Large-eddy simulations of Rayleigh-Taylor instability between miscible fluids

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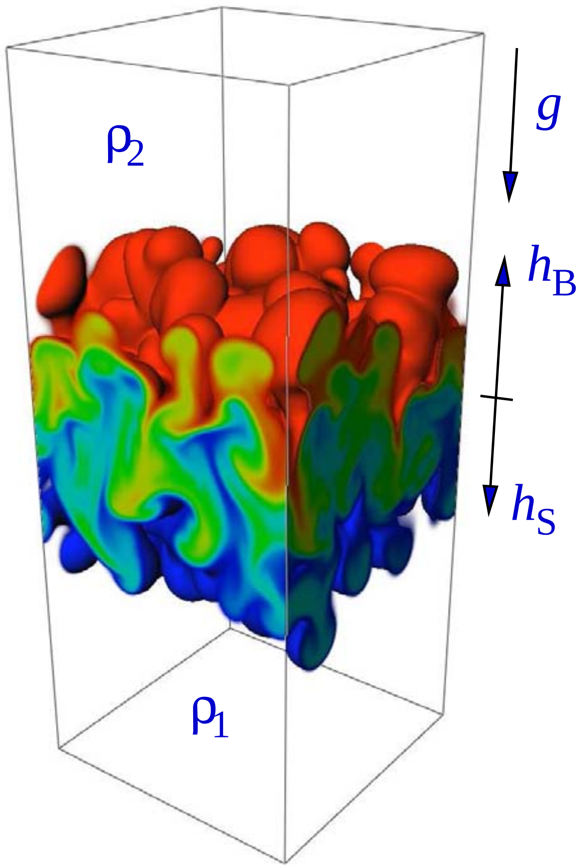
Motivation



- Dimensional analysis:
  - No external length scales
  - Infinite Reynolds/Peclet number

$$\Rightarrow h_{\mathrm{B,S}} = f_{\mathrm{B,S}}\left(\frac{\rho_2}{\rho_1}\right) gt^2 = \alpha_{\mathrm{B,S}}\,\mathcal{A}\,gt^2$$

where $\mathcal{A} = \dfrac{\rho_2 - \rho_1}{\rho_2 + \rho_1}$

- For immiscible fluids, experiment (Dimonte & Schneider, 2000) suggests:
  - α_{S} strongly dependent on $\mathcal{A}$
  - Atwood number effects most significant for $\mathcal{A} \gtrsim 1/2$
- Difficult to attain self-similarity in direct numerical simulation (DNS)

Large eddy simulation (LES) – equations of motion

- Favre-filter: $\widetilde{f} \equiv \overline{\rho f}/\overline{\rho}, \quad \overline{f} \equiv \int G(\boldsymbol{x}-\boldsymbol{x}')f(\boldsymbol{x}')\,\mathrm{d}\boldsymbol{x}'$
- Filtered mole- and mass-fractions: $\overline{X} = \dfrac{\overline{\rho}-\rho_1}{\rho_2-\rho_1}, \quad \dfrac{1}{\overline{\rho}} = \dfrac{\widetilde{Y}}{\rho_2} + \dfrac{1-\widetilde{Y}}{\rho_1}$
- Favre-filtered Navier-Stokes equations:

$$\frac{\partial\overline{\rho}}{\partial t} + \frac{\partial\overline{\rho}\widetilde{u}_j}{\partial x_j} = 0$$

$$\frac{\partial\overline{\rho}\widetilde{Y}}{\partial t} + \frac{\partial\overline{\rho}\widetilde{u}_j\widetilde{Y}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\overline{\rho\mathcal{D}\frac{\partial Y}{\partial x_j}}\right) - \frac{\partial\overline{\rho}q_j}{\partial x_j}$$

$$\frac{\partial\overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial\overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j} = -\frac{\partial\overline{p}}{\partial x_i} + \frac{\partial\overline{\tau}_{ij}}{\partial x_j} - \overline{\rho}g\delta_{i3} - \frac{\partial\overline{\rho}T_{ij}}{\partial x_j}$$

LES – modelled terms

- Compatibility between state, continuity, and scalar transport equations demands

$$\frac{\partial \widetilde{u}_j}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\overline{\frac{\mathcal{D}}{\rho}\frac{\partial \rho}{\partial x_j}}\right) - \left(\frac{1}{\rho_2} - \frac{1}{\rho_1}\right)\frac{\partial \overline{\rho} q_j}{\partial x_j}$$

- Apply stretched-vortex subgrid-scale (SGS) stress and mixing models (Misra & Pullin 1997, Voekl & Pullin 2000, Pullin 2000)

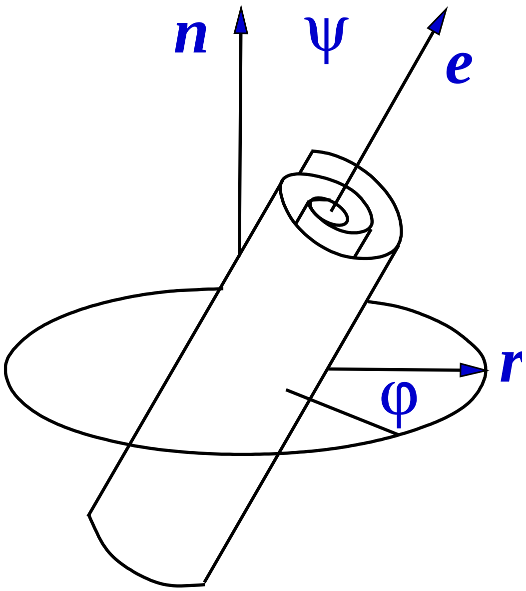
$$T_{ij} = K(\delta_{ij} - e_i e_j)$$

$$q_i = -\frac{1}{2}\Delta K^{1/2}(\delta_{ij} - e_i e_j)\frac{\partial \widetilde{Y}}{\partial x_j}$$

where $K \equiv$ subgrid kinetic energy, $\boldsymbol{e} \equiv$ subgrid vortex orientation, and $\Delta \equiv$ local grid size

$$\Rightarrow \frac{\partial \widetilde{u}_j}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\frac{\mathcal{D}}{\overline{\rho}}\frac{\partial \overline{\rho}}{\partial x_j}\right) - \frac{\partial}{\partial x_j}\left[\frac{1}{2}\Delta K^{1/2}(\delta_{ij} - e_i e_j)\frac{1}{\overline{\rho}}\frac{\partial \overline{\rho}}{\partial x_i}\right]$$

LES – implementation



- Subgrid kinetic energy (Pullin 2000, stretched-spiral Lundgren vortex)

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

where $S_3 = \widetilde{S}_{ij} e_i e_j \equiv$ resolved strain along vortex axis

- $\mathcal{K}_0 \varepsilon^{2/3}$ estimated from approximate expressions (Voekl & Pullin 2000) for the resolved circle-averaged second-order structure function, $F_2^c(r, \boldsymbol{x})$

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

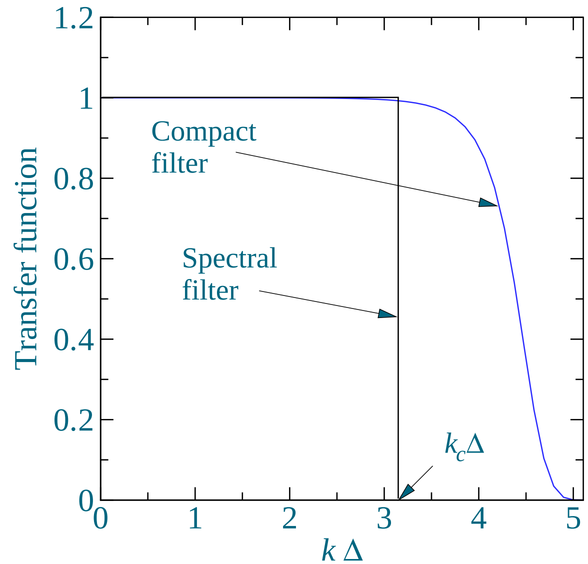
where, in general, $F_2(\boldsymbol{r}, \boldsymbol{x}) = \overline{|\boldsymbol{u}(\boldsymbol{x} + \boldsymbol{r}) - \boldsymbol{u}(\boldsymbol{x})|^2}$

