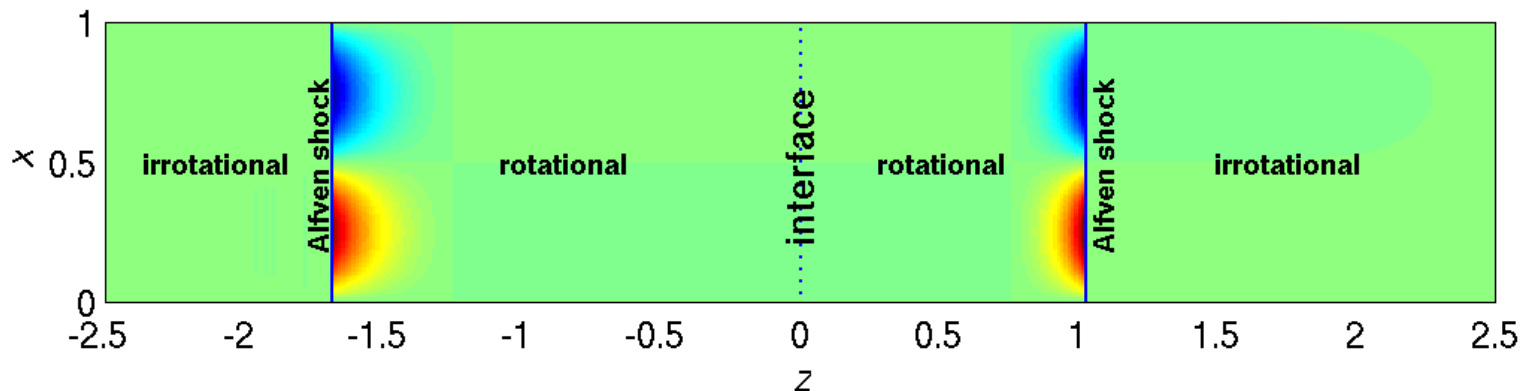
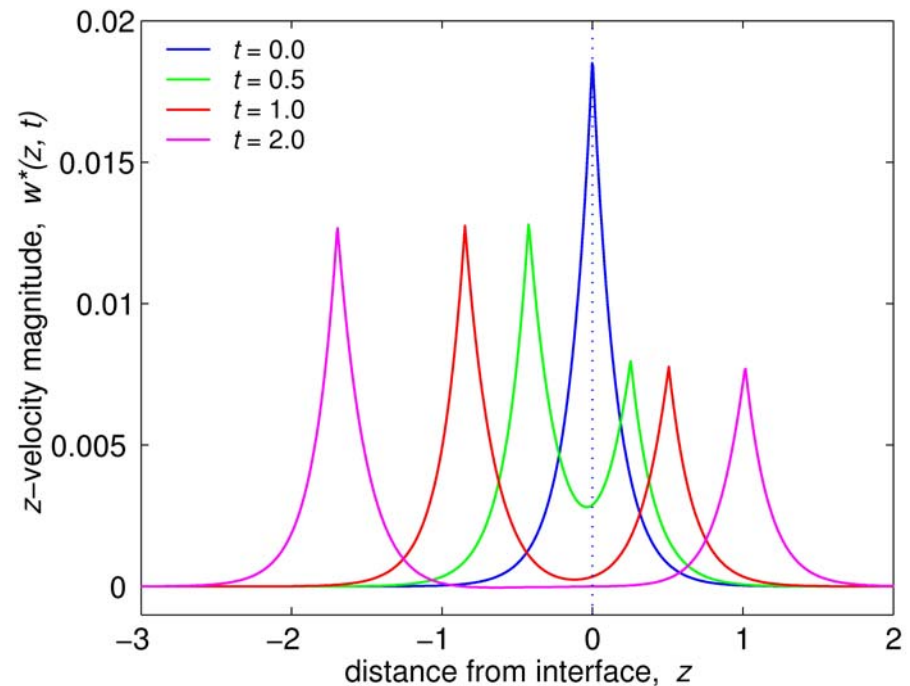
# Analysis: Solution Features: PRL, 2005

Solution consists of:

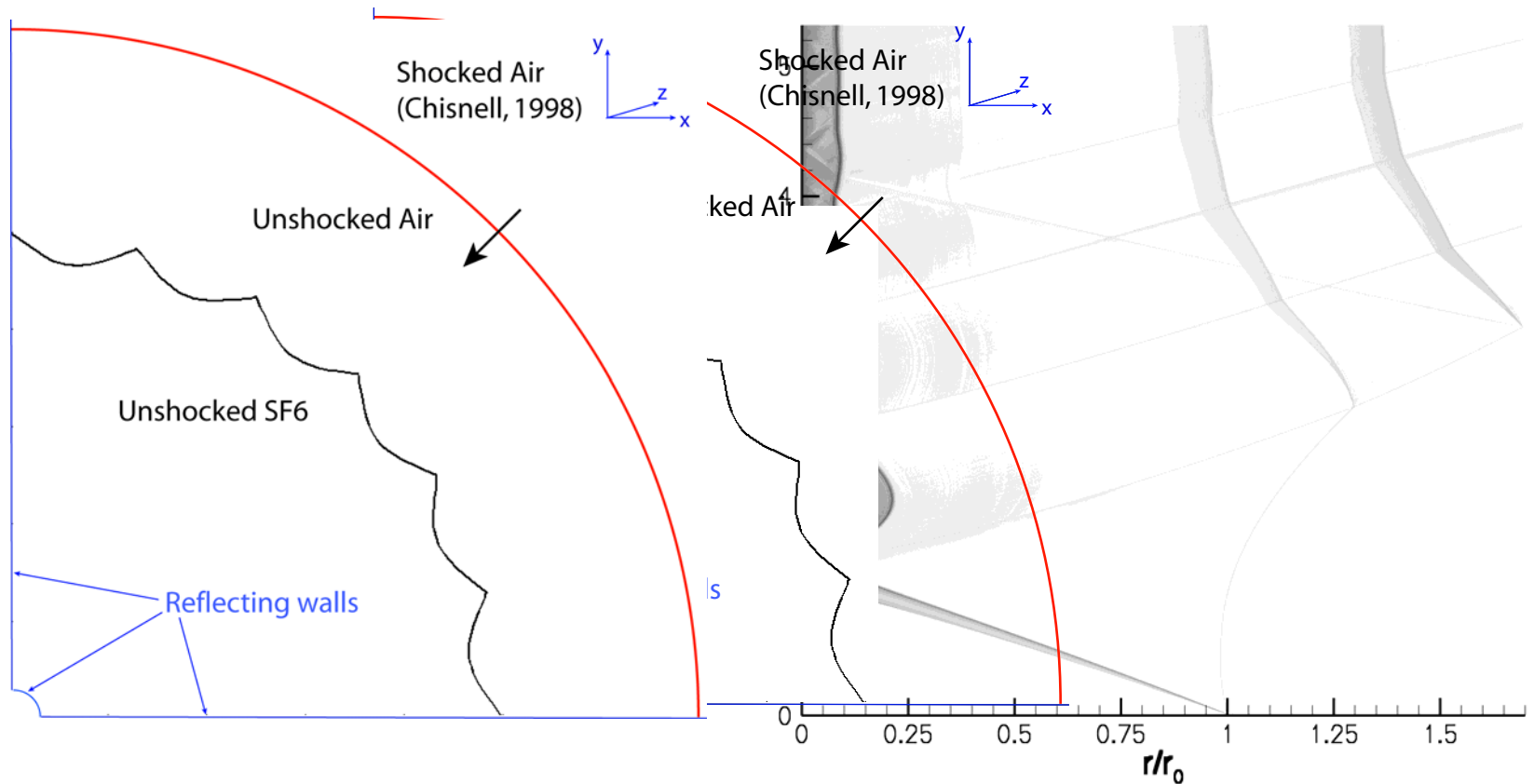
- Inner region of rotational flow
- 2 small amplitude Alfvén shocks that carry circulation
- 2 outer irrotational regions

Notes:

- $w^*(0, t)$  is interfacial growth rate
- this decays to zero as Alfvén shocks propagate away



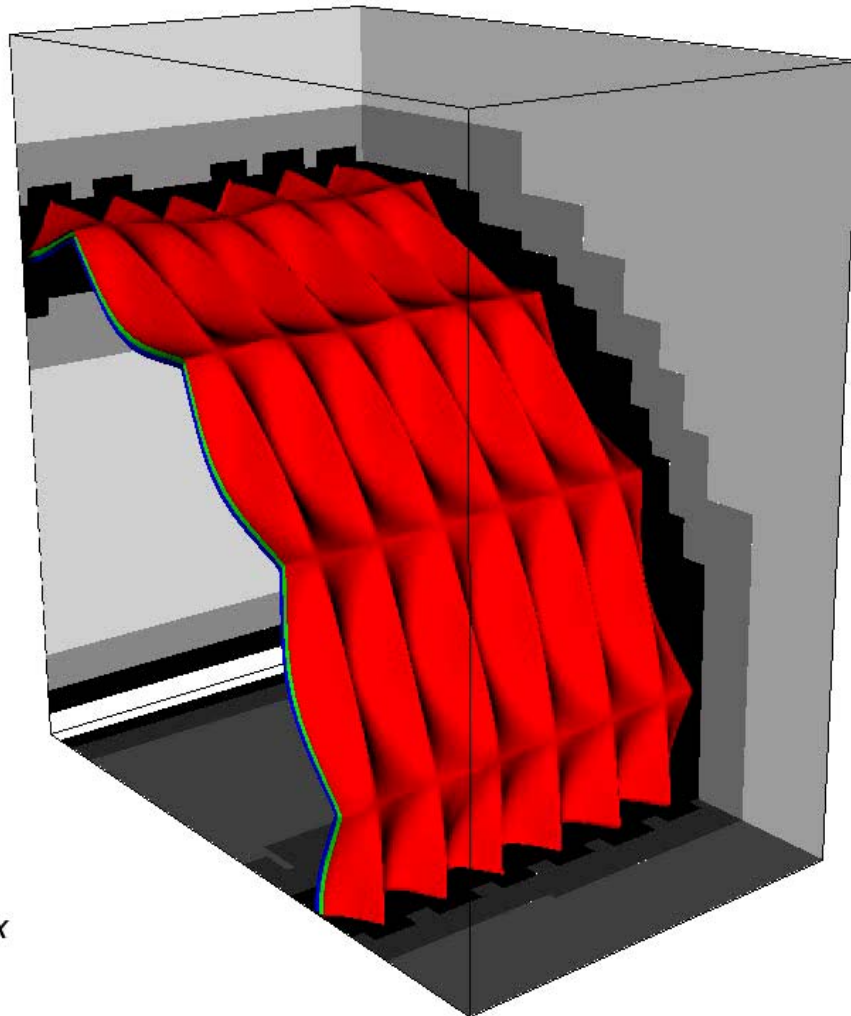
# Cylindrical RMI: Flow Description



Flow conditions and 1-D wave diagram ( $r, t$ )



