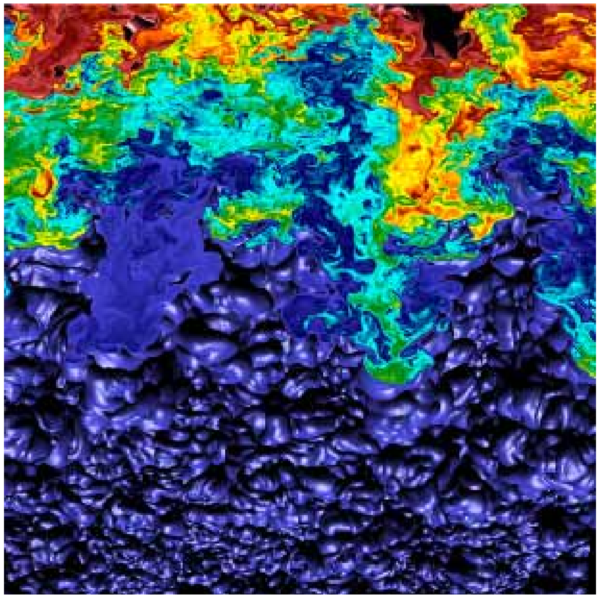
Direct Numerical Simulation of Rayleigh-Taylor Instability

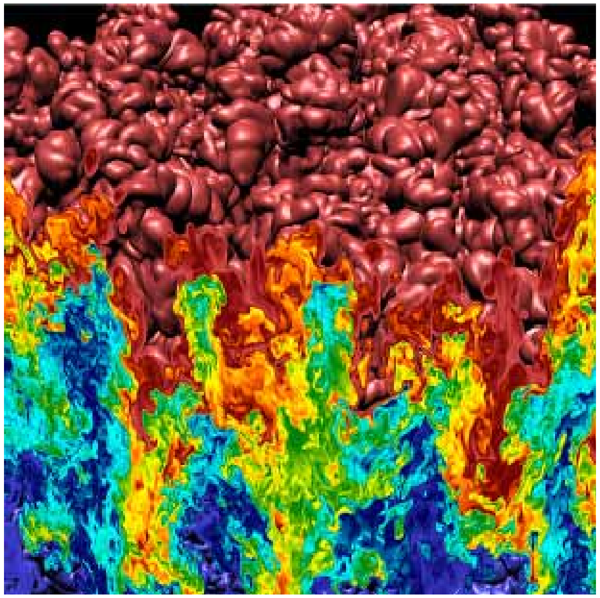


Bill Cabot,

Andy Cook

&

Paul Miller



CS and Viz Support: Mike Welcome (LBL), Brian Miller, Peter Williams, Hank Childs

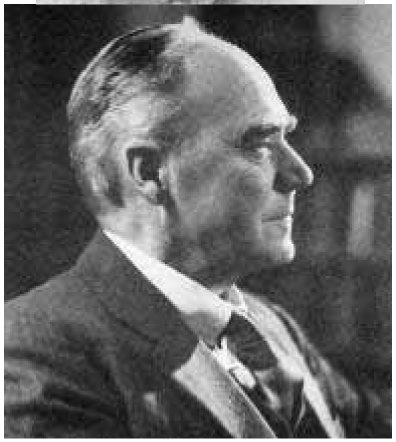
IWPCTM10, Paris

17–21 July 2006

This work was performed under the auspices of the US Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-ENG48.

UCRL-PRES-222608

Rayleigh-Taylor instability is an unsettled issue.



- Does the flow forget its initial conditions?
- Is the flow self-similar?
- What is alpha?
- How does mixing influence the growth rate?
- When does the flow become fully turbulent?
- What is the Reynolds number dependence?
- How should subgrid-scale models be initialized?

Results from high-resolution numerical simulations can be used to elucidate these issues and guide modeling.

The Navier-Stokes equations have been around for 185 years…

$$\frac{\partial \rho}{\partial t} + u_j \frac{\partial \rho}{\partial x_j} = \rho \frac{\partial}{\partial x_j}\left(\frac{D}{\rho} \frac{\partial \rho}{\partial x_j} \right) = -\rho \frac{\partial u_j}{\partial x_j} \ ,$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i \ , \qquad g_i = (0,0,-g)$$

$$\tau_{ij} = \rho \nu \left[\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right]$$

…nevertheless, fluid mechanics is not a dry subject.

The governing equations are solved with high-resolution numerical methods.

- 10^{th}-order compact/Padé spatial derivatives
- 3^{rd}-order predictor-corrector timestepping
- Direct Fourier/Padé Poisson solver
- 8^{th}-order dealiasing filter

- Vertically expanding grid is matched to a potential-flow solution in the far field.

The Crab Nebula is RT unstable.

Paris is the birthplace of the Navier-Stokes equations as well as some key solution methods.

Claude-Louis Navier

George Stokes

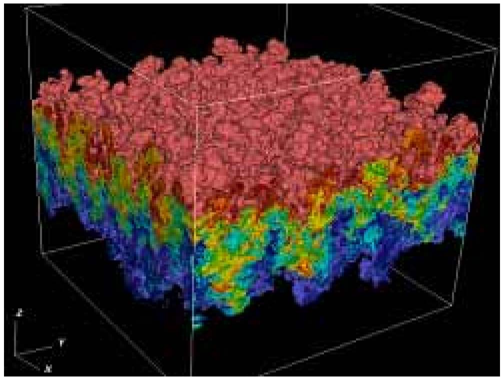
Siméon-Denis Poisson

Joseph Fourier

Who's not French?

Henri Padé

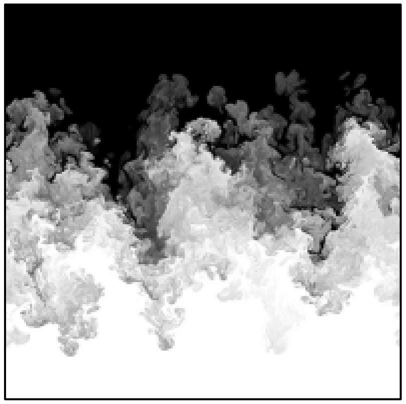
Setup for Rayleigh-Taylor DNS:



- 3:1 density ratio (Atwood number = 0.5)
- Schmidt number = $\nu/D = 1$
- Grid spacing $\Delta \approx \eta$ (Kolmogorov scale)
- 3072 x 3072 x 3072 grid points
- Error function for diffuse initial interface (5 grid points thick) with horizontally perturbed position
- Periodic side boundaries
- Potential-flow vertical boundaries at early times
- Free-slip walls at top and bottom boundaries

Viscous and diffusion scales are resolved.