LES – implementation (cont'd)

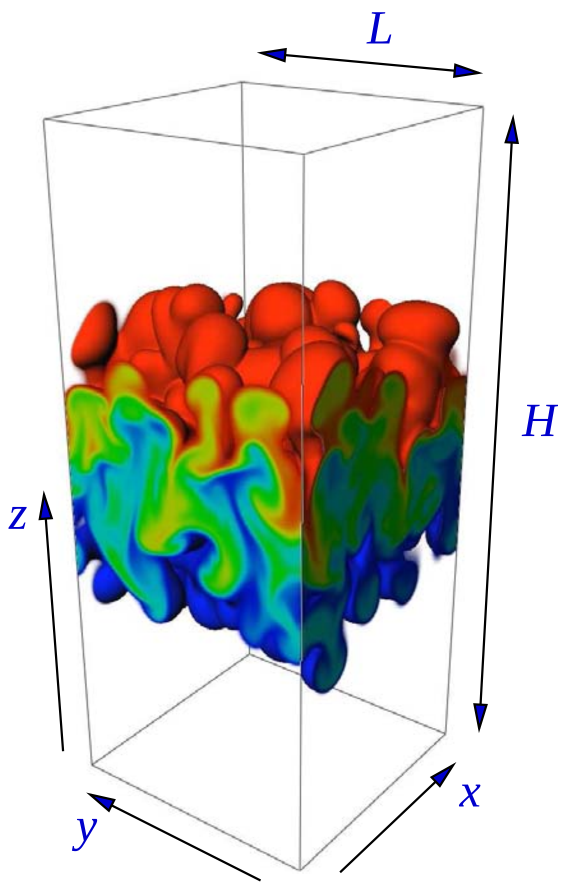
- Subgrid vortex orientation, $\boldsymbol{e}$
  - fraction λ of subgrid vortices aligned with principal extensional eigenvector of resolved rate-of-strain tensor, $\widetilde{S}_{ij}$ (corresponding eigenvalue λ_3)
  - $1-\lambda$ subgrid vortices aligned with resolved vorticity vector, $\boldsymbol{\omega}$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

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

- Explicit filters
  - Circular spectral filter in (x, y)-plane
  - Compact filter in z-direction
  - Only damps wavenumbers above cutoff, $k_c = \pi/\Delta$
  - Accounts for less than 10% of subgrid dissipation

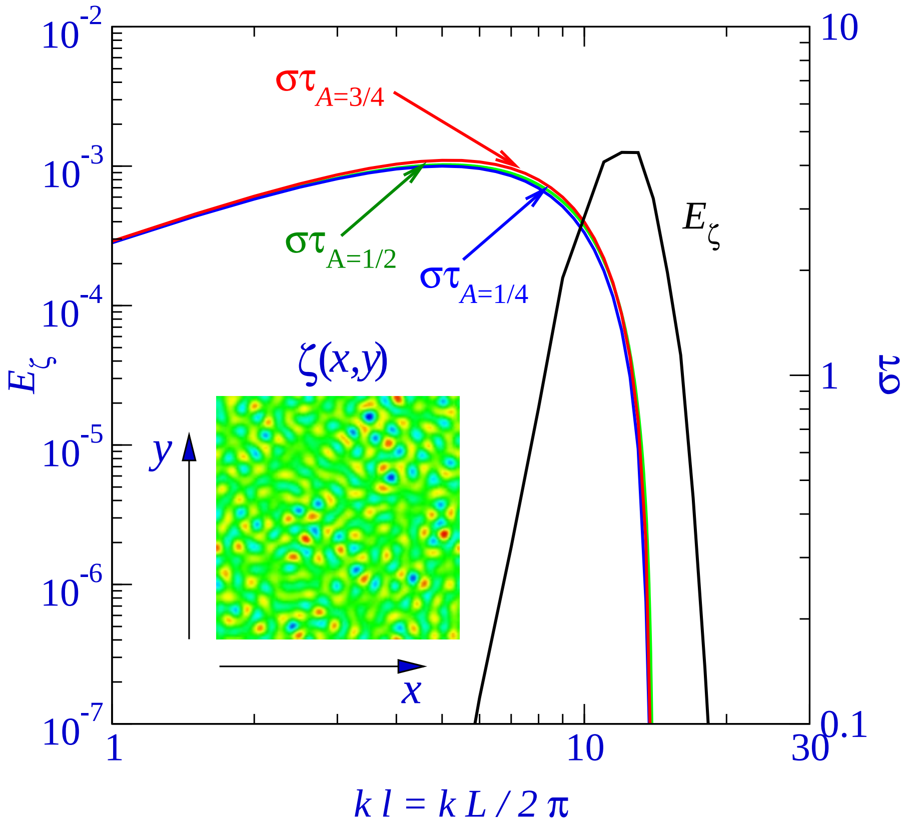


Reference DNS – simulation details



- Boundary conditions:
  - No-slip/penetration top and bottom walls
  - Assume no mixed fluid reaches walls $\Rightarrow$ $X = 1$ (top wall), $X = 0$ (bottom wall)
  - Periodic in homogeneous (x-y) plane
  - $H/L = 32/13 \approx 2.5$
- Discretization:
  - x-y plane: spectral (Fourier)
  - z direction: 8^{th}-order compact finite-difference
  - $\Delta_z/\Delta_{xy} = 8/13$ to approximately match resolution of spatial discretization schemes
  - Grid size: $256 \times 256 \times 1024$
  - Temporal discretization: 3^{rd}-order explicit Adams-Bashforth-Moulton or Runge-Kutta

DNS – simulation details (cont'd)



- Definitions:

$$\overline{\rho} \equiv \frac{\rho_2 + \rho_1}{2},\ L \equiv 2\pi\ell,\ U \equiv \sqrt{g\ell}$$

- Initial conditions:
  - $X = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{z + \zeta(x,y)}{5\Delta_z}\right)\right]$
  - $\boldsymbol{u} = -\mathcal{D}\,\nabla\rho/\rho$
- Parameters:

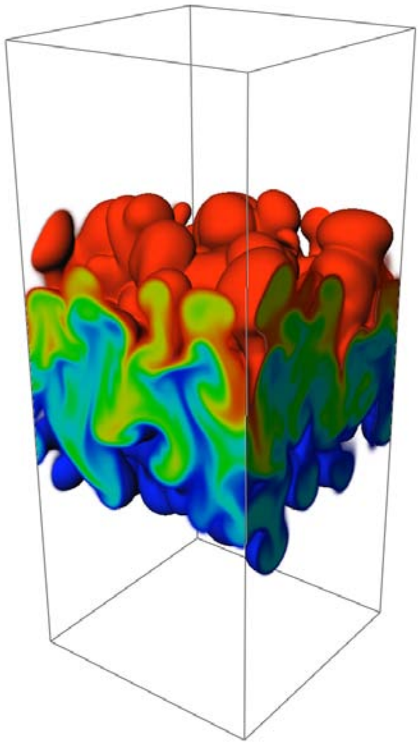
$$Re \equiv \frac{\overline{\rho}\,U\ell}{\mu}, \quad Pe \equiv \frac{U\ell}{\mathcal{D}} = Re\,Sc,$$

- Chosen such that:
  - Same proportion of box used
  - Same final *flow* Reynolds number,

$$Re_h \equiv \frac{\overline{\rho}h\dot{h}}{\mu}$$

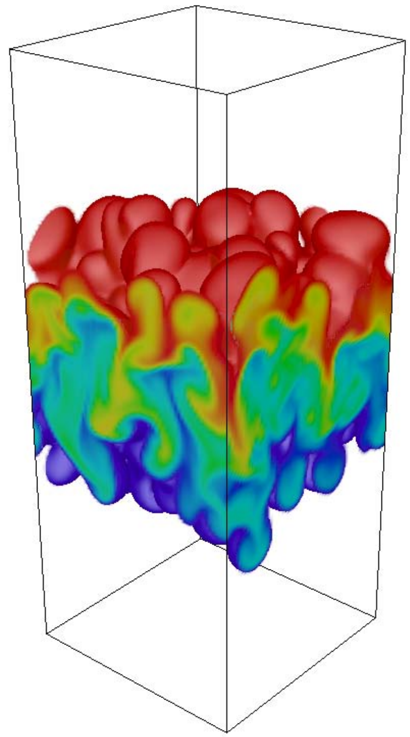
  - Matched linear stability growth rates, $\sigma\tau$, where $\tau \equiv \sqrt{L/\mathcal{A}g}$

