Direct Numerical Simulation of Rayleigh-Taylor Instability

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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…

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

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

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

…nevertheless, fluid mechanics is not a dry subject.
The governing equations are solved with high-resolution numerical methods.

- 10th-order compact/Padé spatial derivatives
- 3rd-order predictor-corrector timestepping
- Direct Fourier/Padé Poisson solver
- 8th-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.
Setup for Rayleigh-Taylor DNS:

- 3:1 density ratio (Atwood number = 0.5)
- Schmidt number = \( v/D = 1 \)
- 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 $\text{Re} > 10^4$ (microscale $\text{Re}_\lambda > 10^2$).

• The range of scales ($\propto$ number of grid points $N$) in any direction is $\Lambda/\eta \sim \text{Re}^{3/4}$; hence the cost of DNS $\sim N^4 \sim \text{Re}^3$ (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: \[ l = 2\pi \frac{\int_0^\infty \frac{E(k)}{k} dk}{\int_0^\infty E(k) dk}, \quad l_0 = l(t = 0) \]

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

Initial spectrum peaked at mode 96.
Outer-scale Reynolds number reaches 32,000.

\[ \text{Re} = \frac{\bar{H} \bar{\dot{H}}}{\nu} \]

H is based on the 1% concentration threshold.

\( \text{Re} \sim 10^4 \) (\( \text{Re}_\lambda \sim 10^2 \)) marks the beginning of the turbulent regime and the formation of an inertial range in the energy spectrum.

Previous DNS at 512 x 512 x 2040 ended here.

\( \text{Re} \) crosses 10,000 around \( t/\tau = 19 \).

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Spectra develop **scale separation and inertial ranges** at late time.

Separation > 10 for $t/\tau > 19$.

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: $$X = \frac{\rho - \rho_1}{\rho_2 - \rho_1} \quad \frac{X_{st}}{2}$$

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

Product thickness: $$h = \int_{-\infty}^{\infty} X_p\left(\langle X \rangle\right) dz$$

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

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 \(\alpha\).
- 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 $\delta P$ is converted to kinetic energy $K$, which cascades down to small scales where it is removed by heat dissipation $\Psi$.

Alpha Group derived

$$K_\tau/\delta P = 12\alpha$$

$K/\delta P$ rises steadily for $Re > 10,000$. 
The mixing rate lags the entrainment rate when the flow enters the turbulent regime.

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

1 → homogenized
0 → segregated

Ever bigger blobs have to be broken down to ever finer scales.
Surface area exhibits weak Re dependence for $\text{Re}>10,000$. 

Area of equimolar surface scales with Taylor microscale.

\[
\frac{a_s}{L^2} \quad \frac{a_s l_o^2}{L^2 \lambda_i \lambda_i}
\]
Self-similarity gives: $\lambda \sim h^{1/4} t^{1/2}, \eta \sim h^{-1/8} t^{-1/4}$ (Ristorcelli & Clark, JFM 2004).

Taylor microscales ($\lambda_i$) stay anisotropic.

Kolmogorov microscales ($\eta_i$) become isotropic by late time.

DNS confirms moment similarity predictions except for $\lambda_z$. 
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).

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

$A = 0.5$

$3072^3$ 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.
DNS of R-T instability at Re up to 32,000 yields some surprises.

- $\alpha$ 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.