# Cylindrical RMI; $M_0=1.3$ , 90 degree wedge (M. Lombardini)

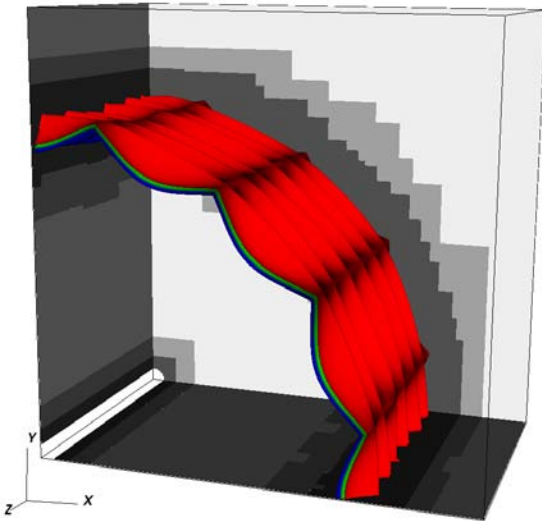


- WENO-TCD with LES (SV model)
- Adaptive Mesh Refinement (AMROC)  
Ghost Fluid Method (inner and outer cylindrical boundaries)
- Initial conditions:
  - $M_0 = 1.3$  or 2.0 or 3.0
  - Air/ $\text{SF}_6$  (Atwood number = 2/3)
  - “egg-carton” + smaller symmetry breaking perturbation with random phase
  - Chisnell’s converging flow behind the shock wave
- Resolution:
  - Base grid 83 x 83 x 51
  - 2 additional levels of refinement
  - Equivalent refined resolution 332 x 332 x 204

Passive scalar contours &  
adaptive levels of refinement

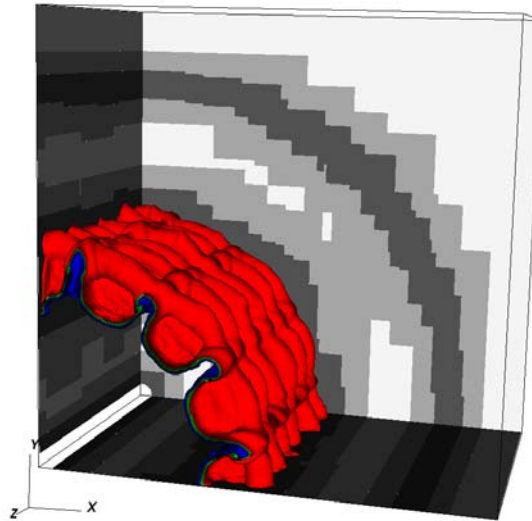


# Growth of turbulent mixing zone ( $M_0=2.0$ )



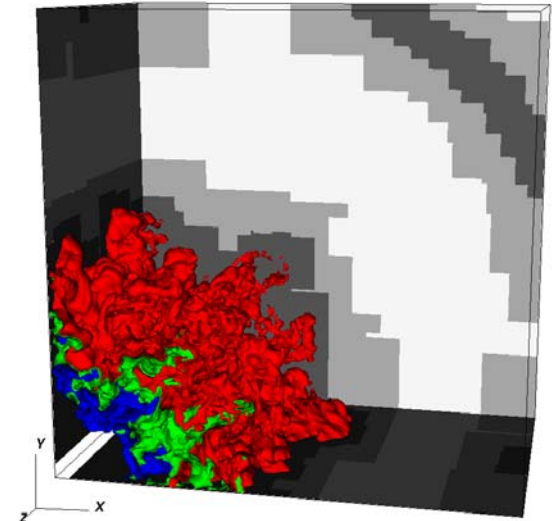
$t = 0$ . ms

Initial condition



$t = 1.45$  ms

After first shock interaction

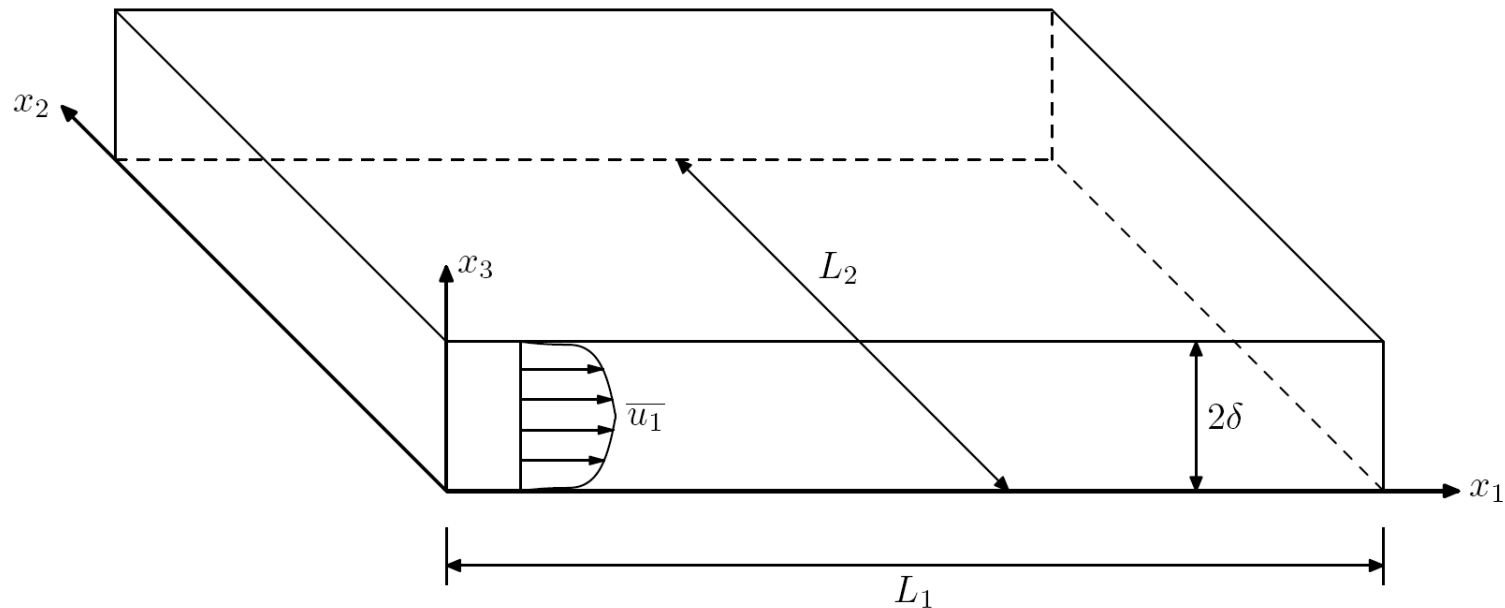


$t = 5.13$  ms

After first reschock



# Turbulent channel flow (work in progress)



$$-\delta \frac{\overline{\partial p}}{\partial x_1} = \nu \left( \frac{\partial \overline{u_1}}{\partial x_3} \right)_{\text{wall}} \equiv u_\tau^2, \quad \text{Re}_\tau = u_\tau \delta / \nu$$



# No large eddies near wall

## Ten questions concerning the large-eddy simulation of turbulent flows

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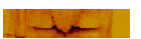
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A second example is high Reynolds number near-wall flows, the simplest specific case being the turbulent boundary layer on a smooth wall. The wall shear stress—all-important in aerodynamic applications—arises from momentum transfer from the outer flow through the boundary layer to the wall. In the viscous near-wall region, the momentum transfer is effected by the near-wall structures, the length scale of which scales with the tiny viscous length scale. As Bradshaw has succinctly put it: in the viscous near-wall region *there are no large eddies*. But, as has been appreciated at least since Chapman [15], the near-wall motions cannot be resolved in high-Reynolds number LES, but must instead be modelled (to avoid impracticable computational requirements that increase as a power of Reynolds number, as in DNS).



