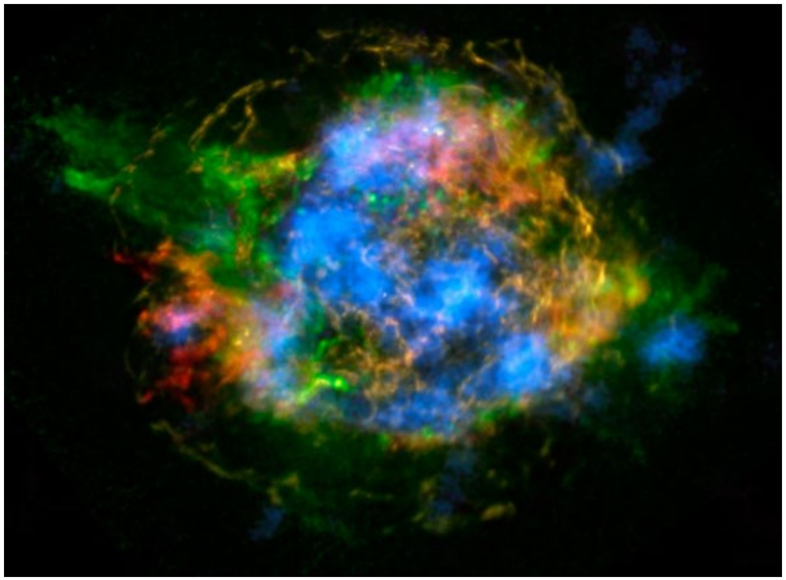
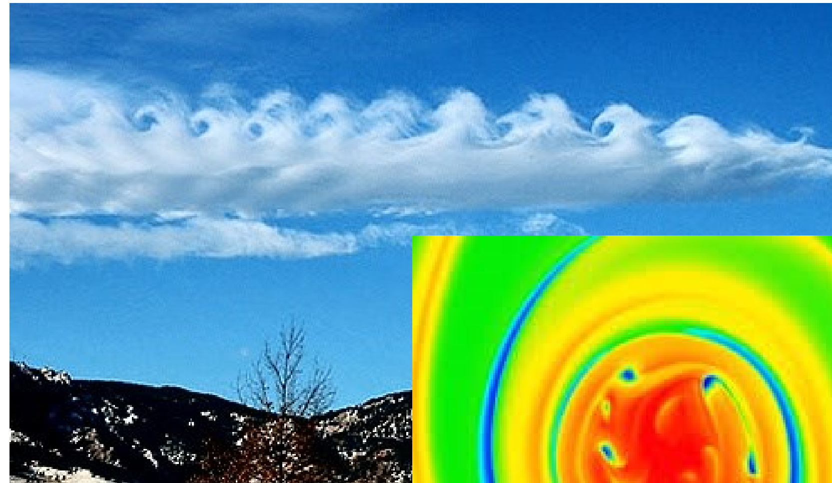
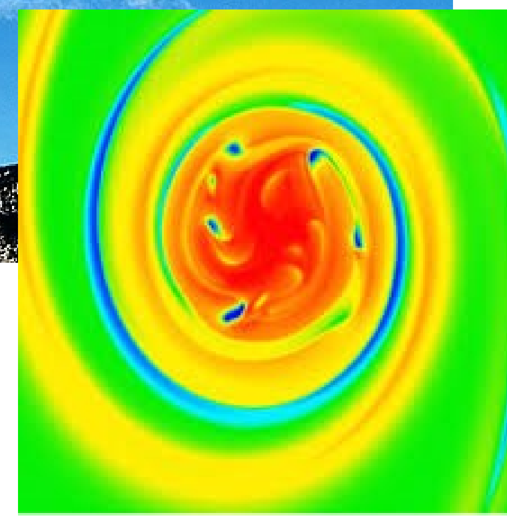
High-Order Eulerian Simulations of Multi-material Flows







Andrew W. Cook

MultiMat

September 2015

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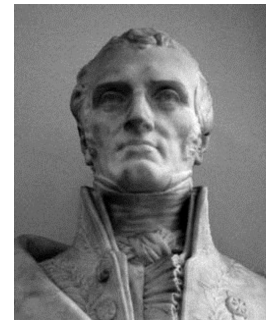
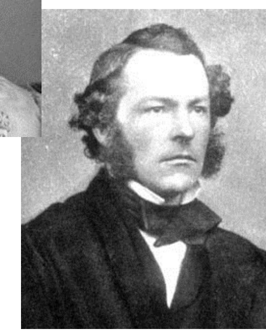
What have we learned from our numerical solutions to the multi-component Navier-Stokes equations?

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \left(\rho Y_i \mathbf{u} \right) = -\nabla \cdot \mathbf{J}_i$$





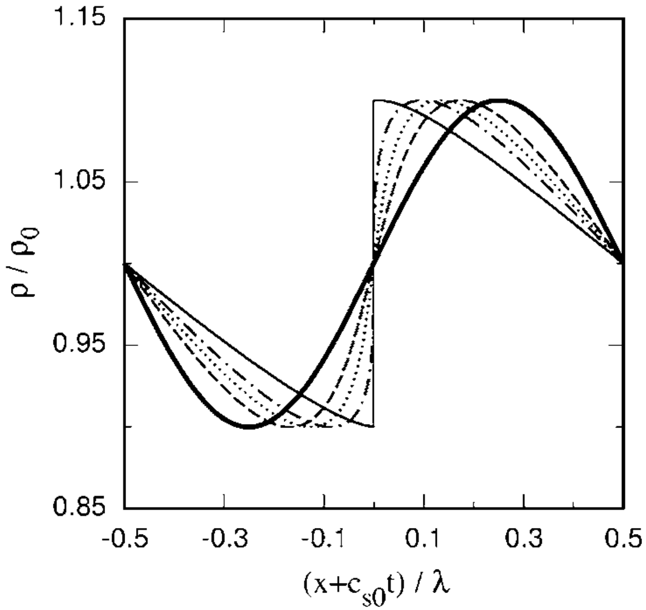
$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \left(\rho \mathbf{u}\,\mathbf{u} + p \underline{\boldsymbol{\delta}} \right) = \nabla \cdot \underline{\boldsymbol{\tau}}$$

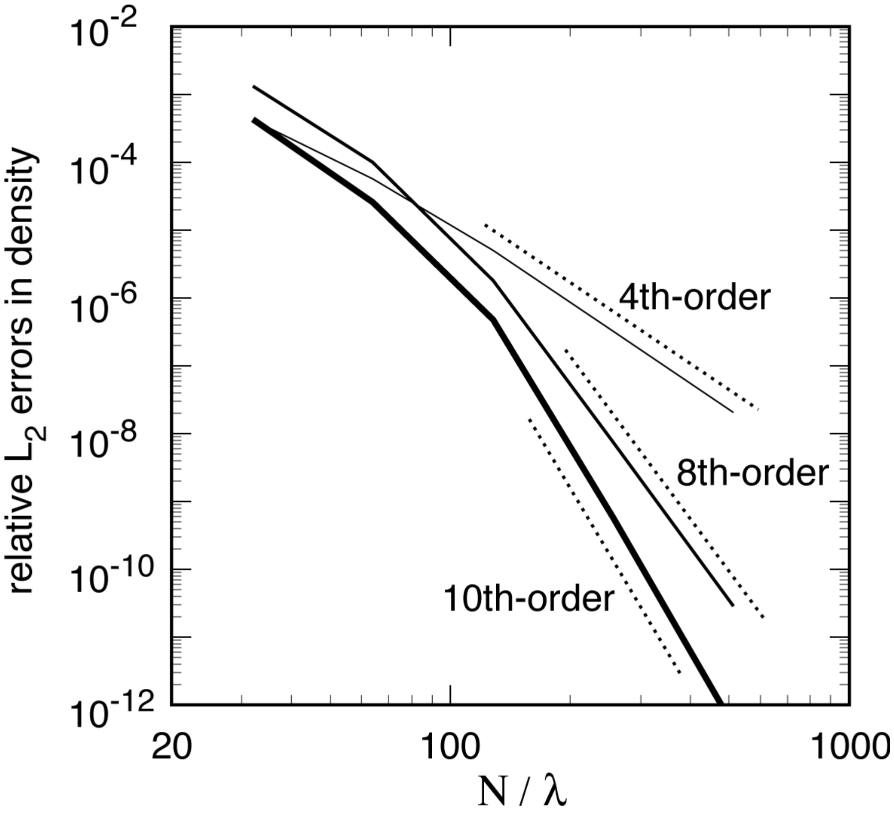
$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left[\left(E + p \right) \mathbf{u} \right] = \nabla \cdot \left(\underline{\boldsymbol{\tau}} \cdot \mathbf{u} - \mathbf{q}_c - \mathbf{q}_d \right)$$

Enthalpy Diffusion: $\mathbf{q}_d = h_i \mathbf{J}_i$

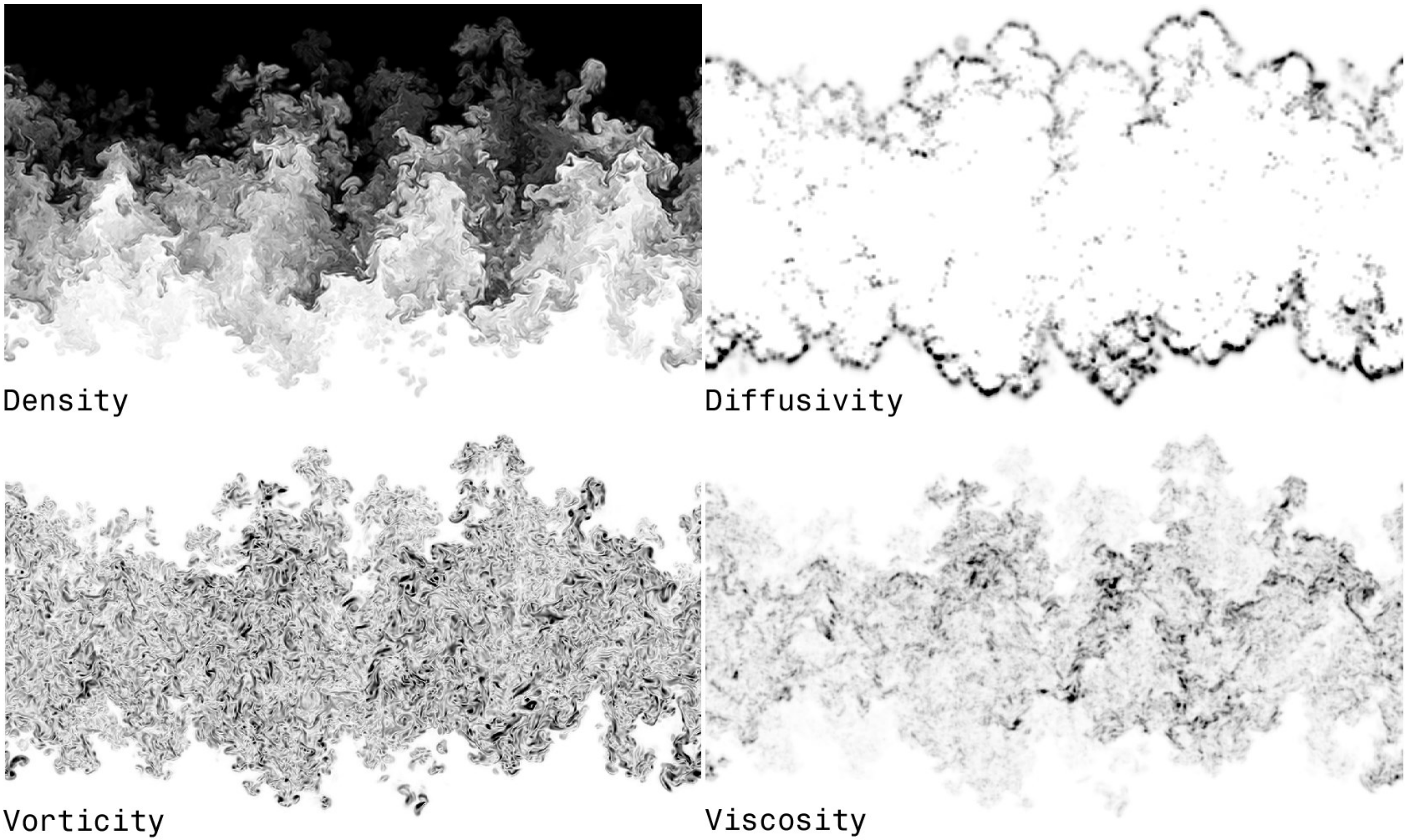
Miranda solves the N-S equations with spectral-like numerics.

- **10^{th}-order compact (Padé) derivatives**
- **4^{th}-order Runge-Kutta timestepping**
- **8^{th}-order dealiasing filter**
- **8^{th}-order hyperviscosity**