LES-DNS comparison – growth



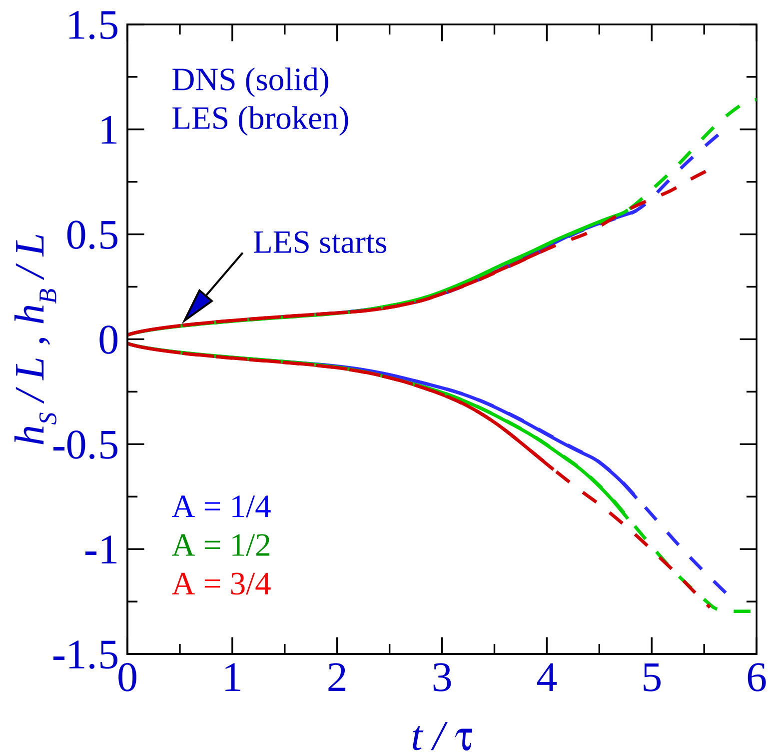
$256 \times 256 \times 1024$

DNS



$64 \times 64 \times 256$

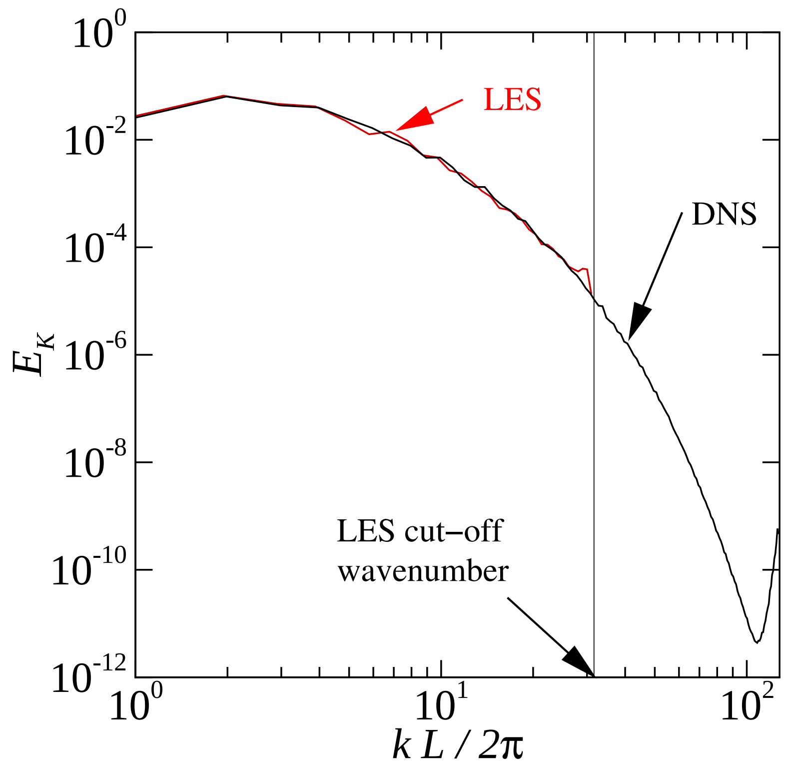
LES



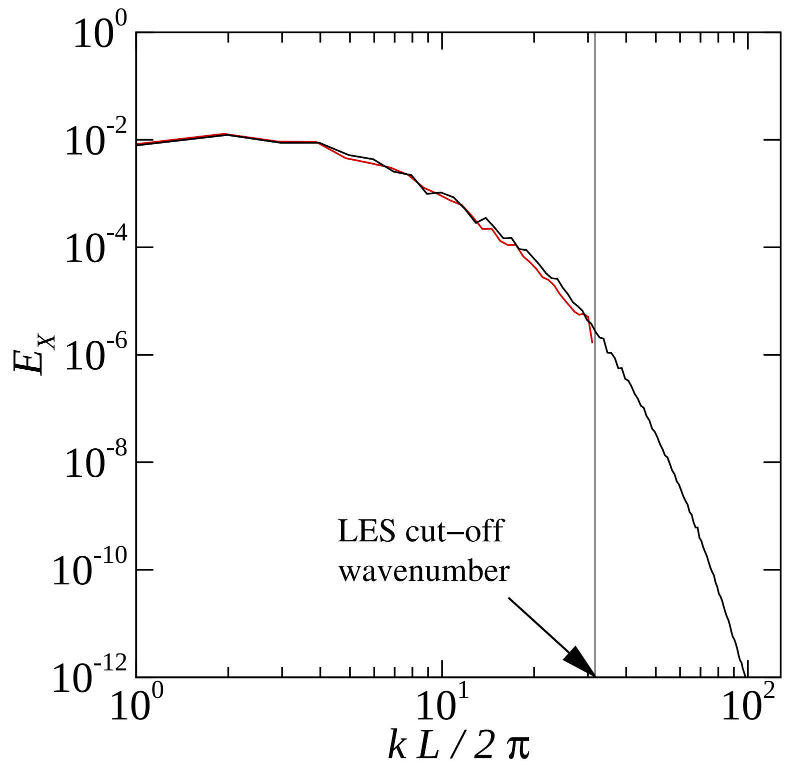
- LES initialized using filtered DNS-data at $t/\tau = 0.5$
  - At this time, DNS data almost resolved on LES grid