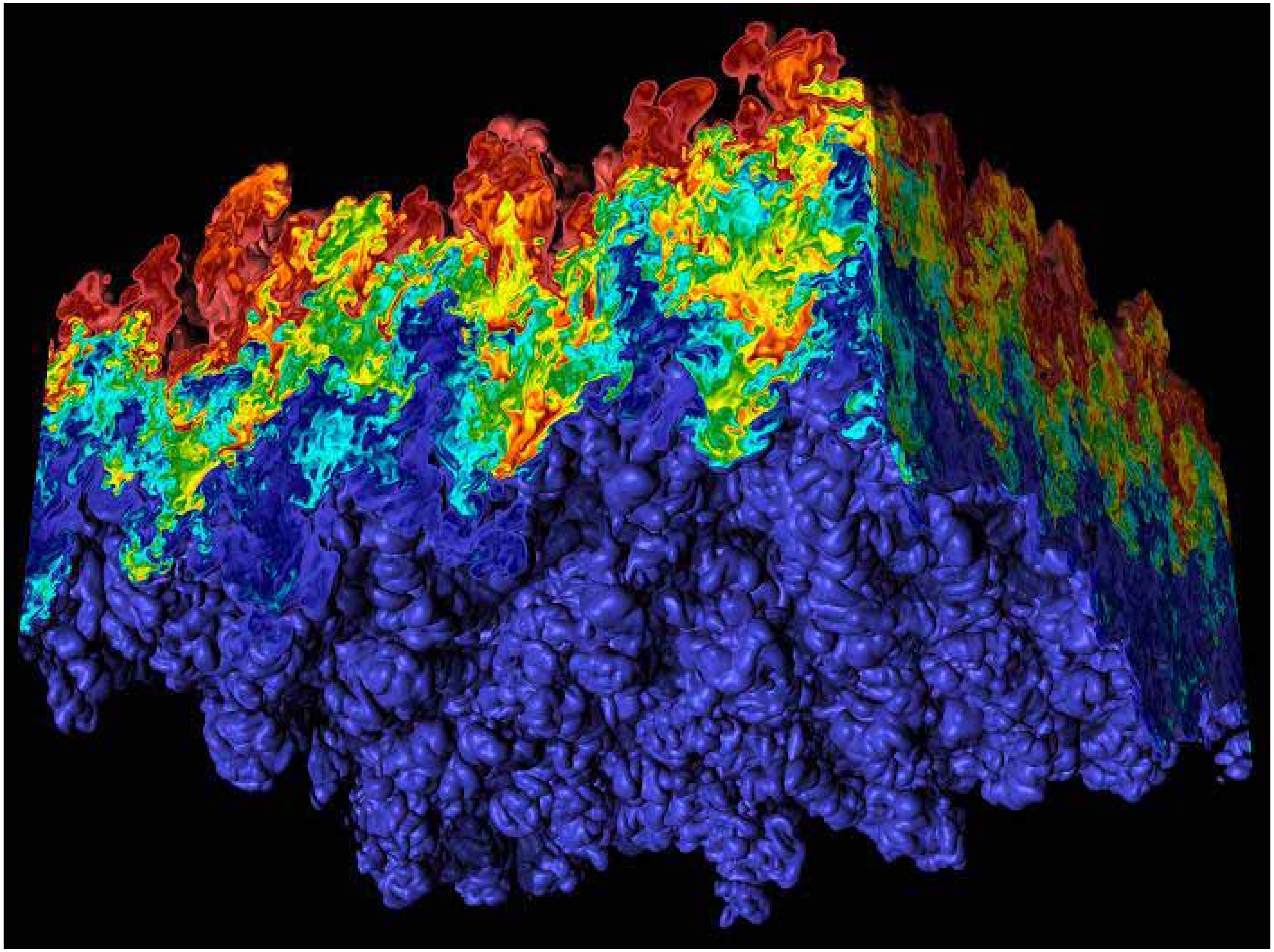
Direct Numerical Simulation serves as a low-Re "numerical experiment"



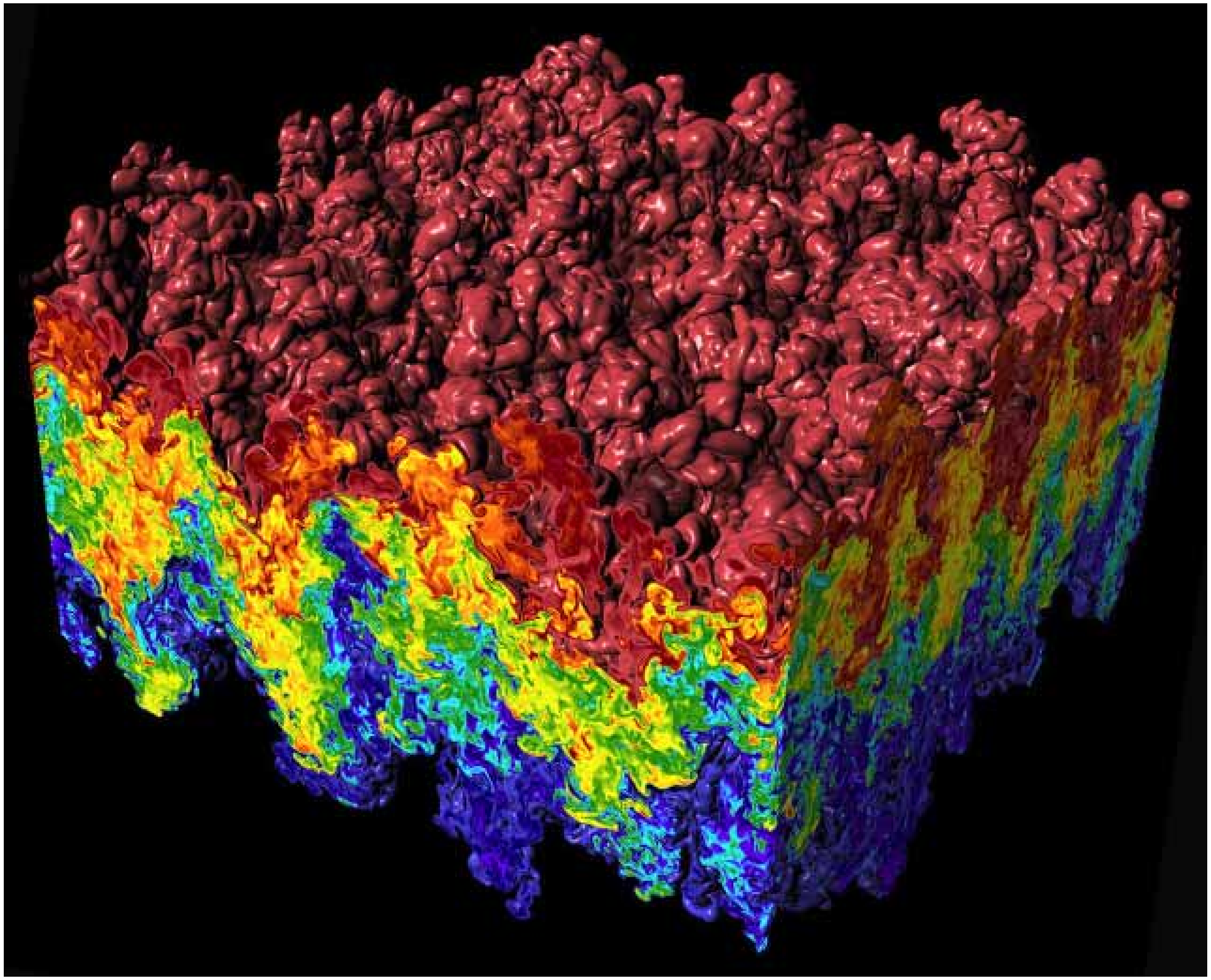
- DNS resolves all relevant scales in turbulent flow (inertial, dissipation, and diffusion); there are no model approximations.
- Turbulence is inherently three-dimensional.
- DNS is limited to low to moderate Reynolds numbers, constrained by computer resources.
- To reach a fully turbulent state (e.g., mixing transition), the outer-scale Reynolds number must exceed $Re > 10^4$ (microscale $Re_\lambda > 10^2$).
- The range of scales ($\propto$ number of grid points N) in any direction is $\Lambda/\eta \sim Re^{3/4}$; hence the cost of DNS $\sim N^4 \sim Re^3$ (assuming perfect parallel scaling).
- DNS needs large resources to reach higher Re.

BG/L is the fastest computer in the world.

There is not much pure heavy fluid in the spikes.



There is not much pure light fluid in the bubbles.



Gravity and initial perturbations set characteristic length and time scales.

