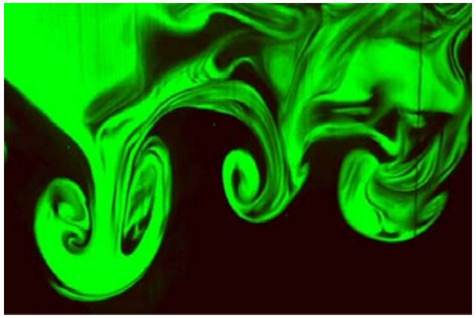
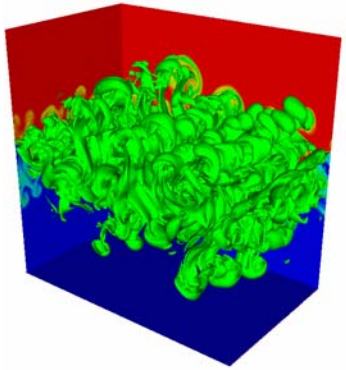
Experimentally-Based Initialization of Direct Numerical Simulations of Miscible, Rayleigh-Taylor Instability-Induced Mixing

Presented at:

9th International Workshop on the Physics of Compressible Turbulent Mixing

Cambridge, UK





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22 July 2004

This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48. This work has also been supported by the Department of Energy as a part of the High Energy Density Science Grant Program under contract #DE-FG03-02NA00060.

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UCRL-PRES-205227

The objective of this research is to couple experimentally-measured initial conditions with high-resolution DNS

- Experimental Objectives
  - Measure initial density and velocity conditions of a small Atwood number, Rayleigh-Taylor driven mixing layer[†]
  - Quantify perturbations in both streamwise and cross-stream directions
  - Measure time-evolution of density statistics, spectra, and molecular mixing parameters
- Numerical Objectives
  - Develop and validate method of initializing DNS (direct numerical simulation) with experimentally-measured data
  - Perform 2D and 3D DNS using measured initial conditions for comparison with experiment[‡] and compare 2D and 3D dynamics
  - Investigate effect of initial conditions on transition from linear to nonlinear mixing layer evolution

[†] P. Ramaprabhu & M. J. Andrews, "Experimental investigation of Rayleigh–Taylor mixing at small Atwood numbers," J. Fluid Mech. 502, 233 (2004)

[‡] P. Ramaprabhu & M. J. Andrews, "On the initialization of Rayleigh-Taylor simulations," Phys. Fluids 16, L59 (2004)