# Near-wall filtering

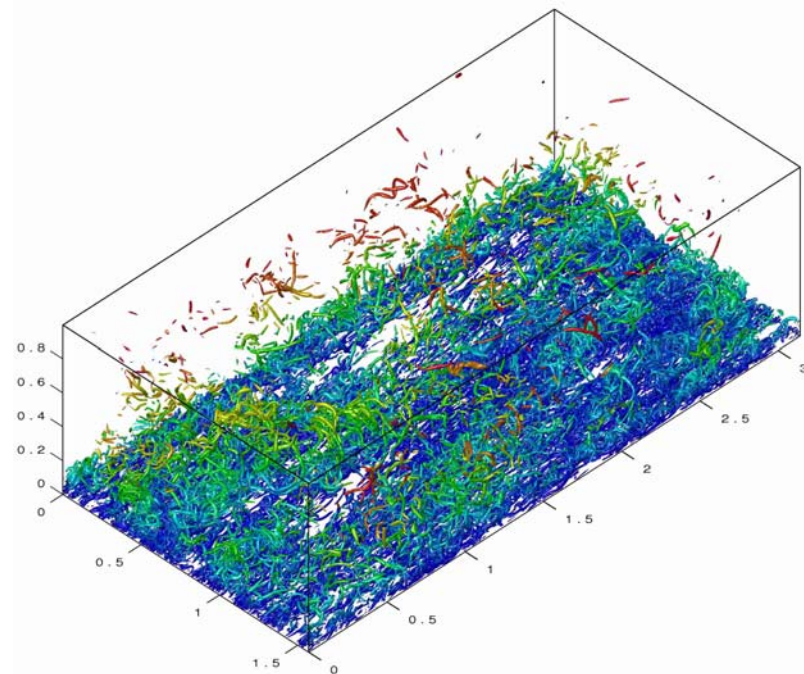
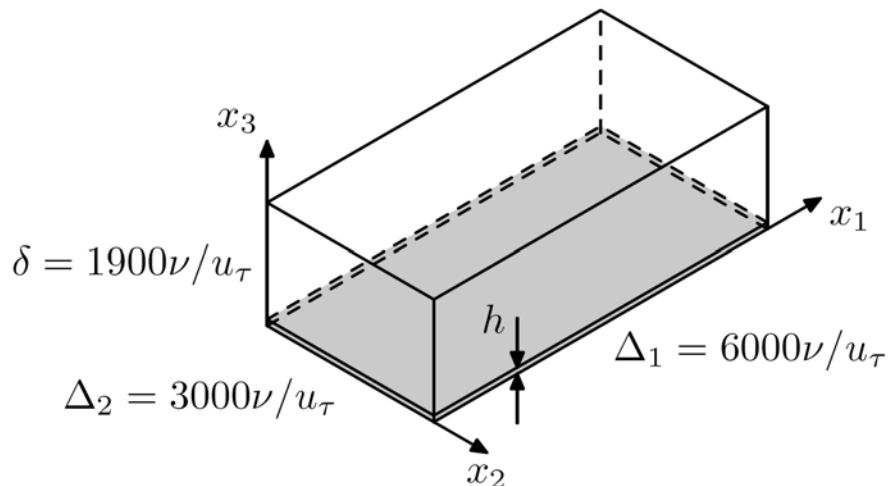
## Streamwise and spanwise Gaussian filter

$$\tilde{Q}(x_1, x_2, x_3, t) \equiv \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} Q(x'_1, x'_2, x_3, t) G_1(x_1, x'_1; \Delta_1) G_2(x_2, x'_2; \Delta_2) dx'_1 dx'_2$$

$$\Delta_1, \Delta_2 \gg \nu/u_\tau$$

## Wall-normal top-hat filter

$$\langle Q \rangle(x_1, x_2, t) \equiv \frac{1}{h} \int_0^h \tilde{Q}(x_1, x_2, x'_3, t) dx'_3$$



# Local inner scaling

Filtered streamwise momentum equation

$$\frac{\partial \langle u_1 \rangle}{\partial t} = \left( -\frac{1}{h} \widetilde{u_3 u_1} - \frac{\partial \widetilde{p}}{\partial x_1} + \frac{\nu}{h} \left[ \frac{\partial \widetilde{u_1}}{\partial x_3} - u'_0 \right] \right)_{x_3=h}$$

$$u'_0(x_1, x_2, t) \equiv \left( \frac{\partial \widetilde{u_1}}{\partial x_3} \right)_{x_3=0} = \widetilde{u_\tau}^2(x_1, x_2, t) / \nu$$



Law of the wall in a local sense

$$\widetilde{u_1}^+ = F(x_3^+) \iff \frac{\widetilde{u_1}(x_1, x_2, x_3, t)}{(\nu u'_0)^{1/2}} = F\left(\frac{x_3}{(\nu/u'_0)^{1/2}}\right)$$

$$\frac{\partial \langle u_1 \rangle}{\partial t} = \frac{(\widetilde{u_1})_{x_3=h}}{2 u'_0} \frac{\partial u'_0}{\partial t}$$



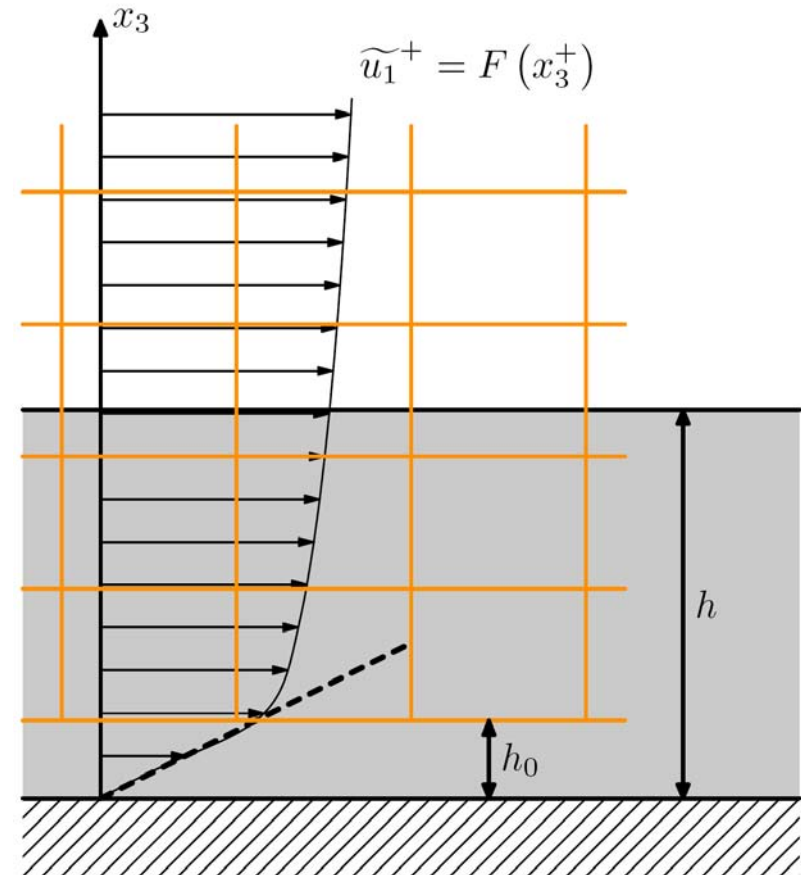
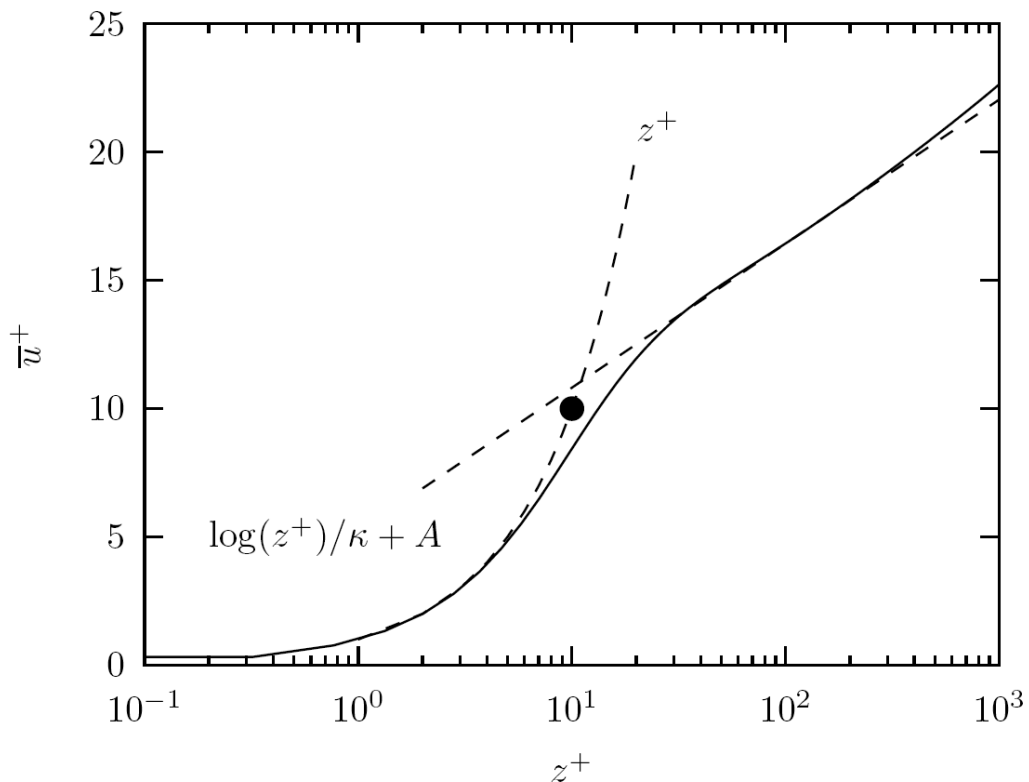
Local shear stress equation

$$\frac{\partial u'_0}{\partial t} = \frac{2 u'_0}{(\widetilde{u_1})_{x_3=h}} \left( -\frac{1}{h} \widetilde{u_3 u_1} - \frac{\partial \widetilde{p}}{\partial x_1} + \frac{\nu}{h} \left[ \frac{\partial \widetilde{u_1}}{\partial x_3} - u'_0 \right] \right)_{x_3=h}$$