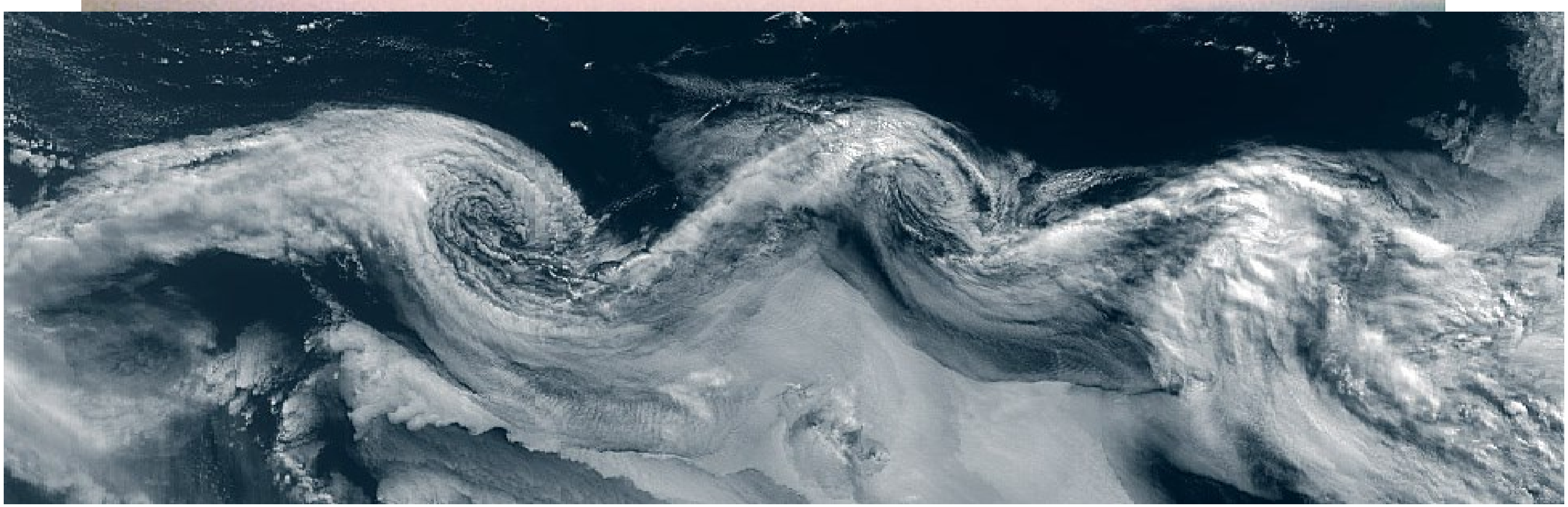




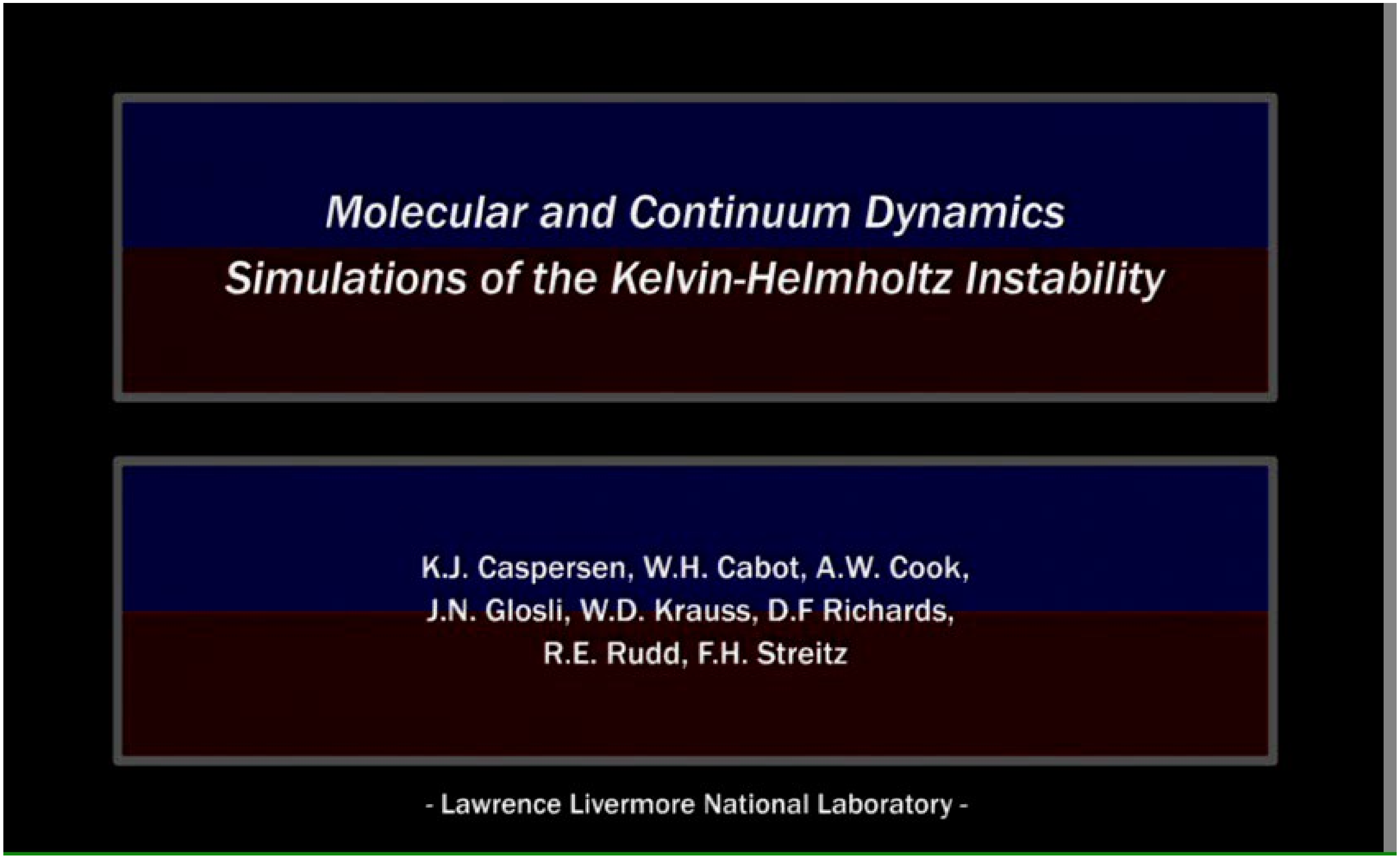
Subgrid-scale models reduce Gibbs oscillations.



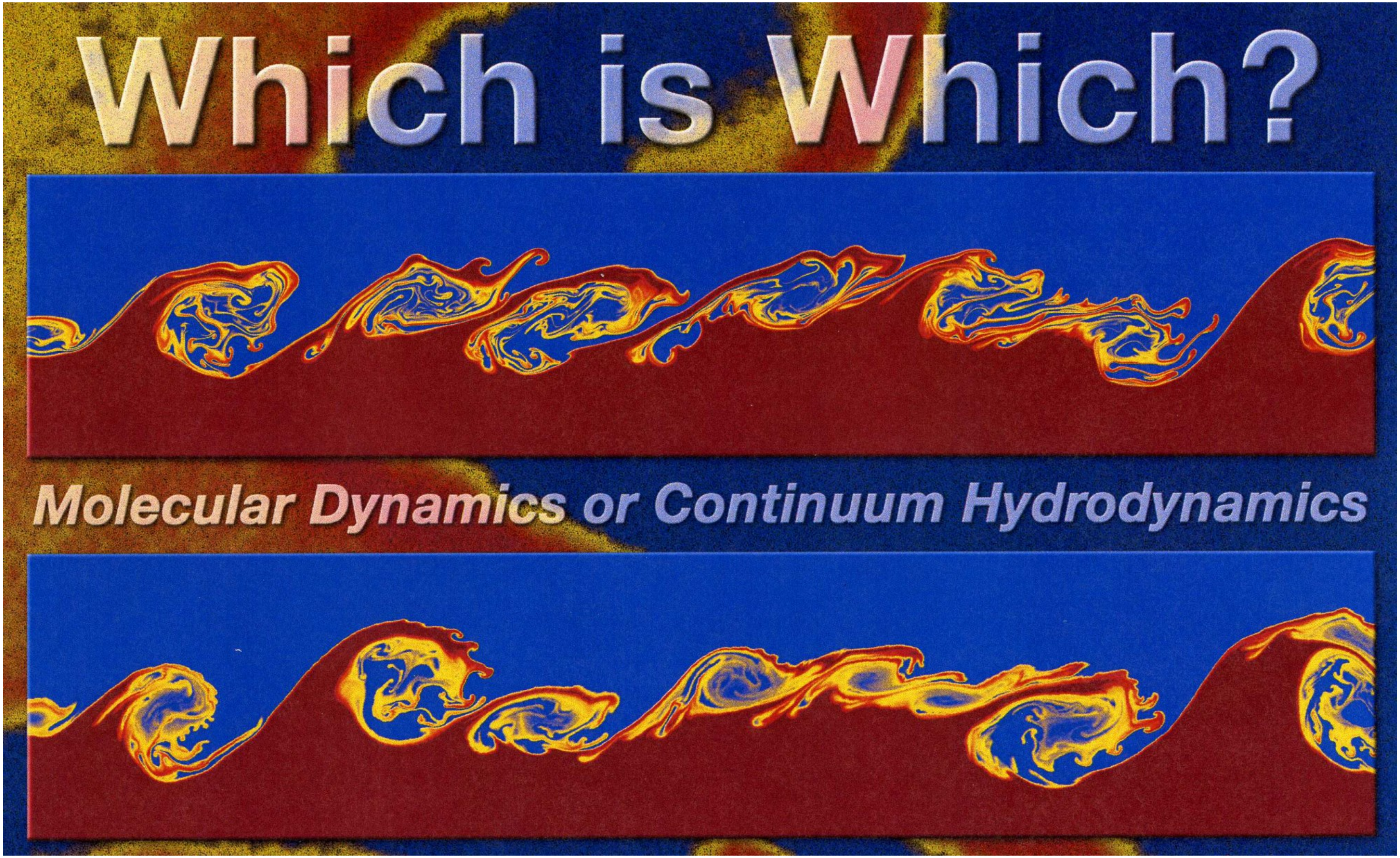
Kelvin-Helmholtz instability is the growth of perturbations to the shearing region between two flows moving past each other.



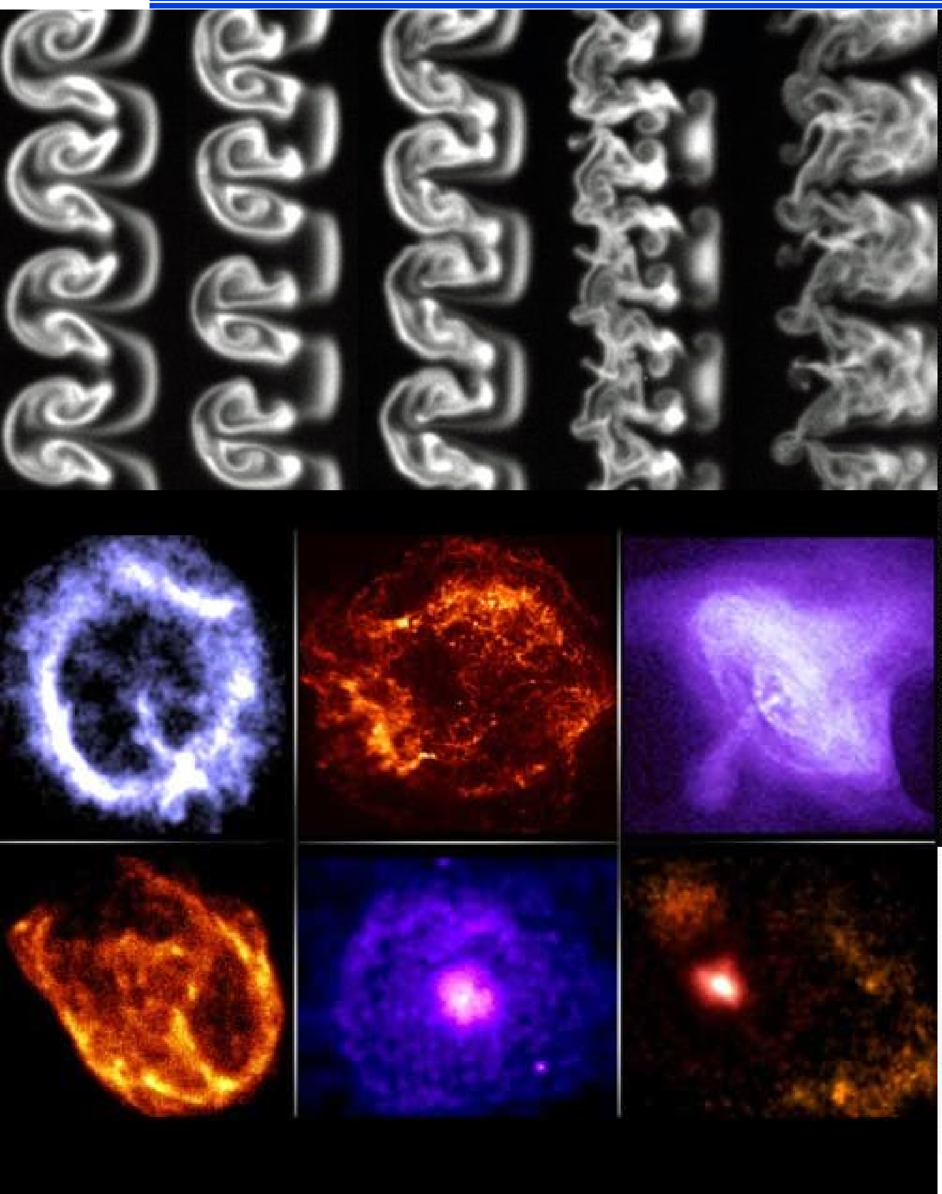
We have compared Direct Numerical Simulations of K-H instability with molecular dynamics.

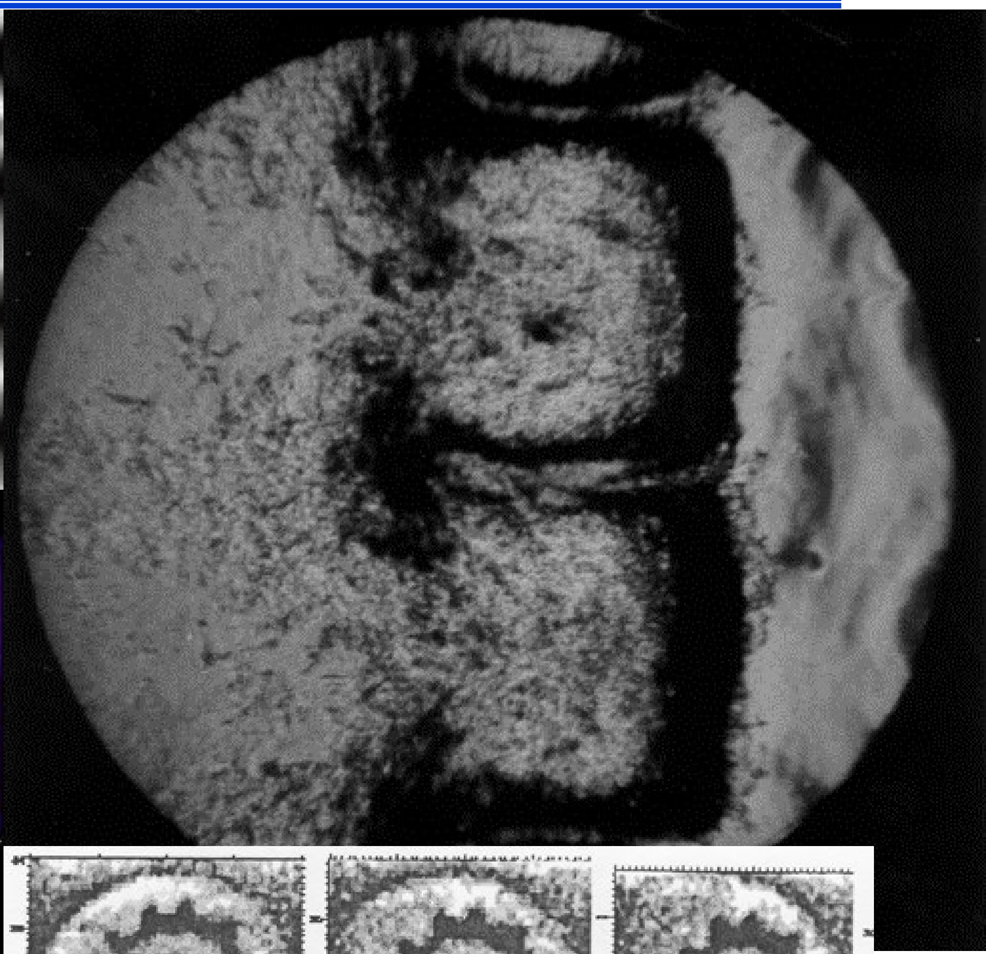


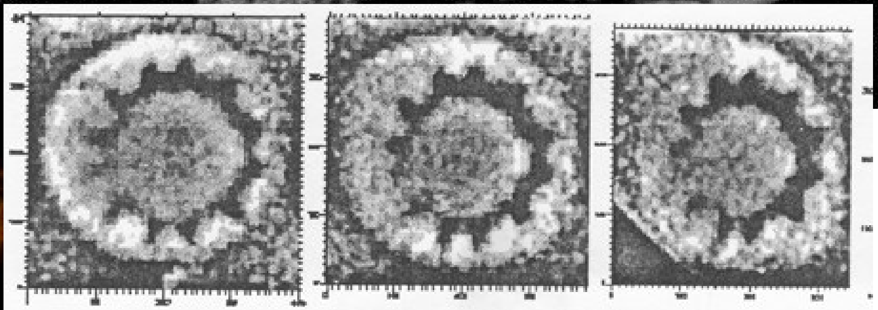
Molecular Dynamics captures thermal fluctuations, which are averaged out in DNS.



Richtmyer-Meshkov instability is the growth of perturbations to a fluid interface after a shock passes through it.