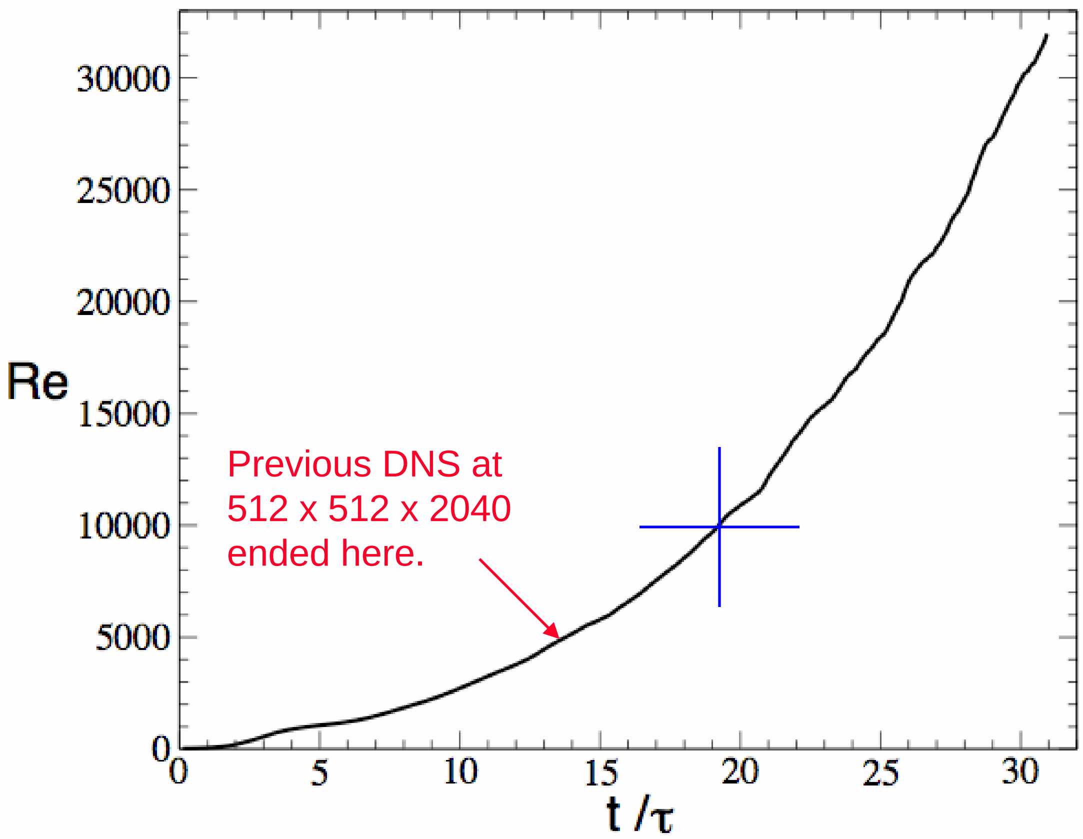
Dominant wavelength: $$l = 2\pi \frac{\int_0^\infty \frac{E(k)}{k}\,dk}{\int_0^\infty E(k)\,dk} \quad , \quad l_0 = l(t=0)$$

Corresponding timescale: $$\tau = \left(\frac{l_0}{Ag}\right)^{1/2} \quad , \quad A = \frac{\rho_2 - \rho_1}{\rho_2 + \rho_1} = 1/2$$

Initial spectrum peaked at mode 96.

Outer-scale Reynolds number reaches 32,000.

$$\mathrm{Re} = H\dot{H} / \nu$$

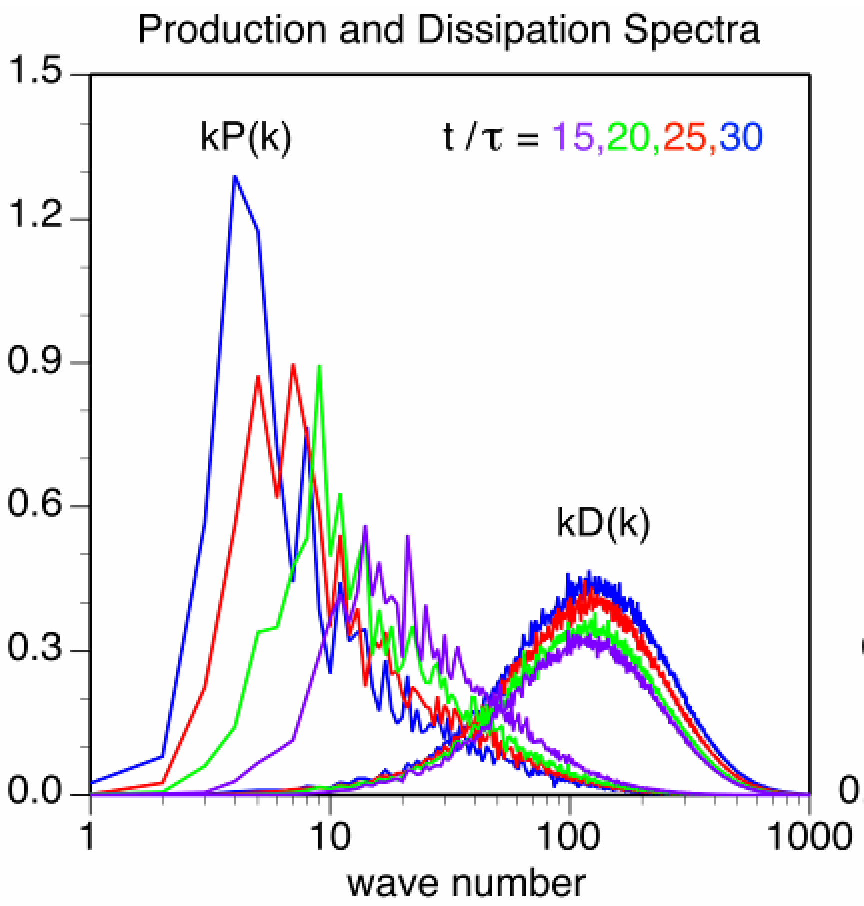


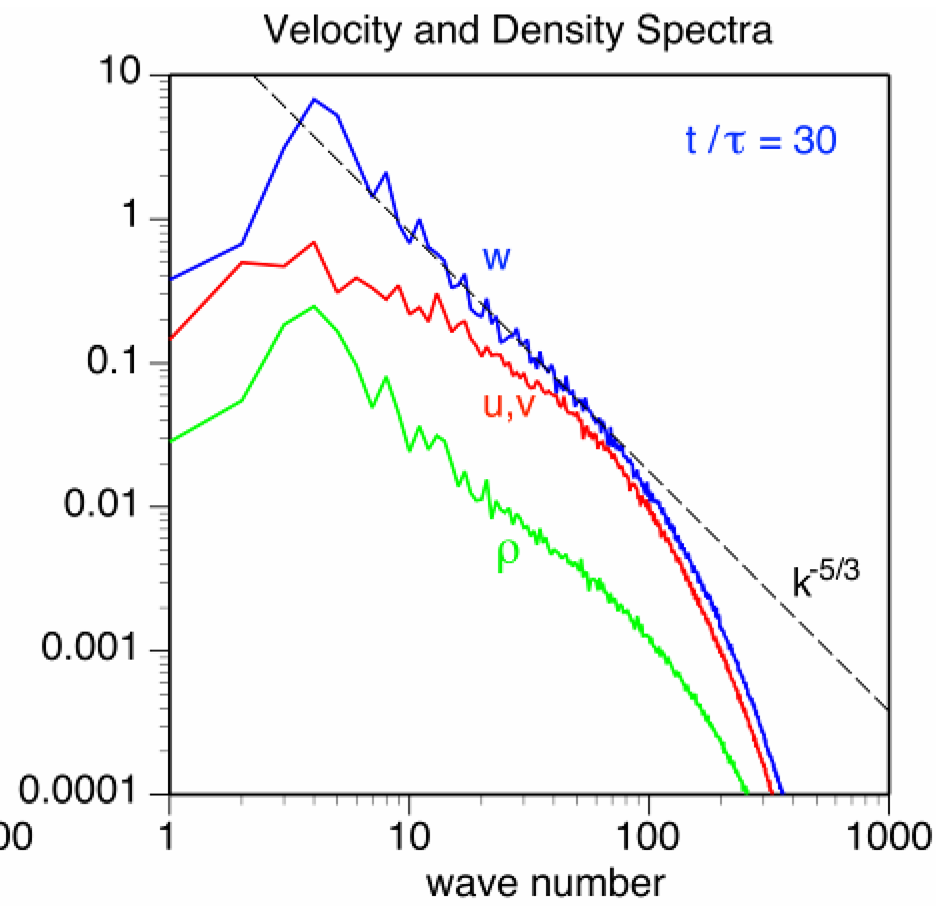
H is based on the 1% concentration threshold.