LES-DNS comparison – spectra

Kinetic energy $\dfrac{\rho u_i^2}{2}$



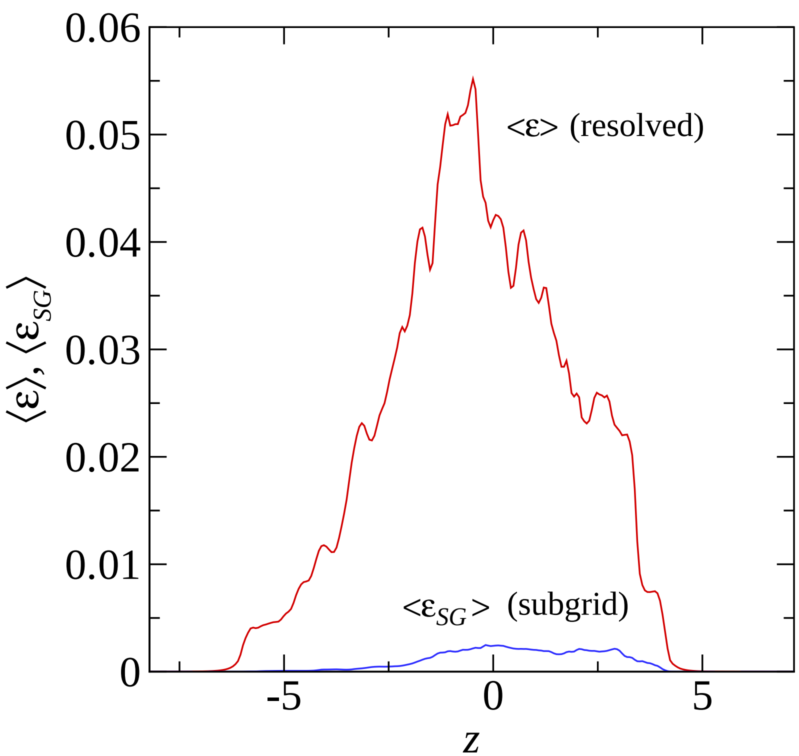
Scalar energy $\dfrac{X^2}{2}$



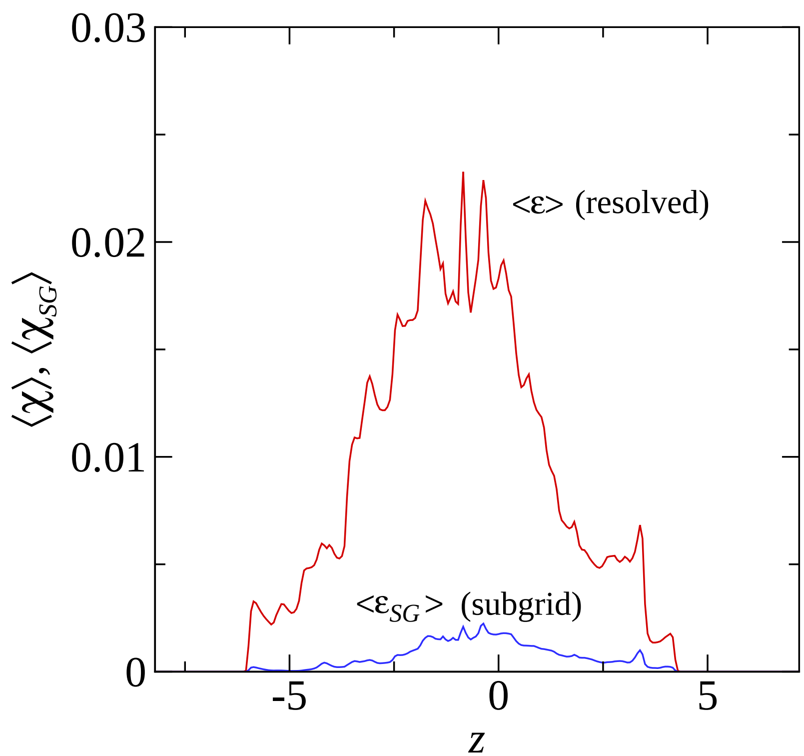
- Model preserves resolved scale features

LES-DNS comparison – dissipation

Kinetic energy dissipation ϵ

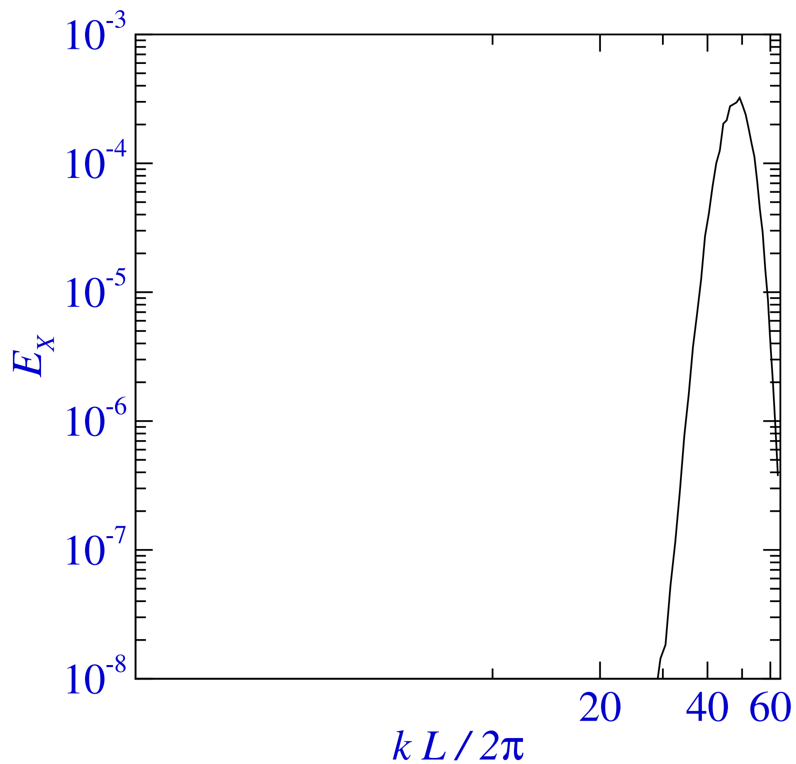


Scalar energy dissipation χ



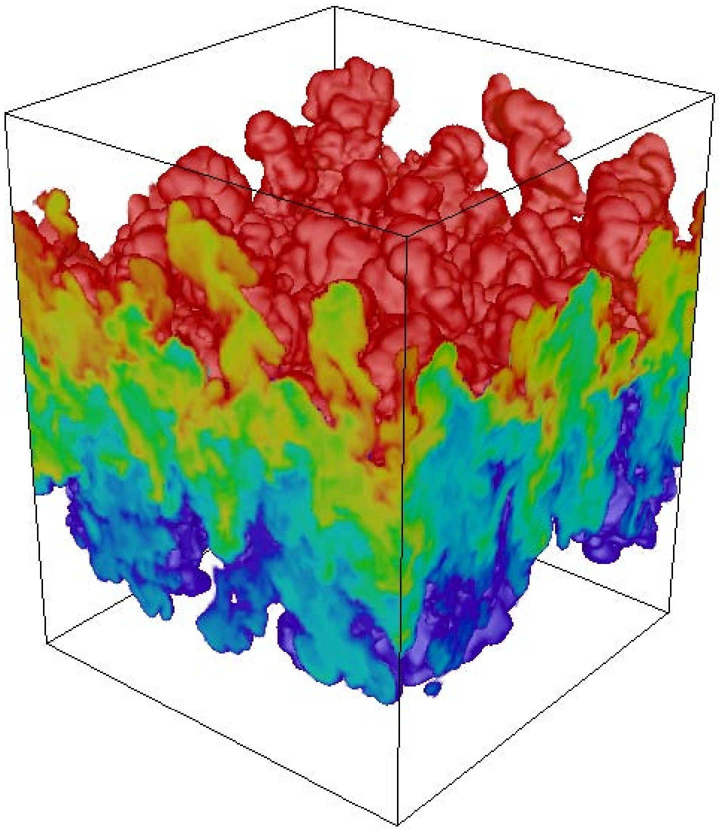
- Resolved-scale dissipation dominates
  - Experiment (or higher Re DNS) required to test model validity

LES – predictions at different density ratios

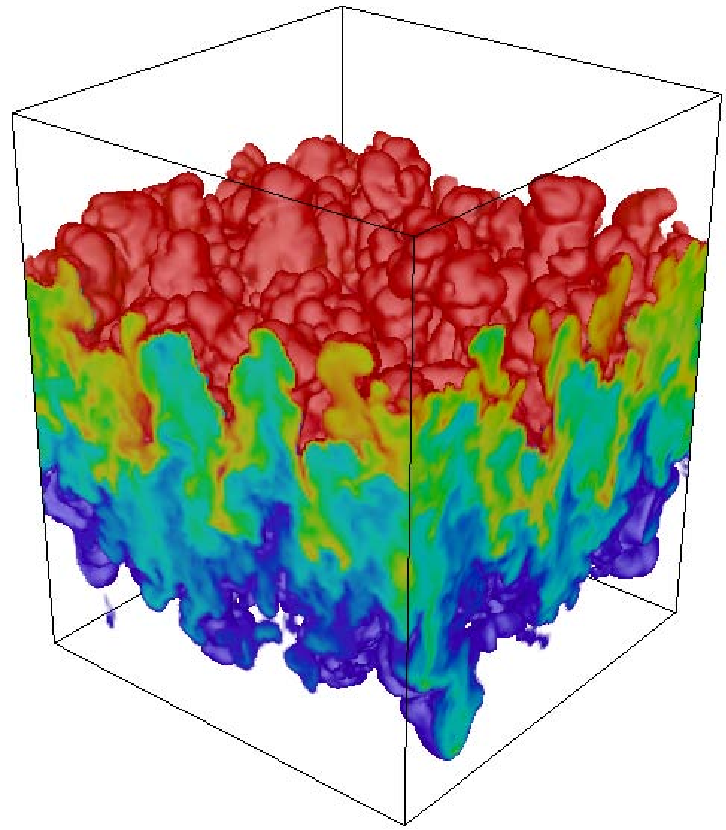


- Initial conditions:
  - $X = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{z + \zeta(x,y)}{5\Delta_z}\right)\right]$
  - $\boldsymbol{u} = -\mathcal{D}\,\nabla\rho/\rho$
- Parameters:
  - $\mathcal{A} = 1/4$, 1/2, 3/4
  - $H/L = 1.23$
  - $Re = \rho_1 U\ell/\mu = 11,215$
  - $Pe = U\ell/\mathcal{D} = 11,215$
  - $Sc = \mu/\rho_1\mathcal{D} = 1$