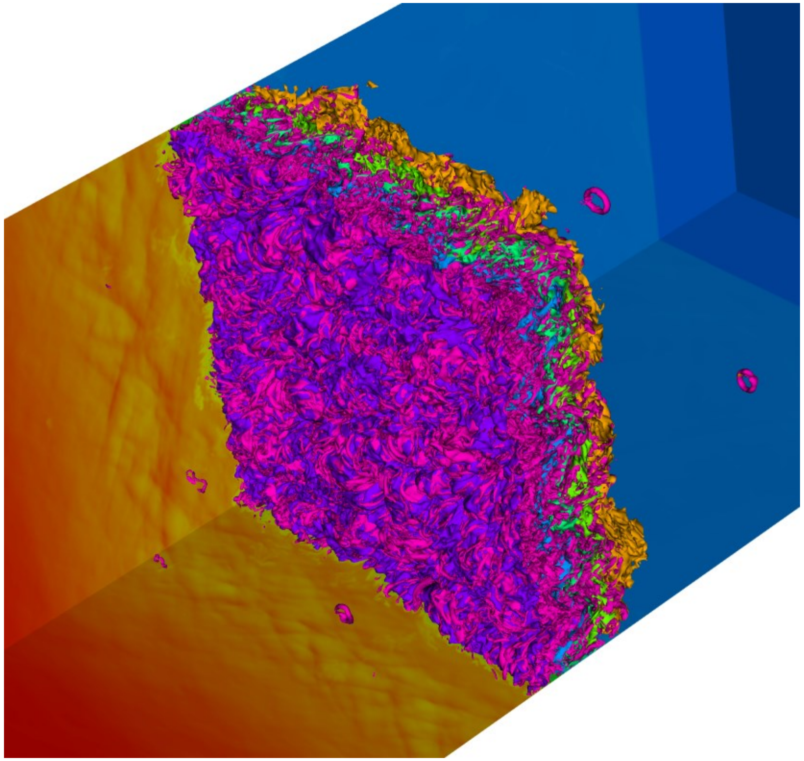
What is the growth rate of Richtmyer-Meshkov instability?

$$h = ct^{\theta}$$

$$h \propto \left(u_s t\right)^{\theta}$$

$$h - h_o \propto \left(t - t_o\right)^{\theta}$$

$$0.2 \leq \theta \leq 0.67$$



h **and *t* must be nondimensionalized for these power laws to work.**

We can directly compute the initial growth rate if the interfacial perturbations are known/measured .

$$\dot{h}_o \approx \dot{h}^+ \equiv \frac{4\langle \rho^+ u^+ \rangle_{x^+}}{\rho_1'' - \rho_2'}$$

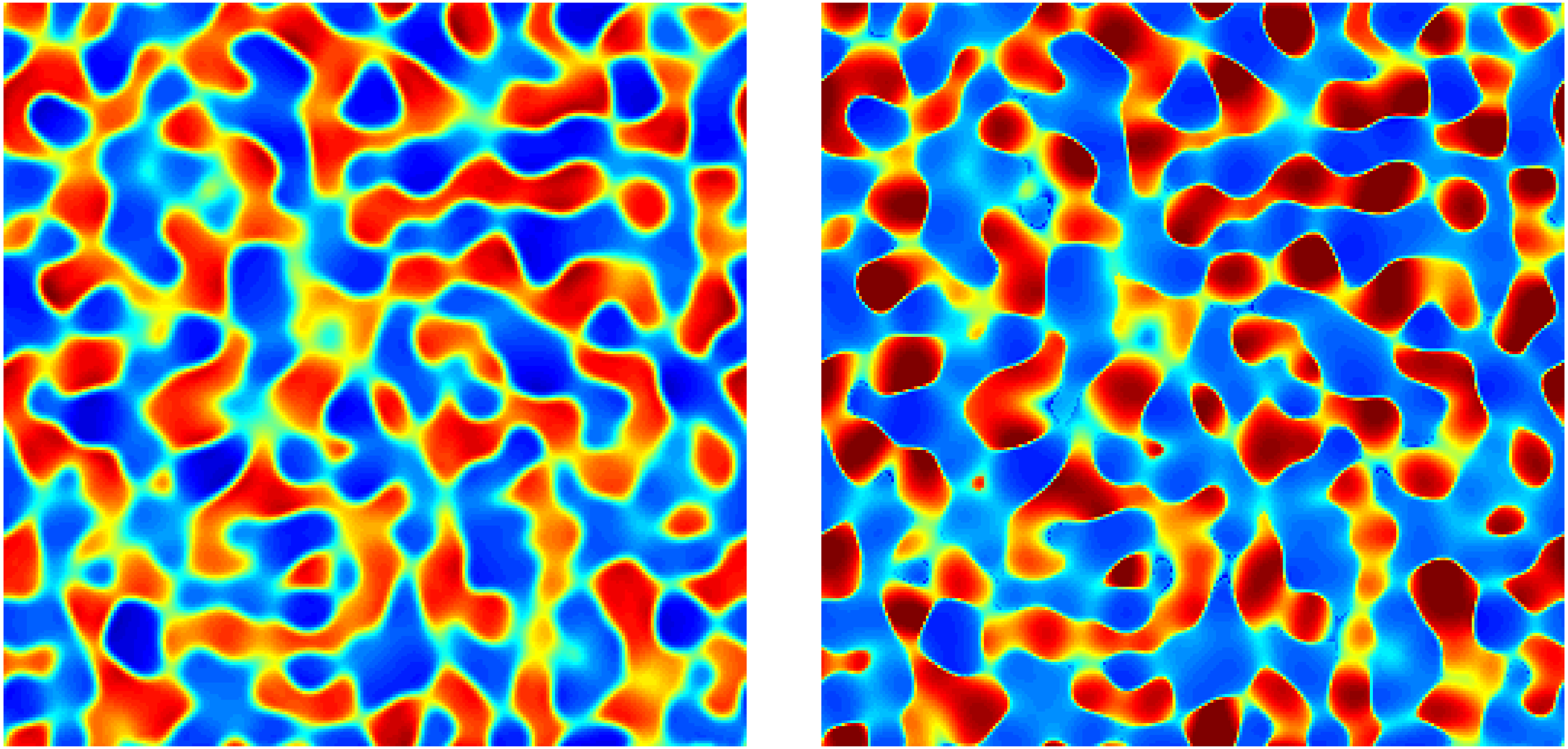
The growth rate is determined by the net mass flux through the equimolar plane.

Using the dominant initial wavelength, a relevant timescale becomes: $\lambda_o / \dot{h}_o$

From baroclinic vorticity deposition:

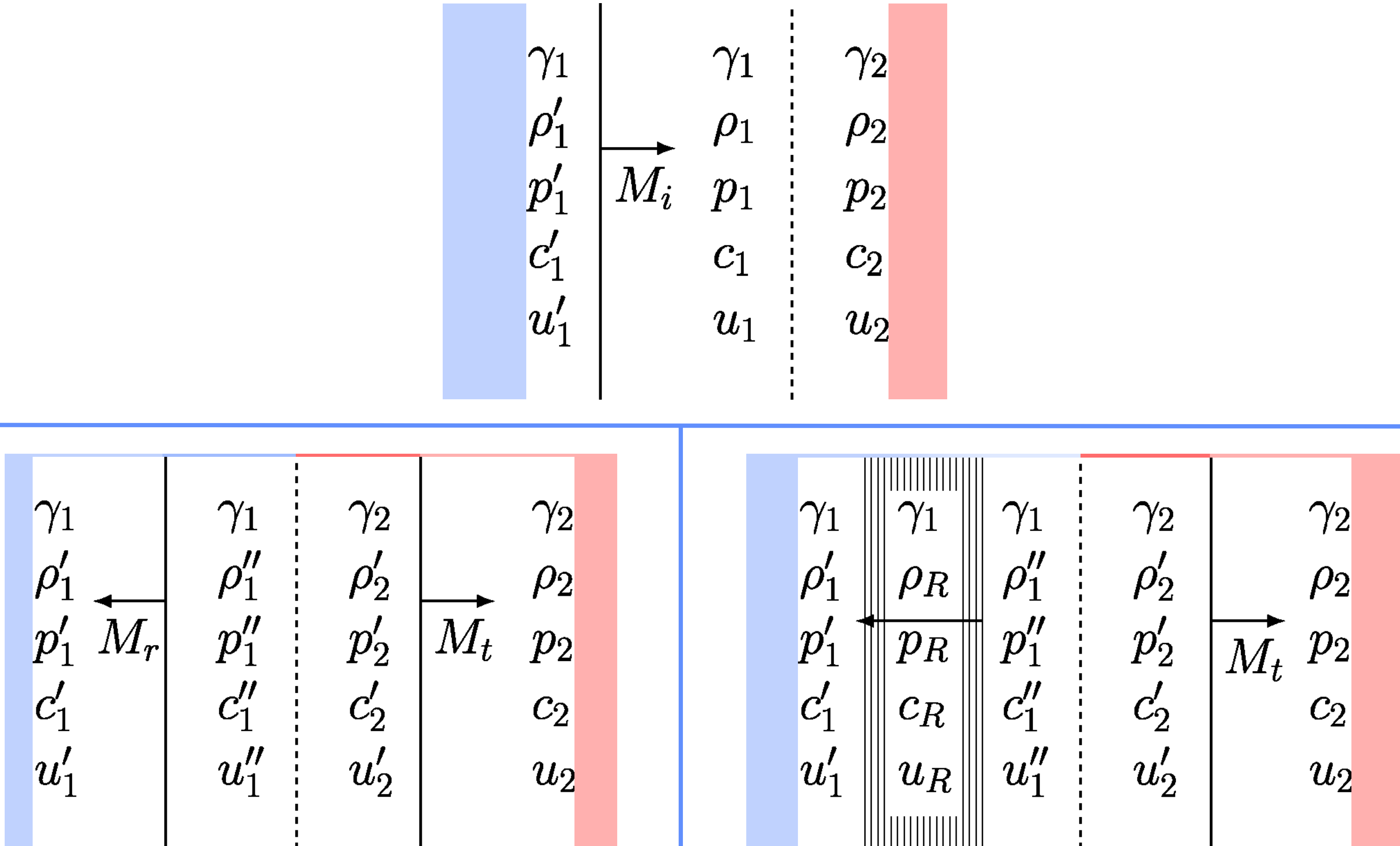
$$u^+ \approx \frac{u_s A^+}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\frac{\partial \eta^+(y^*,z^*)}{\partial y^*}(y - y^*) + \frac{\partial \eta^+(y^*,z^*)}{\partial z^*}(z - z^*)}{[(x - \eta^+(y^*, z^*))^2 + (y - y^*)^2 + (z - z^*)^2]^{3/2}} \, dy^* \, dz^*$$

We can predict the mass flux (ρu) on the equimolar plane after shock passage.



Simulation   Model

Pre and post shock conditions are obtained from the Rankine-Hugoniot jump relations and by matching pressures and velocities across the interface.



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We ran a variety of R-M simulations with different parameters.