# Fluctuating virtual-wall BC

$$\widetilde{u}_1^+(x_1, x_2, h_0, t) = F(h_0^+) = h_0^+, \quad h_0^+ \leq 10$$



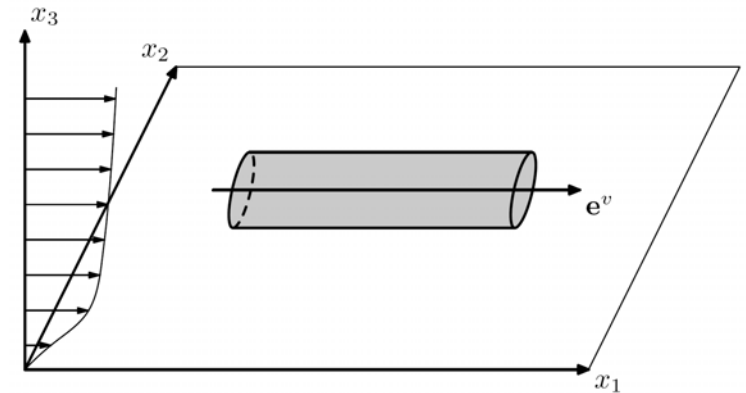
# Extended stretched-vortex SGS model

## LES decomposition

$$u_i(\mathbf{x}, t) = \widetilde{U}_i(\mathbf{x}, t) + U_i(\mathbf{x}, t)$$

## Dynamic alignment of subgrid vortices

$$\frac{\partial e_i^v}{\partial t} = e_j^v \frac{\partial \widetilde{U}_i}{\partial x_j} - e_i^v e_k^v e_j^v \frac{\partial \widetilde{U}_k}{\partial x_j}$$



## Additional stresses from subgrid stretched-vortex wrapping axial velocity.

Pullin, D. I. & Lundgren, T. S. 2001 Axial motion and scalar transport in stretched spiral vortices. Phys. Fluids 13 (9), 2553-2563.

$$\begin{aligned} T_{ij} &= \widetilde{U}_i \widetilde{U}_j + \widetilde{U}_i \widetilde{U}_j + \widetilde{U}_i \widetilde{U}_j \\ &= K (\delta_{ij} - e_i^v e_j^v) - \gamma \frac{1}{2} \Delta_c K^{1/2} \left( e_j^v e_k^v \frac{\partial \widetilde{U}_k}{\partial x_l} (\delta_{li} - e_l^v e_i^v) + e_i^v e_k^v \frac{\partial \widetilde{U}_k}{\partial x_l} (\delta_{lj} - e_l^v e_j^v) \right) \end{aligned}$$

$$(e_1^v, e_2^v, e_3^v) = (1, 0, 0) \quad \Rightarrow \quad T_{13} = -\gamma \frac{1}{2} \Delta_c K^{1/2} \frac{\partial \widetilde{U}_1}{\partial x_3}$$



# LES coupled to wall closure

- 1) Time march local shear stress equation.

$$\frac{\partial u'_0}{\partial t} = \frac{2 u'_0}{(\widetilde{u_1})_{x_3=h}} \left( -\frac{1}{h} \widetilde{u_3 u_1} - \frac{\partial \widetilde{p}}{\partial x_1} + \frac{\nu}{h} \left[ \frac{\partial \widetilde{u_1}}{\partial x_3} - u'_0 \right] \right)_{x_3=h}$$

- 2) Obtain fluctuating slip BC from shear stress.

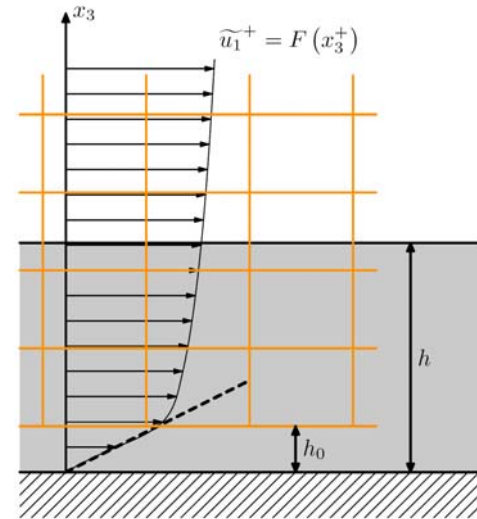
$$\widetilde{u_1}^+ (x_1, x_2, h_0, t) = F(h_0^+) = h_0^+, \quad h_0^+ \leq 10$$

- 3) Time march filtered N-S with extended SGS model.

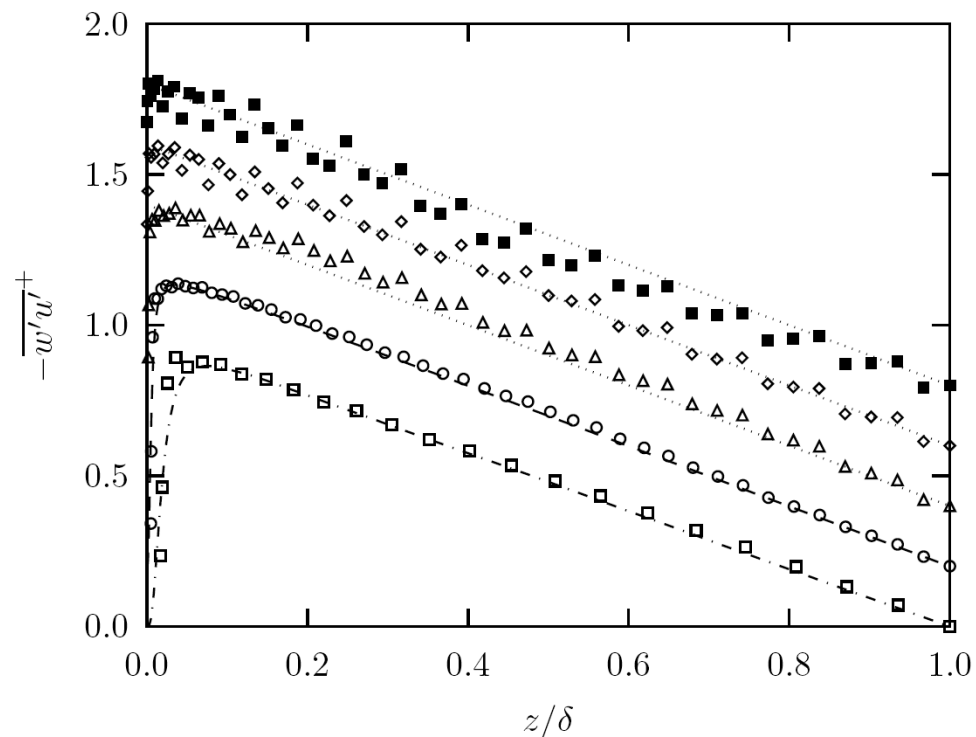
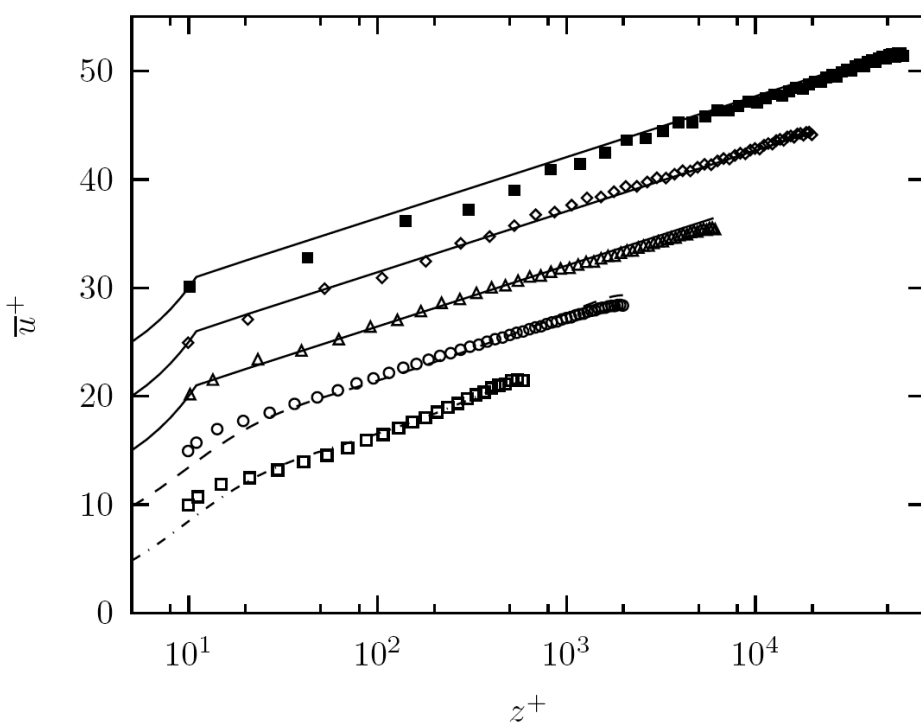
$$\begin{aligned} T_{ij} &= \widetilde{U_i U_j} + \widetilde{U_i \widetilde{U_j}} + \widetilde{\widetilde{U_i} U_j} \\ &= K (\delta_{ij} - e_i^v e_j^v) - \gamma \frac{1}{2} \Delta_c K^{1/2} \left( e_j^v e_k^v \frac{\partial \widetilde{U_k}}{\partial x_l} (\delta_{li} - e_l^v e_i^v) + e_i^v e_k^v \frac{\partial \widetilde{U_k}}{\partial x_l} (\delta_{lj} - e_l^v e_j^v) \right) \end{aligned}$$

- 4) Time march dynamic subgrid vortex alignment model.

$$\frac{\partial e_i^v}{\partial t} = e_j^v \frac{\partial \widetilde{U_i}}{\partial x_j} - e_i^v e_k^v e_j^v \frac{\partial \widetilde{U_k}}{\partial x_j}$$