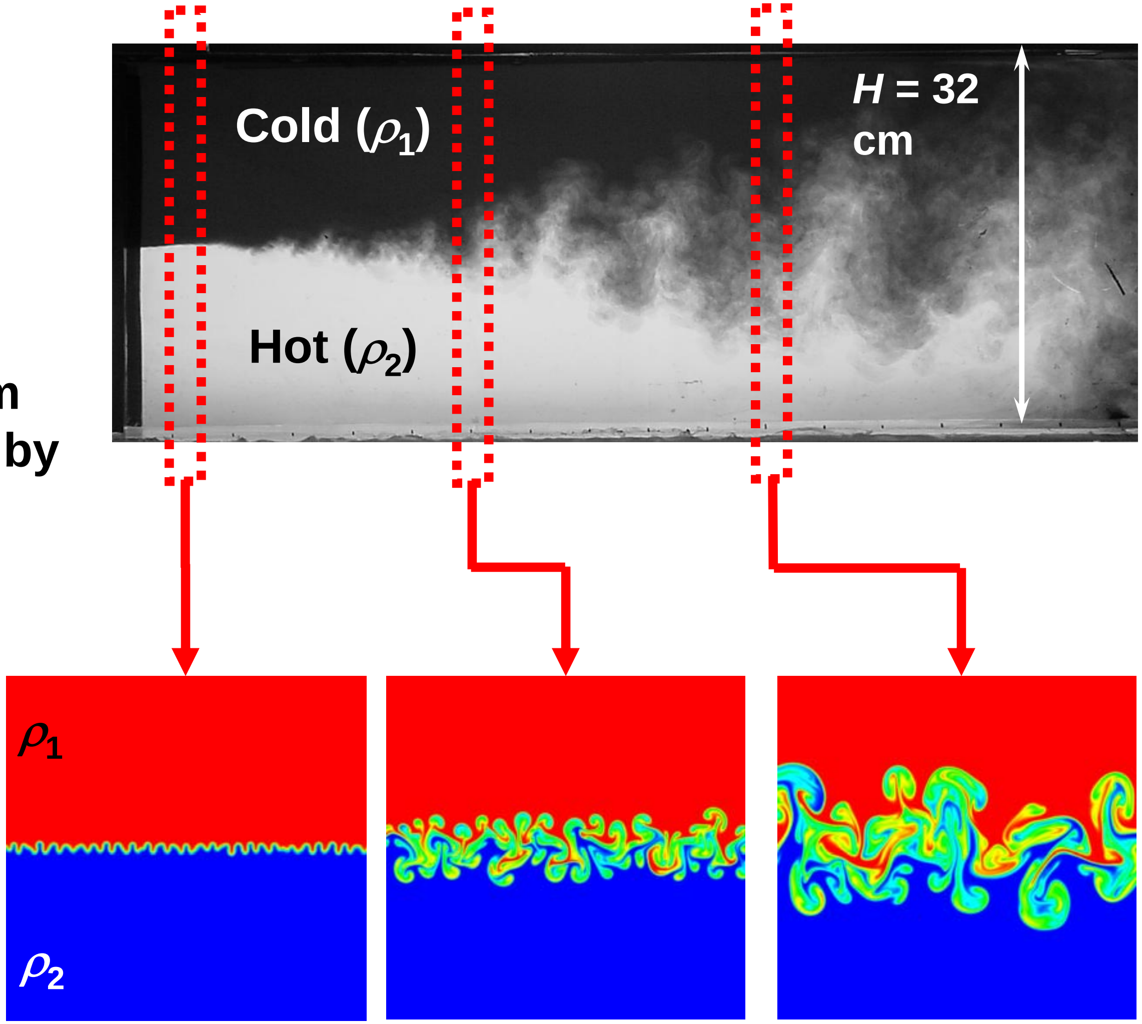
Taylor's hypothesis is used to relate the temporal evolution of statistics to the spatial evolution

- $\Delta T \approx 5°$
- $A = 7.5 \times 10^{-4}$
- $U_m \approx 4.2$ cm/s mean velocity
- $Pr = 7$
- Downstream distance x from splitter plate related to time by

$$t = \frac{x}{U_m}$$

- Dimensionless time

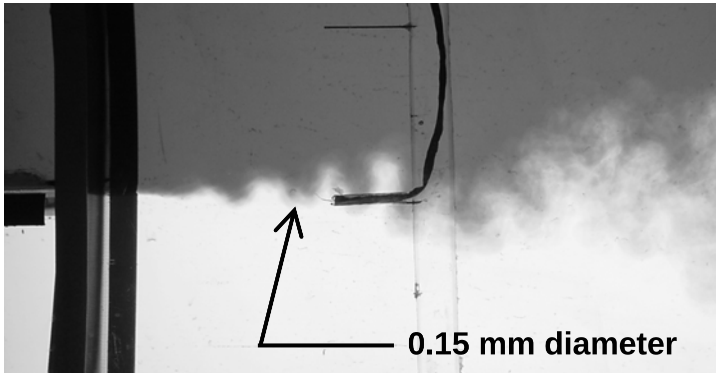
$$\tau = t\sqrt{\frac{gA}{H}} = \frac{x}{U_m}\sqrt{\frac{gA}{H}}$$

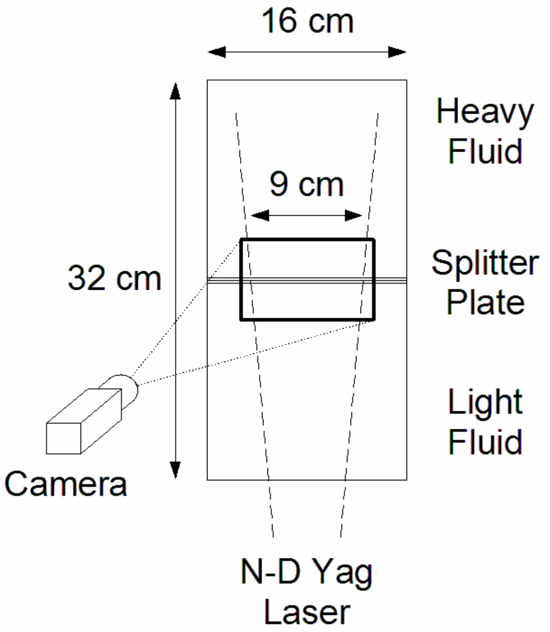


t = 2 s t = 7 s t = 12 s

Density measurements at several downstream locations quantify the evolution of mixing statistics and PLIF diagnostics measured cross-stream perturbation