$t\frac{\dot{h}_o}{\lambda_o} =$ **0** **1** **2** **5** **30**

$A = 0.35$

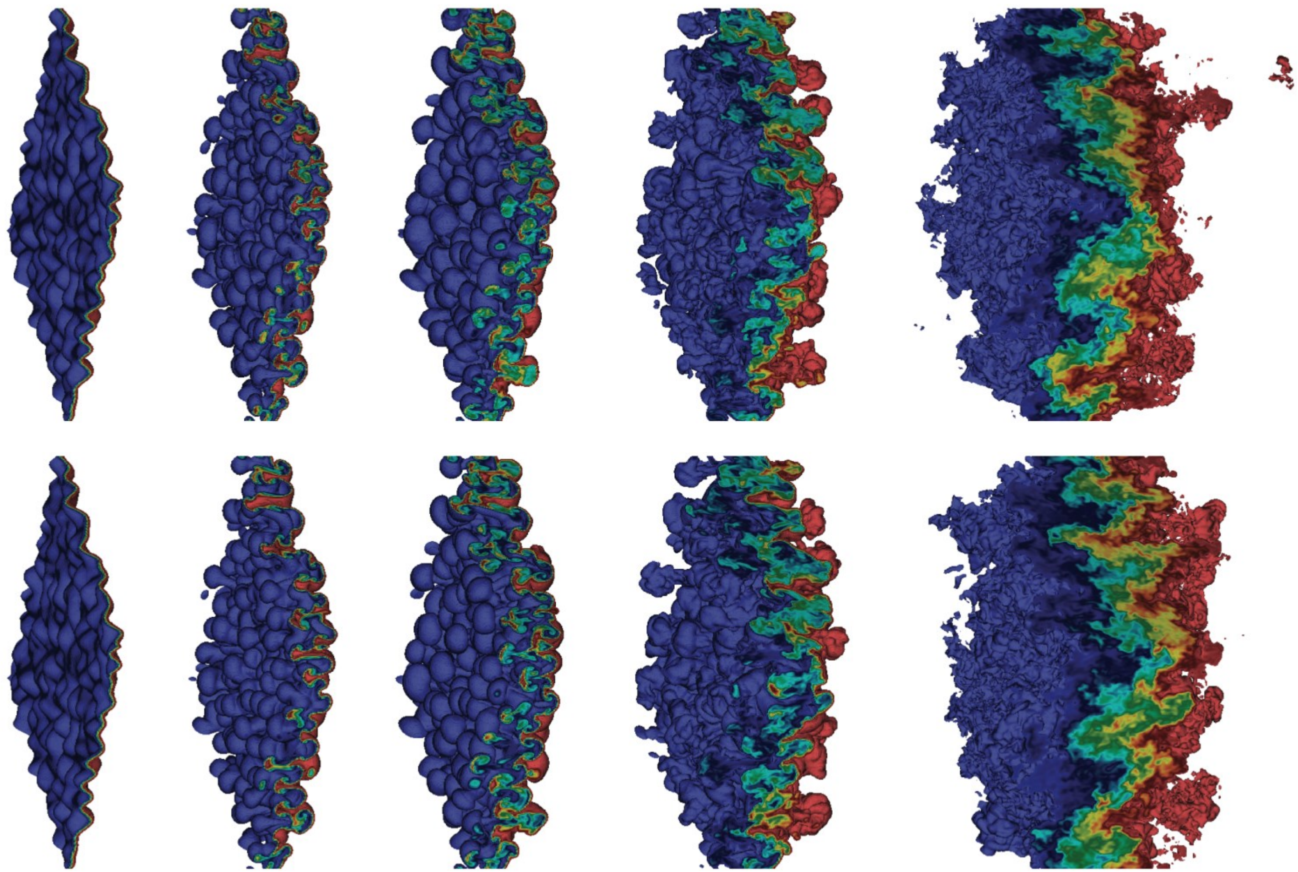
$M_i = 1.5$

$\eta_{rms} / \lambda_o = 0.1$

$A = 0.53$

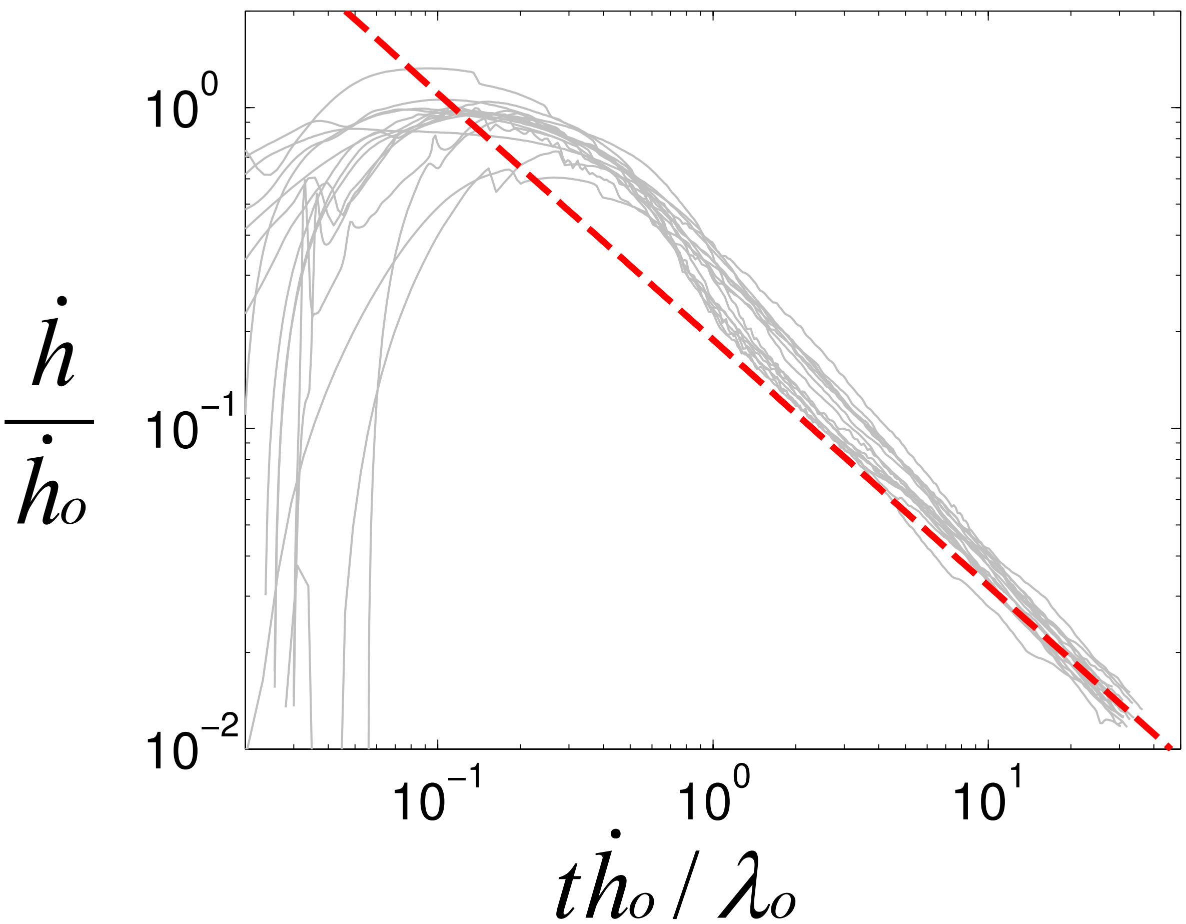
$M_i = 1.1$

$\eta_{rms} / \lambda_o = 0.1$



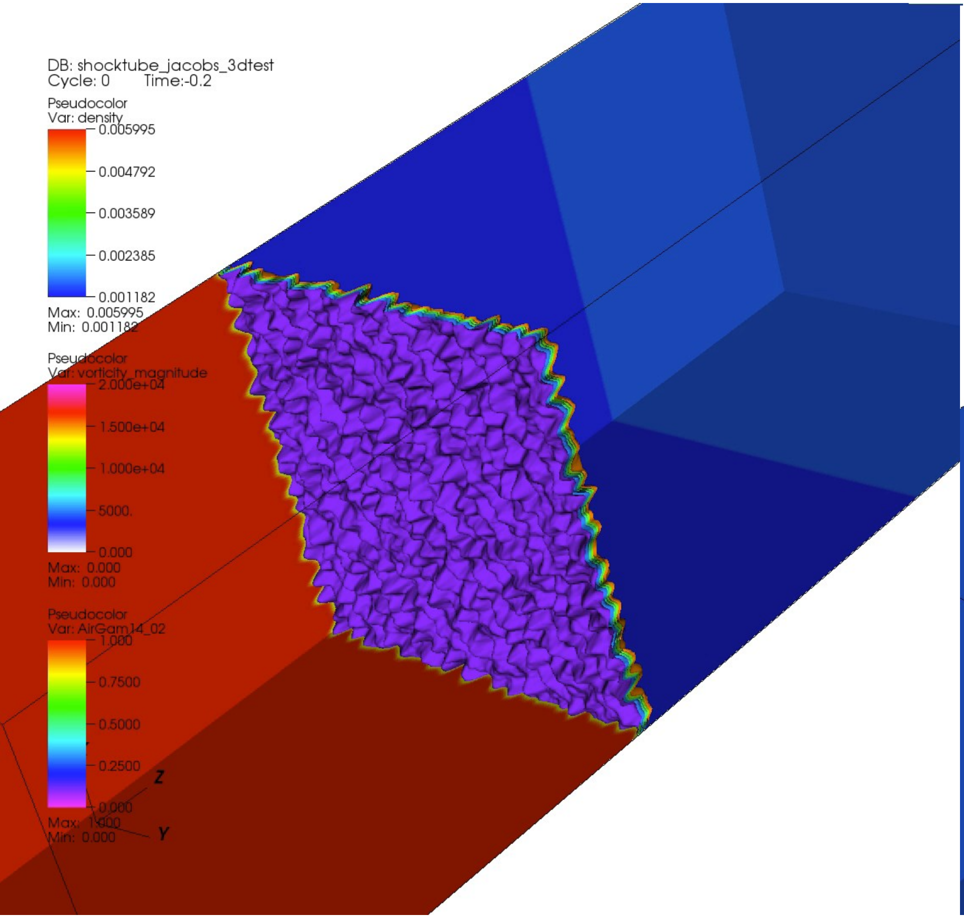
$$0.05 < \xi < 0.95$$

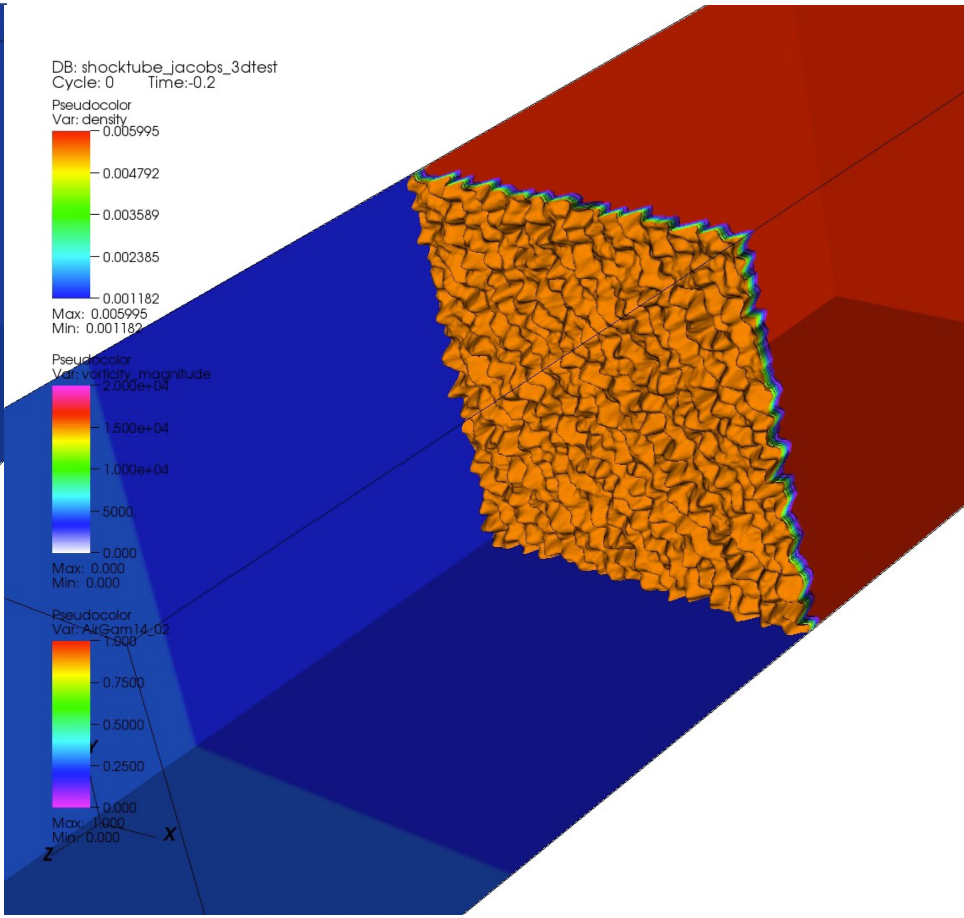
With proper nondimensionalization the growth curves collapse.



$$\theta = 0.233$$

But there are also "vortex projectiles," which defy the growth model.

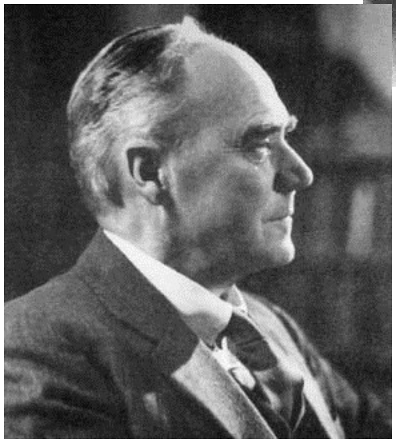


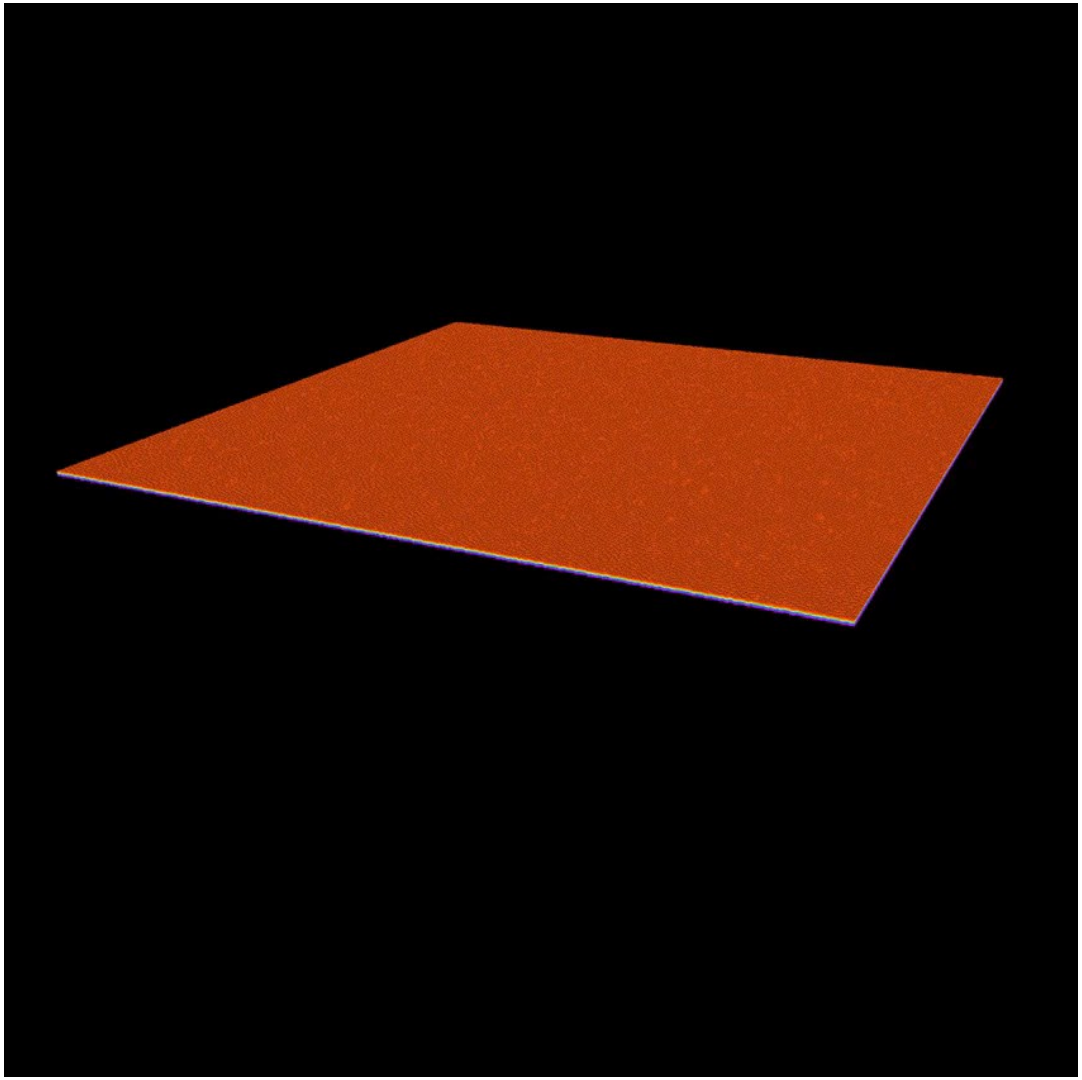


Rayleigh-Taylor instability is the interpenetration of materials that occurs whenever a light fluid pushes on a heavy fluid.

What is the growth rate of Rayleigh-Taylor instability?

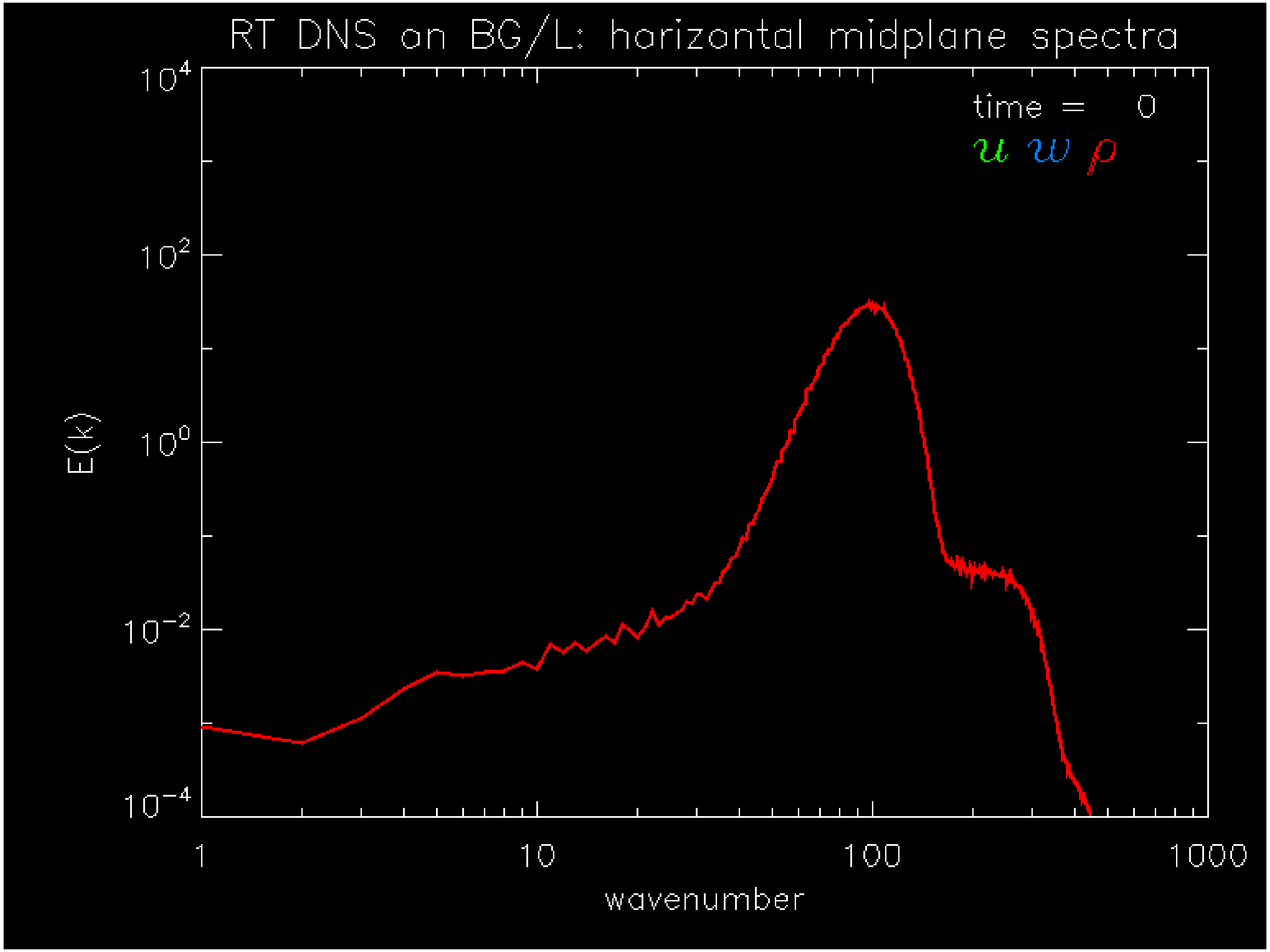
We ran some big simulations (up to 3072^3) to find out.





When does Rayleigh-Taylor instability become self-similar?

R-T instability develops a $k^{-5/3}$ spectrum.