Re ~ 10^4 (Re_λ ~ 10^2) marks the beginning of the turbulent regime and the formation of an inertial range in the energy spectrum.

Re crosses 10,000 around t/τ = 19.

Spectra develop scale separation and inertial ranges at late time.

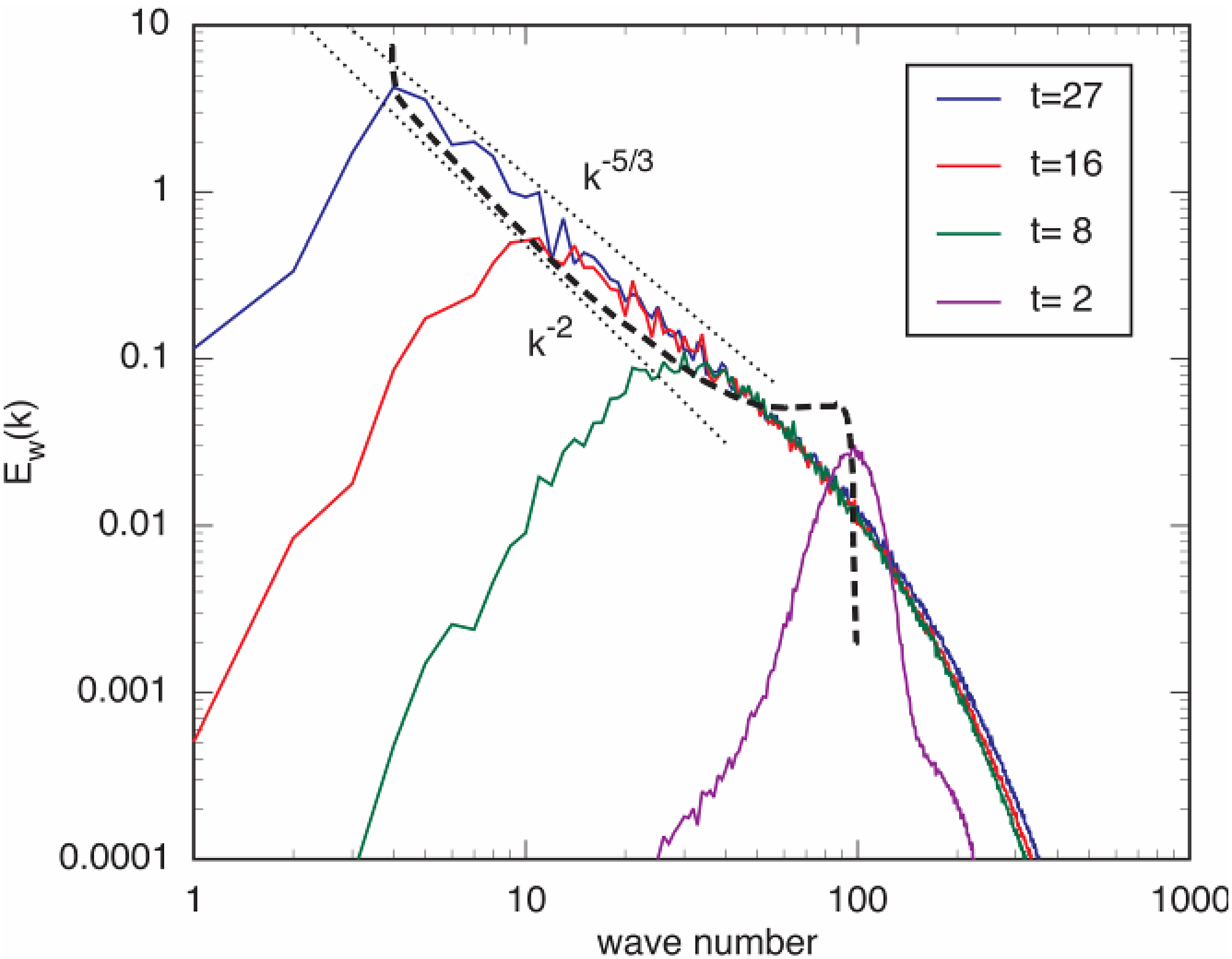


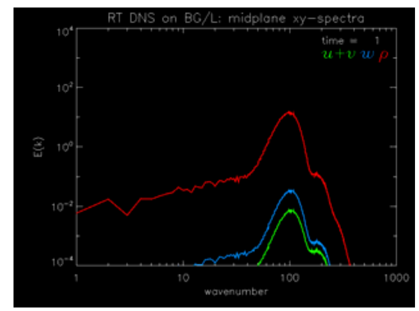


Separation > 10 for t/τ > 19.

Kolmogorov spectrum for w.

Peak of energy spectrum follows a k^{-2} trajectory once the flow becomes self-similar. (see Olivier Poujade's talk)





Growth and mixing are characterized in terms of a product function X_p.

Heavy-fluid mole fraction: $$X = \frac{\rho - \rho_1}{\rho_2 - \rho_1}$$

$$\boxed{X_{st} = \frac{1}{2}}$$

Product (mixed fluid): $$X_p(X) = \begin{cases} X / X_{st} & \text{if } X \le X_{st} \\ (1-X)/(1-X_{st}) & \text{if } X > X_{st} \end{cases}$$

Product thickness:

$$h = \int_{-\infty}^{\infty} X_p(\langle X \rangle)\,dz$$

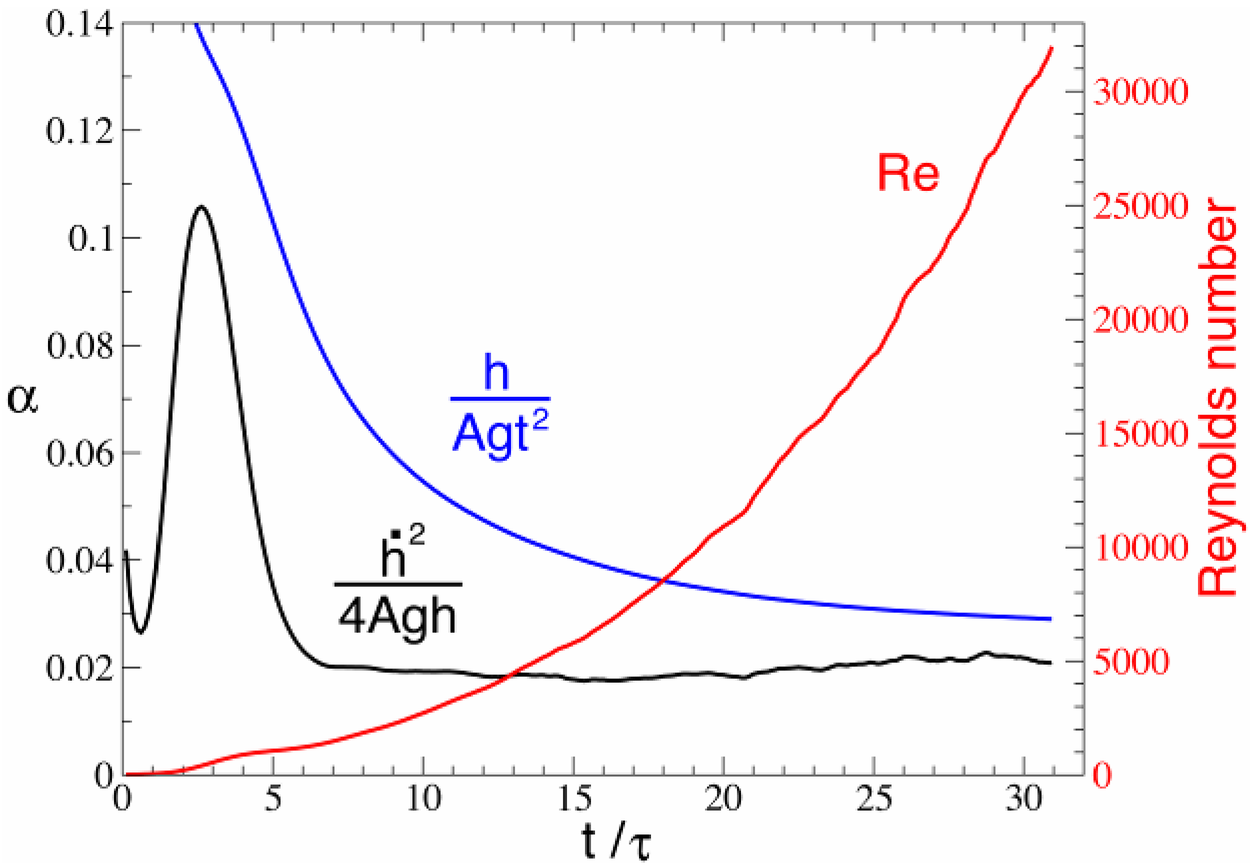
Mixedness:

$$\Xi = \frac{\int_{-\infty}^{\infty} \langle X_p(X) \rangle\,dz}{\int_{-\infty}^{\infty} X_p(\langle X \rangle)\,dz}$$

Integral measure of mix height is insensitive to statistical fluctuations.

In the self-similar regime, $(dh/dt)^2 = 4\alpha Agh$

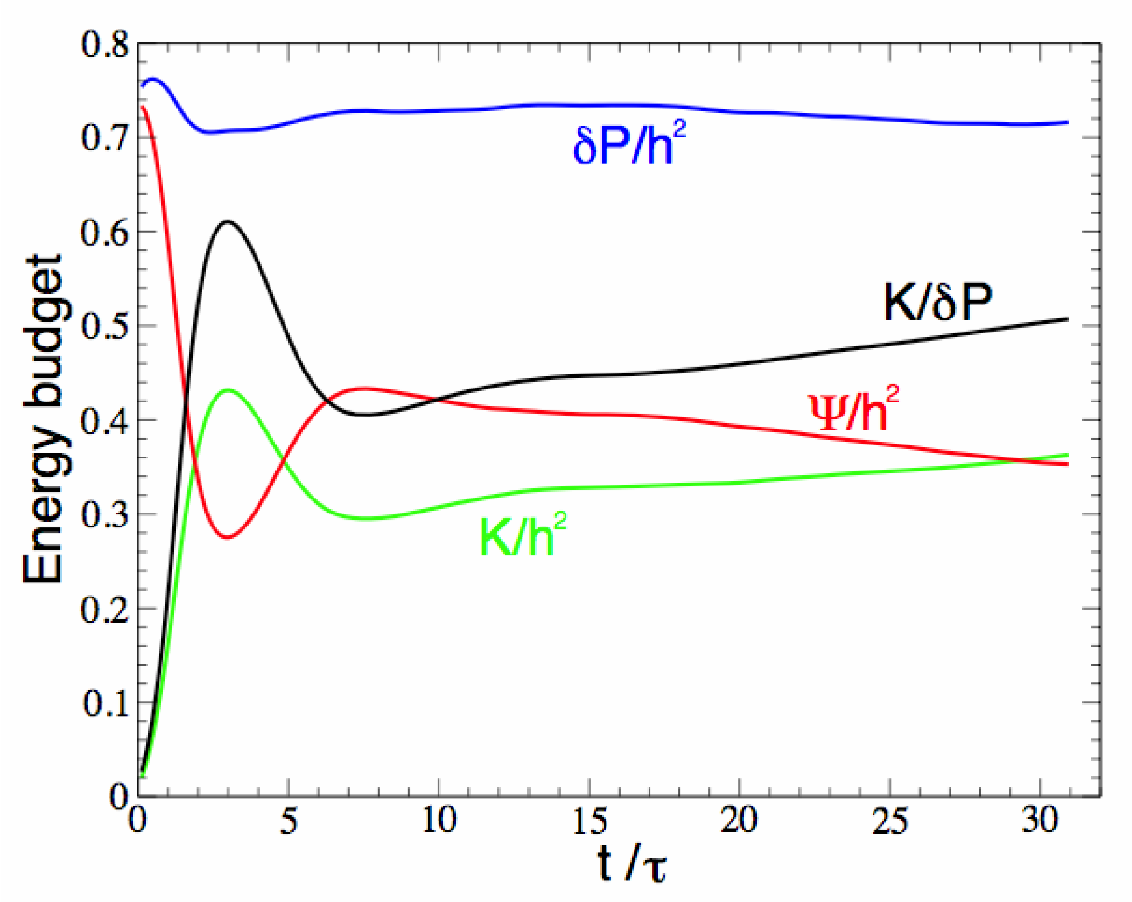
(Ristorcelli & Clark, JFM 2004 and Jacobs & Dalziel, JFM 2005).



- h_o relates to the spectrum of initial perturbations.
- The linear term never completely goes away.
- Using h/Agt^2, larger simulations, run to later times, give smaller α.
- There is a slight but steady increase for Re>10,000.

$$h = \alpha Agt^2 + 2(\alpha Agh_o)^{1/2}t + h_o$$

Many models assume a constant ratio of kinetic energy to released potential energy.