LES – visualizations

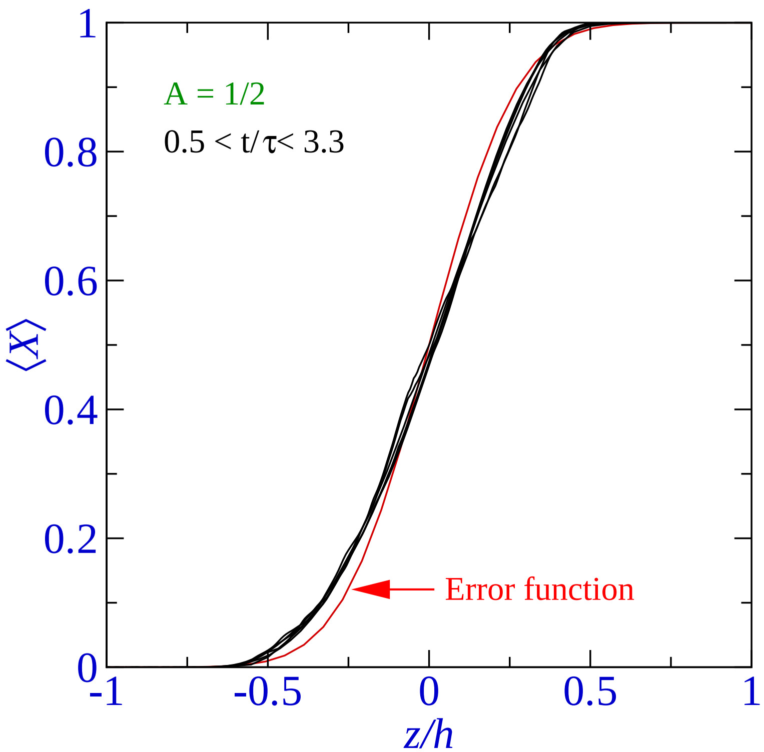


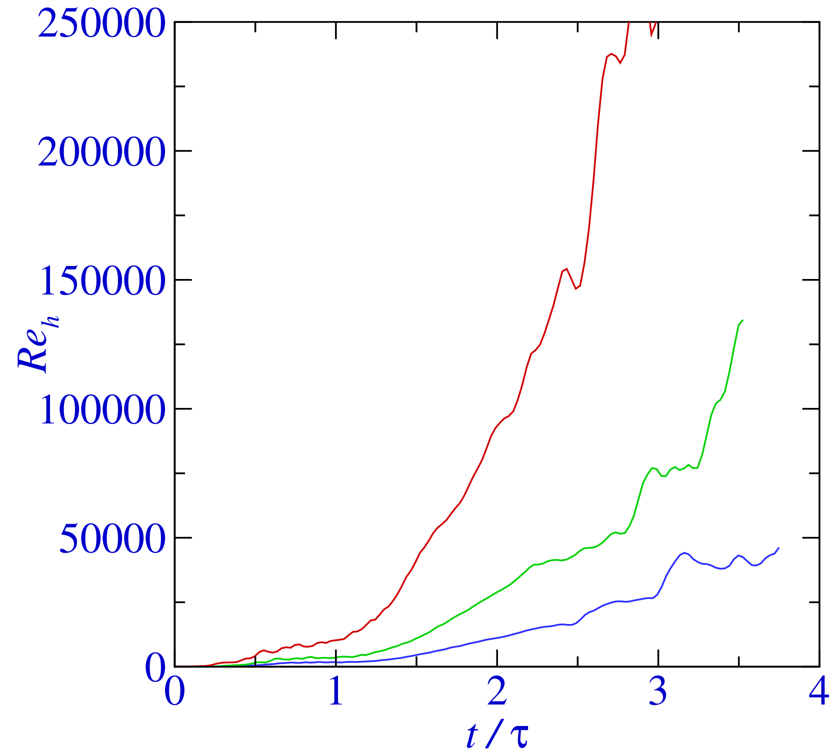
$\mathcal{A} = 1/4$



$\mathcal{A} = 3/4$

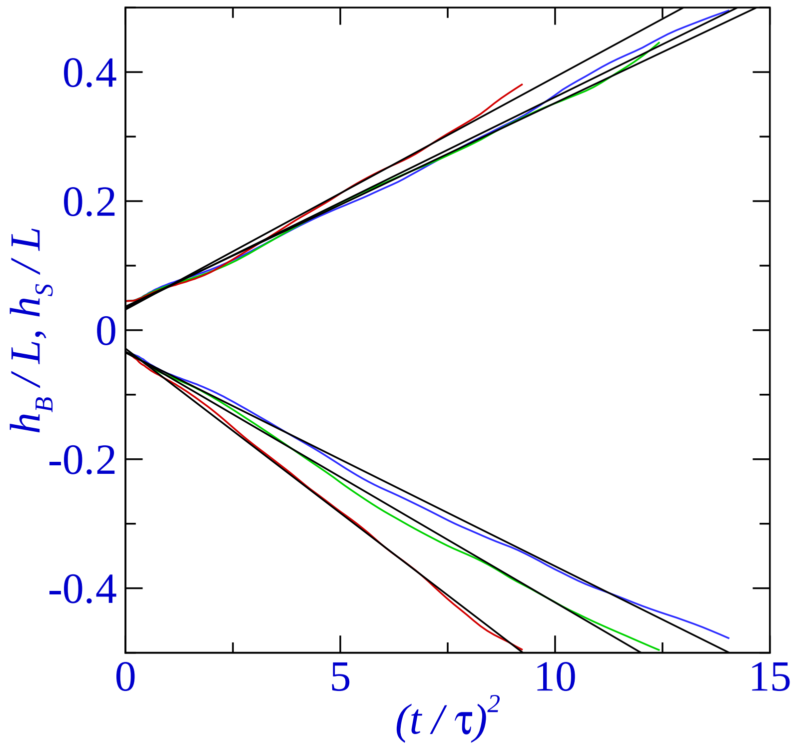
LES – Mole-fraction profiles and Reynolds number

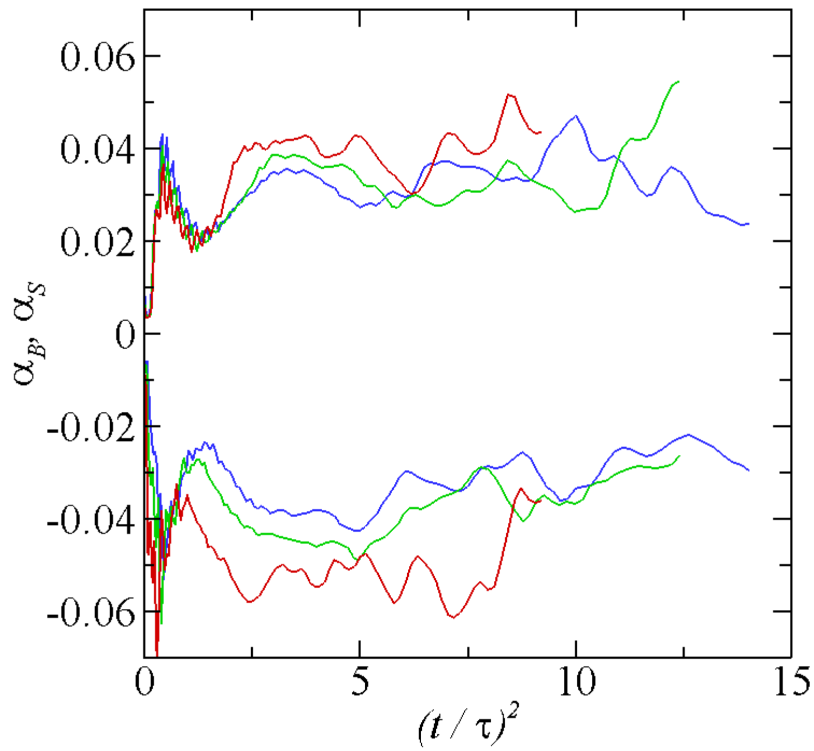




- LES predicts approximately self-similar behavior
  - Bubble/spike penetrations grow by a factor of 8
  - $Re_h > 50,000$