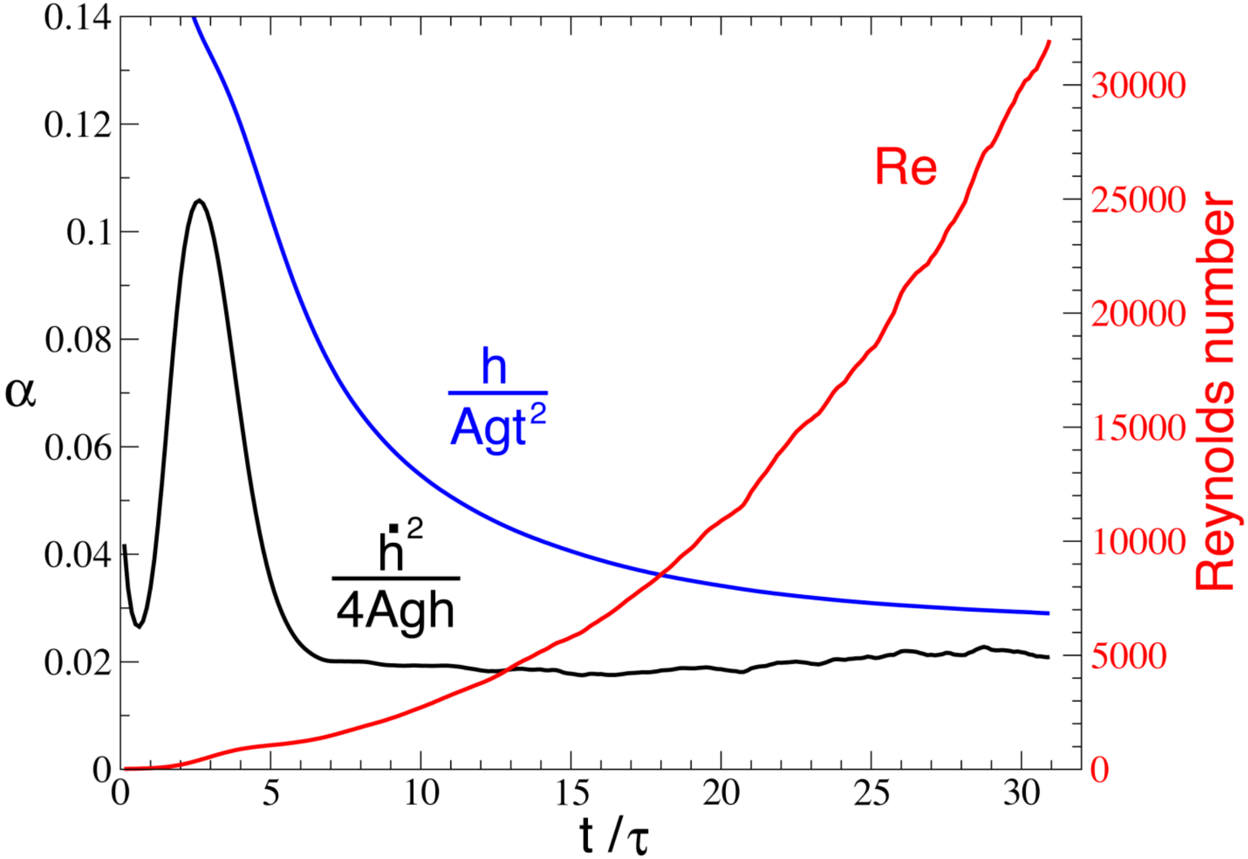
It takes over a billion grid points to reach self-similar growth.

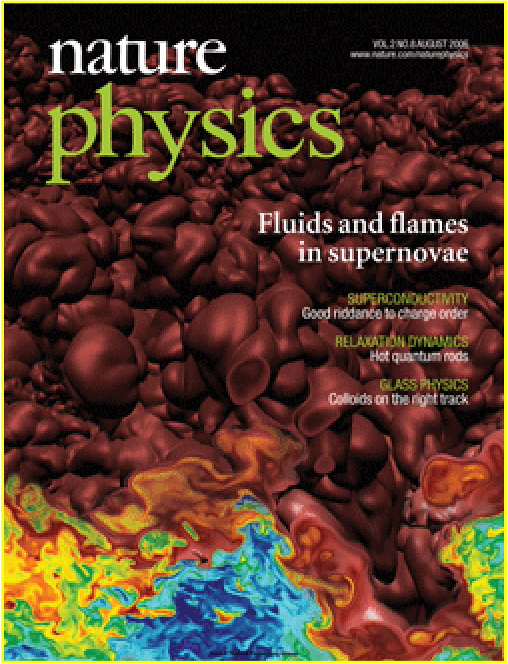
From dimensional analysis:

$$h = \alpha A g t^2$$

From self-similarity and energy balance:

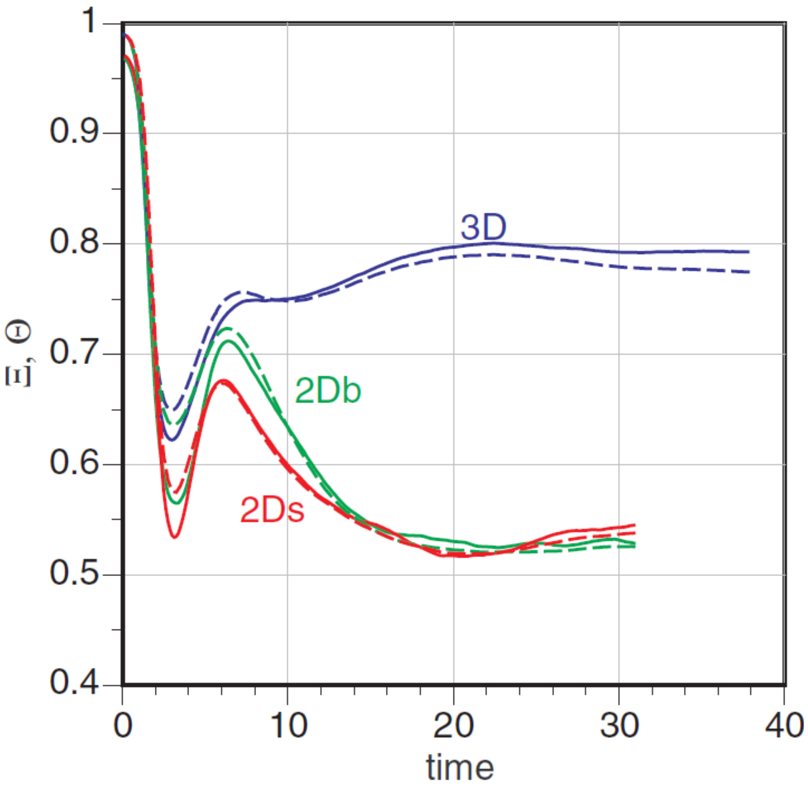
$$(dh/dt)^2 = 4\alpha A g h$$

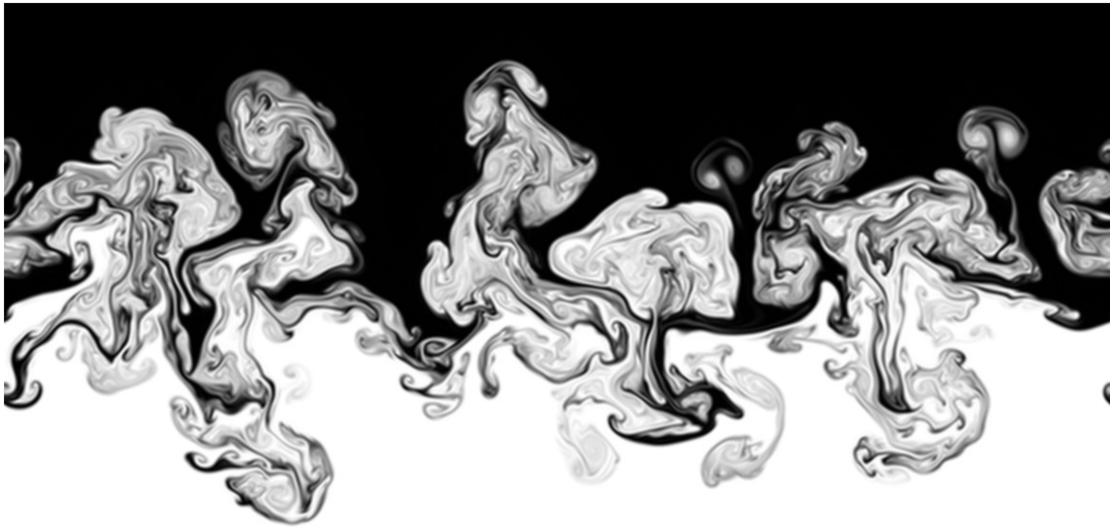


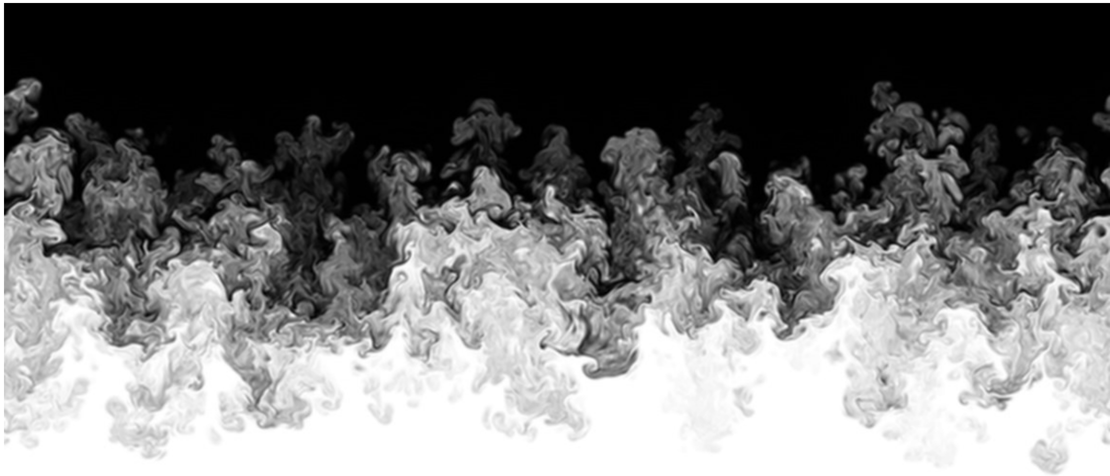


$\alpha = 0.027$

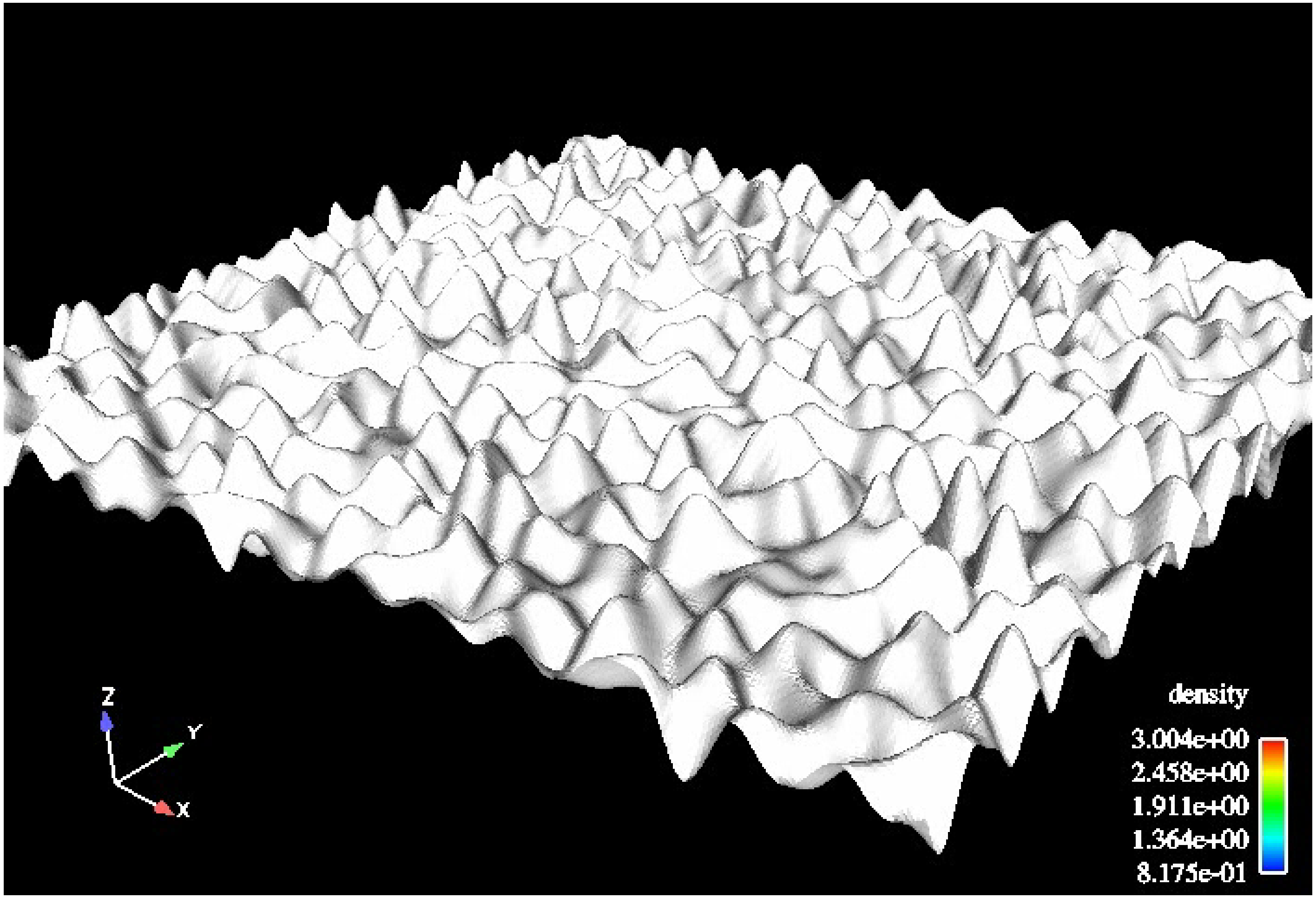
3D flows are better at mixing than 2D flows.



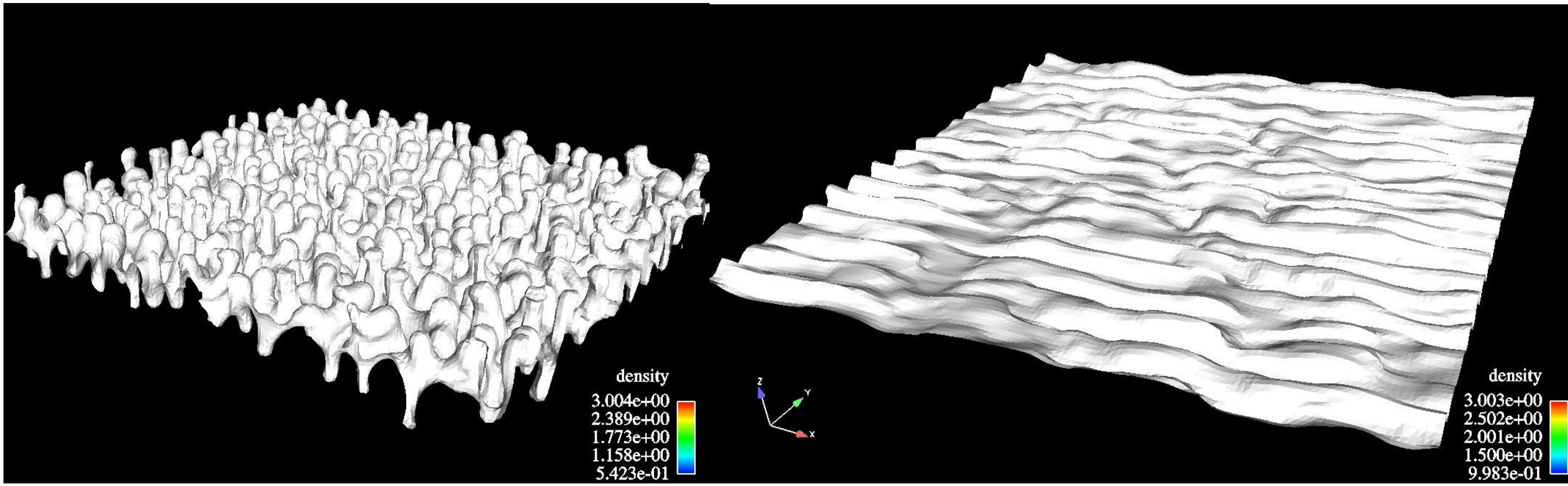


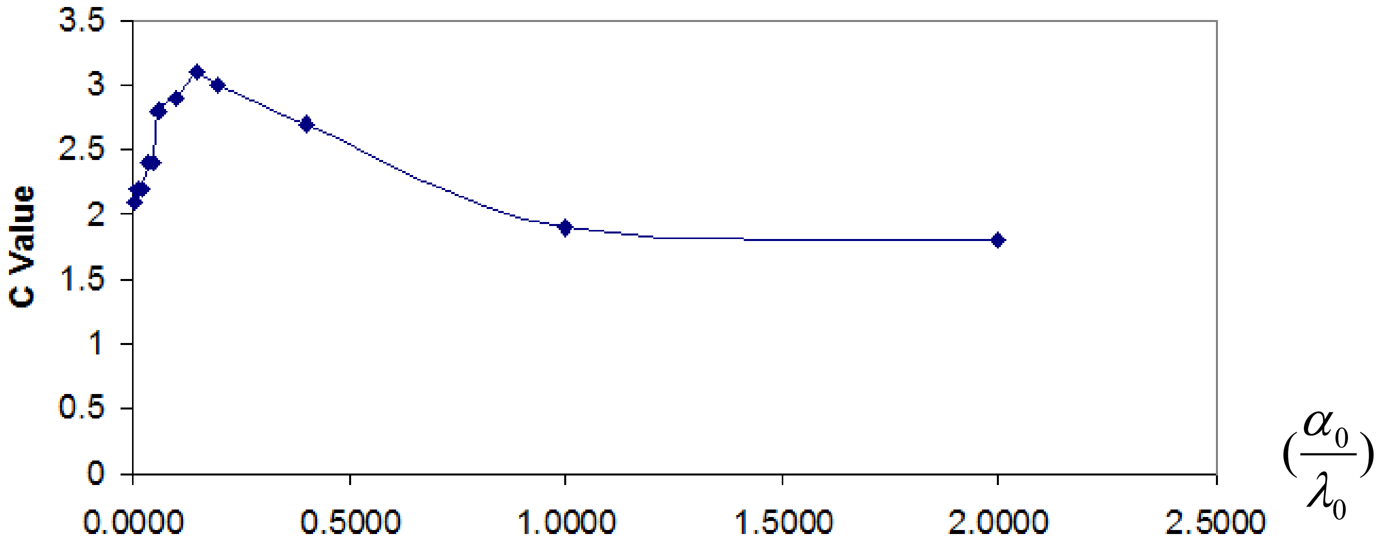


What if we combine Rayleigh-Taylor and Kelvin-Helmholtz instabilities?