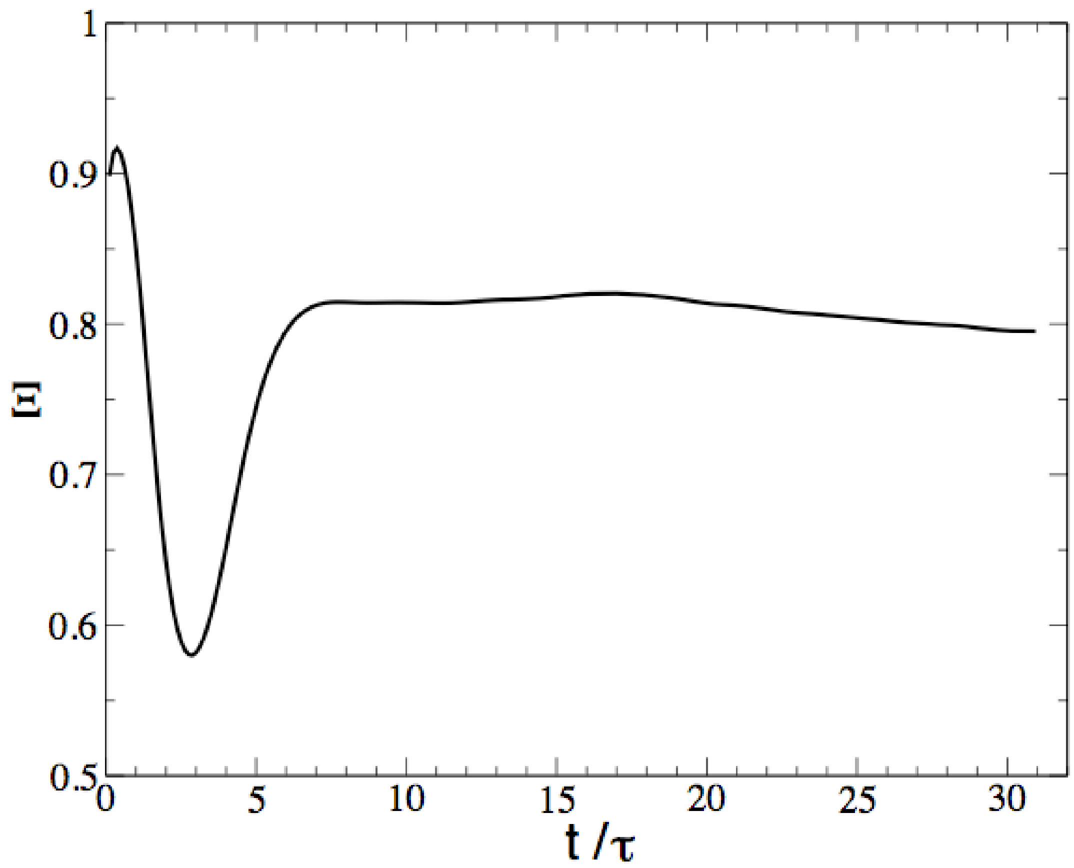
Potential energy δP is converted to **kinetic energy K**, which cascades down to small scales where it is removed by **heat dissipation Ψ**.

Alpha Group derived

$K_z/\delta P = 12\alpha$

K/δP rises steadily for Re > 10,000.

The mixing rate lags the entrainment rate when the flow enters the turbulent regime.



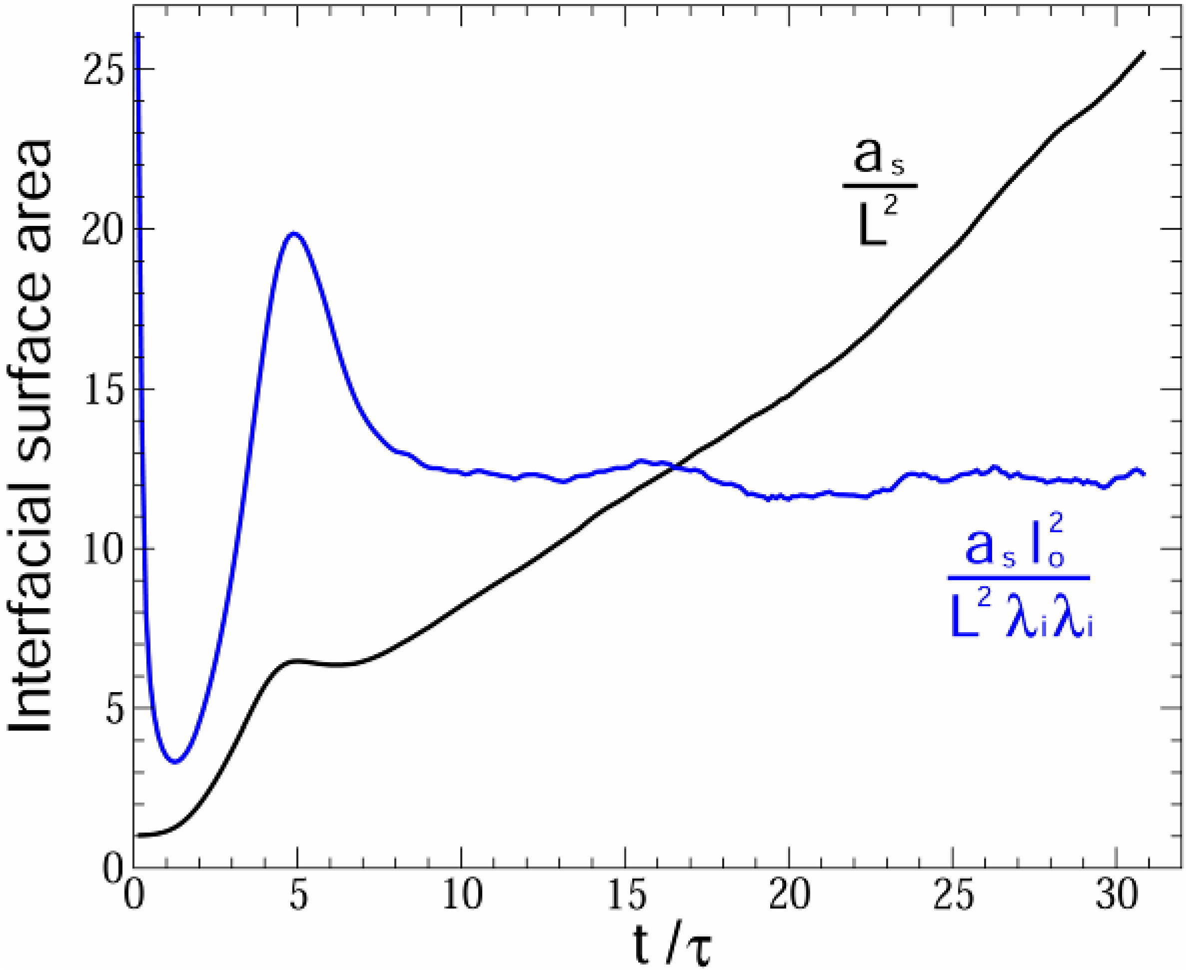
$$\Xi = \frac{\int_{-\infty}^{\infty} \left\langle X_p(X) \right\rangle dz}{\int_{-\infty}^{\infty} X_p\left(\left\langle X \right\rangle\right) dz}$$