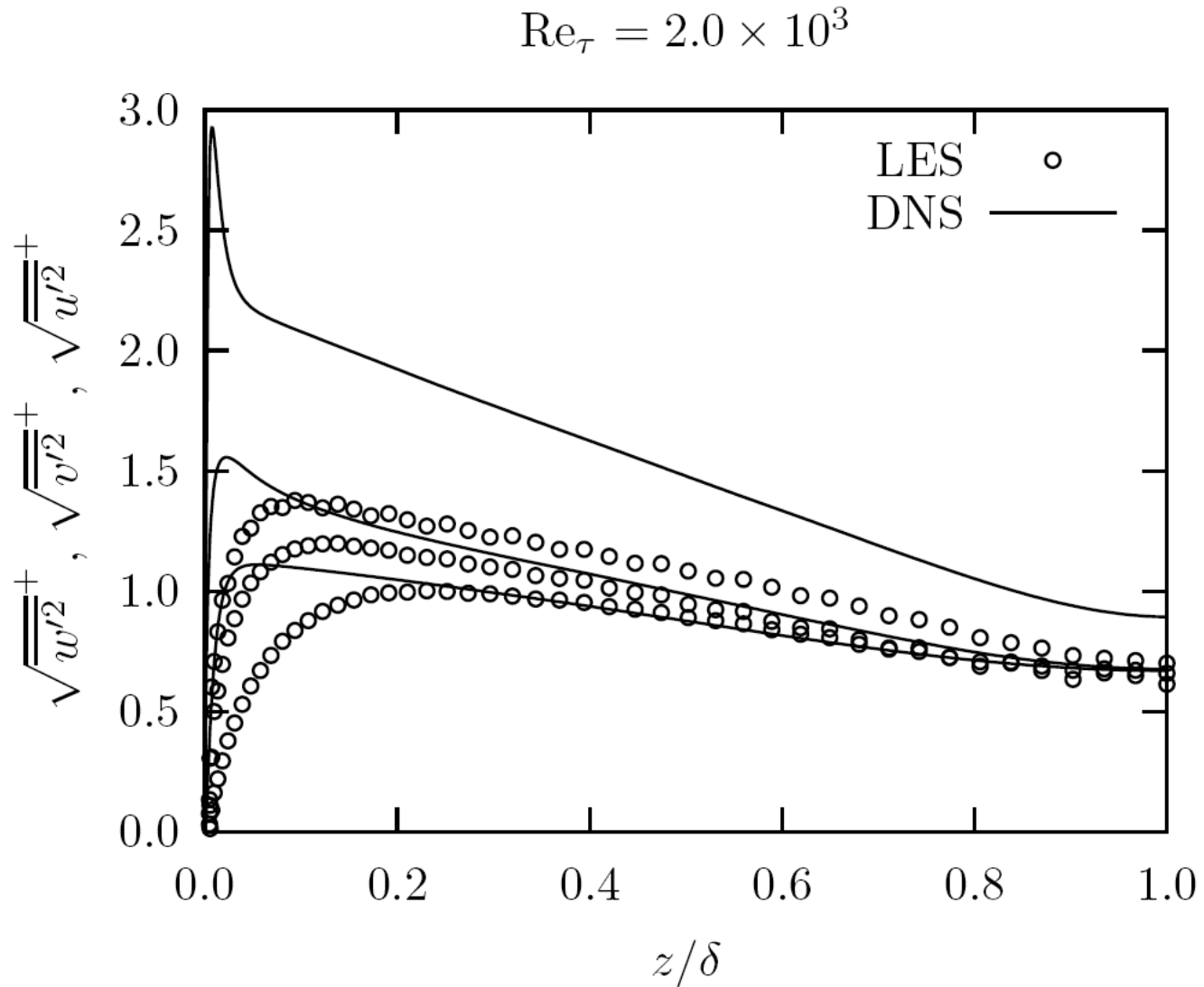
# Results ( $Re_{\tau} = 600$ to $60k$ )



	$Re_{\tau} = u_{\tau}\delta/\nu$	$Re = u_{CL}\delta/\nu$		$N_1 \times N_2 \times N_3$	$L_1 \times L_2$
—			$\log(z^+)/0.41 + 5.2$		
.....			$1 - z/\delta$		
— · —	$5.9 \times 10^2$	$1.2 \times 10^4$	DNS (Moser <i>et al.</i> 1999)	$384 \times 384 \times 257$	$2\pi\delta \times \pi\delta$
---	$2.0 \times 10^3$	$4.9 \times 10^4$	DNS (Hoyas & Jiménez 2006)	$6144 \times 4608 \times 633$	$8\pi\delta \times 3\pi\delta$
□	$5.9 \times 10^2$	$1.2 \times 10^4$	LES	$32 \times 32 \times 33$	$8\pi\delta \times 3\pi\delta$
○	$2.0 \times 10^3$	$4.9 \times 10^4$	LES	$64 \times 64 \times 65$	$8\pi\delta \times 3\pi\delta$
△	$6.0 \times 10^3$	$1.6 \times 10^5$	LES	$64 \times 64 \times 65$	$8\pi\delta \times 3\pi\delta$
◇	$2.0 \times 10^4$	$5.9 \times 10^5$	LES	$64 \times 64 \times 65$	$8\pi\delta \times 3\pi\delta$
■	$6.0 \times 10^4$	$1.9 \times 10^6$	LES	$64 \times 64 \times 65$	$8\pi\delta \times 3\pi\delta$



# Reynolds stresses



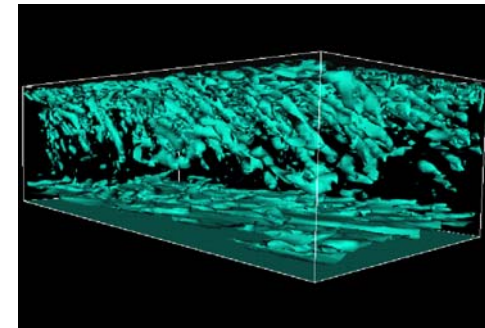
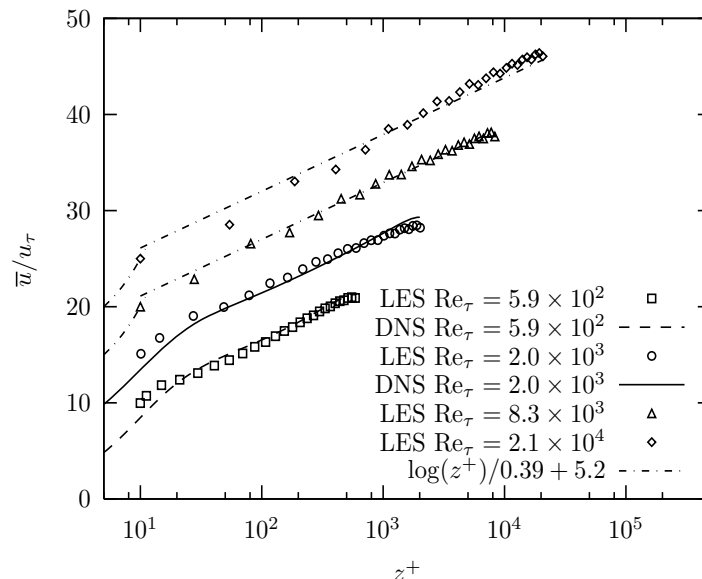
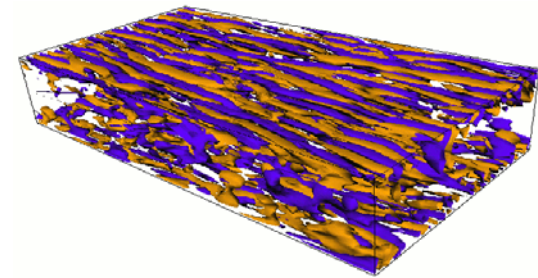
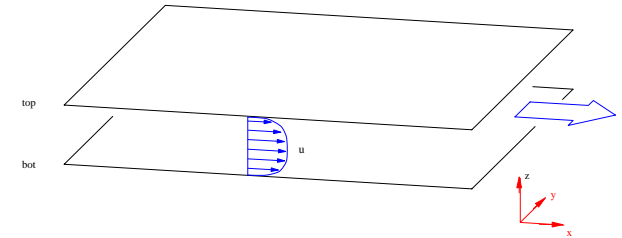
# Future work

- Higher Reynolds number.
- Dynamic gamma from structure function matching.
- Application to flow over airfoil.
- Two-vortex SGS model to improve Reynolds stresses.
- Plug for related presentation:



# LES of turbulent channel flow; virtual wall model

- LES of turbulent channel flow
- Turbulent flow between two parallel plates driven by pressure gradient
  - *Flow contains many features of complex wall-bounded flows*
  - *Viscous sublayer, stream-wise vortices, log layer*
- Stringent test of SGS/LES model for wall-bounded turbulence
- SGS model must accurately model turbulent transport processes
- Near-wall LES; frontier problem in present research
- Special “virtual-wall” near-wall SGS model
- Allow LES of wall bounded flows at large  $Re_{\tau} = 20,000$ ;  $Re_U = 650,000$
- Comparison with DNS;
- $Re_{\tau} = 590$  (Moser et al, 1999)
- $Re_{\tau} = 2000$  (Hoyas et al, 2006)