Rayleigh-Taylor growth is reduced by adding the right amount of shear.





What is the maximum Mach number that a compressible R-T instability can achieve?

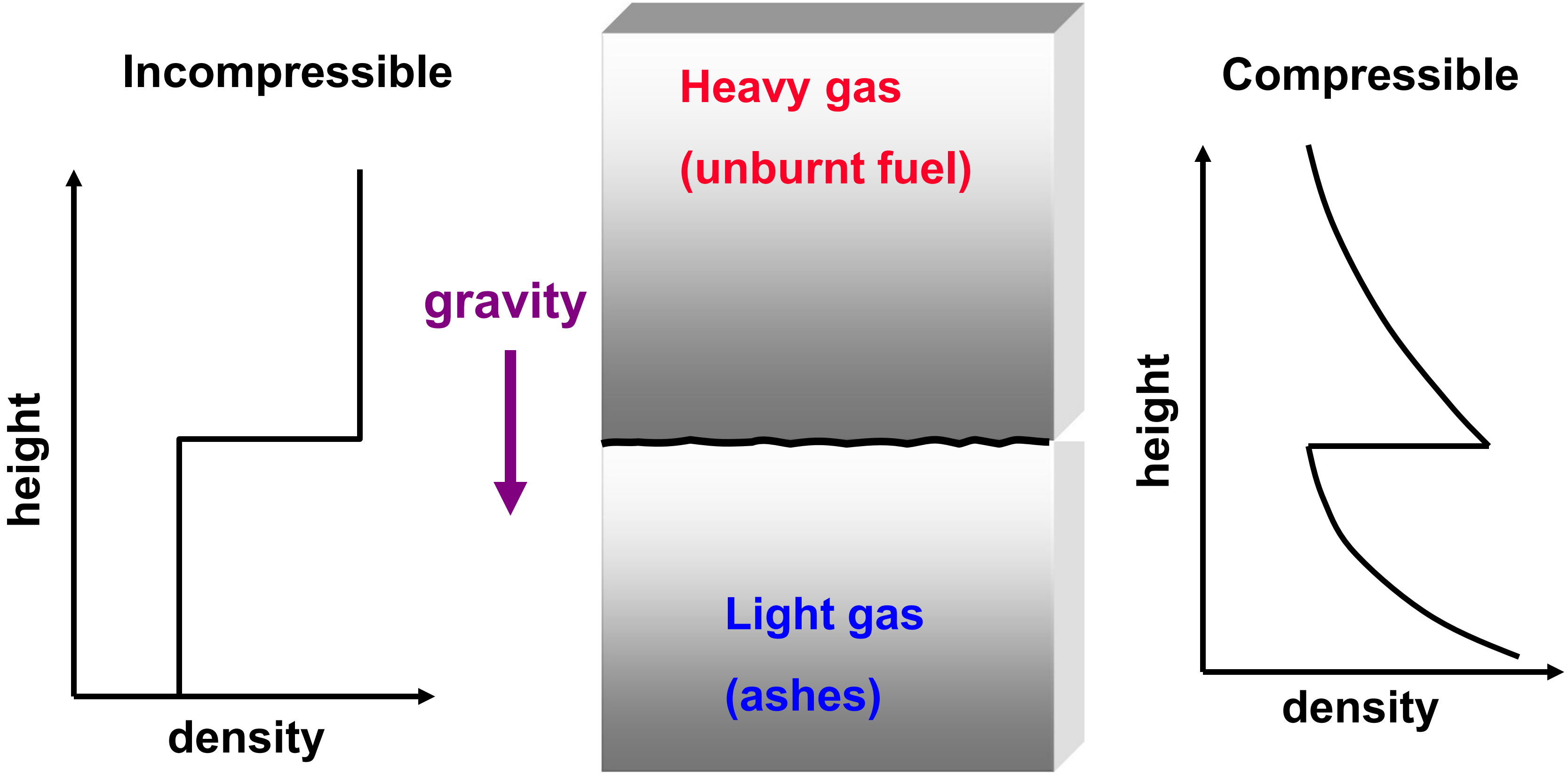
Local Mach Number : $M_l(\vec{x},t) \equiv \dfrac{\|\vec{u}\|}{c}$

Turbulent Mach Number : $M_t(z,t) \equiv \dfrac{\langle\|\vec{u}\|\rangle}{\langle c \rangle}$

Shock Mach Number : $\dfrac{\langle \mathrm{T} \rangle_{\max}}{T_0} = \left[1 + \dfrac{2\gamma}{\gamma+1}\left(M_s^2 - 1\right)\right]\left[\dfrac{2+(\gamma-1)M_s^2}{(\gamma+1)M_s^2}\right]$

Mellado et al. (Phys. Fluids, 17:076101, 2005) found $M_t(0,t) < 0.6$ and concluded that, "the Rayleigh-Taylor problem does not have significant intrinsic compressibility effects."

The density scale height is important in compressible R-T instability.



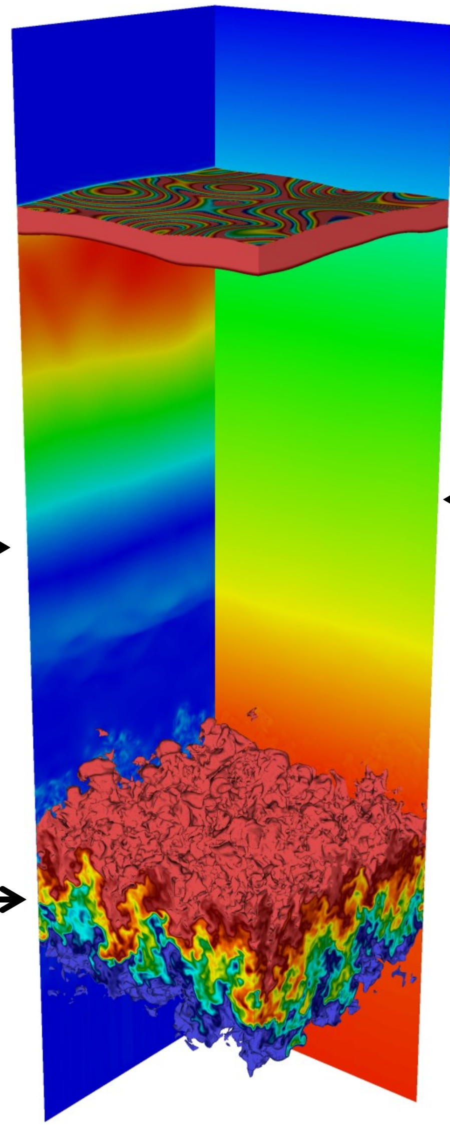
Rayleigh-Taylor instability produces shock waves.

12.8 x 12.8 x 51.2 km

t = 105 s

Temperature

(3,000 ≤ T ≤ 4,400 K)



Xenon

Local Mach Number

($0 \leq M_l \leq 1.98$)

Log Density

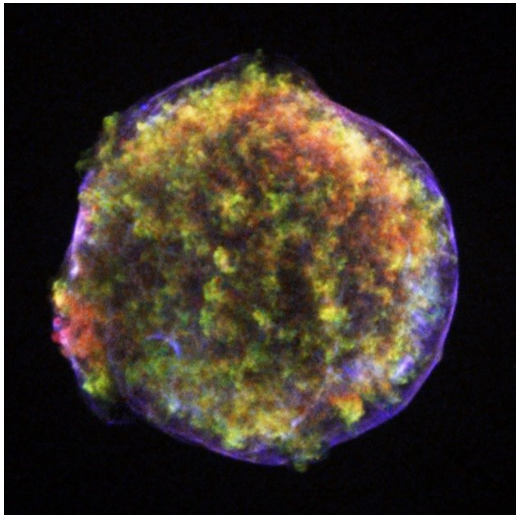
($5.26 \times 10^{-3} \leq \rho \leq 1.68 \times 10^{6}$)

Mixing Region

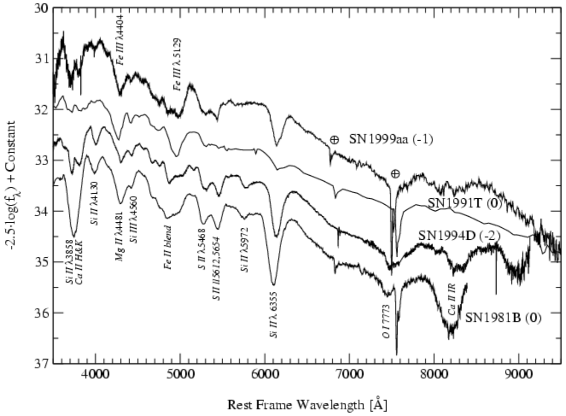
($0.1 \leq Y_{Xe} \leq 0.9$)

Neon **Argon**

Do Rayleigh-Taylor shock waves provide a deflagration-to-detonation mechanism for type Ia supernovae?



- $c \approx 7 \times 10^8$ cm/s
- $g \approx 10^{10}$ cm/s^2
- $A \approx 0.25$
- $\gamma \approx 1.4$
- $L_s \approx 1{,}700$ km
- $R_{wd} \approx 2{,}500$ km



Do the multicomponent Euler equations adequately describe turbulent mixing?

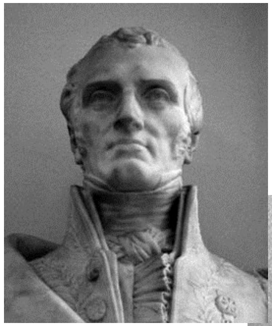
$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \mathbf{u}) = 0$$

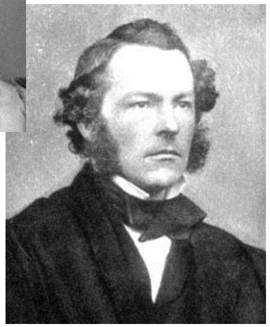
$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\,\mathbf{u} + p \underline{\boldsymbol{\delta}}) = 0$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot [(E + p)\mathbf{u}] = 0$$

Can these equations accurately predict temperature?

What terms are active for quiescent fluids in pressure-temperature equilibrium?





$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \left(\rho Y_i \mathbf{u} \right) = -\nabla \cdot \mathbf{J}_i$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \left(\rho \mathbf{u}\mathbf{u} + p \underline{\boldsymbol{\delta}} \right) = \nabla \cdot \underline{\boldsymbol{\tau}}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \left[\left(E + p \right) \mathbf{u} \right] = \nabla \cdot \left(\underline{\boldsymbol{\tau}} \cdot \mathbf{u} - \mathbf{q}_c - \mathbf{q}_d \right)$$

Enthalpy Diffusion: $\mathbf{q}_d = h_i \mathbf{J}_i$

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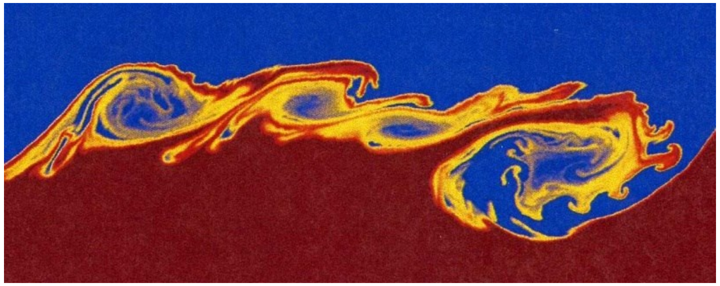
The species diffusion flux (J_i) is present in any simulation wherein mixing occurs.



$\mathbf{J}_i$ can represent:

- molecular diffusion (DNS, physical diffusivity)
- numerical diffusion (Euler solvers, ILES)
- subgrid-scale diffusion (LES, grid-scale transfer)
- turbulent diffusion (RANS, k-ε & k-l models)

If q_d does not balance J_i then the mixture energy will be incorrect.

The role of q_d is illustrated through a simple gedanken experiment.

