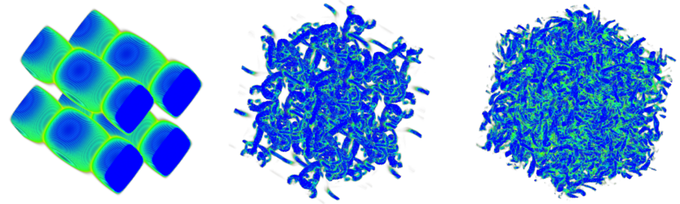
Simulations of Vortex Dynamics,Transition, and Material Mixing in Complex High-Re Flows

t* = 0 t* = 8.89 t* = 29.8



visualizations of λ_2

Fernando F. Grinstein
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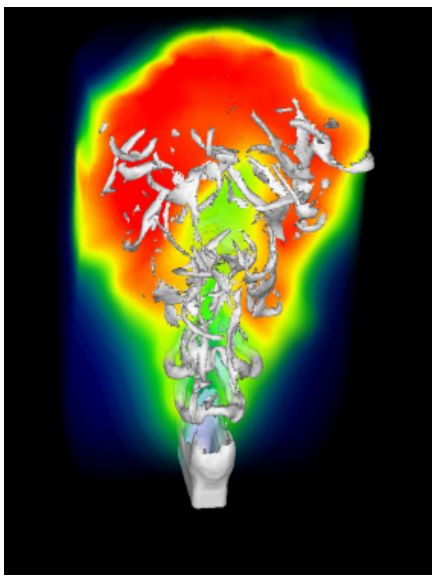

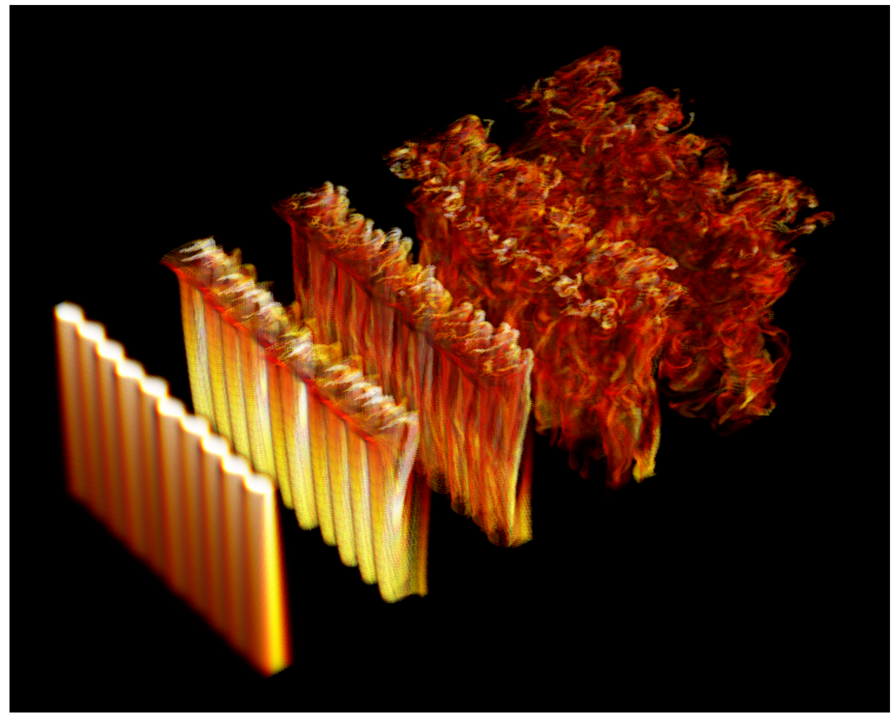

LANL LDRD-DR Program on “Turbulence by Design”
LANL LDRD-ER Program on “LES Modeling for Predictive Mixing

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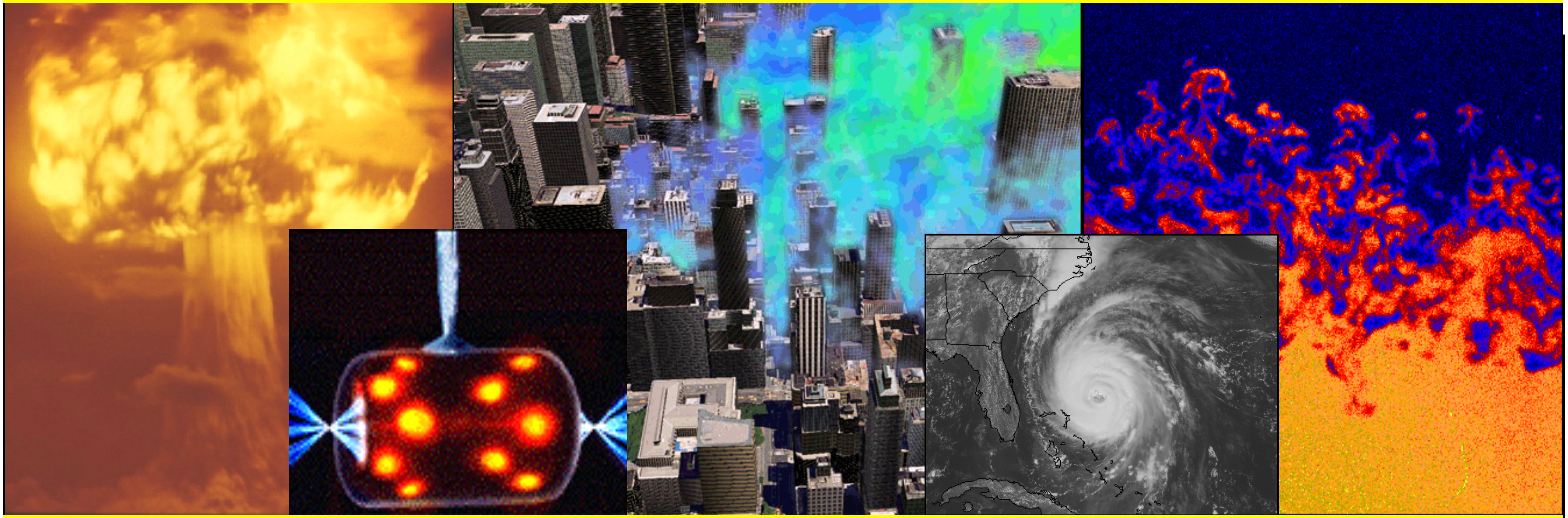
Invited Lecture at the “Workshop on “Models versus Physical Laws / First Principles, or Why Models Work ?”, Wolfgang Pauli Institute, Vienna, February 2-5, 2011

Simulations Based Mixing Prediction in Extremes Conditions

threat reduction, geophysics, inertial confinement fusion, climate modeling, weapons science, astrophysics, …



- **Unavoidably Under-Resolved due to Inherent Complexities**
- **Verification, Validation, and Uncertainty Quantification (VVUQ) Issues**

Simulations are based on augmented Navier-Stokes equations:

3) **Direct Numerical Simulation** (***"resolves all"*** relevant space / time scales)

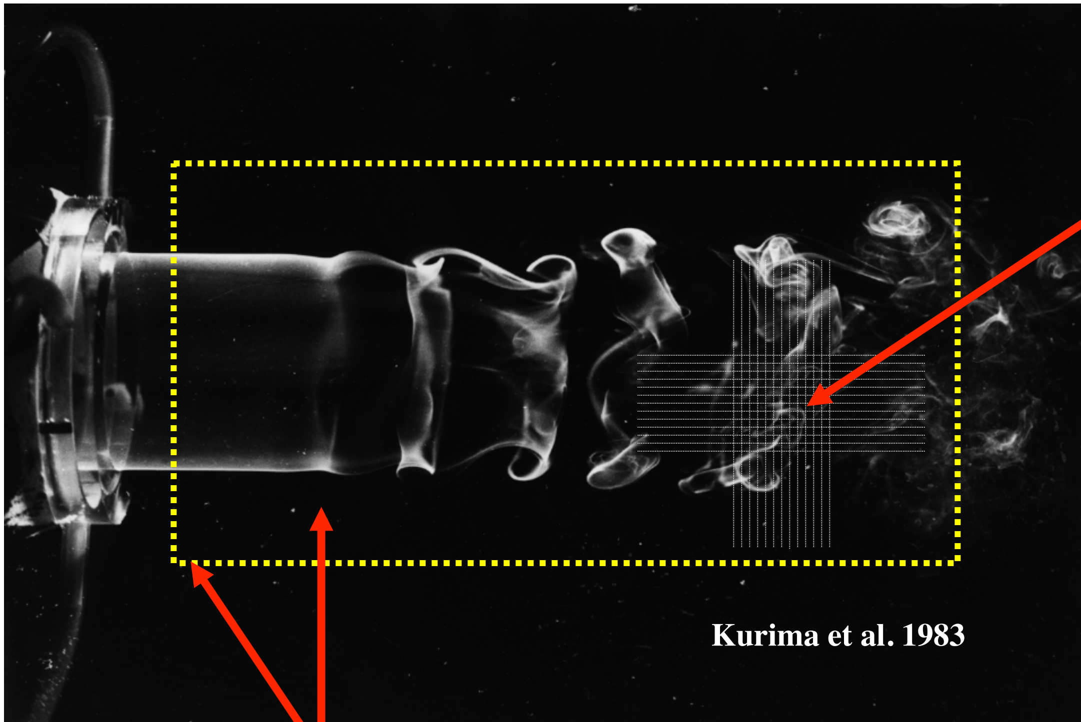
2) **Coarse Grained Simulation** (resolves ***large eddies*** + subgrid scale models)

1) **Moment-Closures / Reynolds Averaged NS** (resolve ***mean quantities***)

cost

Intrusiveness of Flow Experiments

- **Characterization (and Modeling) of Flow Conditions**
- **Uncertainty Quantification (UQ) in V&V Metrics**



Subgrid

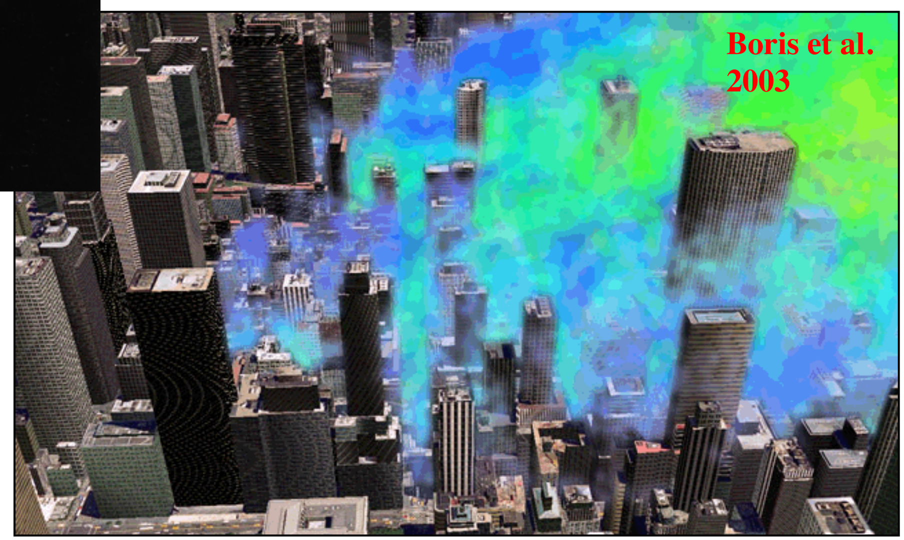
within a computational cell (or CGS filter-length)

within instrumentation size (e.g., hotwire cross-section)

Supergrid

Initial Conditions (ICs) and Boundary Conditions (BCs)

turbulent flow remembers its ICs
(e.g., George & Davidson 2004)



intertwined subgrid & supergrid issues at material interfaces

Coarse Grained Simulations (LES, ILES / MILES): why (and when) do they work ?

CGS: Background & Basis

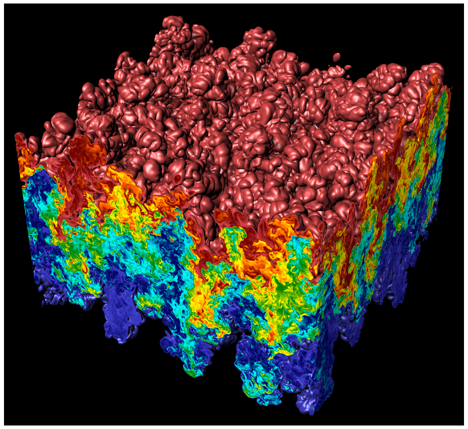
- Vortex dynamics: Inhomogeneous flows
  jets and channel flow
- Transition and Decay: Taylor-Green vortex
- Material mixing
  material interface characterization & modeling
  shock-driven turbulence

Outlook

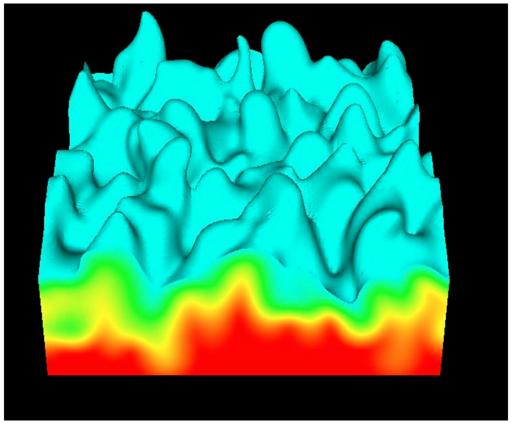
Instantaneous, Filtered, Ensemble Averaged, DNS, Coarse Grained Solutions, Moment closures

- **Direct Numerical Simulation:** resolve all ***relevant*** space / time scales
- **Moments methods:** ensemble - averages over many realizations within some constraint on initial and boundary conditions.
- **CGS** (LES, ILES / MILES): spatial filtering or averaging with either closure for effects of small scales or designed numerical dissipation.