# Summary

- LES methodology
  - *Two-component Favre-filtered Navier-Stokes equations*
  - *Stretched-vortex subgrid-scale (SGS) model; structure based*
- Computational method: hybrid WENO-TCD
  - *Shock capturing low numerical dissipation*
  - *Verification*
    - *Decaying compressible turbulence*
    - *Riemann 1D wave (Exact Euler)*
- Large-eddy simulation of Richtmyer-Meshkov instability with reshock
  - *RM instability in plane channel with end wall; Air-SF6*
  - *Modeled on experiments of Vetter & Sturtevant (1995)*
- Traditional Statistics
  - *Mixing-layer growth*
  - *Turbulence statistics, velocity, density & scalar spectra*
- “Multi-scale modeling”
  - *Subgrid continuation statistics; spectra and anisotropy*
  - *Scalar p.d.f.s, including subgrid contribution*
  - *Effect of Schmidt number*
- Adaptive Mesh Refinement (AMROC)
  - *Berger & Colella’s algorithm for conservation laws*
  - *Hierarchical data structure*
  - *WENO-TCD and stretched-vortex SGS model implemented*

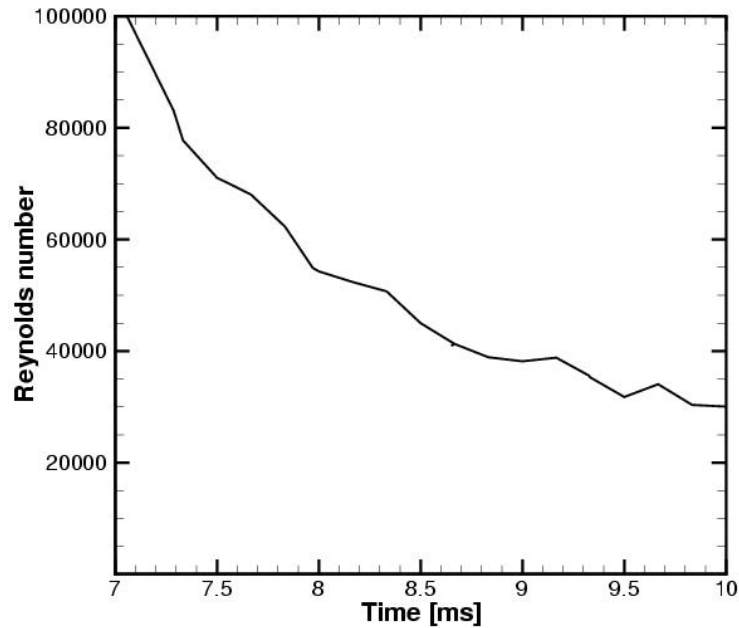


# Conclusions

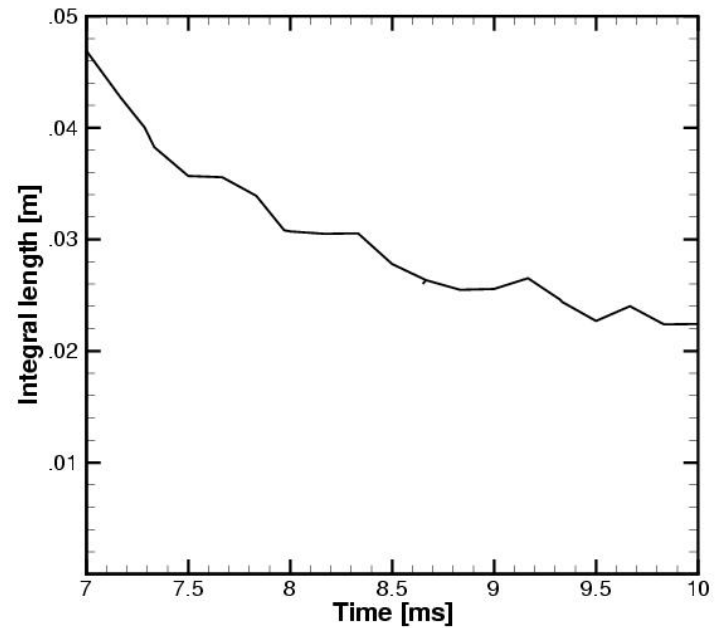
- Large-eddy simulation of plane Richtmyer-Meshkov instability with reshock
  - *Hybrid WENO-TCD scheme with SV SGS model*
  - *Air-SF<sub>6</sub>; modeled on experiments of Vetter & Sturtevant (1995)*
- Growth of mixing-layer width
  - *Initial linear growth of interface following first shock impact*
  - *Period of nonlinear bubble/spike growth*
  - *Reshock produces rapid transition to turbulent mixing layer*
  - *Strong mixing layer growth*
  - *Enhanced by interaction with reflected expansion*
  - *Eventual saturation of growth*
- Traditional Statistics
  - *Mixing-layer growth*
  - *turbulence statistics, velocity, density & scalar spectra*
- “Multi-scale modeling”
  - *SV SGS model provides basis for subgrid continuation statistics; spectra and anisotropy*
  - *Scalar p.d.f.s, including subgrid contribution*
  - *log-dependence of scalar p.d.f. on Schmidt number*



# Reynolds number and integral length



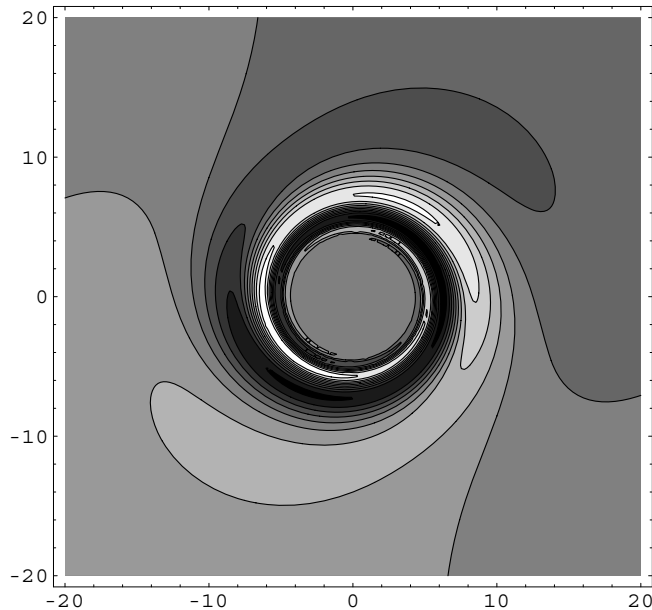
*Decay on Reynolds number*



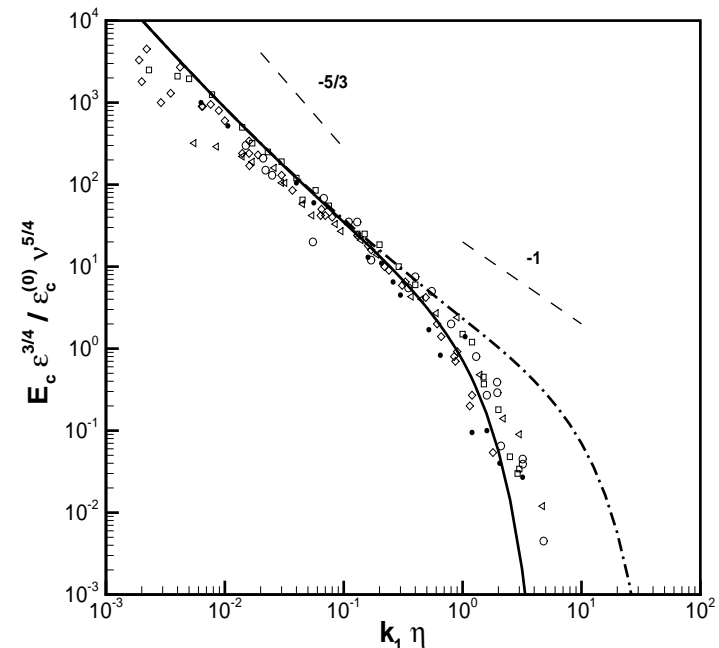
*Decay of integral length*



# Scalar spectrum from stretched-spiral vortex



Schematic showing winding of scalar field by 'subgrid vortex'.  
Contours of passive scalar



1-D scalar spectrum for homogeneous turbulence, Pullin & Lundgren (2001)

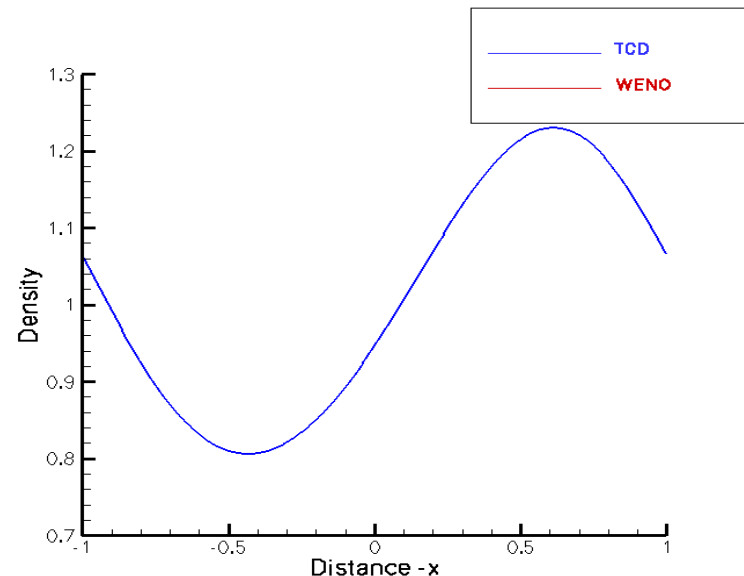
————  $Sc = 7$ , -----  $Sc = 700$ . Symbols, Data  
(Gibson & Schwarz 1963)