LES – growth

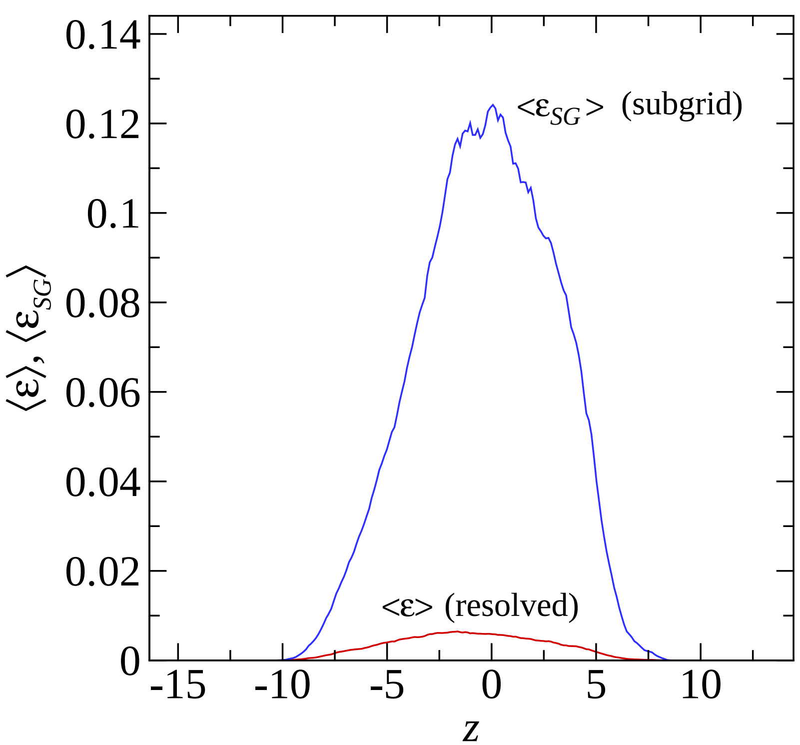




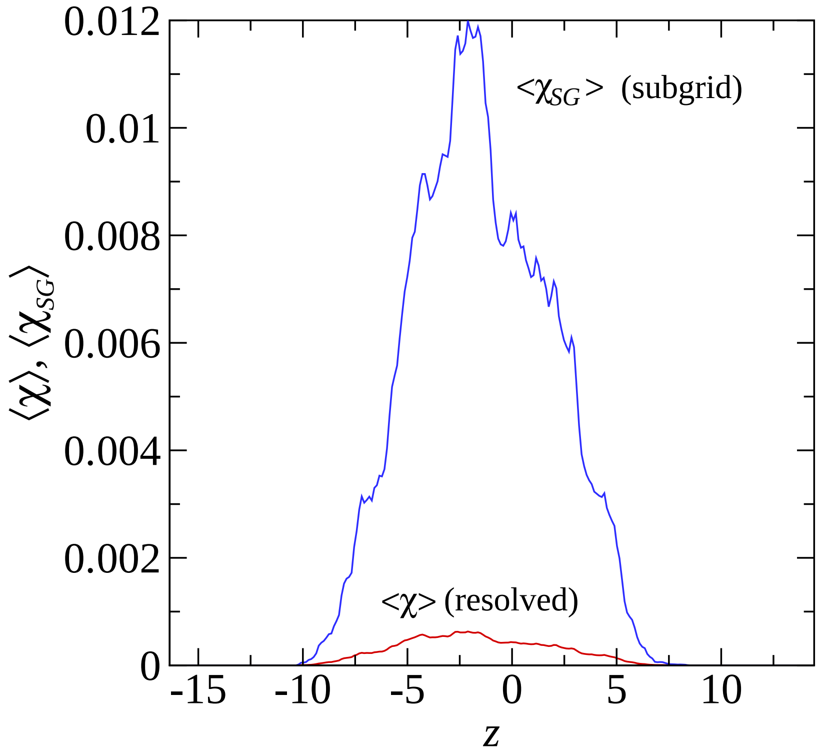
- LES predicts approximately self-similar behavior
  - Approximately quadratic growth
  - Only weak Atwood number effects