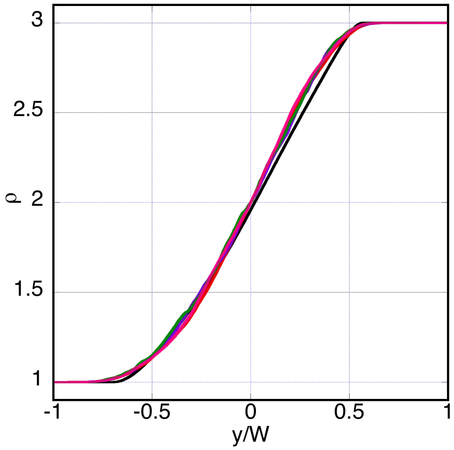
  depends on explicit or implicit filter-length (typically grid size)
- **COST:** DNS > CGS >> moment closures



DNS : 3D



CGS (LES, ILES) : 3D



Moment closures for applications (e.g., BHR): 1D

CGS for Turbulent Flow & Mix Prediction
Example: Incompressible flow & scalar mixing

CGS (LES) Ingredients

- **Low-pass filter**
- **Discretization (Finite Volume preferred …)**

$$\bar{f}(\mathbf{x}_P) = \frac{1}{\delta V_P} \int_{\Omega_P} f(\mathbf{x}')G(\mathbf{x}' - \mathbf{x}_P, \Delta)\,dV'$$

Modified Equation Analysis (satisfied by computed solutions)

$$\partial_t(\overline{\mathbf{v}}) + \nabla\cdot(\overline{\mathbf{v}}\otimes\overline{\mathbf{v}}) + \nabla\,\overline{p} - \nu\nabla\cdot\overline{\mathbf{S}} = -\nabla\cdot\mathbf{T}_{\mathbf{v}} + \nabla\cdot\boldsymbol{\tau}_{\mathbf{v}} + \mathbf{m}_{\mathbf{v}}$$

$Sc=\nu/\kappa$

$$\partial_t(\overline{\theta}) + \nabla\cdot(\overline{\theta}\,\overline{\mathbf{v}}) - \kappa\nabla^2\overline{\theta} = -\nabla\cdot\mathbf{T}_{\theta} + \nabla\cdot\boldsymbol{\tau}_{\theta} + \mathbf{m}_{\theta}$$

truncation and commutation "error" terms

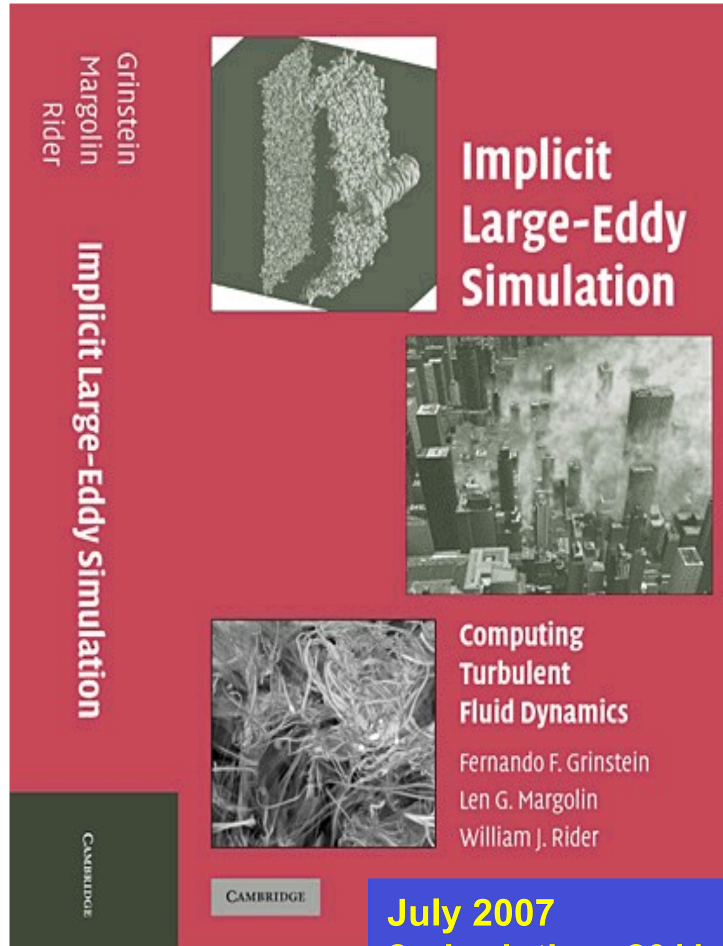
explicitly modeled in LES

"well resolved" LES requires : $\nabla\cdot\boldsymbol{\tau} << \nabla\cdot\mathbf{T} + \mathbf{m}$

- **Ghosal '96 -- *Models and* "errors"are *comparable* in *typical LES***
  --> motivates Implicit LES (ILES, MILES)

Coarse Grained Simulation
based on Euler, N-S, or augmented N-S, …

- **Resolve energy containing large scale physics**
- **Model subgrid scales**
  - **no universal theory**
  - **no exact solutions**
  - **pragmatic practice**



July 2007
2nd printing: 2011

Classical LES:

explicit subgrid models (eddy-viscosity, …, mixed, …)

Numerical LES (NLES):

relies on subgrid models implicitly provided by the numerics

Implicit LES (ILES, MILES):
(a very specific NLES !)

relies on non-oscillatory finite-volume numerics (FCT, PPM, Godunov, …)
--> Boris, Youngs, … ILES Book '07

Implicit Large Eddy Simulation

ILES, MILES --> is not free lunch !

$$\partial(\bar{\mathbf{v}}) + \nabla\cdot(\bar{\mathbf{v}}\otimes\bar{\mathbf{v}}) + \nabla\bar{p} - \nabla\cdot\bar{\mathbf{S}} = -\cancel{\nabla\cdot\mathbf{T}} + \nabla\cdot\boldsymbol{\tau} + \cancel{\mathbf{m}}$$

$$\boxed{\mathbf{T} = \overline{\mathbf{v}\otimes\mathbf{v}} - \bar{\mathbf{v}}\otimes\bar{\mathbf{v}}}$$

- **Finite Volumes ⇒ discretization "error" appears in div. form "∇.τ "**
- ***No explicit filtering:*** no commutation error term "**m**",

FV discretization provides top-hat implicit filtering

$$\boxed{\bar{f}_P \equiv \frac{1}{\delta V_P}\int_{\Omega_P} f dV}$$

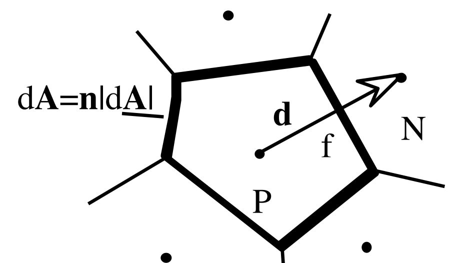
- **T=0:** ***minimal-choice -->*** **models convection driven physics**
(uses Non-Oscillatory FV numerics: FCT, PPM, Godunov, TVD, hybrid)

Depending on Re, Sc, Da…, additional models and / or numerics are needed with ILES (or any LES !) **to address**
near-wall flow, material mixing, combustion, …

MEA Example: Flux-Limiting ILES vs. Classical LES

momentum equation, 2nd. order fluxes,
1st-order upwind / 2nd-order central

$$\mathbf{v}_f^C = \Gamma \mathbf{v}_f^{C,H} + (1-\Gamma)\mathbf{v}_f^{C,L}, \quad \Gamma = \Gamma(\mathbf{v},\mathbf{x},t)$$



$$\boxed{\chi = (1-\Gamma) \sim \alpha\,|\mathbf{d}|}$$

$$\partial_t(\rho\mathbf{v}) + \nabla\cdot(\rho\mathbf{v}\otimes\mathbf{v}) = -\nabla p + \nabla\cdot(\tfrac{1}{3}\mu(\nabla\cdot\mathbf{v})\mathbf{I} - \mu(\nabla\mathbf{v}+\nabla\mathbf{v}^T)) + \rho\mathbf{f}$$

$$\boxed{+\nabla\cdot\Big(\rho\big[\chi(\mathbf{v}\otimes\mathbf{d})\,(\nabla\mathbf{v})^T + \chi(\nabla\mathbf{v})(\mathbf{v}\otimes\mathbf{d})^T + \chi^2(\nabla\mathbf{v})\mathbf{d}\otimes(\nabla\mathbf{v})\mathbf{d}\big]\Big) + \ldots}$$

lead-order convective truncation

generalized eddy-viscosity — *anisotropic scale-similarity*

$$+\nabla\cdot\Big(\tfrac{1}{8}\rho\big[\mathbf{v}\otimes((\nabla^2\mathbf{v})(\mathbf{d}\otimes\mathbf{d})) + ((\nabla^2\mathbf{v})(\mathbf{d}\otimes\mathbf{d}))\otimes\mathbf{v}\big]\Big) + \ldots$$

Clark-type term due to 2nd order FV scheme

lead-order viscous truncation

$$+\nabla\cdot\Big(\tfrac{1}{24}\mu(\nabla^3\mathbf{v})(\mathbf{d}\otimes\mathbf{d})\Big) + \ldots$$

hyperviscosity

Grinstein & Fureby, JCP 2002, JFE 2007

Classical LES MEA for 2nd order central + explicit SGS model

lead truncation terms

$$\partial_t(\tilde{\rho}\bar{\mathbf{v}}) + \nabla\cdot(\tilde{\rho}\bar{\mathbf{v}}\otimes\bar{\mathbf{v}}) = -\nabla\bar{p} + \nabla\cdot(\tfrac{1}{3}\mu(\nabla\cdot\bar{\mathbf{v}})\mathbf{I} - \mu(\nabla\bar{\mathbf{v}}+\nabla\bar{\mathbf{v}}^T)) + \tilde{\rho}\mathbf{f}$$

$$\boxed{+\nabla\cdot(\mathbf{T})}$$

$$+\nabla\cdot\Big(\tfrac{1}{8}\tilde{\rho}\big[\bar{\mathbf{v}}\otimes((\nabla^2\bar{\mathbf{v}})(\mathbf{d}\otimes\mathbf{d})) + ((\nabla^2\bar{\mathbf{v}})(\mathbf{d}\otimes\mathbf{d}))\otimes\bar{\mathbf{v}}\big]\Big)$$

$$+\nabla\cdot\Big(\tfrac{1}{24}\mu(\nabla^3\bar{\mathbf{v}})(\mathbf{d}\otimes\mathbf{d})\Big) + \ldots$$

T~O(d^p), with 2/3<p<2 !

ILES Rationale: Connection with Finite-Scale Equations

Margolin & Rider, IJNMF ‘02; **Margolin, Rider, FFG**: JoT ’06; … Ristorcelli, Margolin & FFG ‘11

- **MEA of NFV approximations to Burgers and NS equations**
- **analytically derived finite scale (avgd. over V=L^3 & T) Burgers & NS eqs.**

$$
\begin{aligned}
\frac{\partial}{\partial t}\bar{c} + \bar{u}_j\,\bar{c}_{,j} &= \mathcal{D}\bar{c}_{jj} - L^2[\bar{u}_{j,k}\,\bar{c}_{,k}]_{,j} - T^2[\bar{u}_{j,t}\,\bar{c}_{,t}]_{,j} \\
\frac{\partial}{\partial t}\bar{u}_i + \bar{u}_j\,\bar{u}_{i,j} &= -\bar{p}_{,i} - L^2[\bar{u}_{j,k}\,\bar{u}_{i,k}]_{,j} - T^2[\bar{u}_{j,t}\,\bar{u}_{i,t}]_{,j} + \nu\bar{u}_{i,kk} \\
-\nabla^2\bar{p} &= \bar{u}_{j,i}\,\bar{u}_{i,j} + L^2\bar{u}_{j,ik}\,\bar{u}_{i,jk} + T^2\bar{u}_{j,ti}\,\bar{u}_{i,tj}\ .
\end{aligned}
$$

“… leading order truncation “errors” introduced by **non-oscillatory finite volume (NFV)** schemes represent physical flow regularization, providing necessary modifications to the governing equations that arise when the motion of **finite scale observables** is considered”.

Kinetic theory $\longrightarrow$ *integral* $\longrightarrow$ *Continuum NS eqs.*

NFV discretizations $\sim$ *Finite Scale eqs. for physical observables*

Coarse Grained Simulations (LES, ILES / MILES)
why (and when) do they work ?

CGS: Background & Basis

- **Inhomogeneous free & wall-bounded flows**

  jets, channel flow
- Transition & Decay: Taylor-Green vortex
- Material mixing: shock-driven turbulence

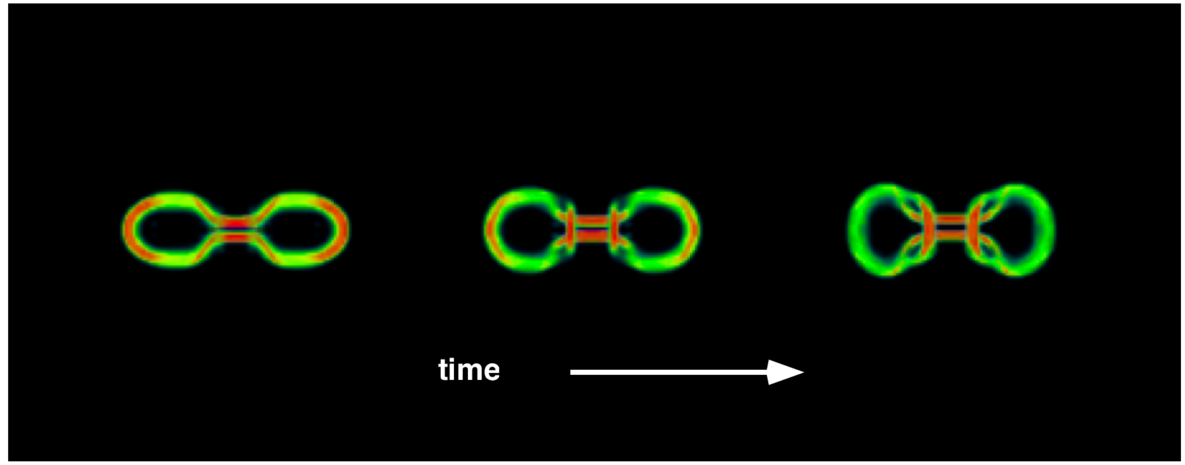
Outlook

ILES-FCT of M=0.6 Jet Vortex Dynamics

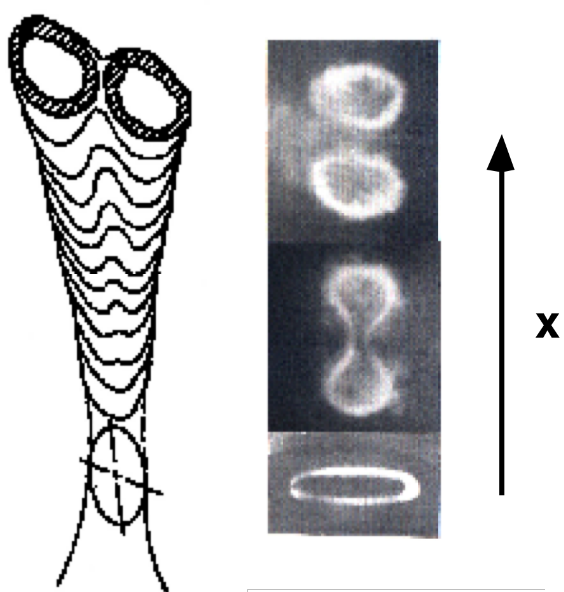
Axis-Switching, Reconnection, Bifurcation, and Transition

AR=4, simulated jet

FFG, Phys. Fluids (1995).