# Numerical algorithm (D. Hill, C. Pantano)

- WENO-TCD hybrid method (Hill & Pullin, JCP, 2004)
  - *Tuned-Centered Difference (TCD); away from shocks exploit smoothness of flow*
  - *Order of accuracy traded for minimization of one-step truncation error in LES equations (Ghosal, 1995)*
  - *5-point stencil -> 2-nd order accuracy*
  - *At shocks (only) revert to full WENO*
  - *Optimal WENO stencil matched to TCD stencil*
- Flux-based finite difference
  - *Naturally integrated in AMROC*
  - *Conservative, skew-symmetri*
- Skew-symmetric
  - *Energy conserving*
  - *Satisfies summation-by-parts*
- Tested in 1D, 2D, 3D
  - *Decaying compressible turbulence*
- No explicit filtering

*Riemann 1D Wave*  
*Exact solution of 1D Euler*



# Idea: Improve $K(k)$ for center-difference

- Finite-difference operator

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

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

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

- Tuned 5-point with parameter  $\alpha$

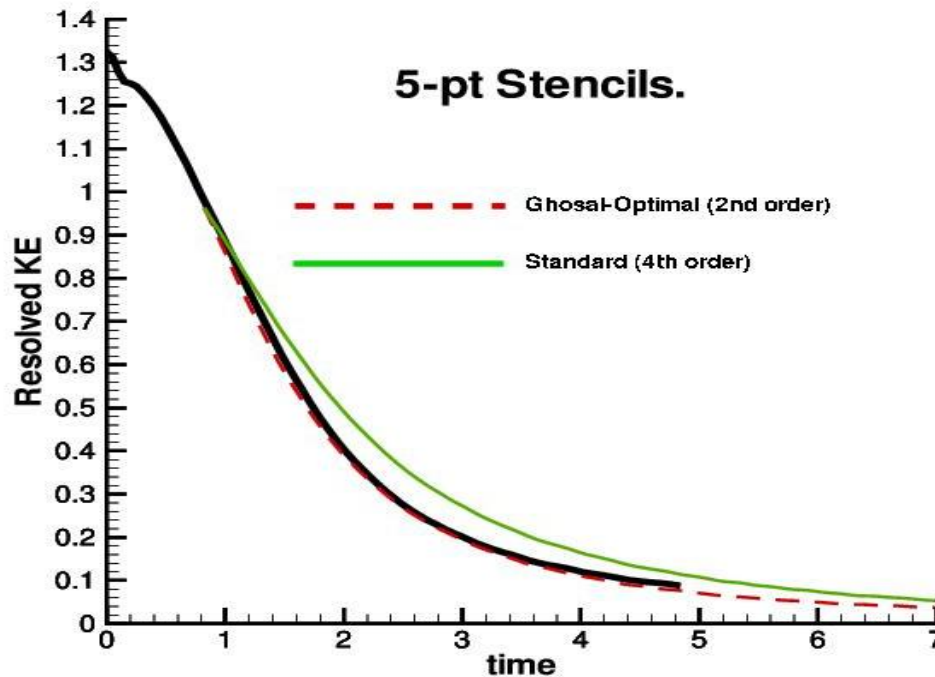
$$d_1 = \frac{1}{2} - 2\alpha, \quad d_2 = \alpha, \quad d_3 = 0, \quad \rightarrow 5 - pt, \quad 2^{nd} \text{ order}$$

- Tuned 7-point with parameter  $\alpha$

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



# Performance for LES of decaying turbulence



DNS and LES of Decaying compressible turbulence,  $M_t = 0.488$ ,  $R_\lambda = 70$ .

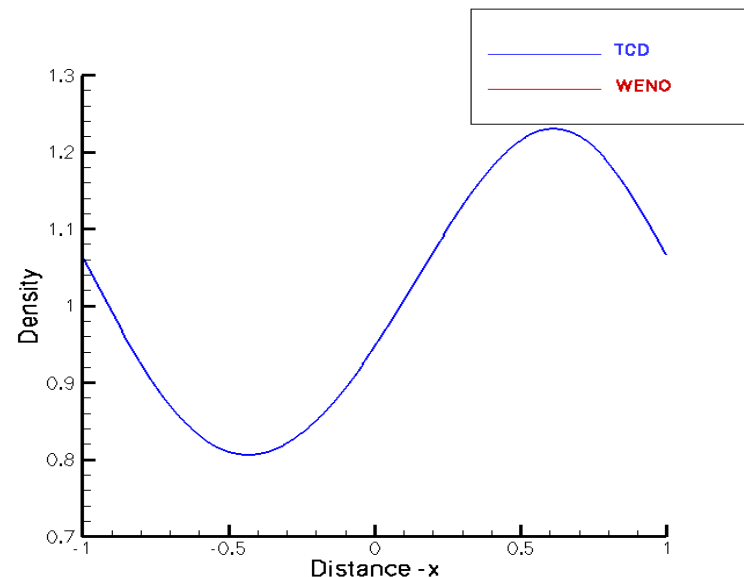
Decay of total TKE. Black;  $256^3$  DNS (10-th order Pade)



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*Riemann 1D Wave*  
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# Conservation and time adaptation

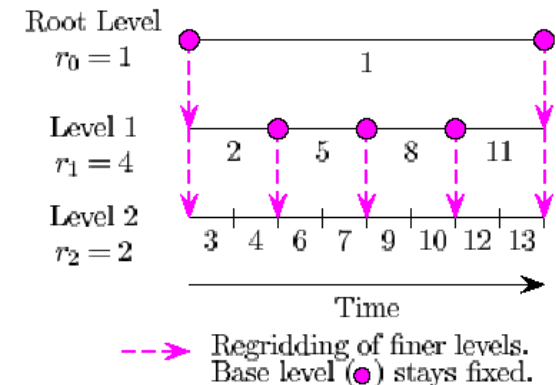
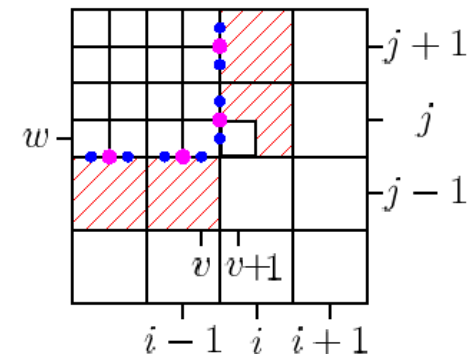
- Hanging nodes exist because cells at different levels are logically conforming
- A special correction, fixup, must be applied to satisfy global conservation
- Fluxes at coarse cells next to fine cells are replaced by the sum of those fluxes at the fine cells

$$\delta \mathbf{F}_{i-\frac{1}{2},j}^{1,l+1} := \delta \mathbf{F}_{i-\frac{1}{2},j}^{1,l+1} + \frac{1}{r_{l+1}^2} \sum_{m=0}^{r_{l+1}-1} \mathbf{F}_{v+\frac{1}{2},w+m}^{1,l+1}(t + \kappa \Delta t_{l+1})$$

- This correction impacts the spatial as well as temporal integration scheme

$$\tilde{Q}_{ij}^{n+1} := Q_{ij}^{n+1} + \frac{\Delta t_l}{\Delta x_{1,l}} \delta \mathbf{F}_{i-\frac{1}{2},j}^{1,l+1}$$

- Ghost cell values of fine patches are obtained by linear time interpolation from the coarse patch solution



# LES in the absence of strong shocks and density contacts

- The nonlinear term  $\frac{\partial}{\partial x_i}(\rho u_i u_j)$  is responsible primarily for the energy cascade
- The most successful Eulerian methods are global
  - *Spectral*
  - *High-Order Pade*
- Good response across all (*spectral*) or most (*Pade*) of the resolved scales, i.e. modified wavenumber

$$\mathbf{F}(\partial / \partial x) = ik$$

$$\mathbf{F}(D_x) = i\hat{K}(k)$$

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



# Conservation and time adaptation

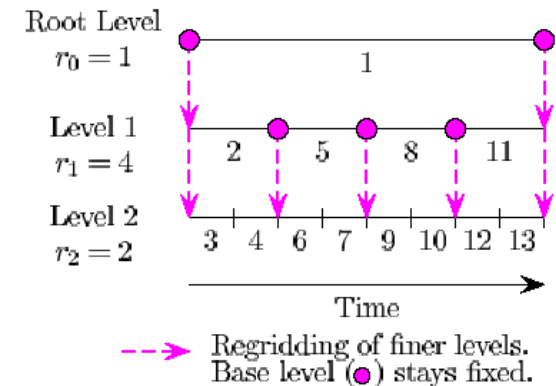
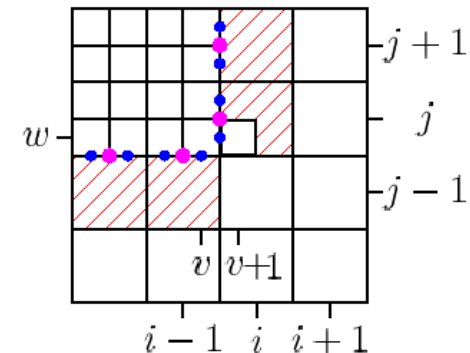
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$$d_1 = \frac{3}{4}, \quad d_2 = -\frac{1}{10}, \quad d_3 = -1/2, \quad \rightarrow 7 - pt, \quad 6^{th} \text{ order}$$

- Tuned 5-point with parameter  $\alpha$

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- Tuned 7-point with parameter  $\alpha$