1 → homogenized

0 → segregated

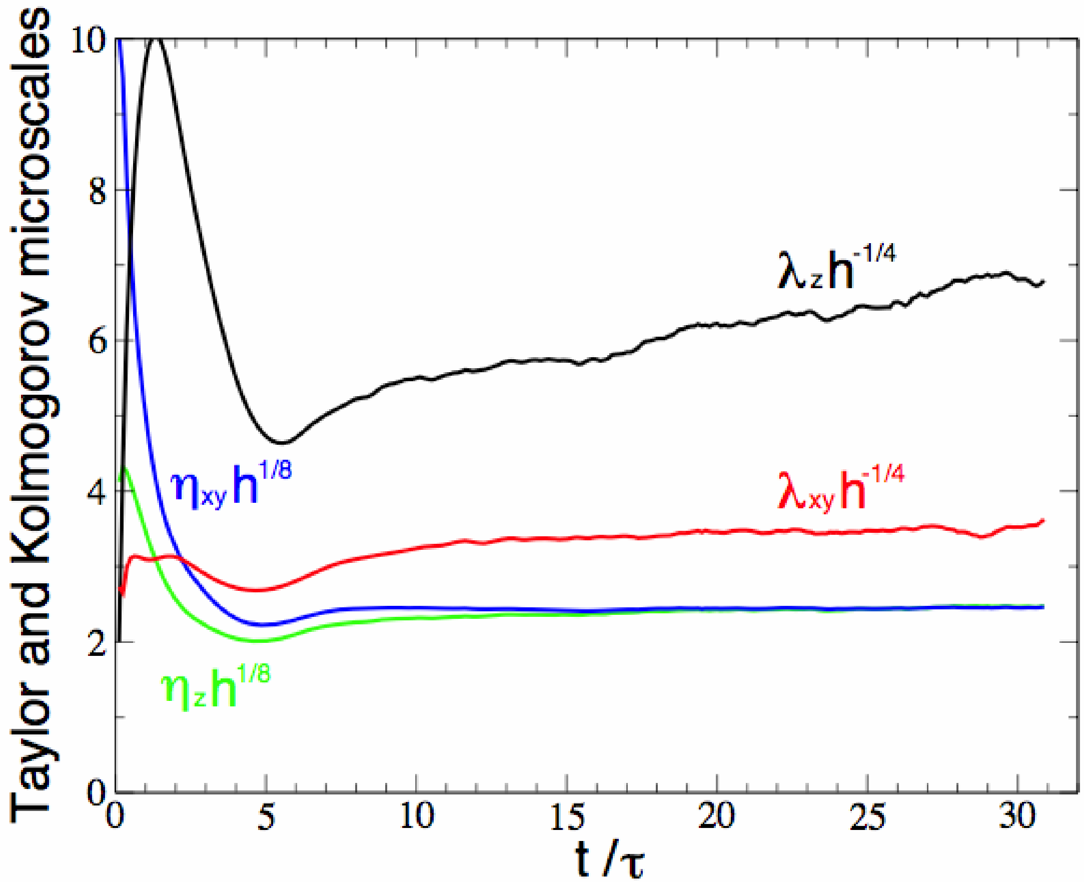
Ever bigger blobs have to be broken down to ever finer scales.

Surface area exhibits weak Re dependence for Re>10,000.



Area of equimolar surface scales with Taylor microscale.

Self-similarity gives: $\lambda \sim h^{1/4} \sim t^{1/2}$, $\eta \sim h^{-1/8} \sim t^{-1/4}$ (Ristorcelli & Clark, JFM 2004).

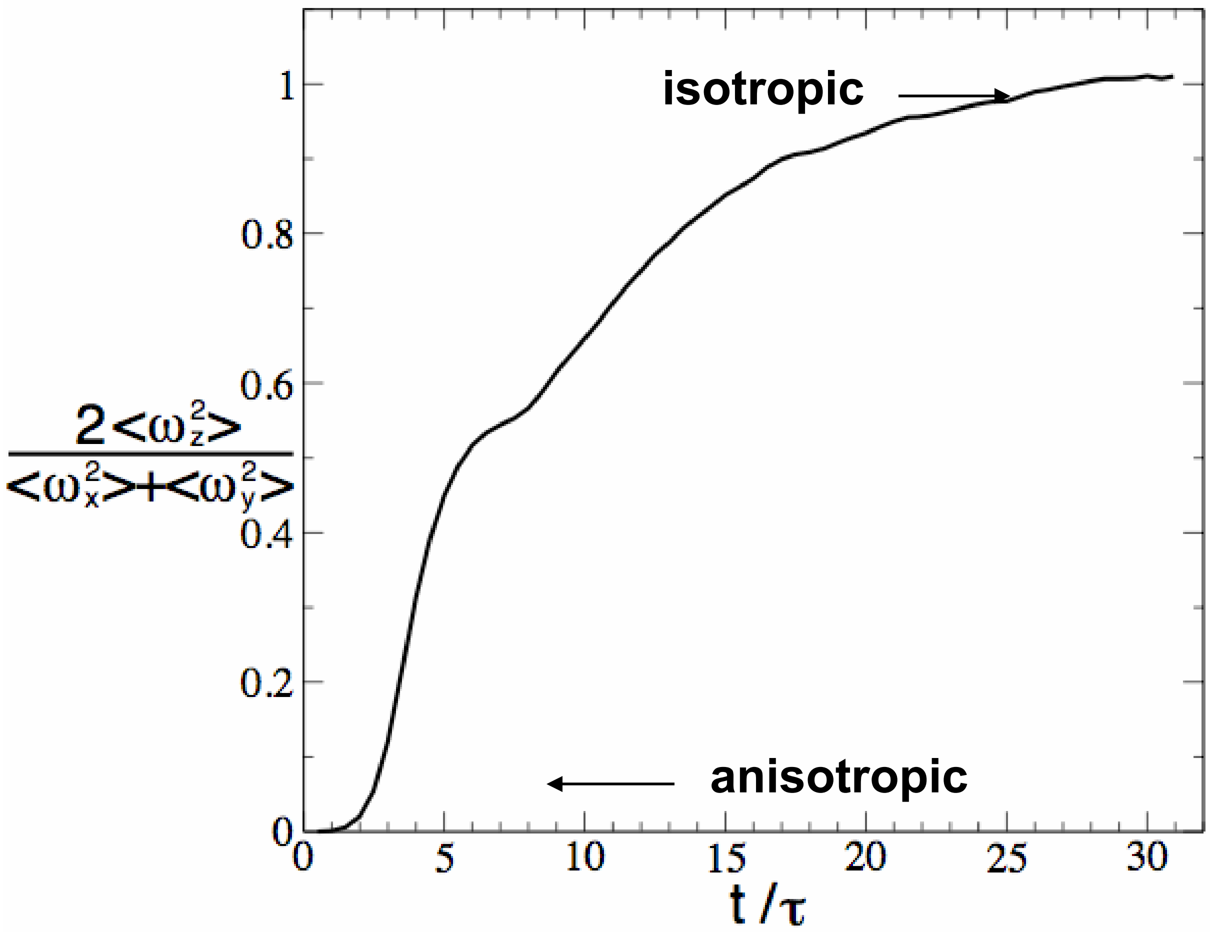


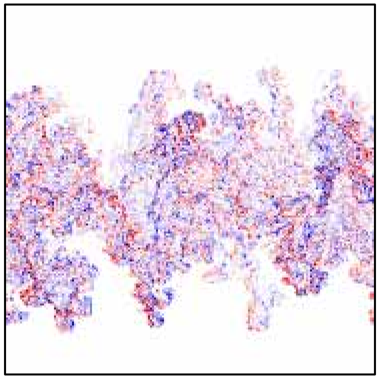
Taylor microscales (λ_i) stay anisotropic.

Kolmogorov microscales (η_i) become isotropic by late time.

DNS confirms moment similarity predictions except for λ_z.