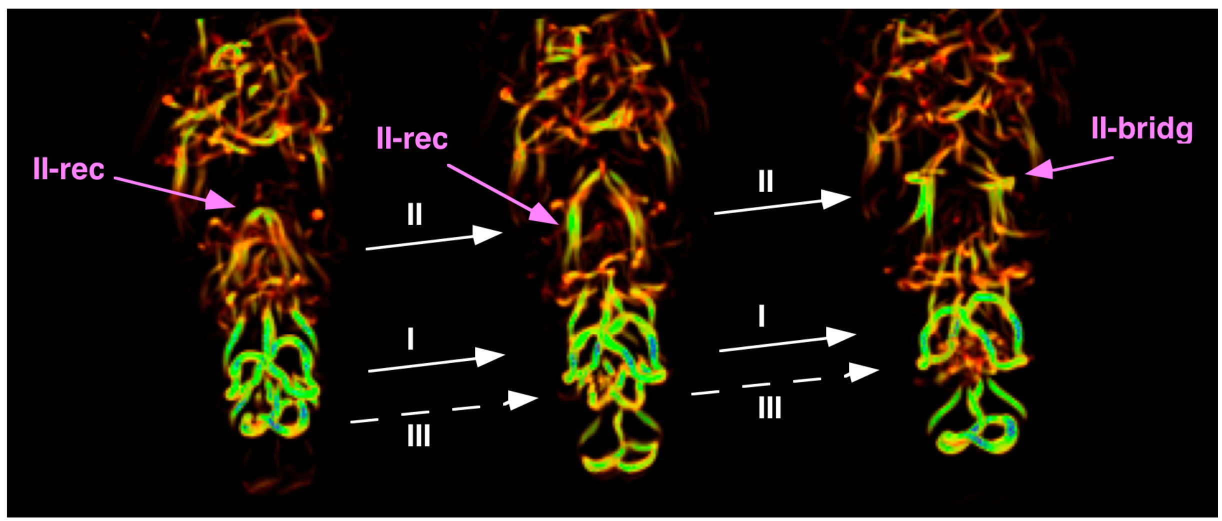
axis-switching
& bifurcation



AR=4, laboratory jet flow visualization
Hussain & Husain, JFM (1989).

Volume visualizations of λ_2

λ_2 = second-largest eigenvalue of $S^2 + \Omega^2$



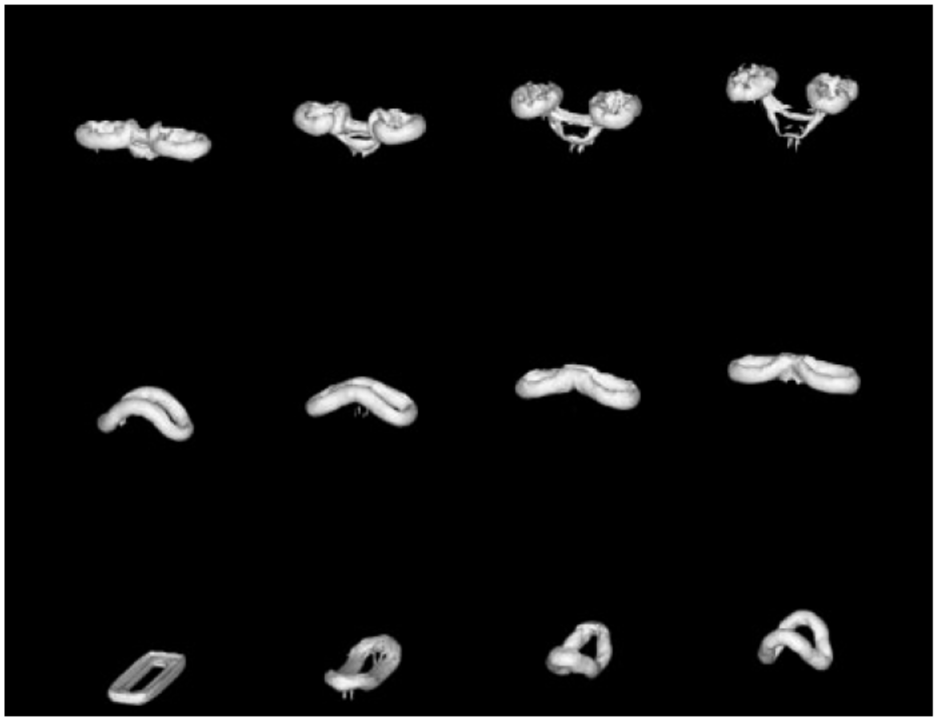
AR=3, simulated jet

FFG, J. Fluid Mechanics (2001).

FCT-based MILES of Rectangular Jets
with 2D⊗1D splitting (transverse ⊗ streamwise)

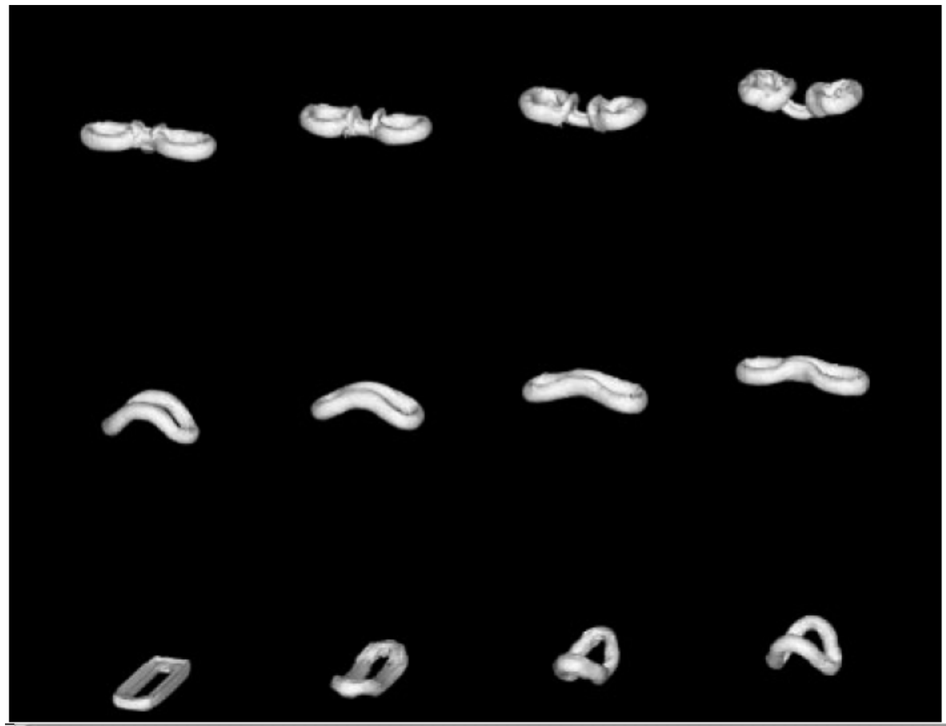
FFG, Fureby & DeVore, IJNMF 2005

positivity- but not monotonicity-preserving
(more effectively built-in backscatter …)



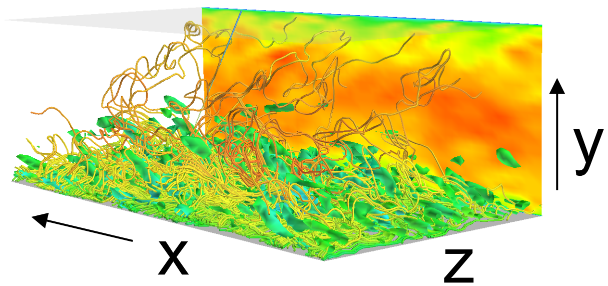
using Zalesak's 2D FCT limiter

with additional pre-limiting step enforcing local monotonicity in each direction



using DeVore's 2D FCT limiter

How much and what kind of backscatter is desirable ?
How much vortex dynamics detail should be captured ?
Need suitable well designed lab experiments & VVUQ metrics to decide …



Under-Resolved Near-Wall (Sc = ∞) Flow

robust *outer* flow **CGS**; ***mature VVUQ metrics***

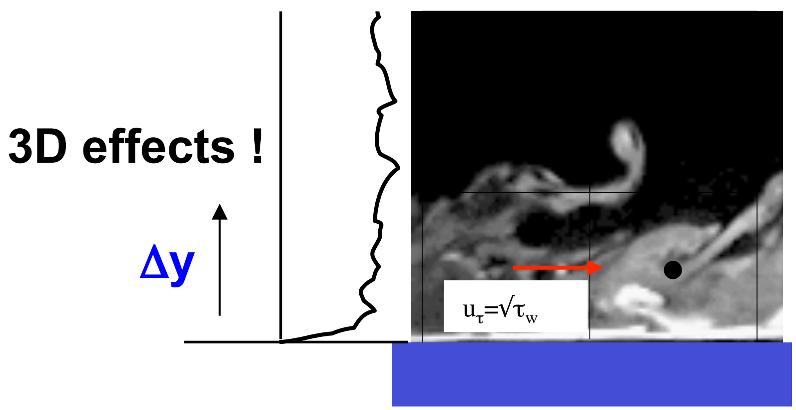
Developed Turbulent Channel Flow, Fureby et al. AIAA J. 2004

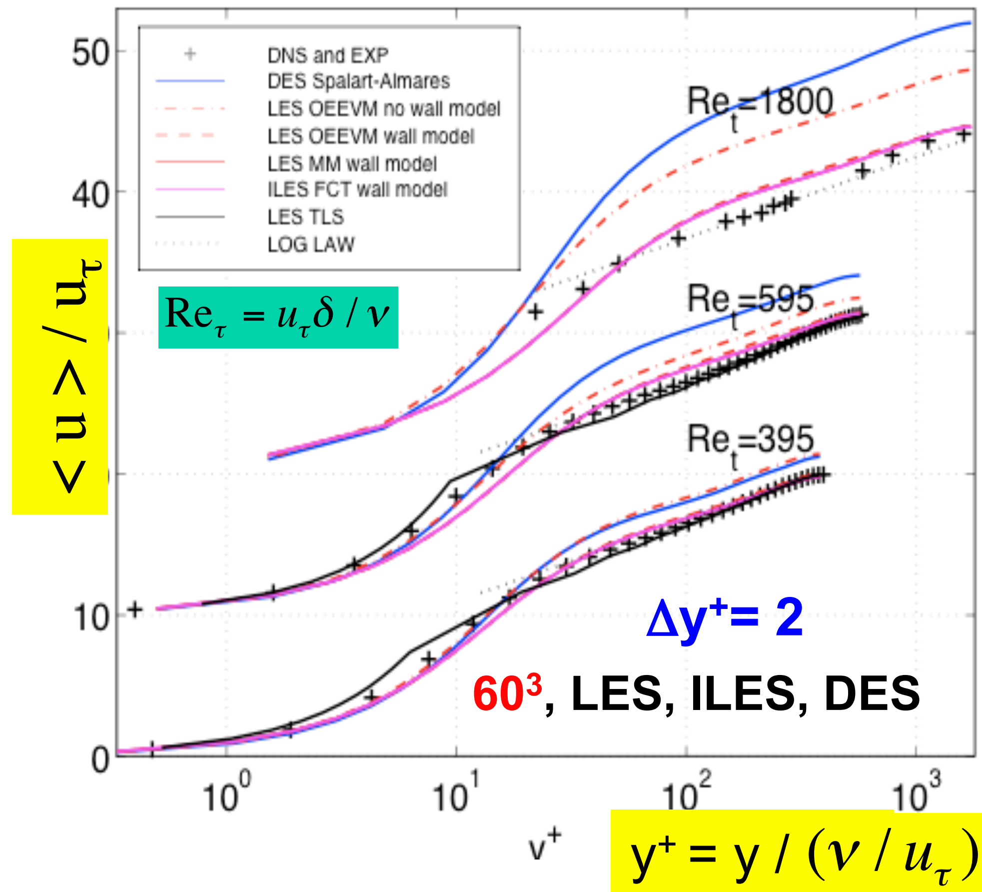
Prohibitive number of grid points to resolve near-wall dynamics

for DNS: ~ $(Re_\tau)^3$, $\Delta y^+ << 1$;

for LES: ~ $(Re_\tau)^2$, $\Delta y^+ < \sim 1$

+: scaled by viscous length scale





State-of-the-art strategies

- Hybrid RANS / LES (e.g., DES)
- Wall shear stress BC models, $\tau_w = \tau_w(\mathbf{v})$