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



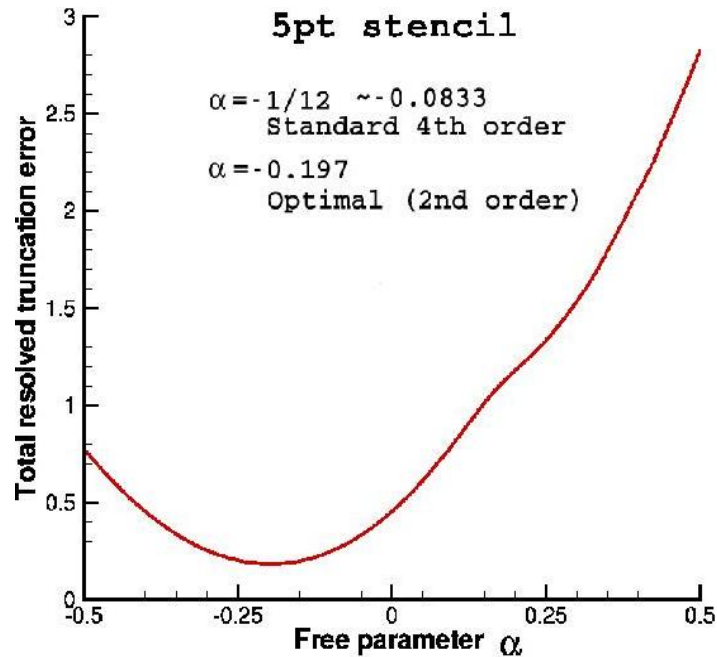
# Tuned Center-Difference Stencil (TCD)

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

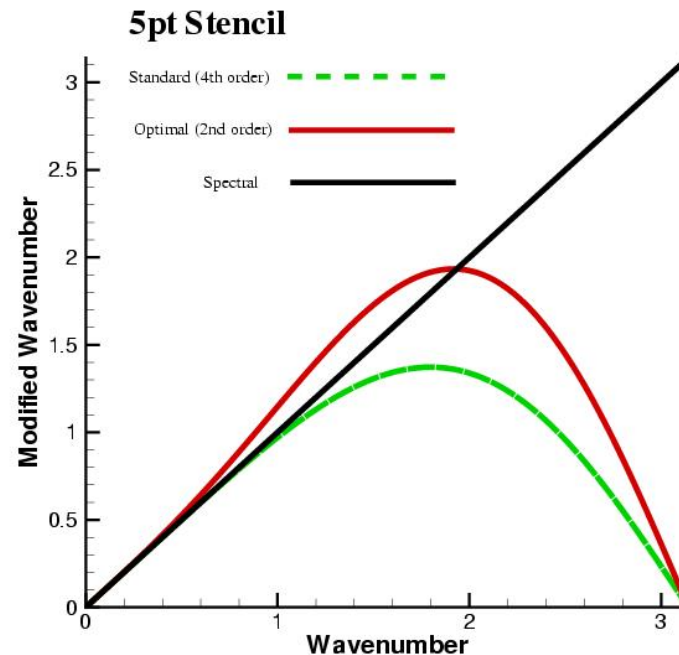
$$E_G(\alpha) = \int_0^{\frac{\pi}{\Delta x}} \mathcal{E}^{(FD)}(\kappa, \tilde{\kappa}(\kappa, \alpha)) d\kappa$$



## Optimized 5-point TCD stencil (second order)



Truncation error

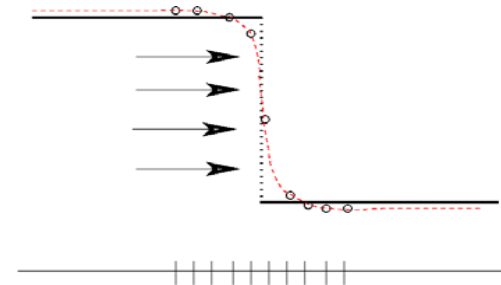


Modified wavenumber of  
minimal error stencil



# Shock capturing solvers; WENO

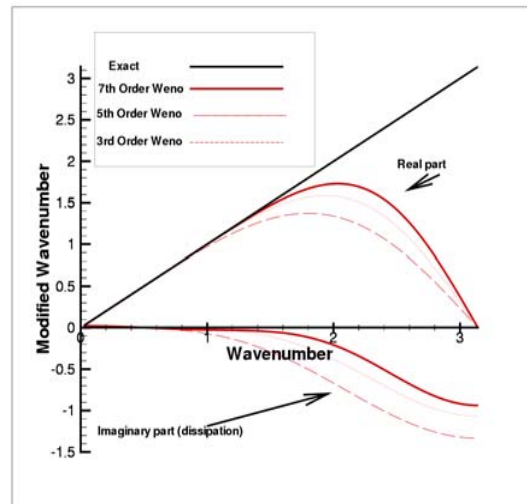
- True shocks have a thickness on the mean free path order
- The shocks are not resolved: Euler equations are solved in conservative form
- Euler solver shocks are 'captured', i.e. smeared across a few cells – first-order accurate at shocks



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

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

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



Weighted Essentially Non-Oscillatory (WENO) method (Osher)



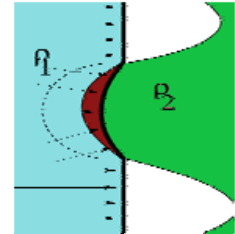
# Hybrid WENO-TCDS algorithm: LES and strong shocks (D. Hill)

- 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**

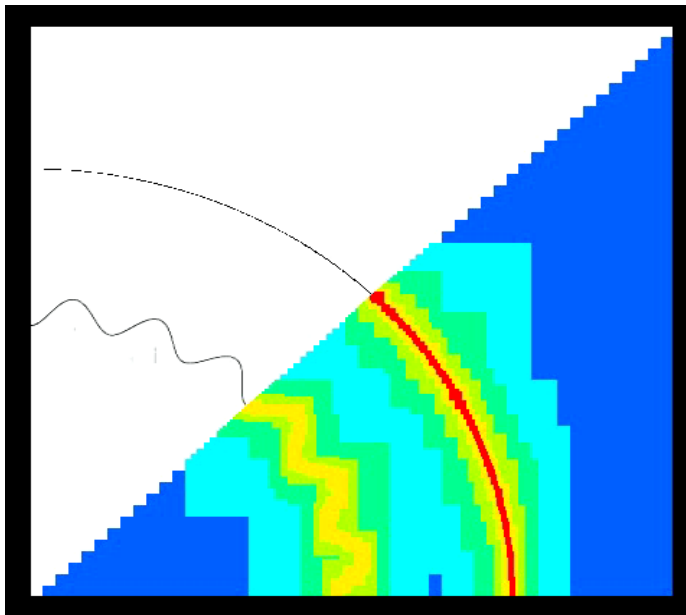


# Cylindrical RM instability with AMROC (R.Deiterding)

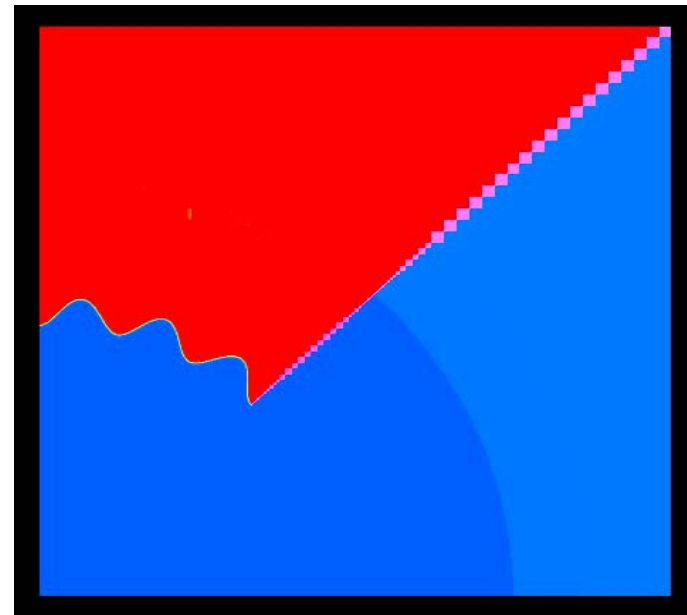
- AMROC – Adaptive Mesh Refinement engine
- Exploratory 2D Richtmyer-Meshkov instability with reshock in wedge geometry
- Passage of the shock results in vorticity deposition by means of baroclinic generation
- Canonical model of phase 2 experiments
- Incident shock modeled by Chisnell (1998) approximation to Guderley solution for similarity shock
- Euler simulation
- Initial density interface ; sinusoidal perturbation corresponding to  $n = 24$  on circle



Schlieren



Scalar



Refinement

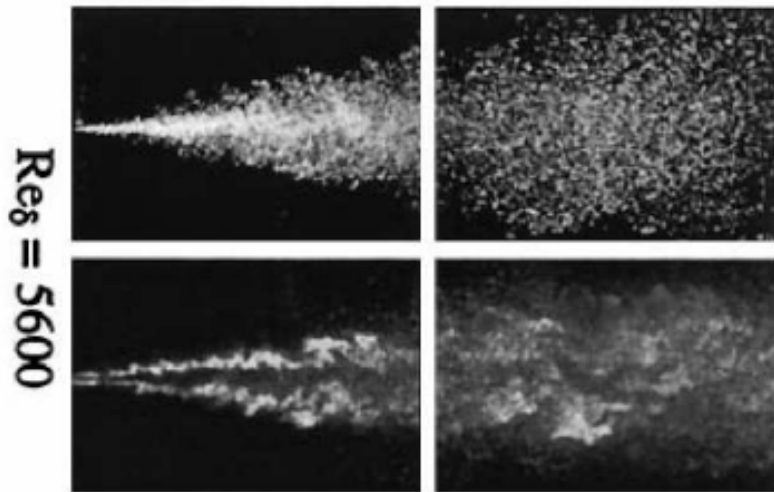
Pressure



# Reacting Hydrogen Jet flame (C. Pantano)

- Planar hydrogen jet flame of Rehm & Clemens (1999), Mach=0.28
- $5 \times 10^6$  grid cells and 4 levels of refinement
- 128 processors at LLNL ALC, 50,000 cpu/hours
- Cantera chemistry solver by D. Goodwin for flamelet model

experiment



simulation