Light gas

Molecular weight: M_L

Mass fraction: $Y_L = 1$

Temperature: $T^< = T_0$

$n_L \rightarrow$

$\leftarrow n_H$

Heavy gas

Molecular weight: M_H

Mass fraction: $Y_H = 1$

Temperature: $T^> = T_0$

If $q_d=0$ there can be no net mass flux; hence, $n_L M_L = n_H M_H$

Mixed gas in left partition

$T^< = T_0/(Y_L + Y_H M_L/M_H) > T_0$

$\Delta S^< > 0$

Mixed gas in right partition

$T^> = T_0/(Y_L M_H/M_L + Y_H) < T_0$

$\Delta S^> < 0$

$$\Delta S = \Delta S^< + \Delta S^> < 0$$

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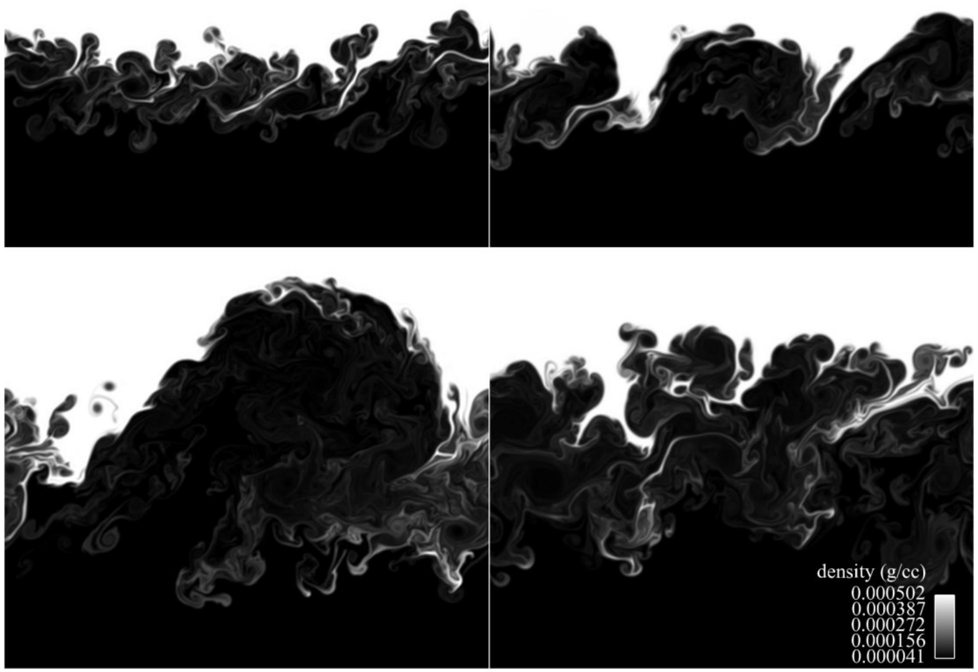
Shear layers evolve differently, depending on the presence of $q_{d.}$

OFF | ON

1 ms

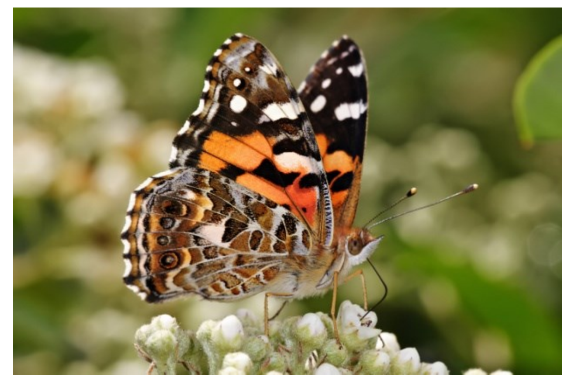
5 ms

10 ms

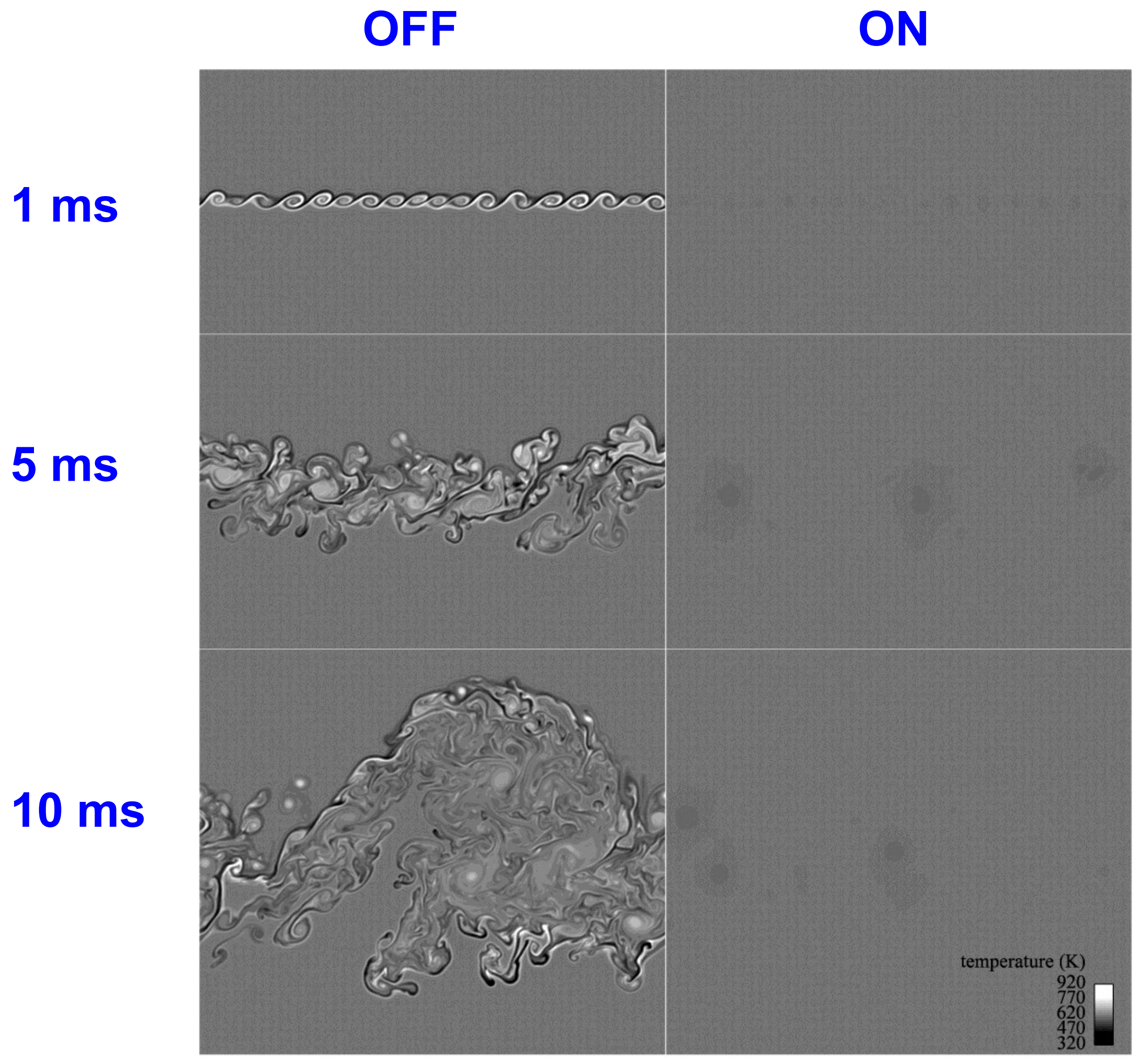


Air →

H_2 ←



Temperature can be extremely sensitive to enthalpy diffusion.

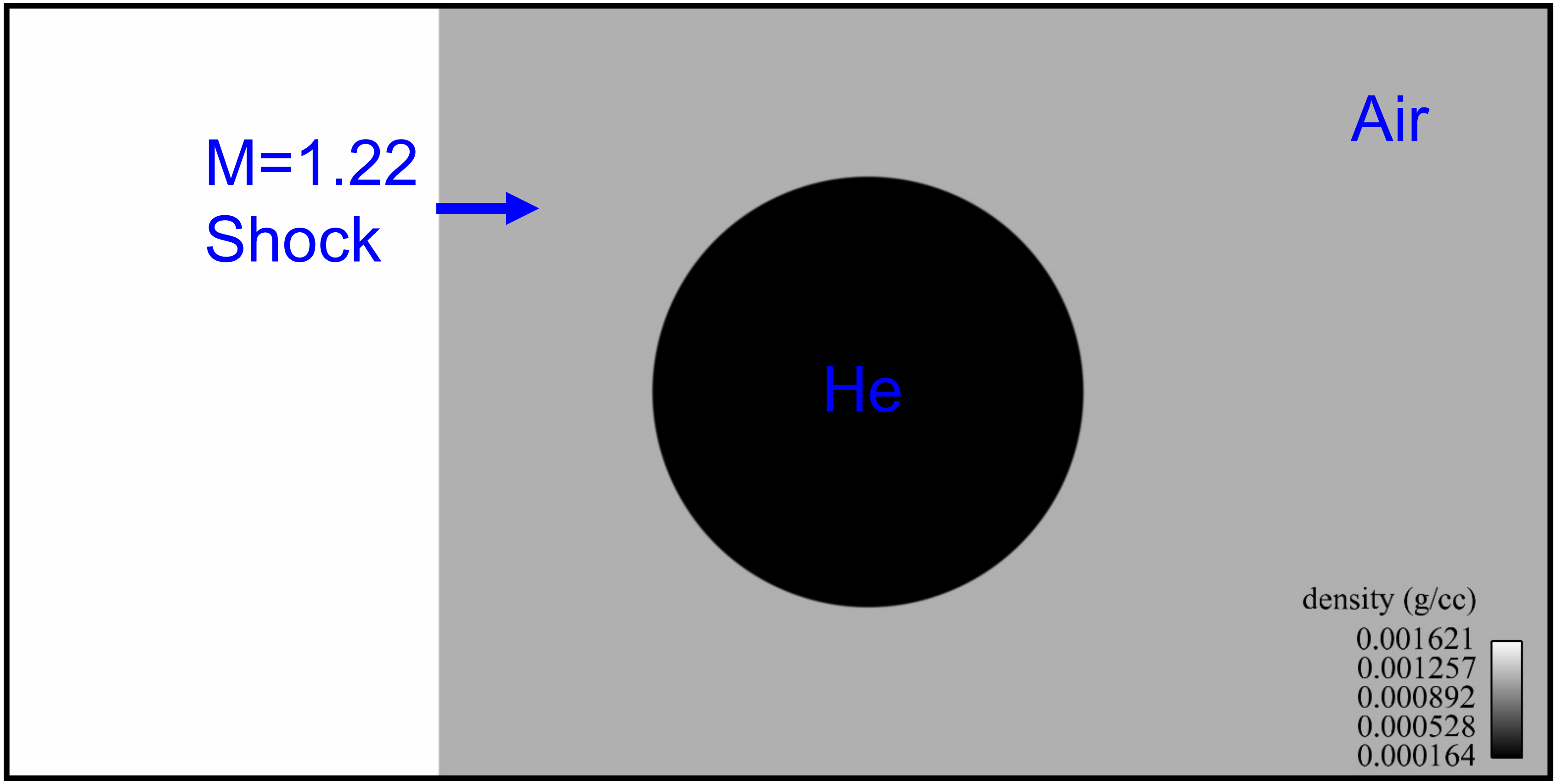


Air →

H_2 ←

White regions exceed ignition temperature.

The Haas-Sturtevant shock-bubble experiment provides a good test of the importance of q_d.



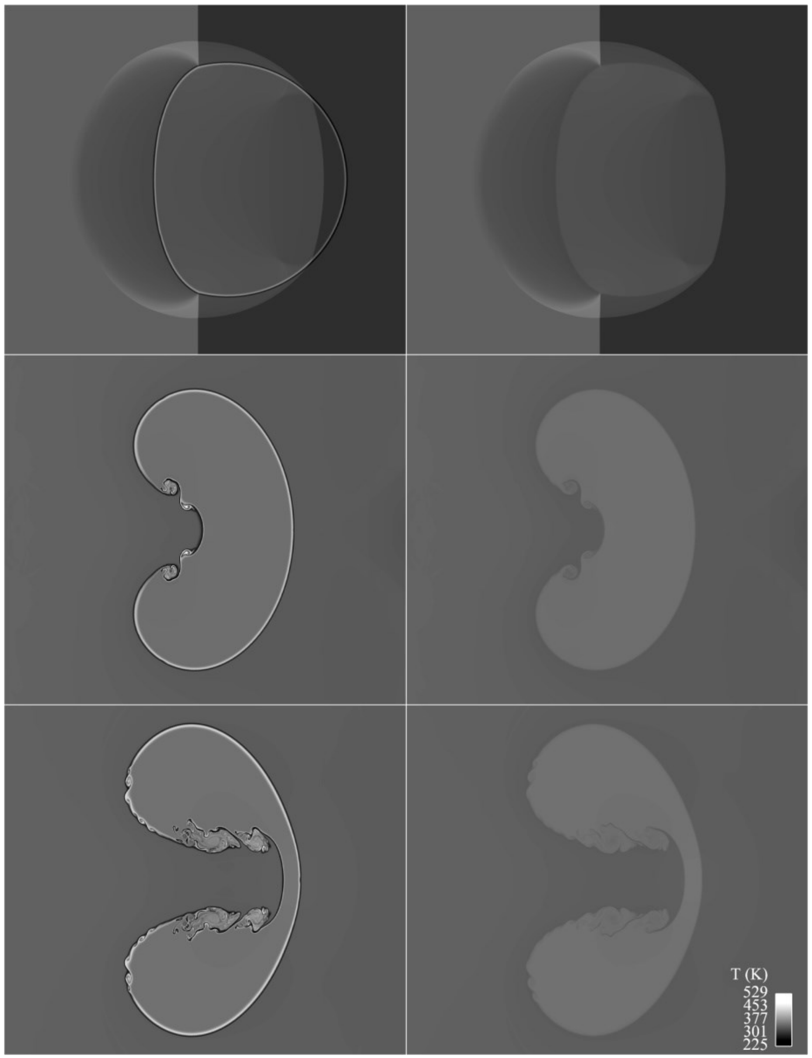
Without q_d, anomalous temperature gradients form in mixing regions.

OFF ON

100 ms

300 ms

500 ms



<u>Numerical simulation of shock-cylinder interactions</u>

J. Comput. Phys., 122:244-265 (1995)...

"Haas and Sturtevant's shock-helium cylinder interaction is well simulated by an Euler code"

"the temperature T is found to require a slightly heavier smoothing"

For Hydrogen-Air case…

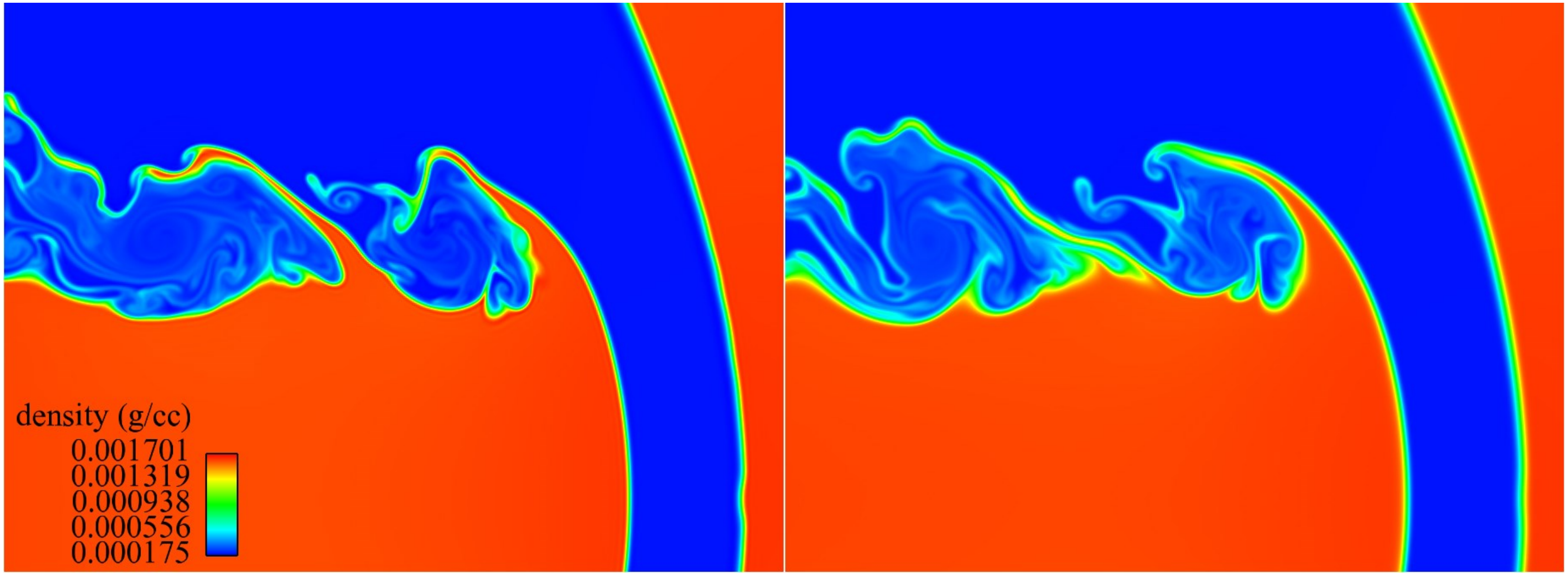
"the general features are quite similar for both the Euler and the reactive Navier-Stokes simulations"