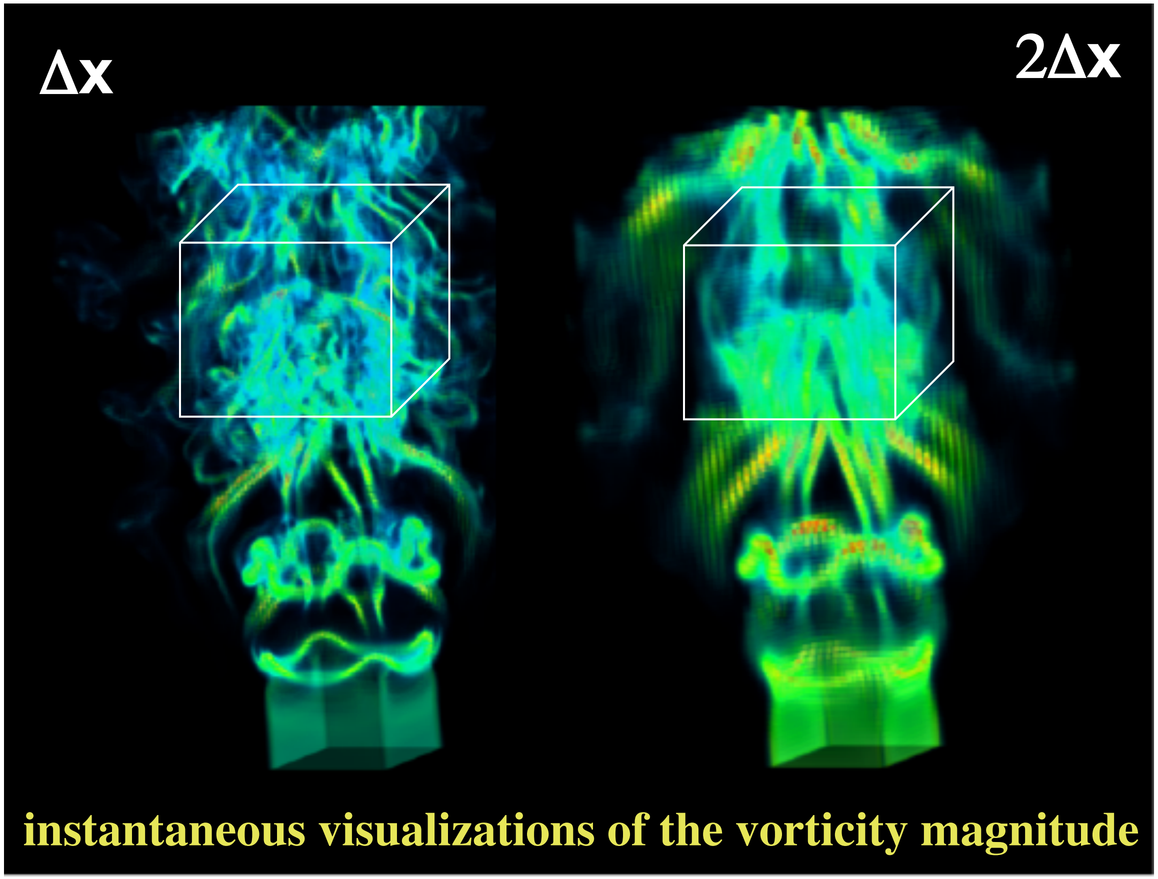
$u_\tau = \sqrt{\tau_w}$ = friction velocity

δ= boundary layer thickness

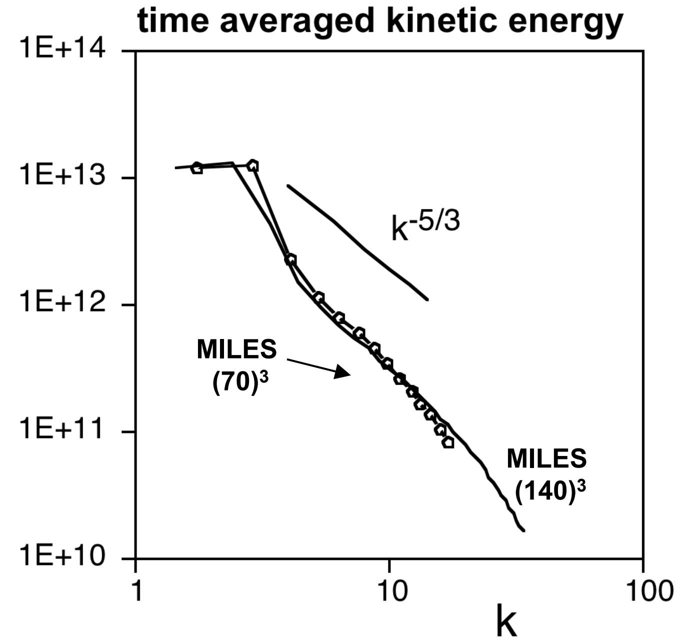
- Re = 395, 595, DNS by Moser et al. '95
- Re = 2030-50, expts. by Wei & Willmarth '89

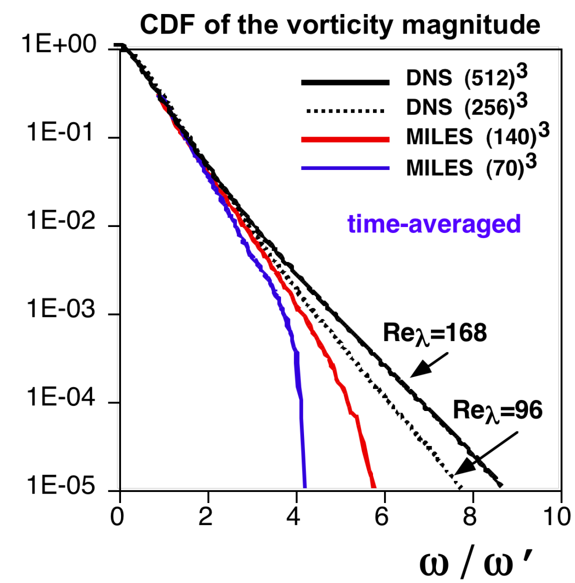
Coarse Grained Simulation "Convergence"

weakly forced jets, small-scale analysis



ILES by Grinstein & Devore PoF 1996, Grinstein JFM 2001;
DNS by Jimenez JFM 1993





Coarse Grained "observations" are affected by (explicit or implicit) filter-length cutoff …
--> must be incorporated in V&V metrics

Coarse Grained Simulations (LES, ILES / MILES)
why (and when) do they work ?

- CGS: Background & Basis
- Inhomogeneous free & wall-bounded flows
  - jets, channel flow
- **Transition & Decay: Taylor-Green vortex**
- Material mixing: shock-driven turbulence

Outlook

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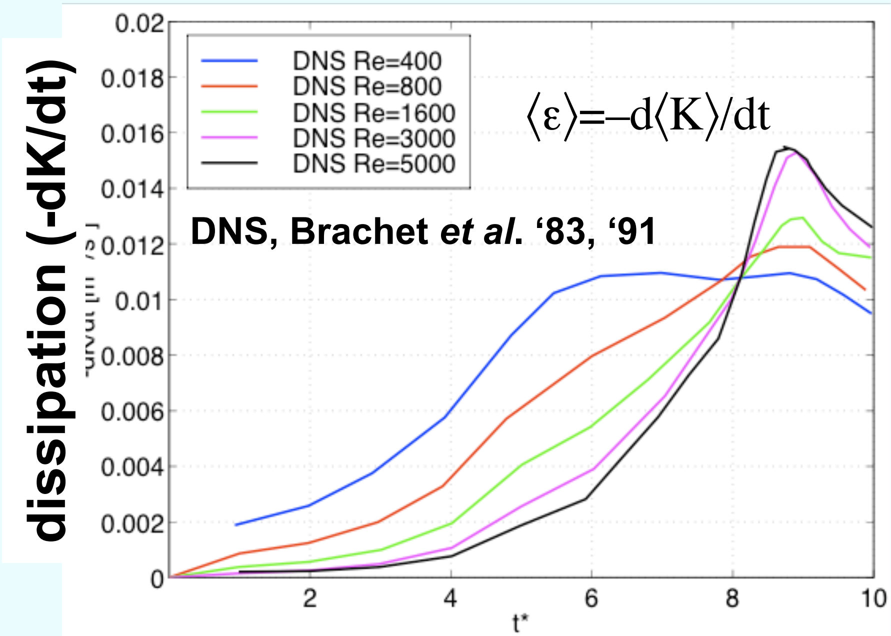
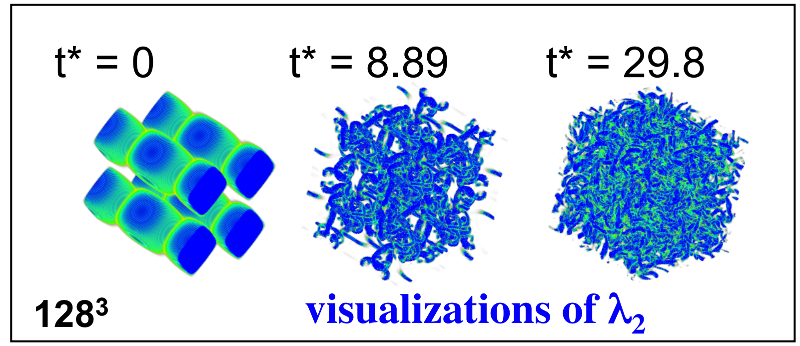
Taylor-Green Vortex

Simulations of Transition and Turbulence Decay

LES, ILES, DNS: Grinstein et al. JoT '07, **DNS,** Bracher *et al.* '83, '91

ILES effectively captures high-Re physics of transition and decay rates





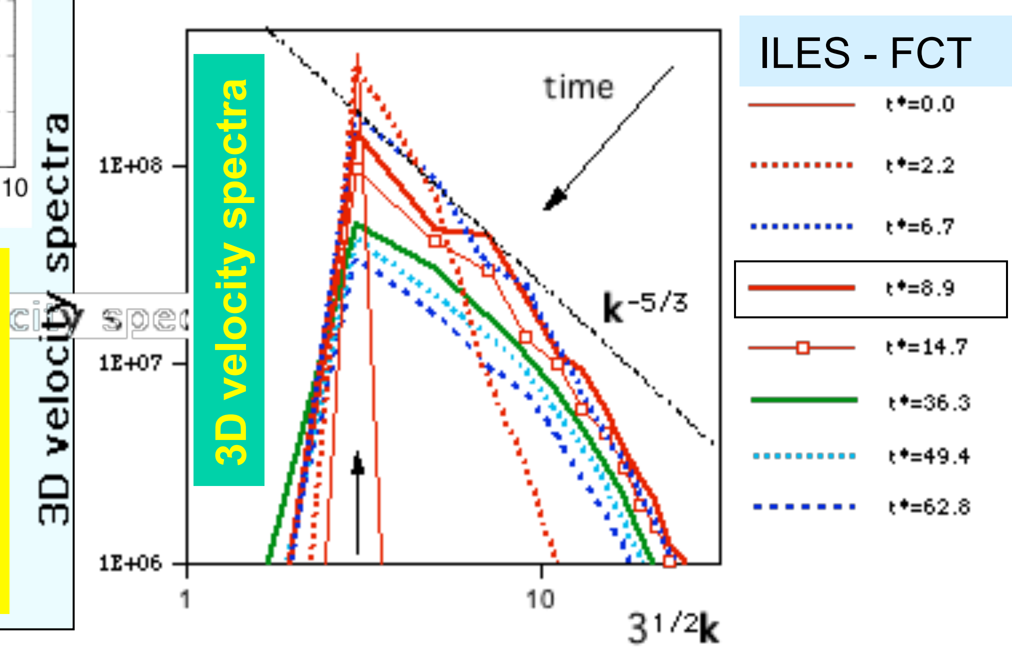
Robust dissipation peak at t*≈9

⇒ **onset of inviscid instability**

⇒ **viscosity independent limit**

⇒ **to be captured by CGS**

transition time, dissipation rate



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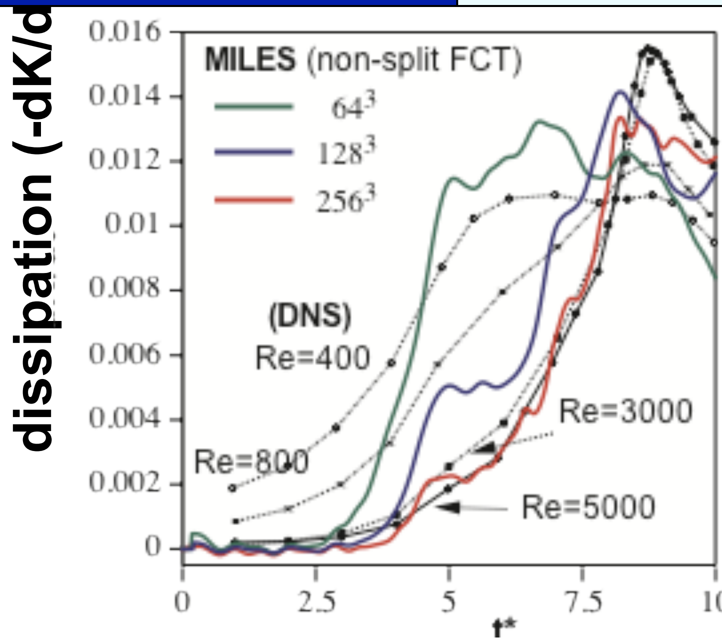
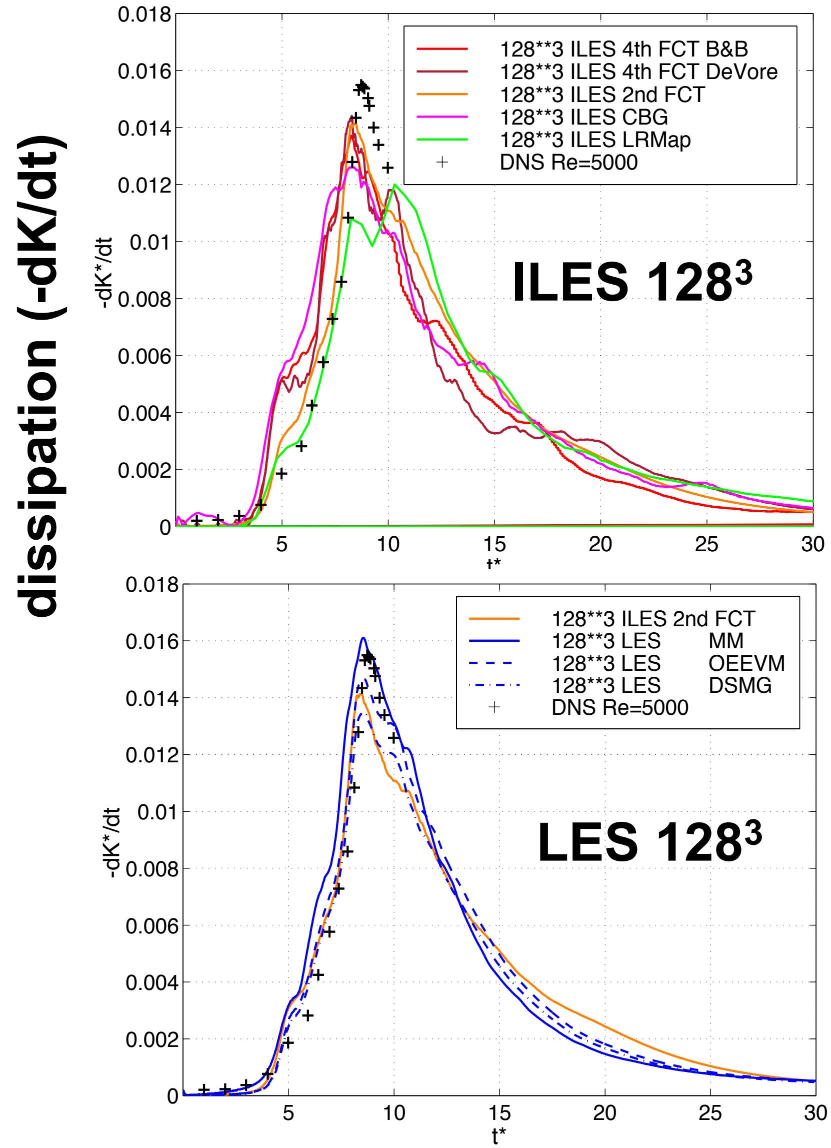
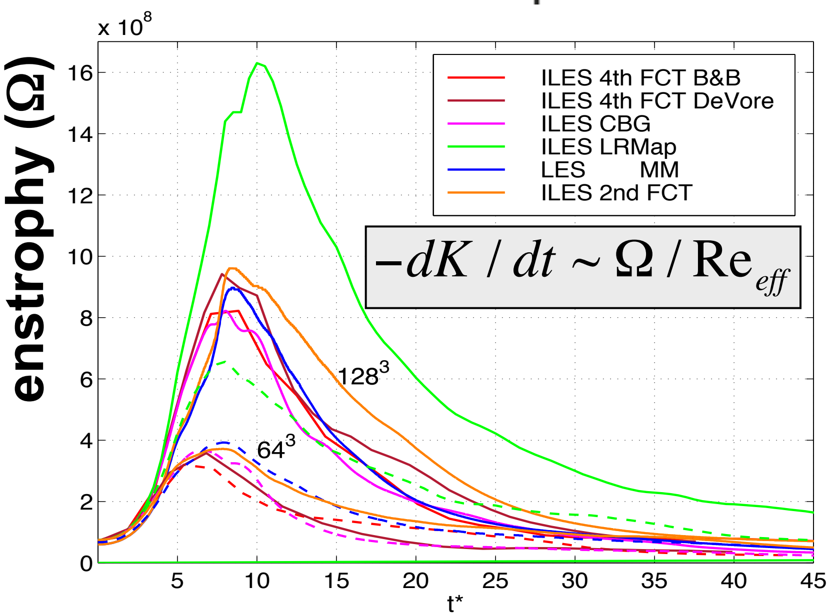
Taylor-Green Vortex Integral Measures