- **Thermocouple measurements**
  - **Converted to density measurements through H_20 equation of state**
  - **Smaller weld bead in new experiments decreased probe *volume* by 90%**
- **Planar Laser-Induced Fluorescence (PLIF) used to measure cross-stream (*y*-direction) perturbations off splitter plate**
  - **First experimental measurement of *y*-direction perturbation in Rayleigh-Taylor instability**





The initial multi-mode interfacial perturbation $\zeta(x,y)$ is modeled by two Fourier series

- Initial density assumed to have an error function profile

$$\rho(x,y,z,t=0)=\frac{\rho_1+\rho_2}{2}+\frac{\rho_1-\rho_2}{2}\,\mathrm{erf}\left[\frac{z+\zeta(x,y)}{\varepsilon}\right]$$

where $\varepsilon = \delta/2$ and δ is width of initial diffusion layer

$$\zeta(x,y)\equiv\left[\sum_{m=0}^{N_x}a_m\cos\left(\frac{2\pi m}{\lambda_x}x\right)+b_m\sin\left(\frac{2\pi m}{\lambda_x}x\right)\right]+\left[\sum_{n=0}^{N_y}c_n\cos\left(\frac{2\pi n}{\lambda_y}y\right)+d_n\sin\left(\frac{2\pi n}{\lambda_y}y\right)\right].$$

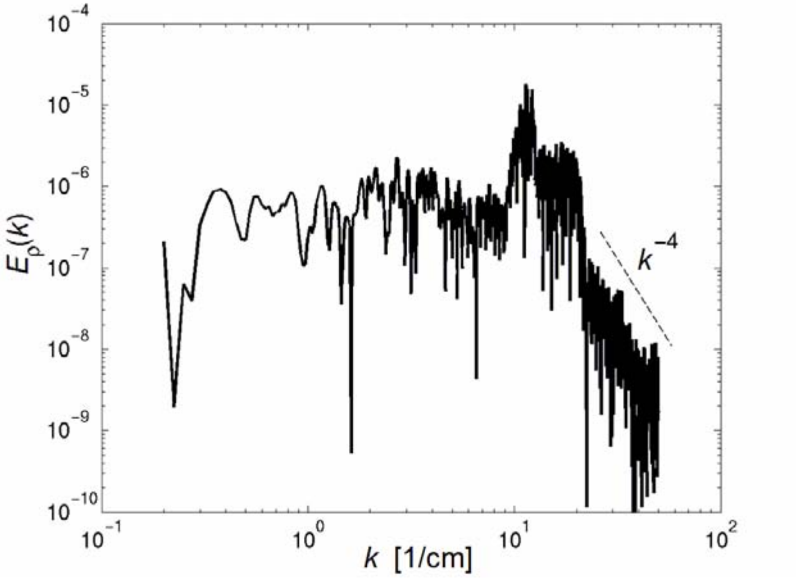
- Fourier coefficients taken directly from fluctuating density spectrum at x = 0.1 cm from splitter plate
- Initial diffusion velocity field required to satisfy continuity is

$$u_i=-\frac{D}{\rho}\frac{\partial\rho}{\partial x_i}$$

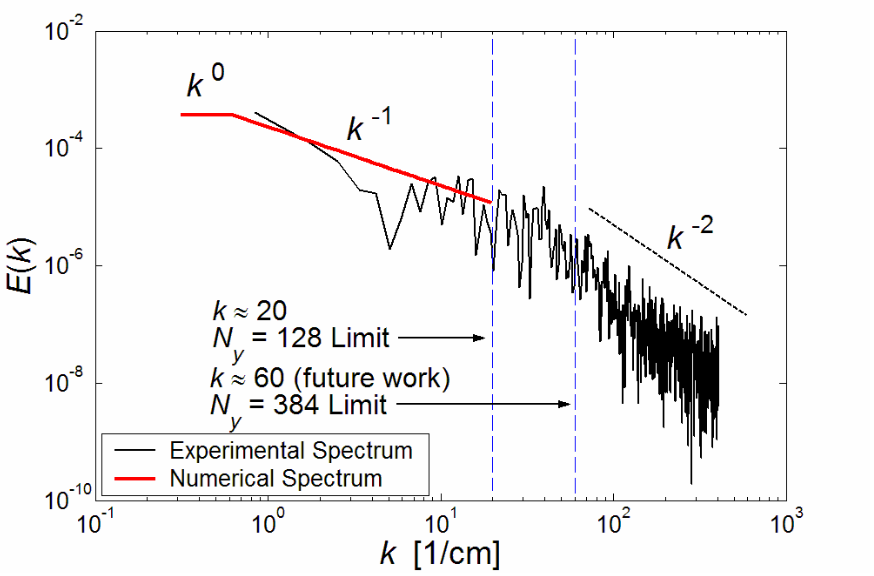
The initial density spectra in *x*- and *y*-directions include short- and long-wavelength perturbations