LES – model dissipation

Kinetic energy dissipation ϵ

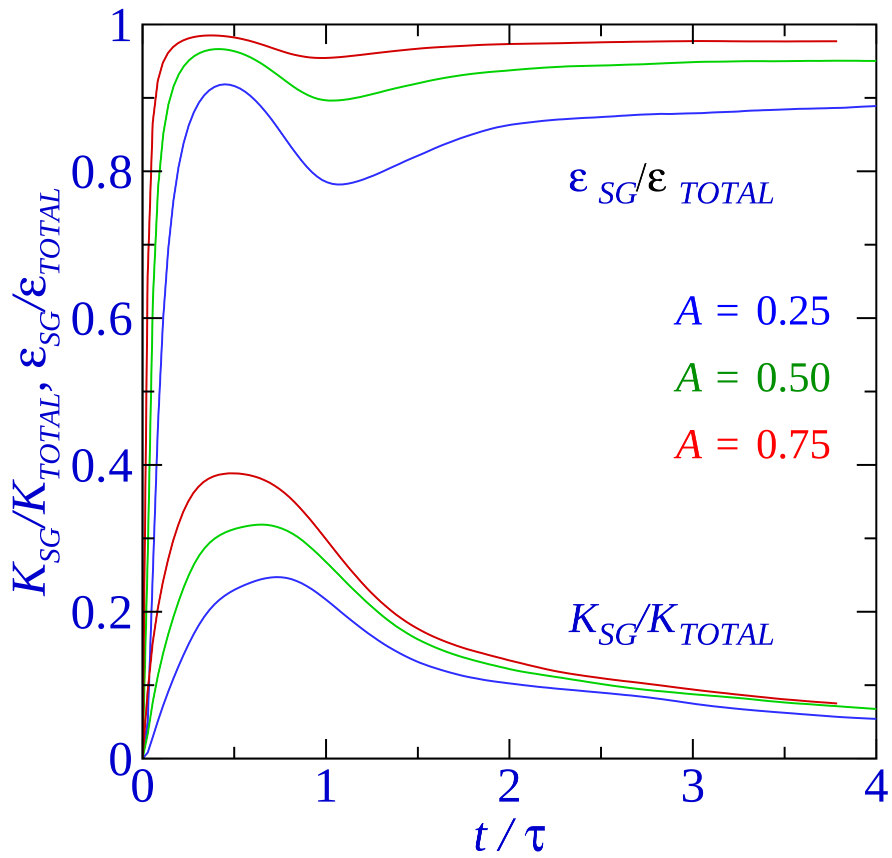


Scalar energy dissipation χ



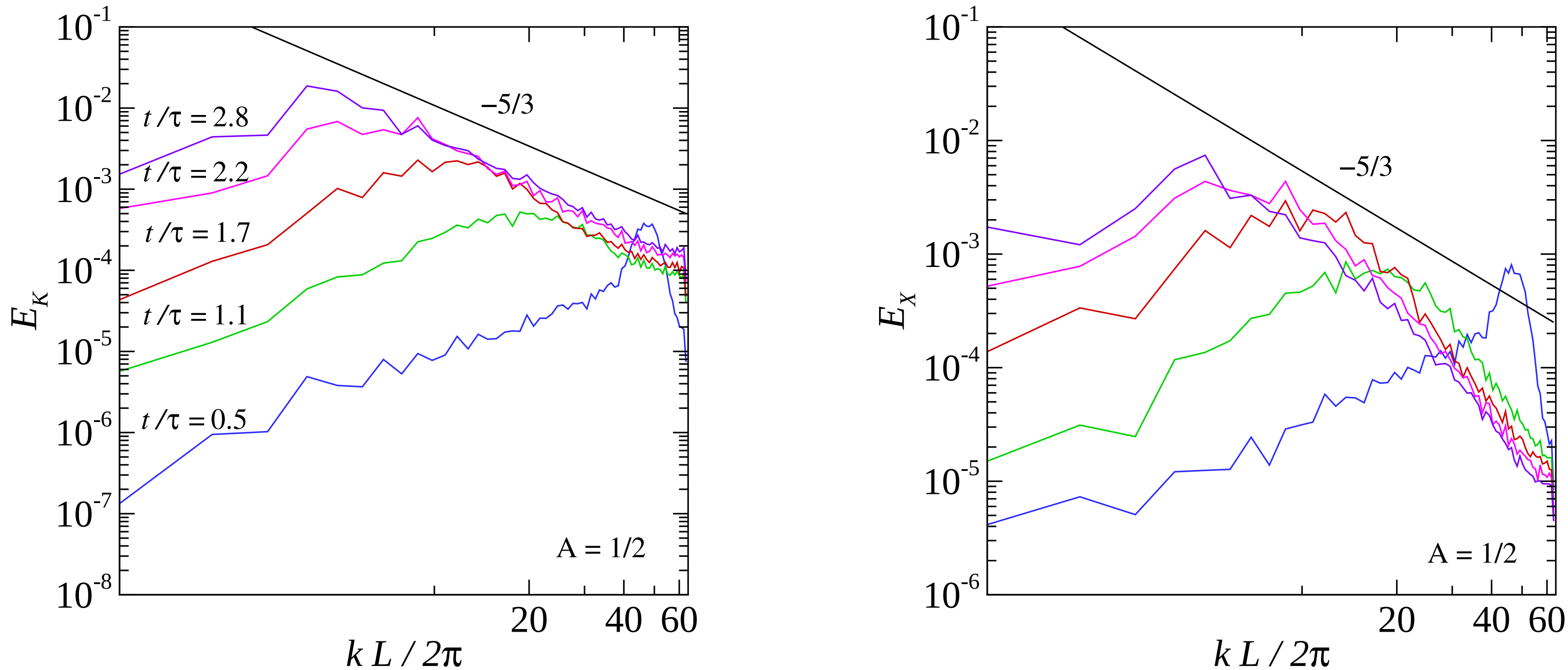
- Subgrid-scale dissipation dominates

LES – subgrid kinetic energy



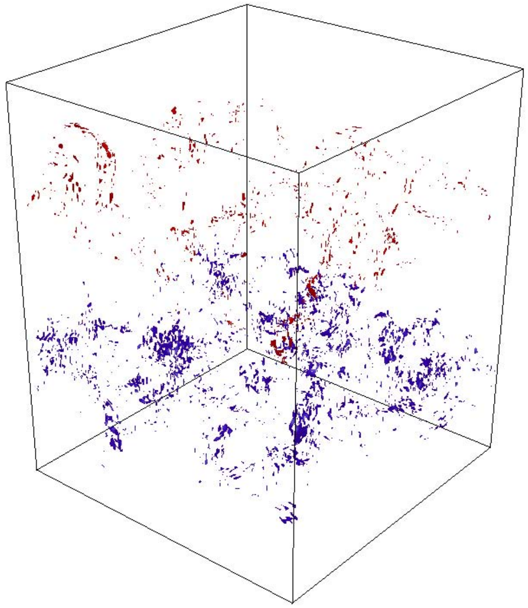
LES – spectra

Kinetic energy $\dfrac{\rho u_i^2}{2}$ Scalar energy $\dfrac{X^2}{2}$

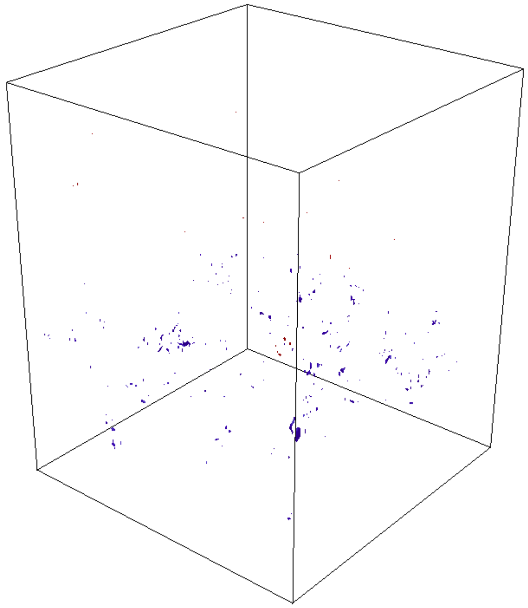


- Kinetic energy spectrum approximately asymptotes to Kolmogorov -5/3 slope
- Scalar energy spectrum decays faster than -5/3

LES – scalar excursions



$X = -0.01, 1.01$



$X = -0.02, 1.02$

- 'Unphysical' scalar excursions:
  - Occupy small volume fraction
  - Average out in statistics
  - More serious at high density ratio, *e.g.*, $\frac{\rho}{\rho_1} = \frac{\Delta\rho}{\rho_1} X + 1$

Conclusions

- Used subgrid vortex model to simulate Rayleigh-Taylor instability
- DNS–LES comparison:
  - Model preserves resolved scales
  - Higher Re experiment or DNS required to definitively test model
- Encouraging behaviour observed:
  - Self-similar mole-fraction profiles
  - Approximately quadratic growth
  - Approximate -5/3 slope in resolved kinetic energy spectra
- Scalar excursions are an outstanding issue for very high density ratio simulations

Acknowledgements

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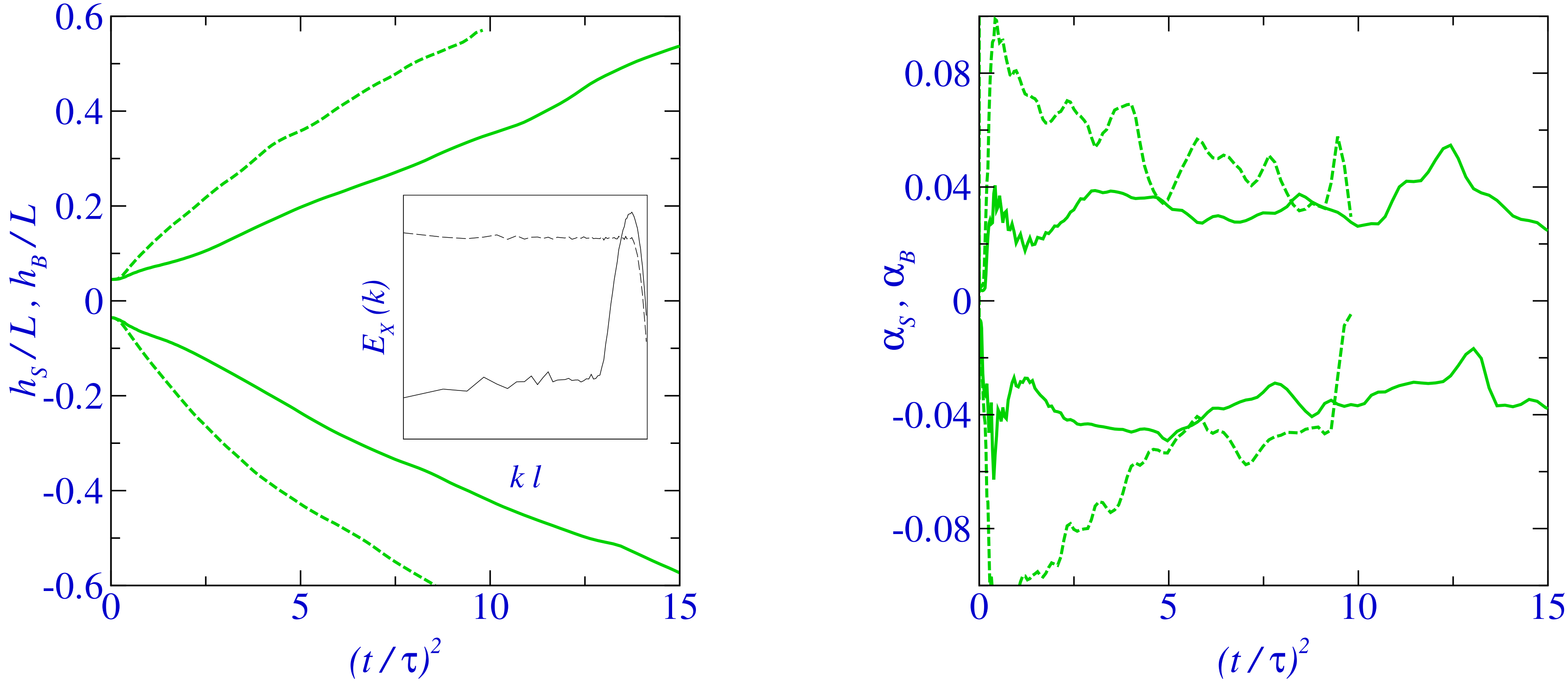
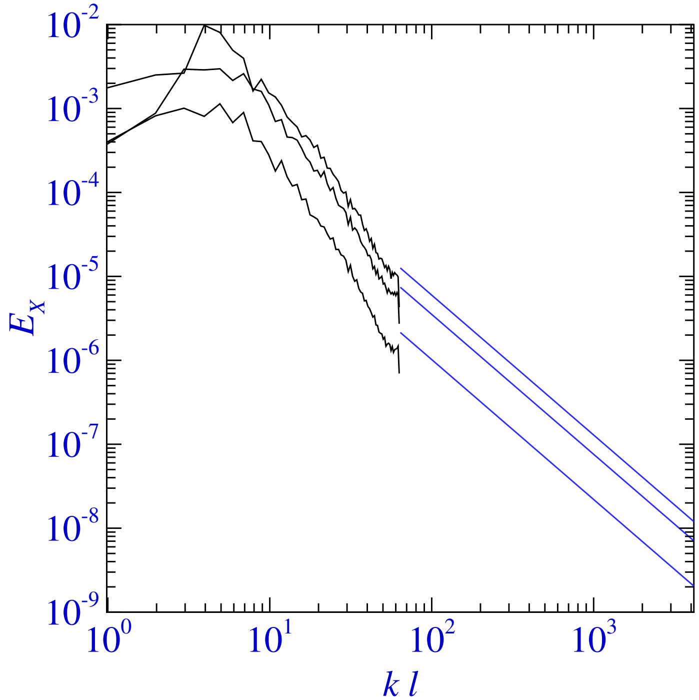
DOE/ASC
AFOSR