Effective Re associated with resolution

LES & ILES: Grinstein et al. JoT ’07, **DNS,** Brachet *et al*. ‘83, ‘91

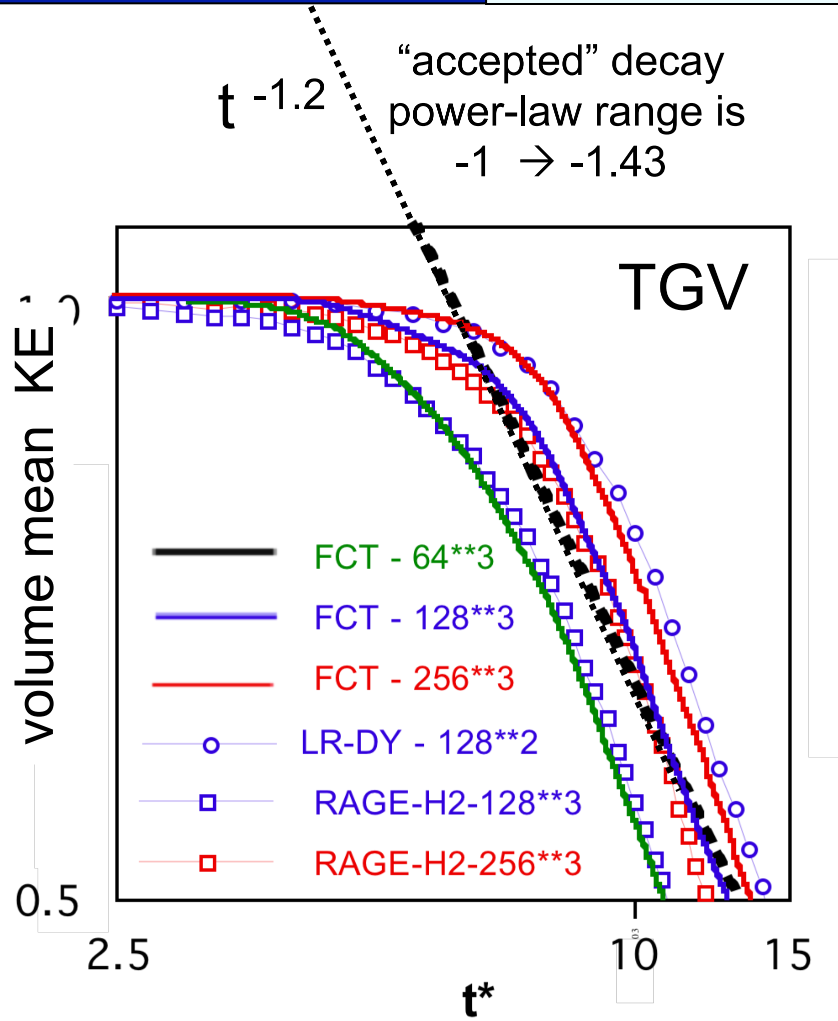




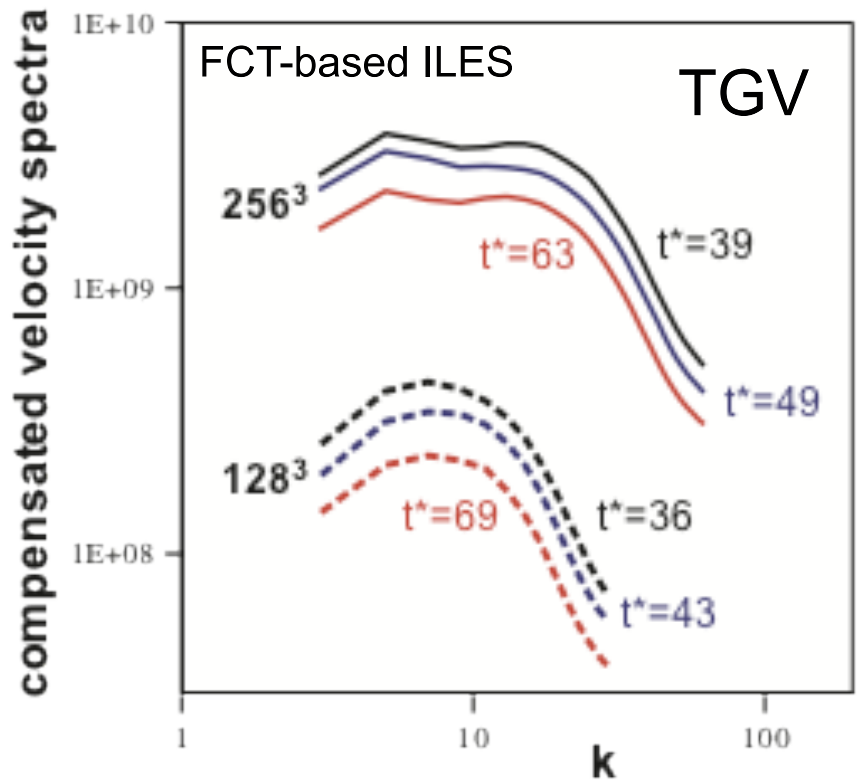


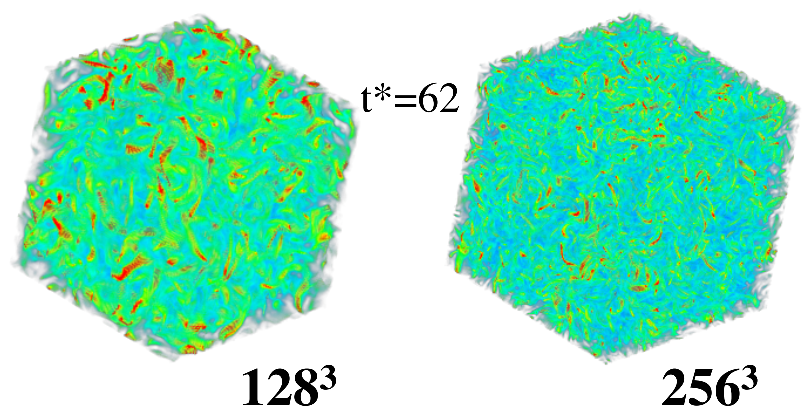
KE Decay Rate vs. Numerics

TGV, Grinstein et al. JoT '07



FCT (4th order), RAGE-Godunov (2nd order)
LR: D. Youngs Lagrange-Remap, uses van Leer (3rd order) at remap phase





Coarse Grained Simulations (LES, ILES / MILES)
why (and when) do they work ?

CGS: Background & Basis

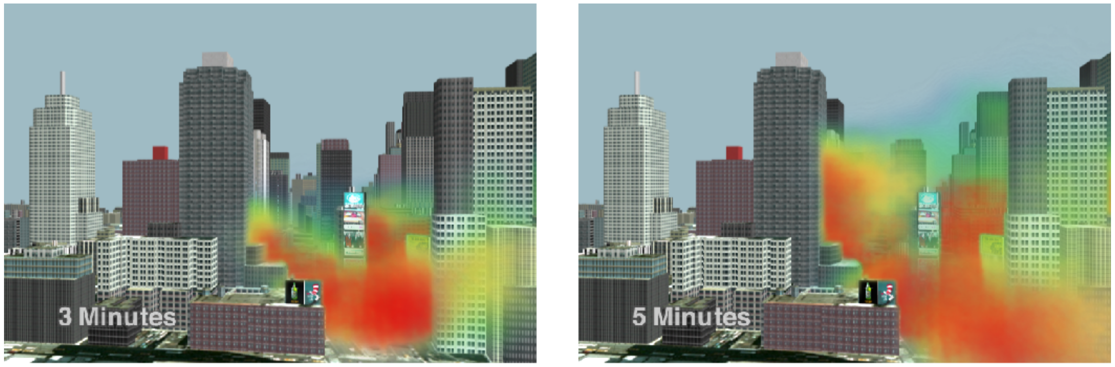
Inhomogeneous free & wall-bounded flows

- jets, channel flow

- Transition & Decay: Taylor-Green vortex
- **Material mixing**
  - **shock-driven turbulence**

Outlook

Predictive Mix Simulation



"Numerical mix" is unavoidable in under-resolved simulations of complex turbulent flows !

➔ **What physical mix can be emulated numerically ?**

➔ **When is a subgrid mix model needed ?**

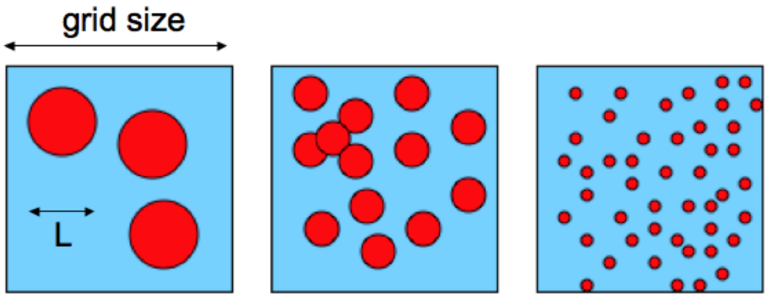


Figure 1. Three different realizations of fluid mixing that all have the same volume fractions.

Fundamental mix issues:

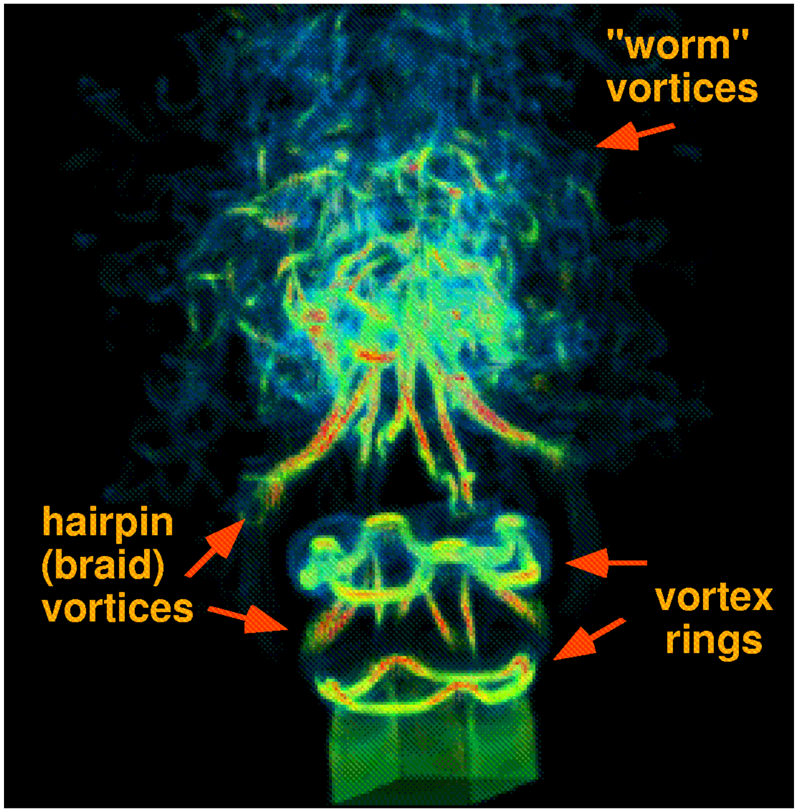
Can we predict *integral consequences* of small-scale scalar mix ?

resolve *integral mix effects* due to Initial Conditions ?

How to improve under-resolved mix modeling when it "breaks" ?