- **Smallest perturbation present limited by current simulation resolutions**
- **Density spectra (thermocouple) and interfacial perturbation spectra (PLIF) related through interfacial thickness δ**

Density Spectrum
***x*-direction perturbation (thermocouple)**



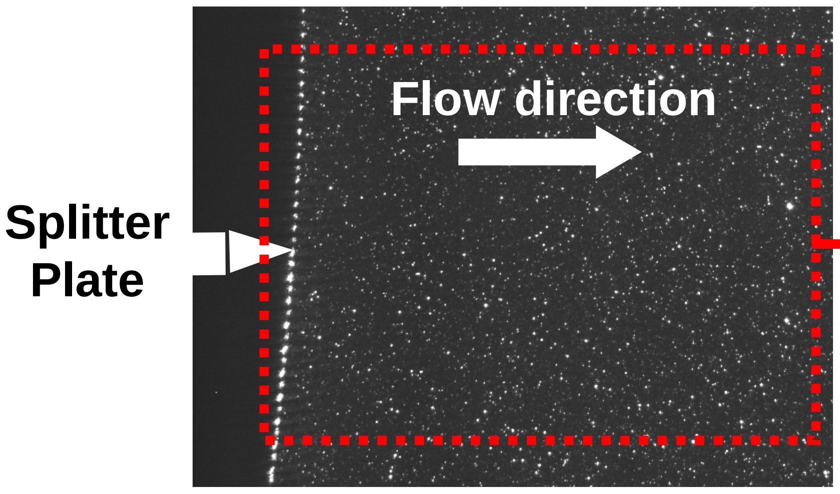
Interfacial Perturbation Spectrum
***y*-direction perturbation (PLIF)**



Particle image velocimetry (PIV) was used to measure initial streamwise velocity perturbation

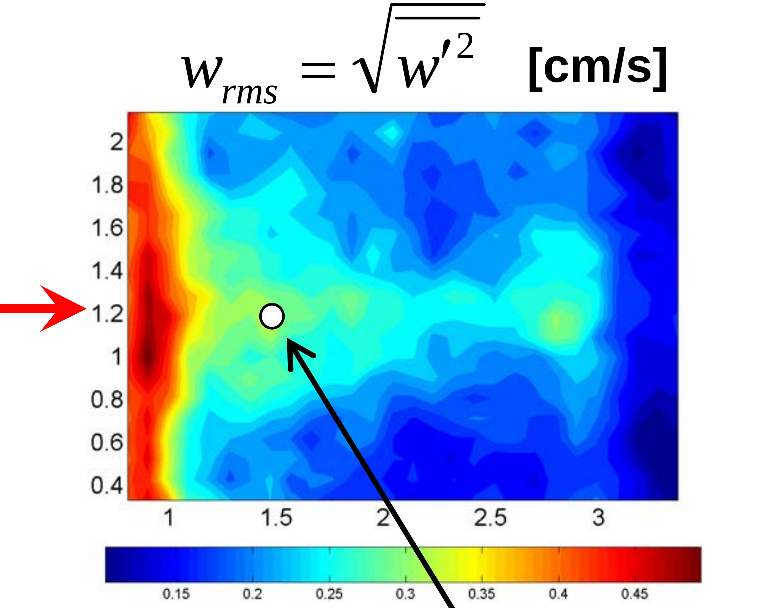
- **Velocity measurements performed without buoyancy isolate momentum input generated by splitter plate**
- **Fluctuating vertical velocity (*w*′) at *x* = 0.75 cm from edge of splitter plate characterize initial velocity conditions**