but

T (ambient) = 1000 K
T (ignition) = 853 K

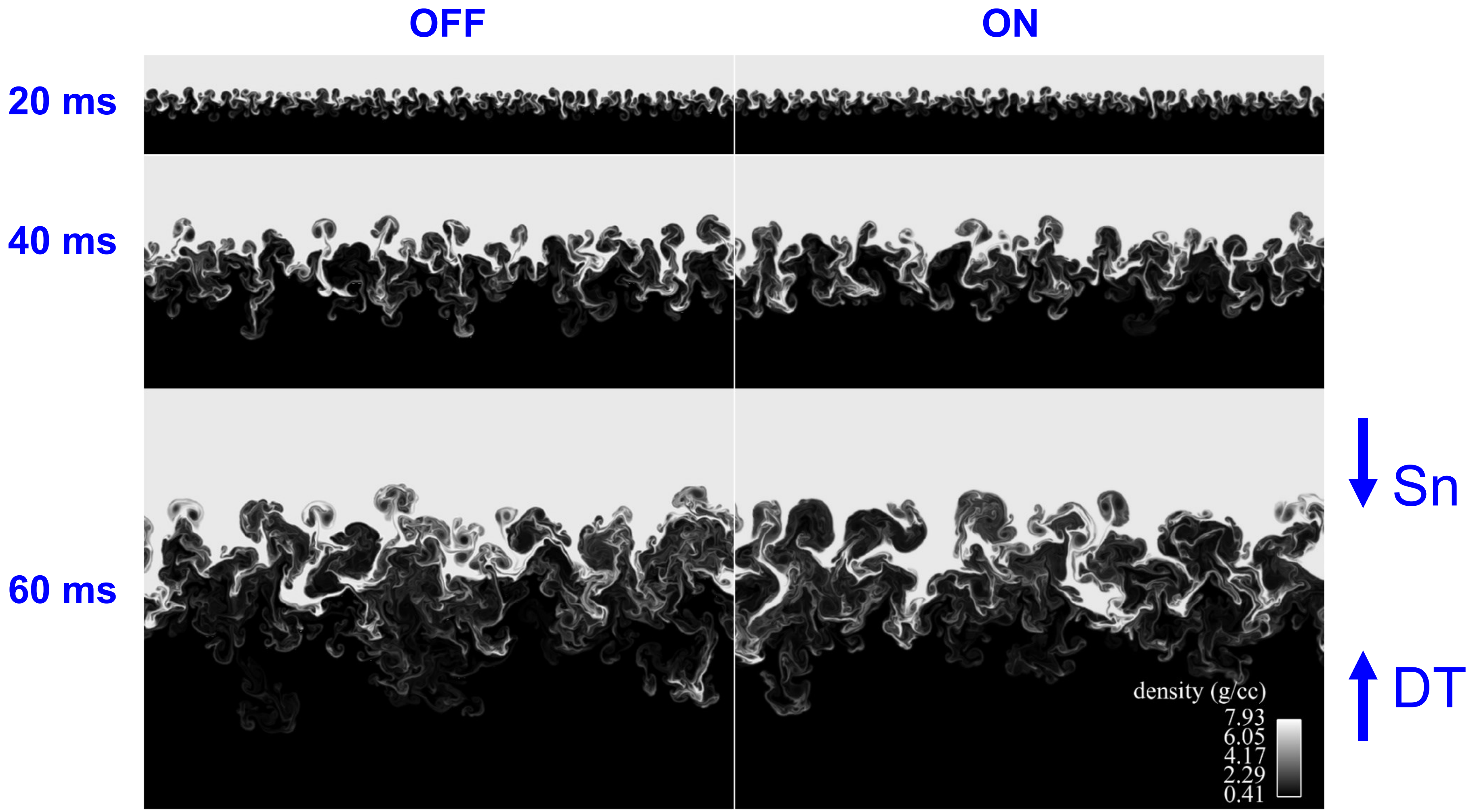
Enthalpy diffusion indirectly results in a smoother density field.

OFF **ON**



Density does not diffuse! Smoothing of the density field is brought About by a local divergence in the velocity field, which is here influenced by both heat conduction and enthalpy diffusion.

The Rayleigh-Taylor instability evolves differently, depending on the presence of q_d.



A = 0.87

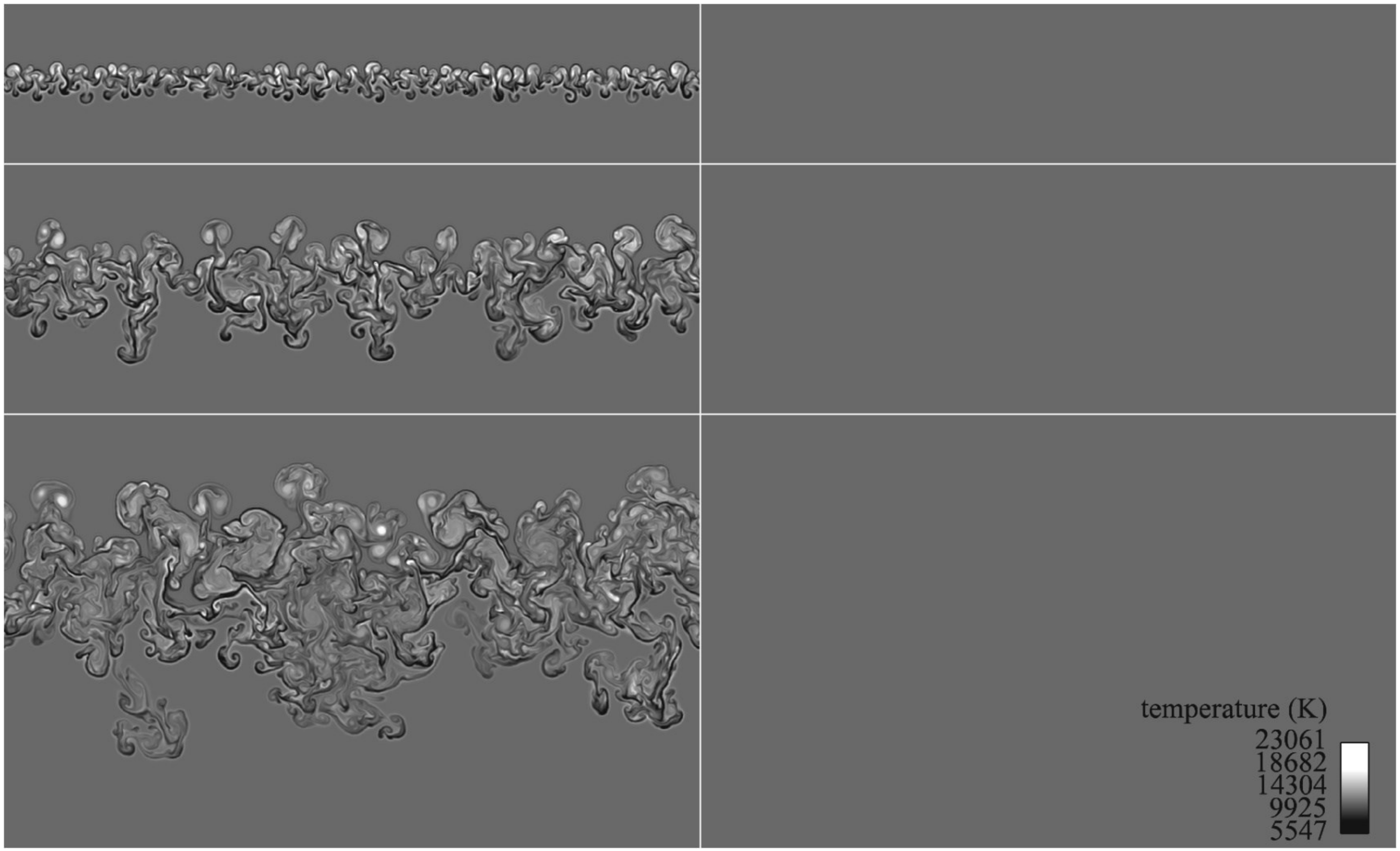
Including q_d, $\Delta T<0.0052$ eV
Excluding q_d, $0.5 \text{ eV} < T < 2 \text{ eV}$

OFF | **ON**

20 ms

40 ms

60 ms

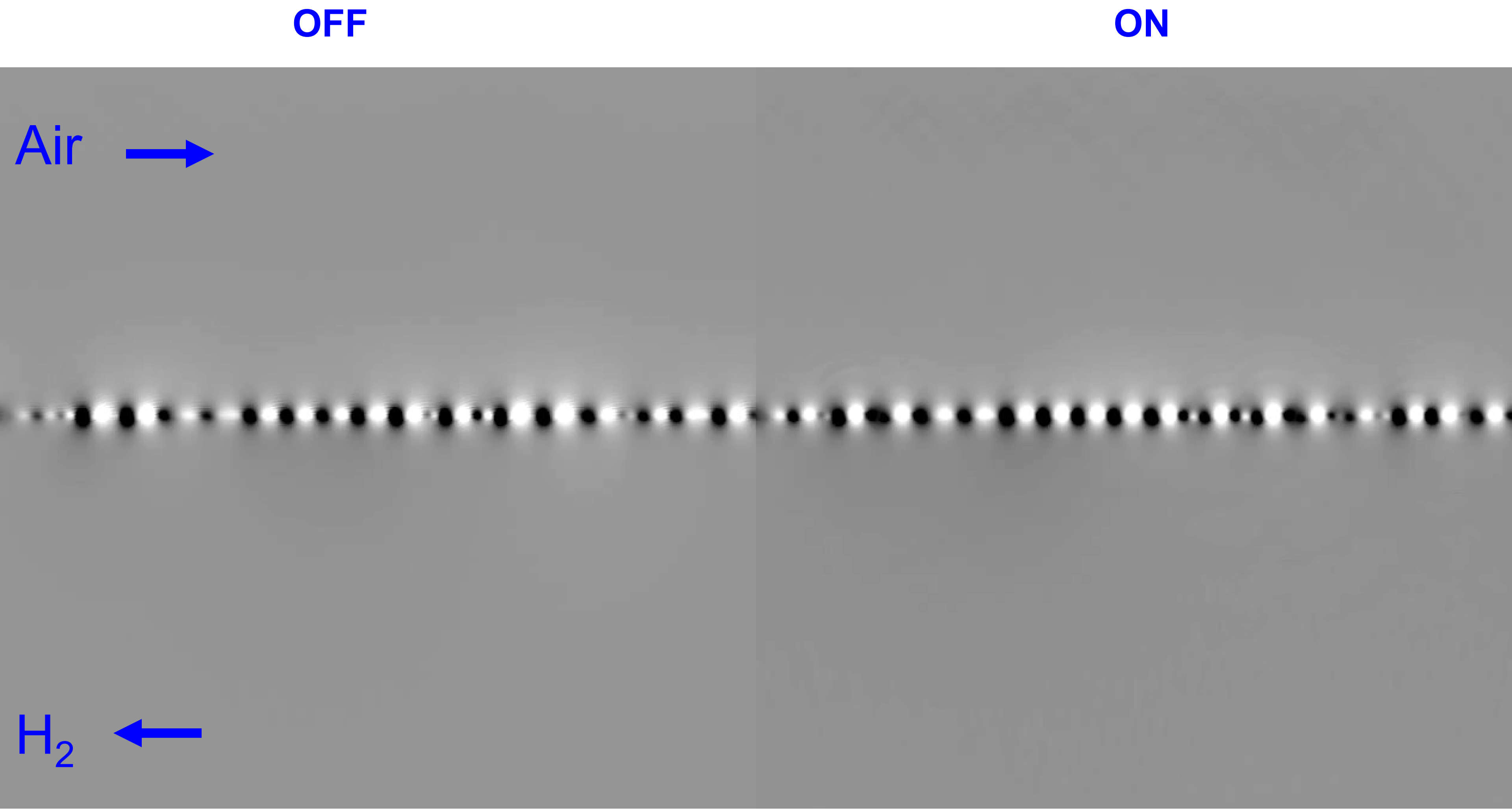


Sn

DT

T_o=1 eV (to match Dimonte-Tipton, PF 18:085101)

Enthalpy diffusion enhances the formation of sound waves in Kelvin-Helmholtz instability.

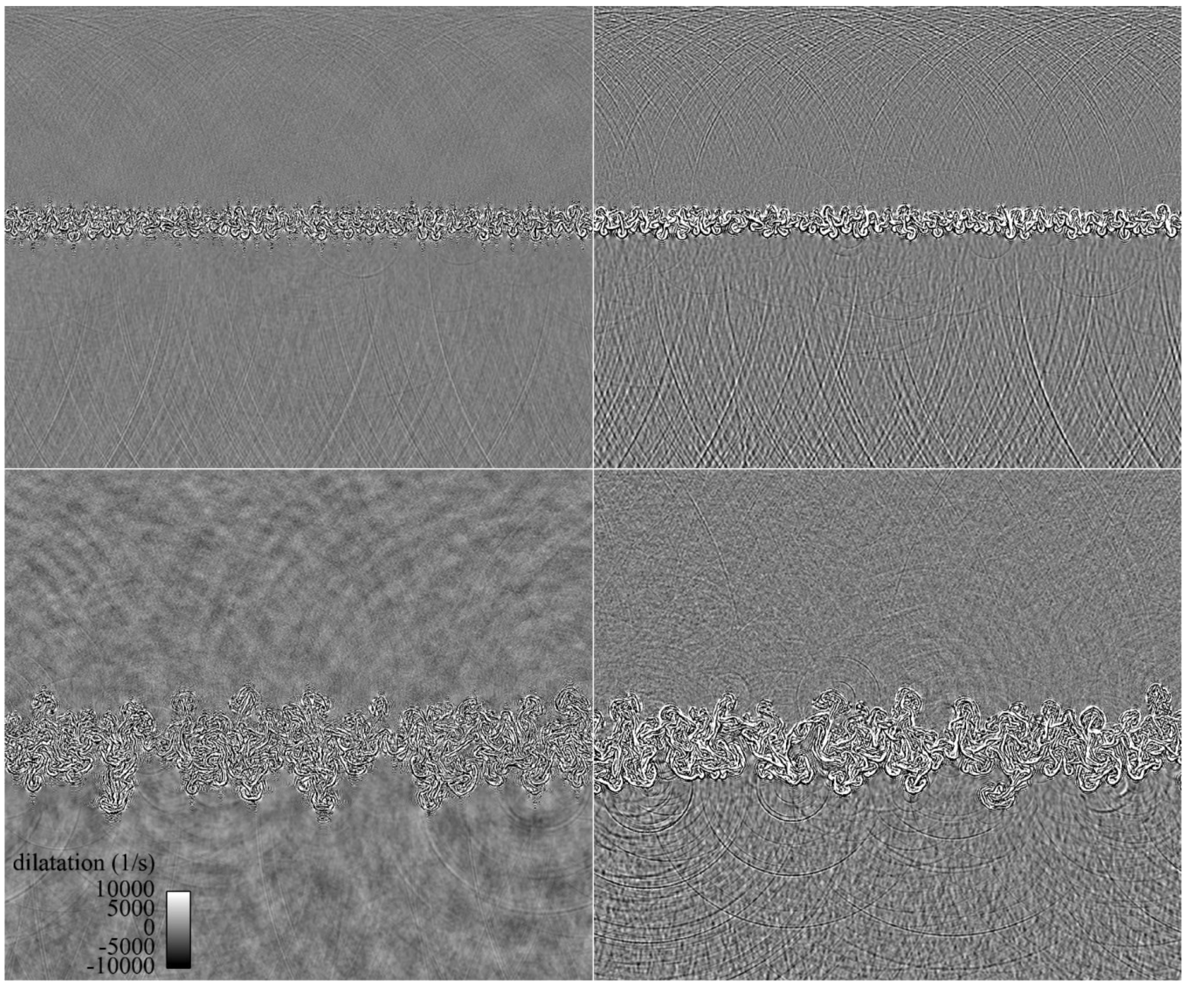


Enthalpy diffusion generates acoustic noise in Rayleigh-Taylor instability.

OFF | ON

20 ms

40 ms



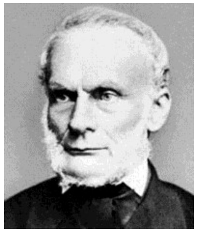
↓ Sn

↑ DT

q_d perturbs pressure which perturbs velocity

Conclusions

Rudolf Clausius
originator of the
concept of entropy



1. The growth rates of RT, RM and KH instabilities are determined by the net mass flux through the equimolar plane.
2. Growth rates are universal only if the flows forget their initial conditions and do not feel their boundaries.
3. RT growth can be reduced by adding shear.
4. RT instability can produce shock waves
5. Enthalpy diffusion preserves the second law of thermodynamics.
6. In addition to temperature, enthalpy diffusion affects density, dilatation and other fields in subtle ways.