(effective *mixed implicit / explicit* subgrid modeling)

CHARACTERISTIC MIXING PROCESSES

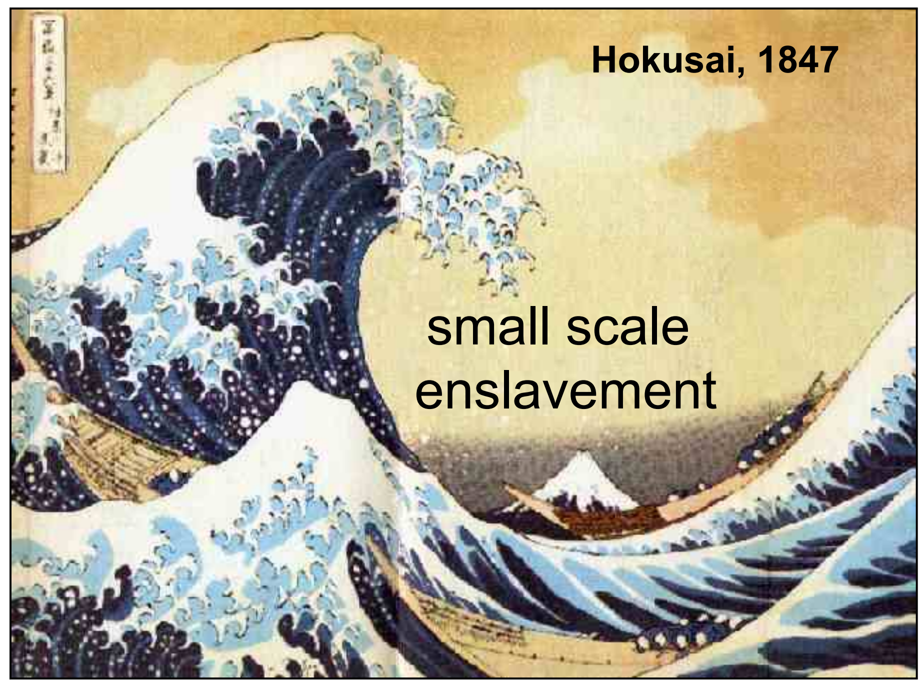


FFG, ILES, jfm ‘01

1) **large scale entrainment**

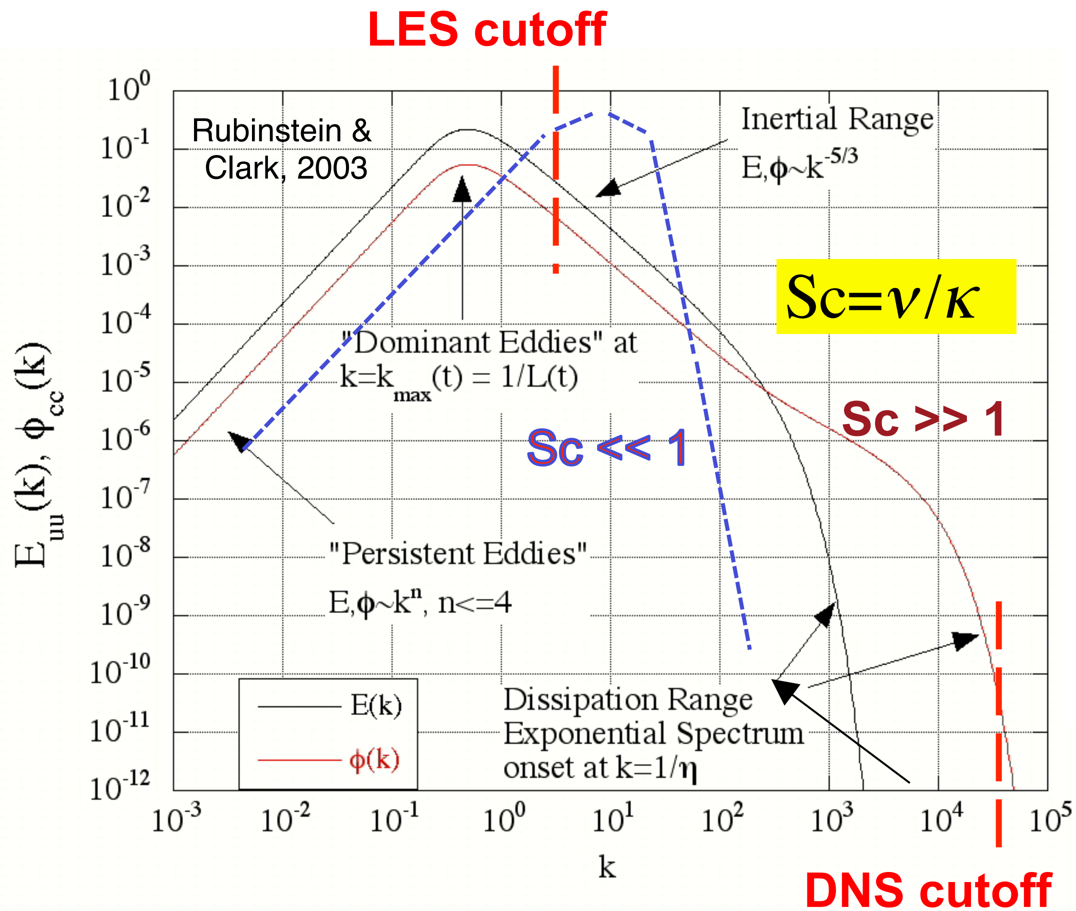
2) **intermediate / small scale stirring due to velocity fluctuations**

3) **smaller scale molecular diffusion**
(less important for high Re and Sc~1)

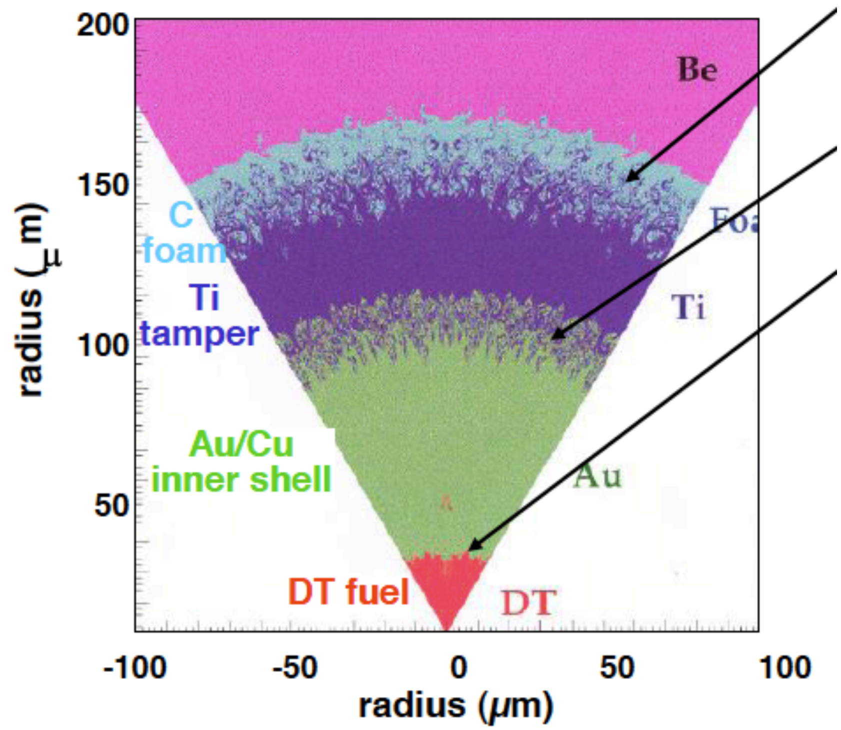


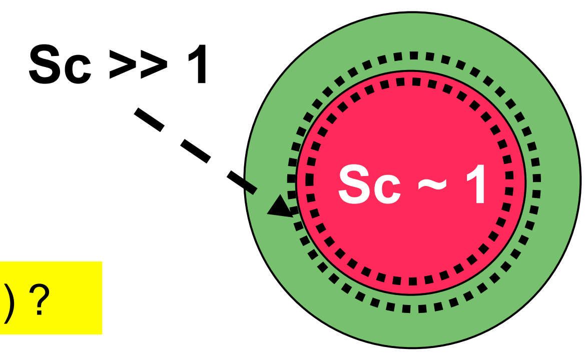
Under-Resolved Sc effects in Extremes

TKE & Scalar spectral features *vs.* Sc



2D HYDRA simulation of NIF-scale ignition double shell capsule

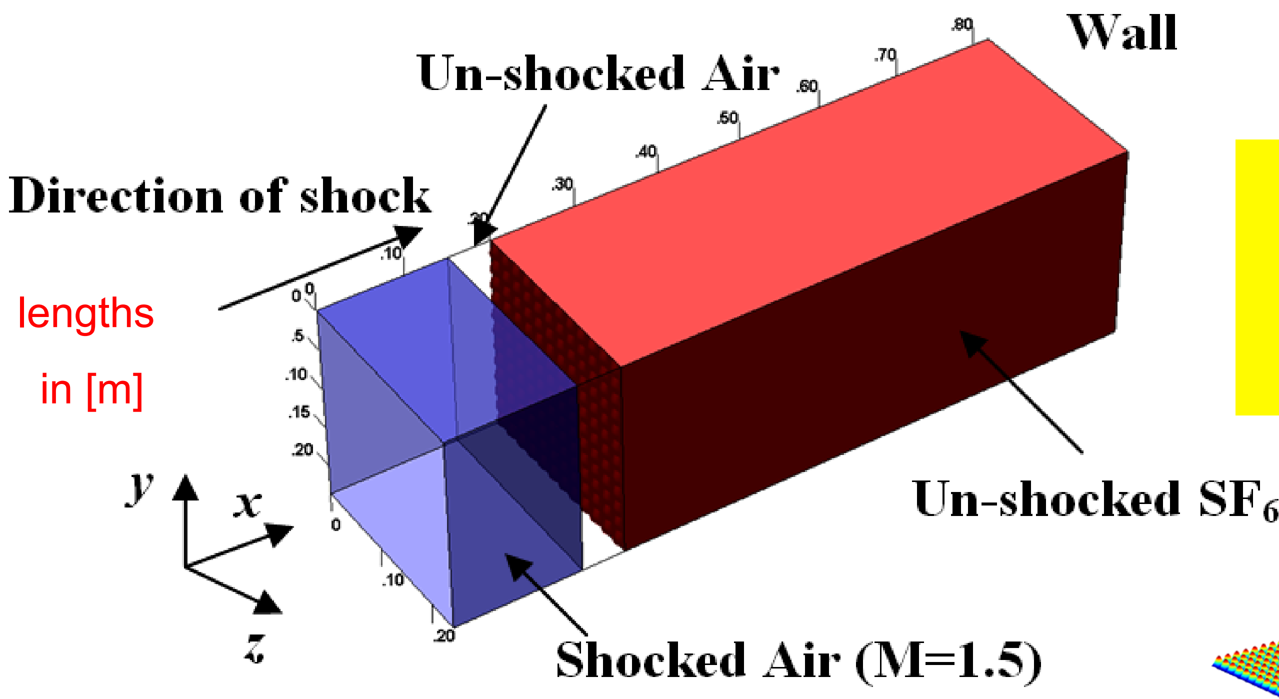




VVUQ of Material Interface Treatments (VOF, IP, …) ?

Shock-Driven Turbulent Mixing

Shocks and Turbulence must be Captured !

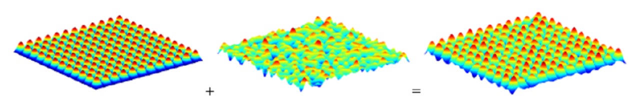


lengths

in [m]

Up to three-levels of adaptive mesh refinement (AMR)
smallest grid sizes:
h=0.2, 0.1, 0.05, 0.025 cm

ϕ: random (spectral content & s.d.)



S : egg crate, λ_o **interface IC**

- **Vetter & Sturtevant -- shocktube experiments,** *Shock Waves* 1995
- **Pullin et al. -- hybrid WENO / classical LES,** *JFM* 2006
- **Grinstein et al. -- ILES RAGE,** *PoF* 2011, to appear

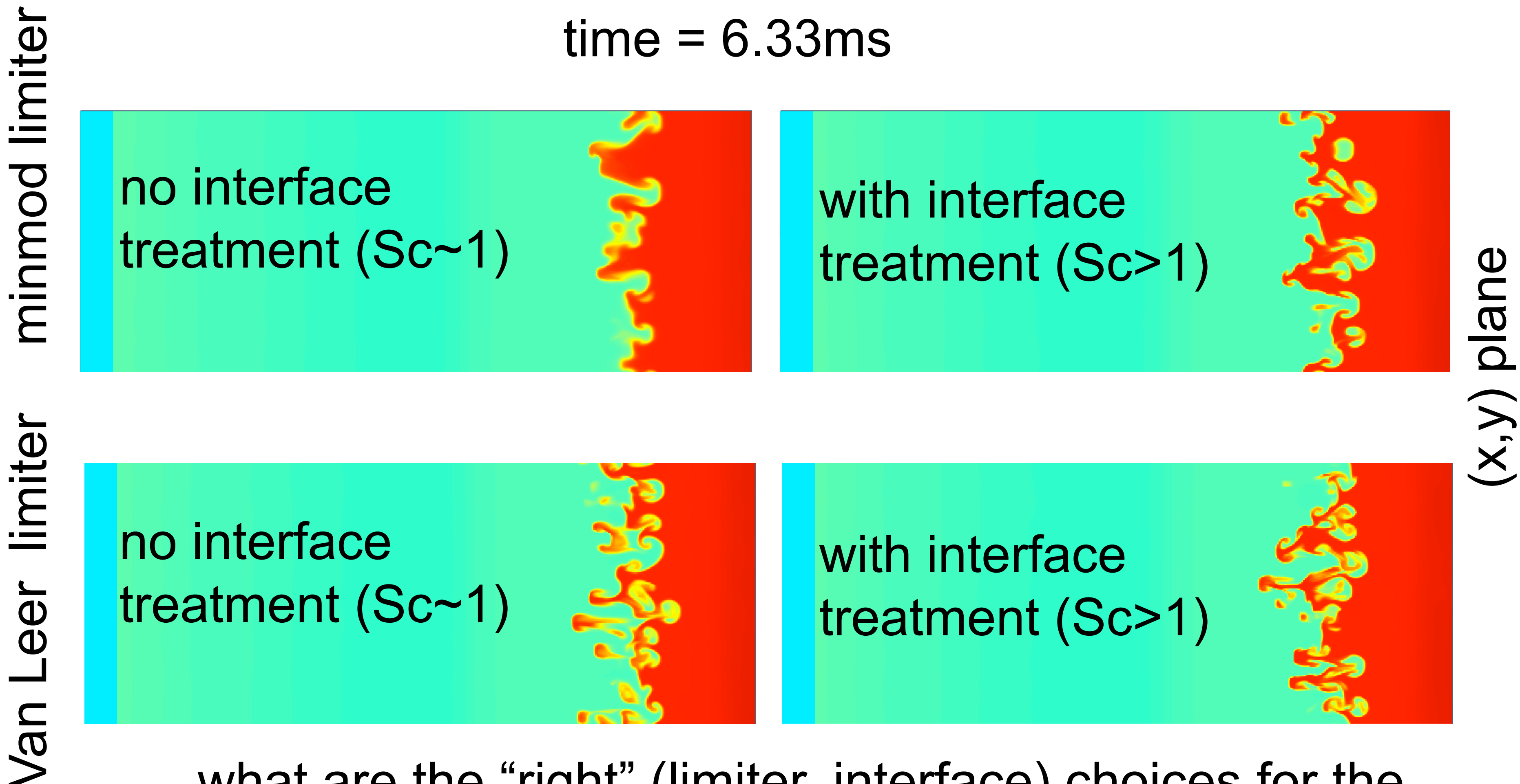
Challenge for any LES : simulating *under-resolved* mixing driven by *under-resolved* velocities *and* *under-resolved* initial conditions

Planar RM Simulations (RAGE)

Dealing with Under-Resolved Sc effects …

uniform grid, h=0.2cm, 410x160x160, varying limiter & interface treatment

time = 6.33ms



what are the “right” (limiter, interface) choices for the problem of interest ? --> VVUQ metrics ?