LES – initial conditions



- For broad spectrum initial conditions, LES predicts
  - Faster growth
  - Flow not self-similar

LES – Subgrid scalar energy estimate



- Assume:

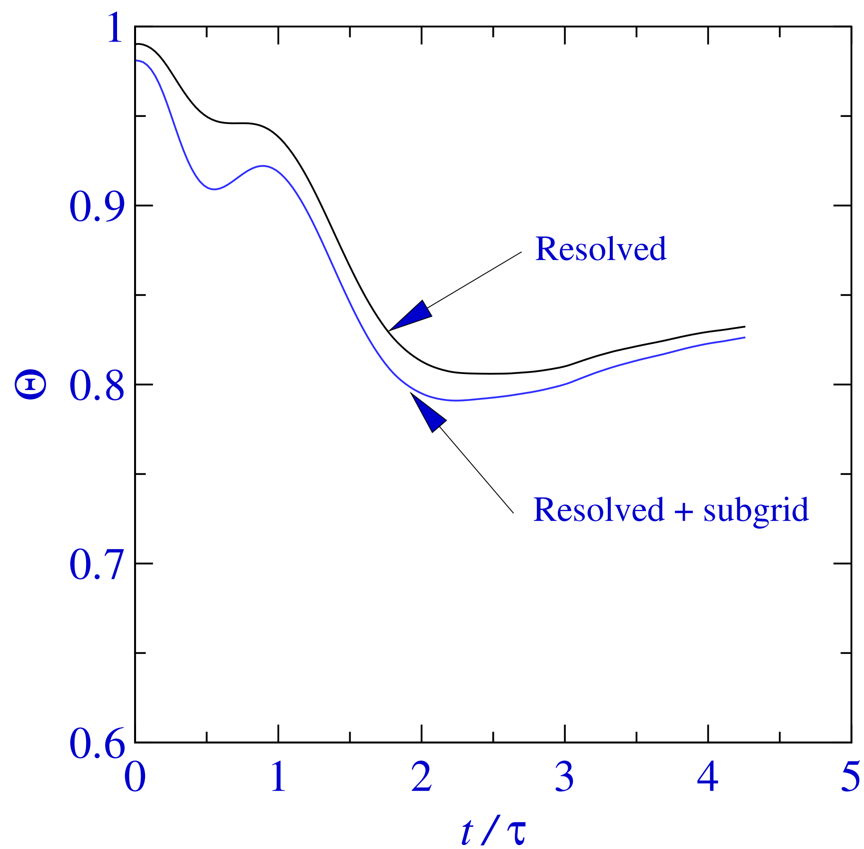
$$E_X(k) = \beta\epsilon^{-1/3}\epsilon_X k^{-5/3}$$

- $\beta\epsilon^{-1/3}\epsilon_X$ computing using analogous expressions for the second-order scalar structure function

- Subgrid variance:

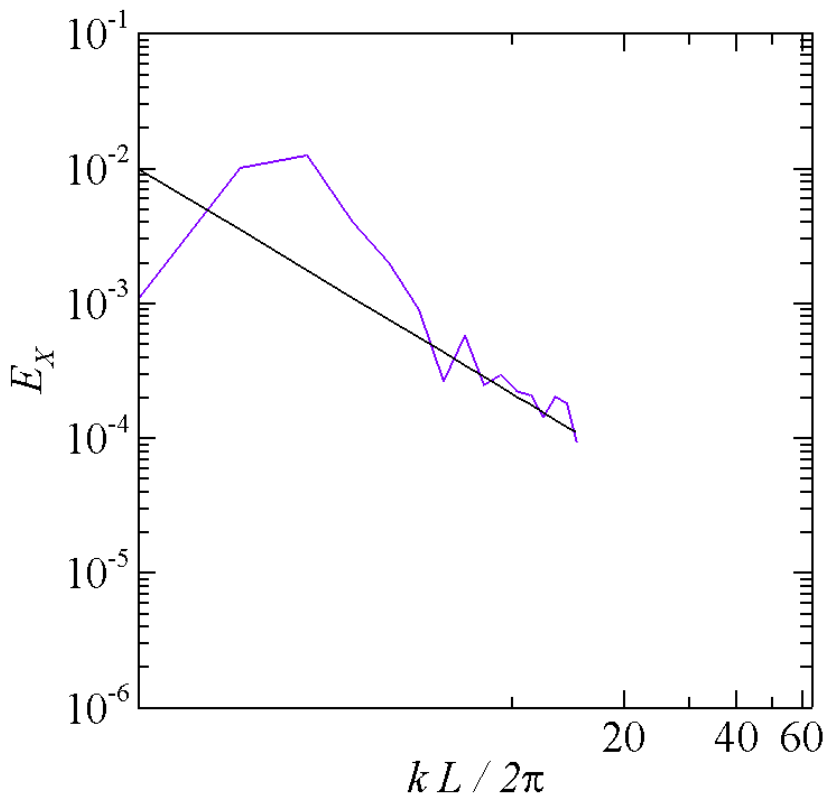
$$\overline{X^2} - \overline{X}^2 = \frac{3}{2}\beta\epsilon^{-1/3}\epsilon_X k_c^{-2/3}$$

LES – Youngs molecular mixing fraction



$$\Theta = \frac{\int_0^H \langle X(1-X)\rangle \, \mathrm{d}z}{\int_0^H \langle X\rangle\langle 1-X\rangle \, \mathrm{d}z} = \frac{\int_0^H \langle \overline{X}(1-\overline{X})\rangle - \langle \overline{X^2} - \overline{X}^2\rangle \, \mathrm{d}z}{\int_0^H \langle \overline{X}\rangle\langle 1-\overline{X}\rangle \, \mathrm{d}z}$$

LES – dynamic scalar-flux model



- Model originally contains a parameter, γ, which is estimated statically

$$q_i = -\frac{\gamma}{2}\Delta K^{1/2}(\delta_{ij} - e_i e_j)\frac{\partial \widetilde{Y}}{\partial x_j}$$

- Also possible to estimate γ dynamically