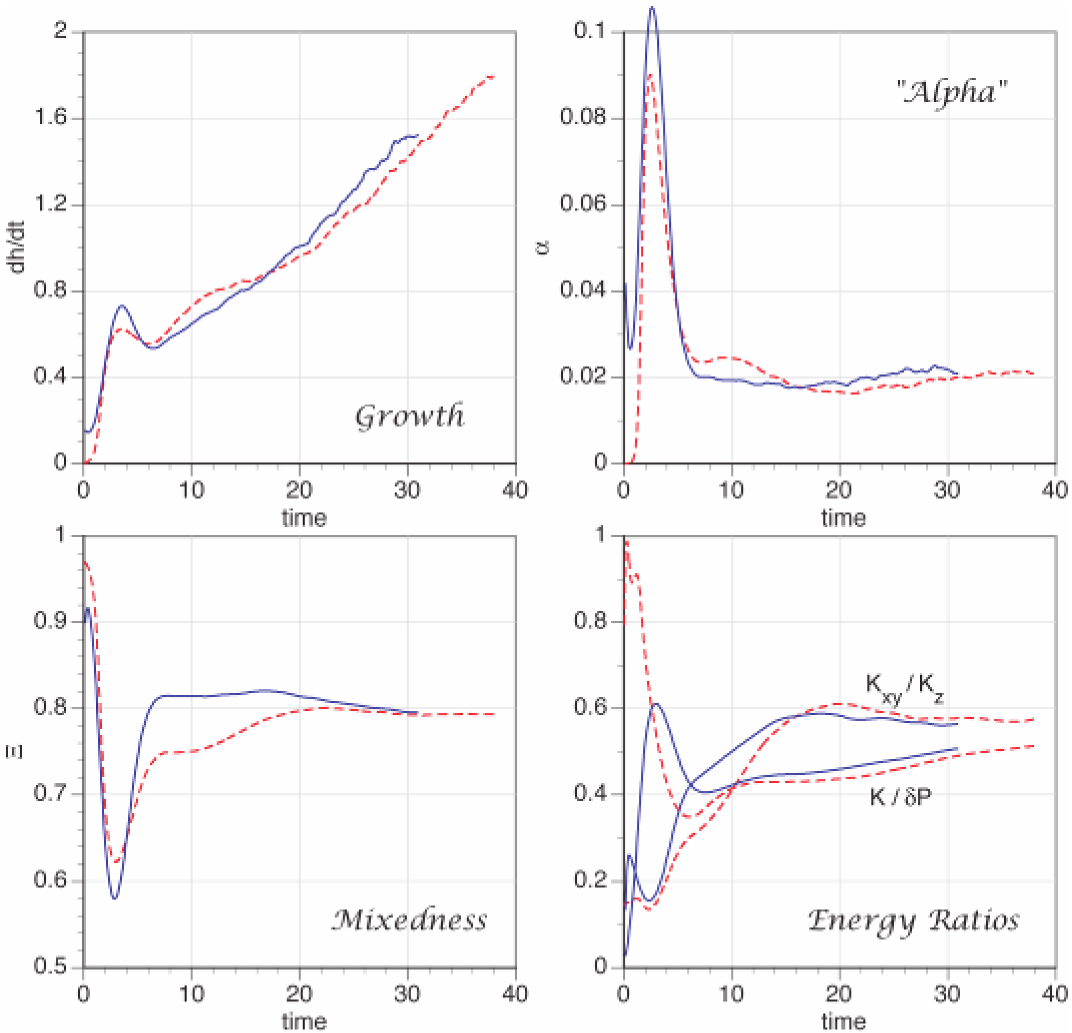
Enstrophy becomes isotropic near midplane only at very late time.





Flow near bubble and spike fronts is always highly anisotropic.

Similar trends were observed in a previous 1152^3 LES (Cook, Cabot & Miller, JFM 2004).



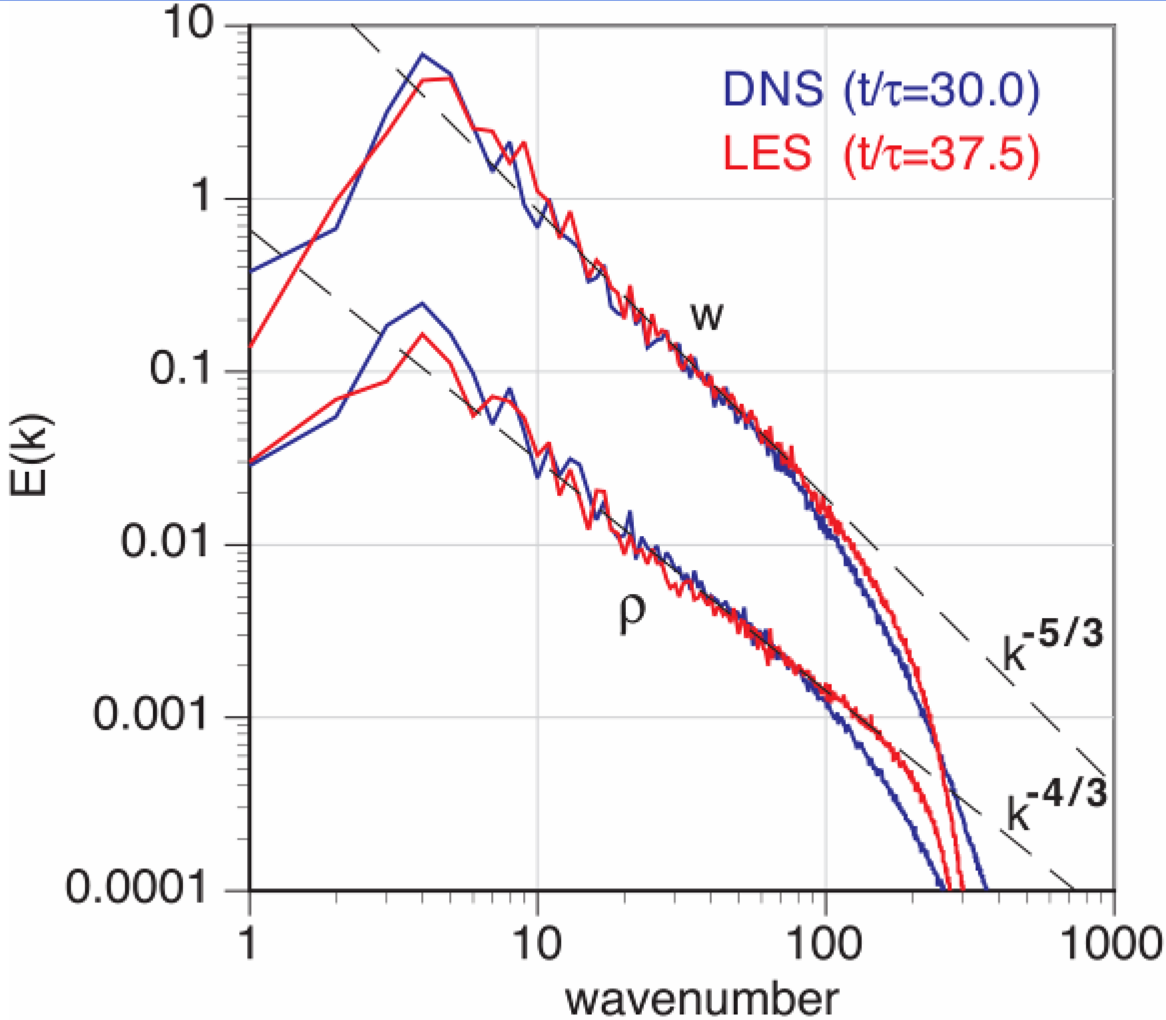
A = 0.5

3072^3 DNS

1152^3 LES

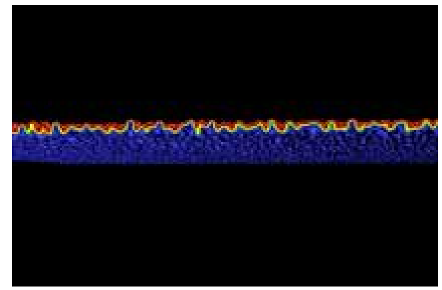
LES results suggest that some quantities may asymptote at later times.

Shallower slope of density spectrum is observed in both DNS and LES.



3072³ DNS, 1152³ LES

DNS of R-T instability at Re up to 32,000 yields some surprises.



- α cannot be determined by plotting h vs. Agt^2.
- Kinetic/Potential energy ratio keeps rising.
- Taylor microscales are always anisotropic.
- Kolmogorov scales and enstrophy eventually become isotropic.
- Flow is weakly Reynolds number dependent for Re>10,000.
- How should growth and mixing curves be extrapolated to very high Reynolds number regimes?

Extremely large simulations are required to escape initial, boundary, and low-Re effects and obtain good statistical samples.