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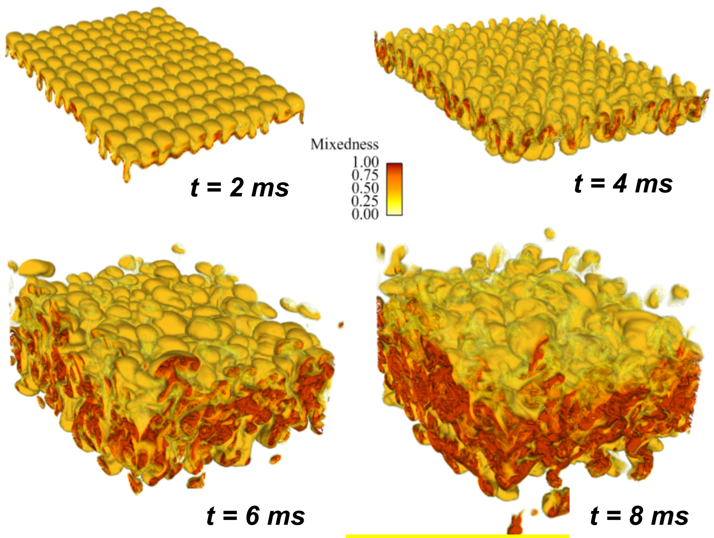
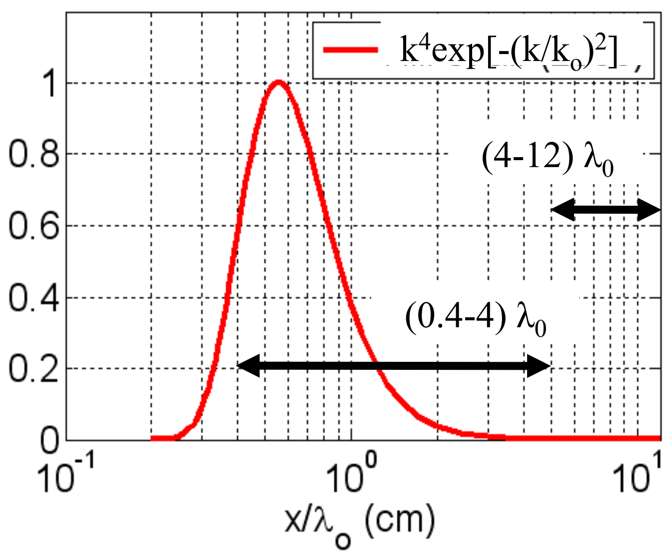
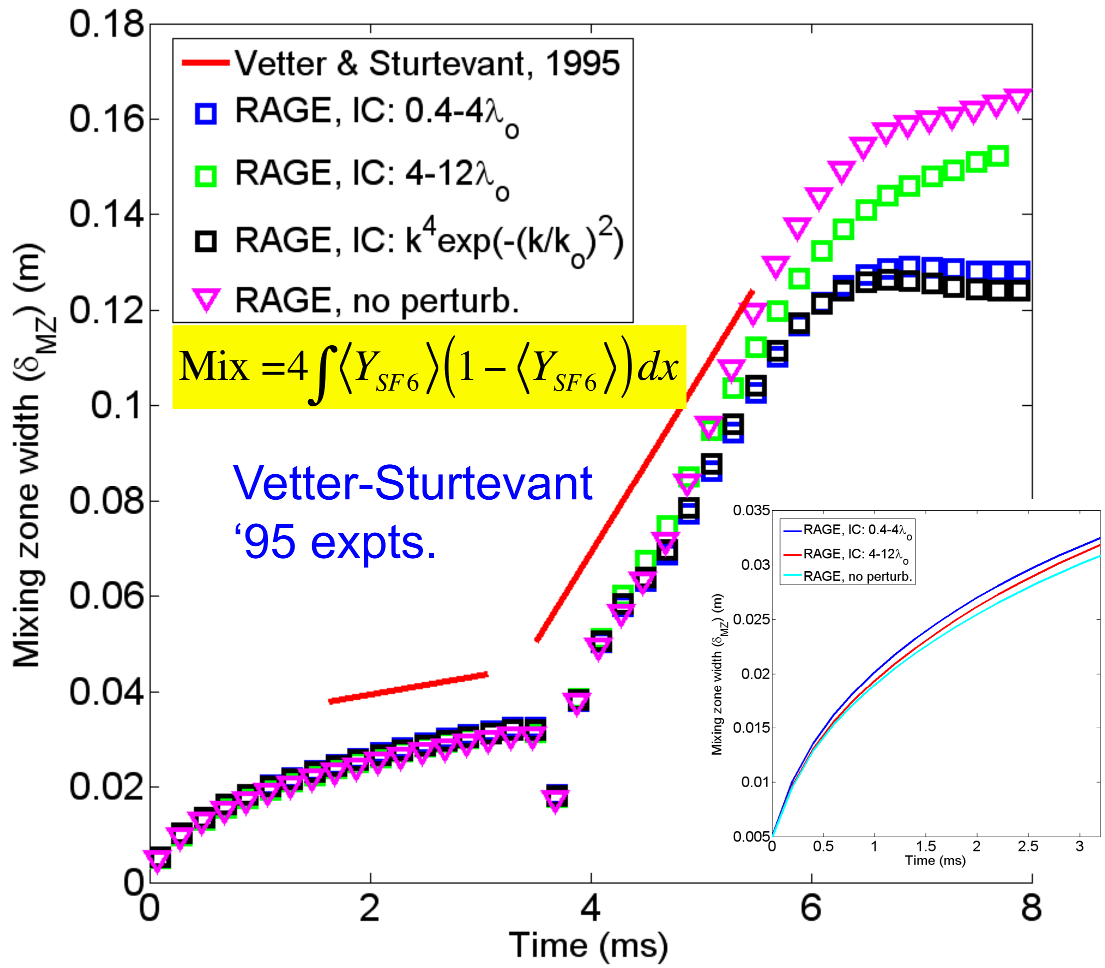
ILES RAGE of reshocked Planar RM
IC spectral content effects, PoF 2011



$\theta = (1 - Y_{SF6})Y_{SF6}$

Initial interface perturbation





- **consistent *growth rates***
- **late-time sensitive to IC specifics**

  faster growth associated with "long" ICs
  (as known for RT)

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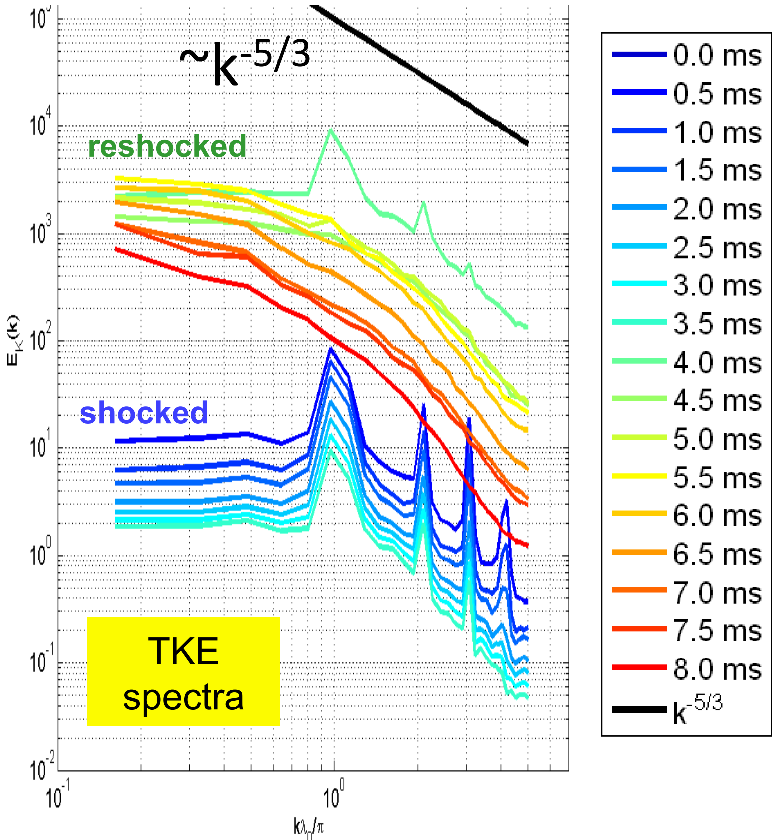
Planar RM -- RAGE Simulations

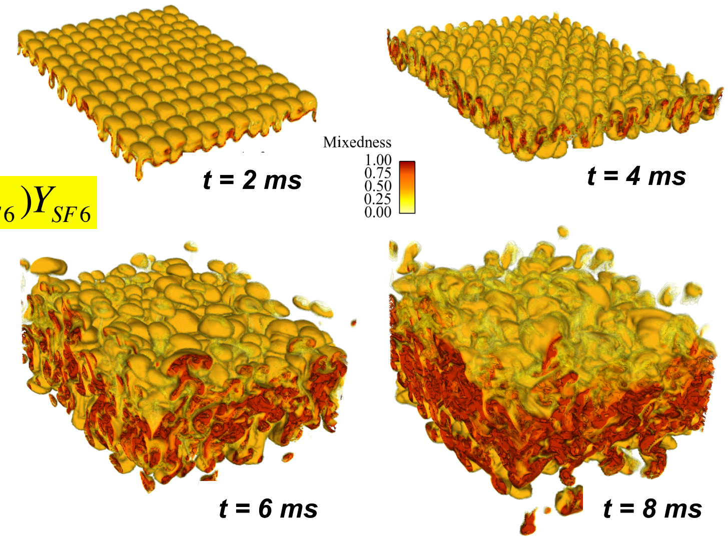
short-perturbed ICs : transition to turbulence

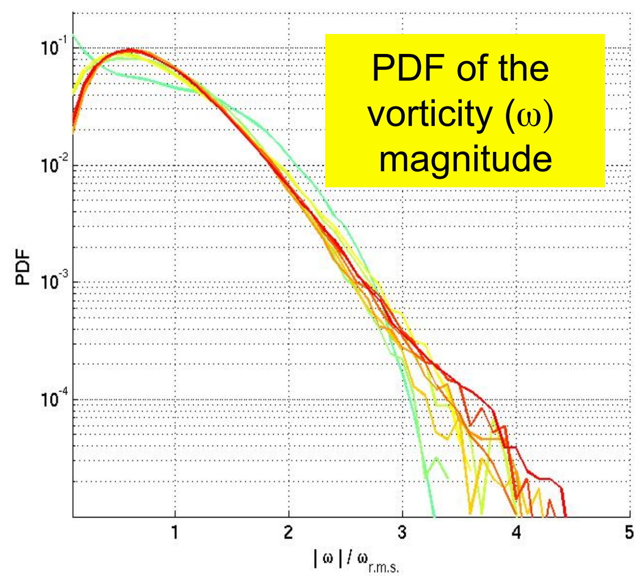


0.1 cm grid

late-time self-similarity suggested

$$\theta = (1 - Y_{SF6})Y_{SF6}$$





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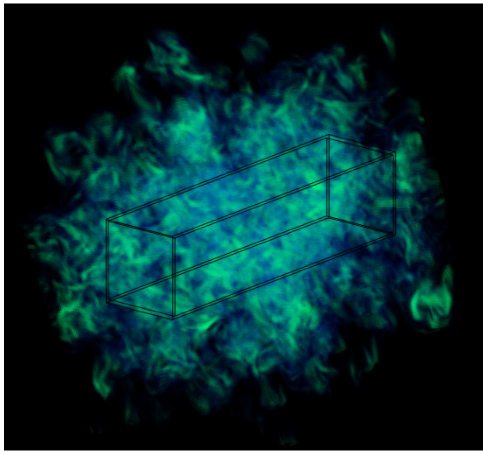
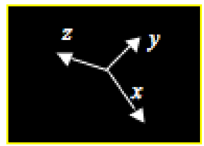
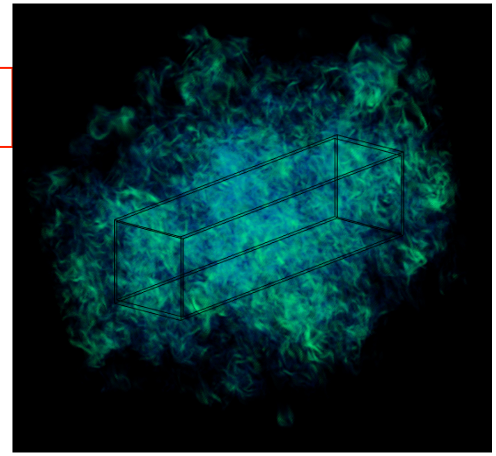
Planar RM – ILES RAGE

short IC, late time velocity-derivative PDF analysis

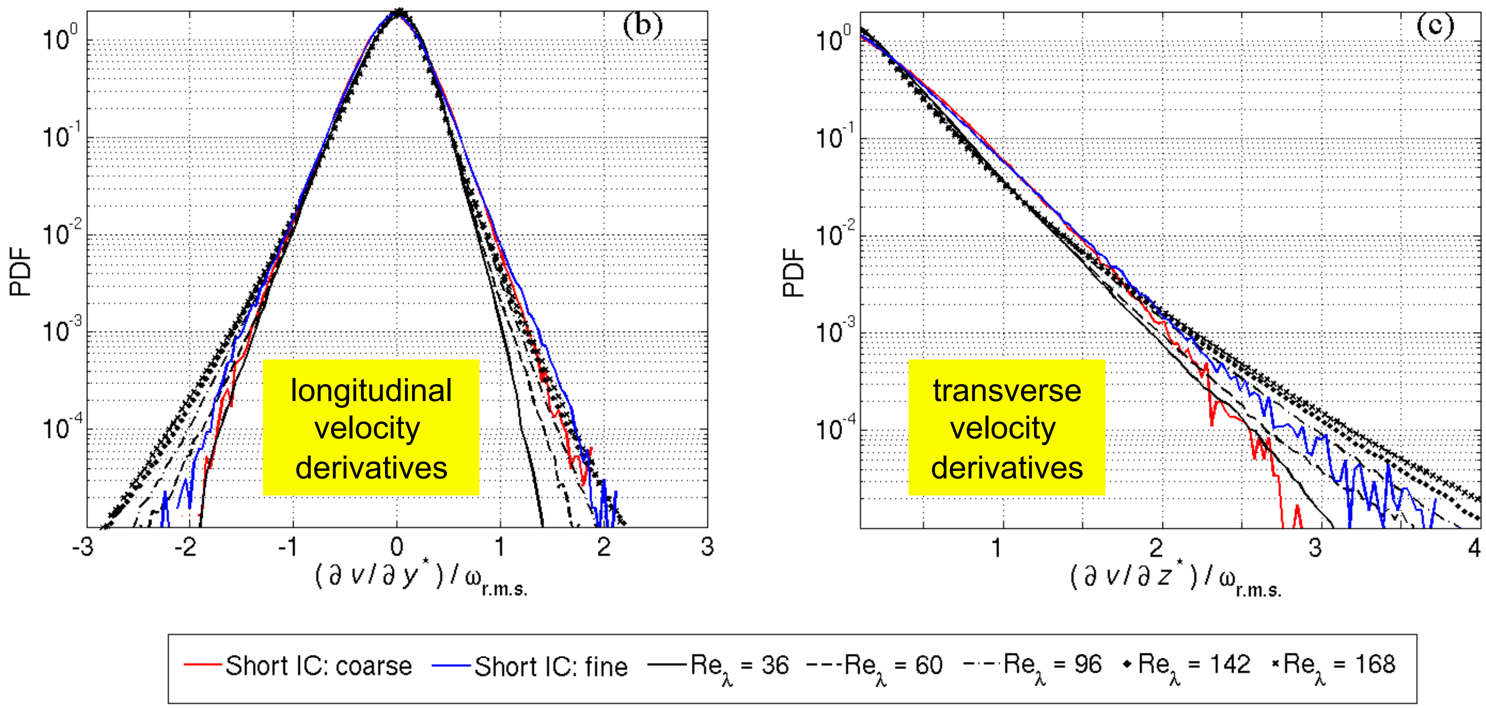


t = 8ms





- **late-time self-similarity**
- **non-gaussian PDF tails**
  (consistent with DNS)
- **higher resolution**
  → **higher effective Re**



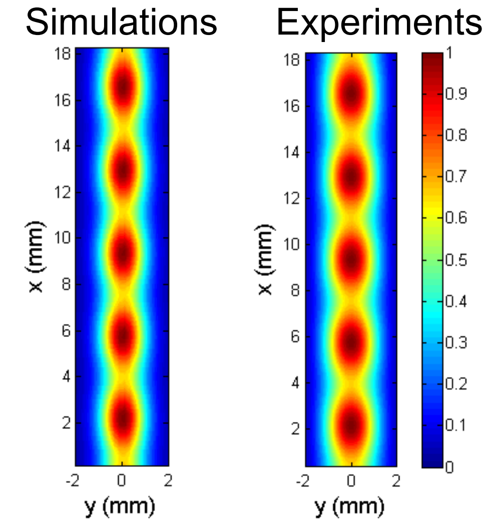
ILES

DNS (isotropic turbulence)
Jiménez et al. JFM '93

ILES of Shocked Gas-Curtain

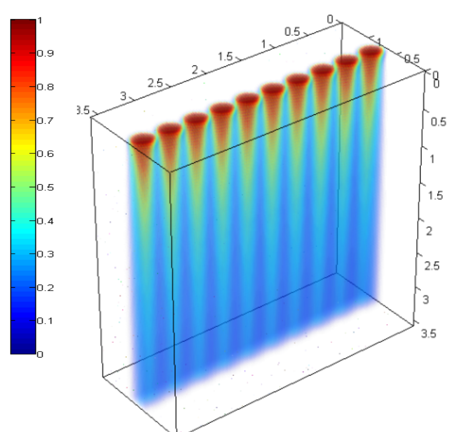
FFG et al., AIAA ASM (2010), PoF in preparation

LDRD innovation for our nation

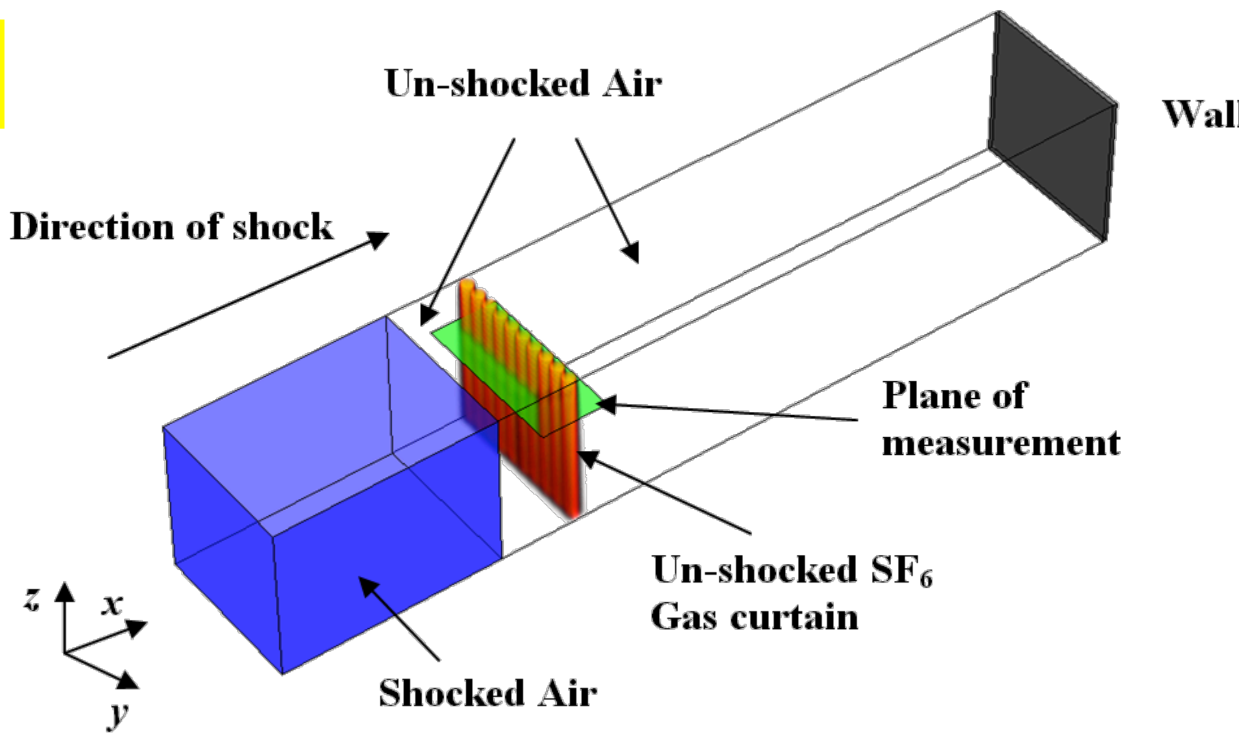


- **3D gas curtain** (ICs for RM simulations) is insufficiently characterized in laboratory expts.
- **Initial 3D *gas curtain simulated*** using separate incompressible NS-Boussinesq code and available info from LANL P-23 expts.

NS-Boussinesq simulated initial 3D Gas curtain



SF_6 Volume Fraction distributions



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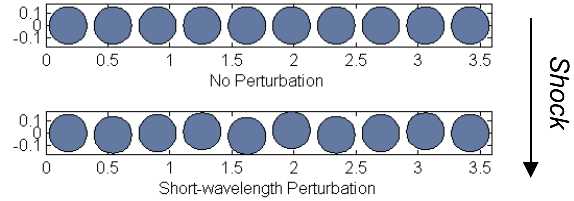
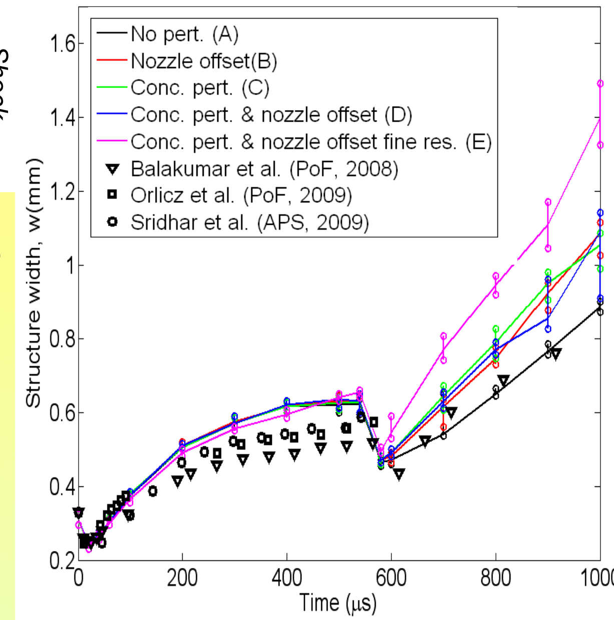
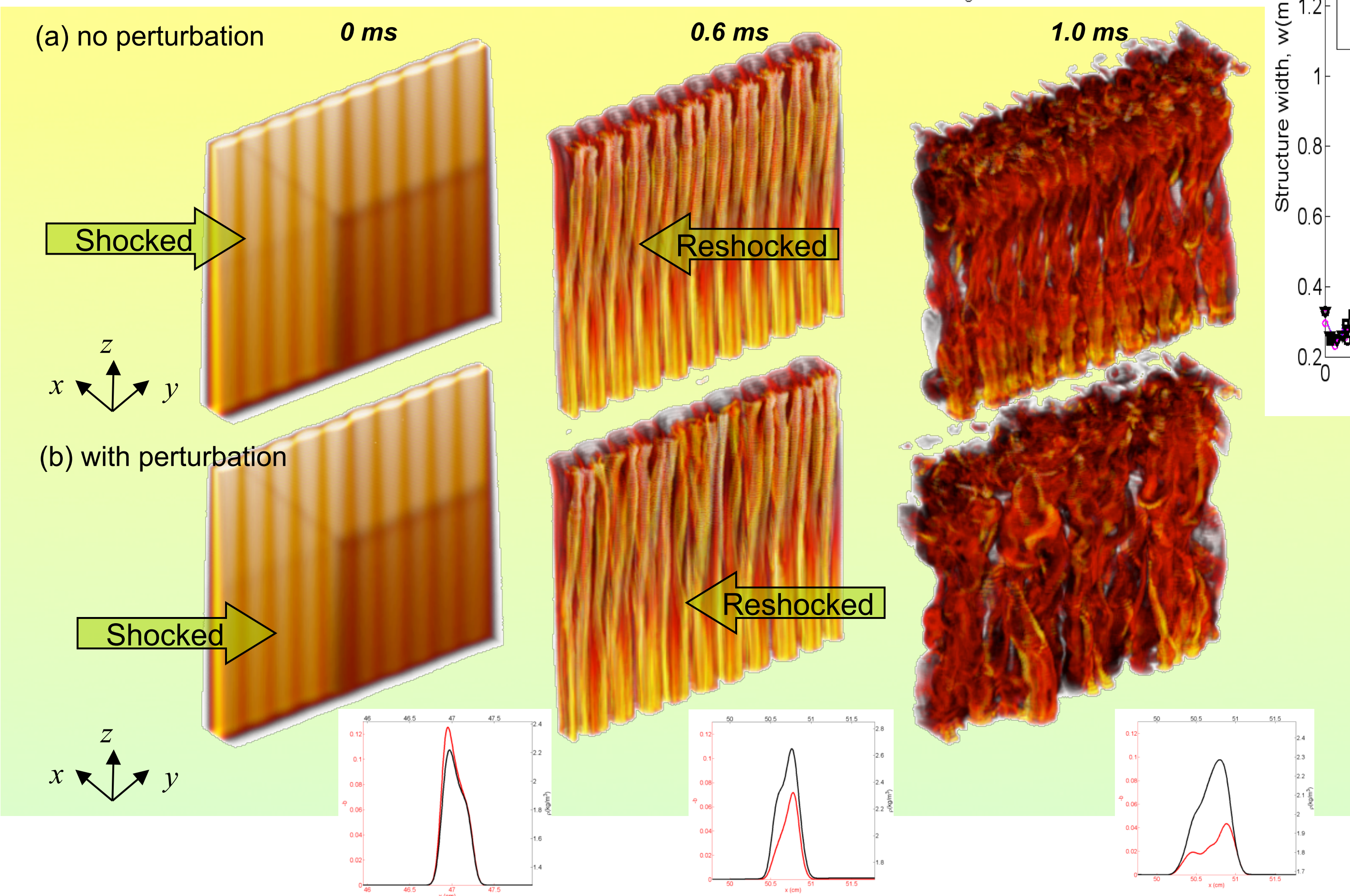
ILES RAGE of Shocked Gas-Curtain
IC Effects on Mixing

Nozzle centers are randomly offset in the shock direction in the perturbed IC case







Mean mass density ρ, mass density self-correlation b (→ for BHR turbulent mixing modeling)

$$b = -\overline{\rho' \times \left(\frac{1}{\rho}\right)'}$$

Significantly more complex ICs *in perturbed arrangement* lead to enhanced vortex interactions and mixing

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Transition & Material Mixing in high-Re inhomogeneous, under-resolved Extreme Turbulent Flows --> CGS

- **Modified Equation Analysis**

to assess / reverse-engineer subgrid features

- ➢ finite scale vs. continuum
- ➢ mixed explicit / implicit models

- **Material Interface dynamics VVUQ**
  - ➢ difficult: mathematics is sketchy
  - ➢ extreme sensitivity to ICs
  - ➢ equations of state … expts. …

- **UQ for "predictive" simulations**

characterize & model intrusiveness of

laboratory & computational expts.

2D HYDRA simulation of NIF-scale ignition double shell capsule