Raw PIV Image



Laser light on screen mesh

$$w_{rms} = \sqrt{\overline{w'^2}} \quad \text{[cm/s]}$$



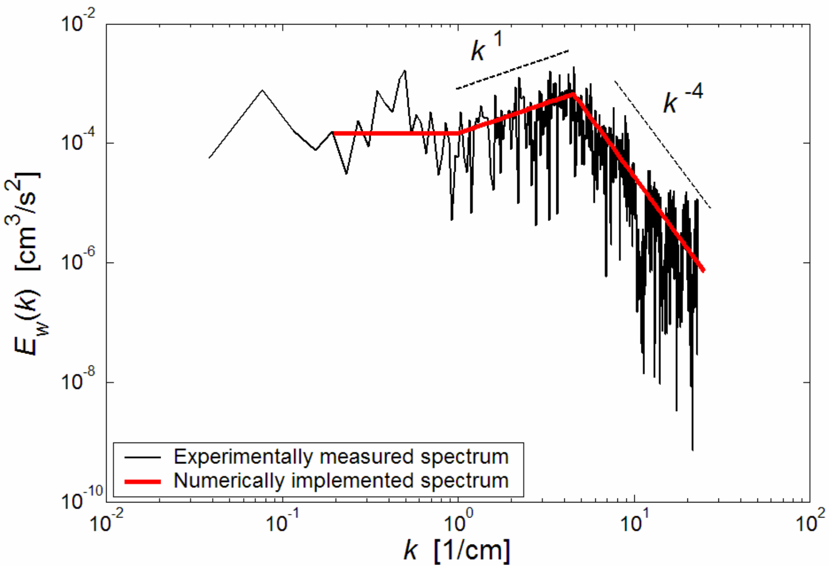
Point used for initialization of velocity conditions

The initial potential field is constructed from the measured initial vertical velocity spectrum

- **Potential field** [†] $\phi(x,z) = a_0 \sum_{k=k_{\min}}^{k_{\max}} \frac{A(k)}{k} \sin(kx) \exp(-k|z|)$ **created using spectral coefficients *A*(*k*) from measured vertical velocity spectrum**
- **Initial velocity defined as**

$$u_i = \frac{\partial\phi}{\partial x_i} - \frac{D}{\rho}\frac{\partial\rho}{\partial x_i}$$

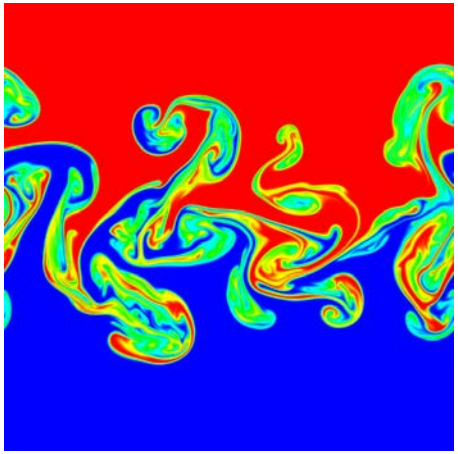
- **Initial velocity conditions DNS have PLIF measured perturbation in *y*-direction and no ρ perturbation in *x*-direction**
- **Initial potential field for 2D and 3D DNS is 2D, as no velocity perturbation is measured in *y*-direction**



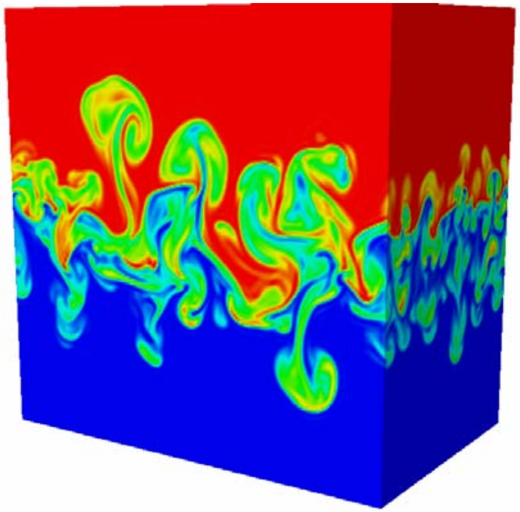
[†] **P. G. Drazin & W. H. Reid, *Hydrodynamic Stability*, Cambridge University Press (1982)**

Simulations have been performed with both initial density and velocity conditions

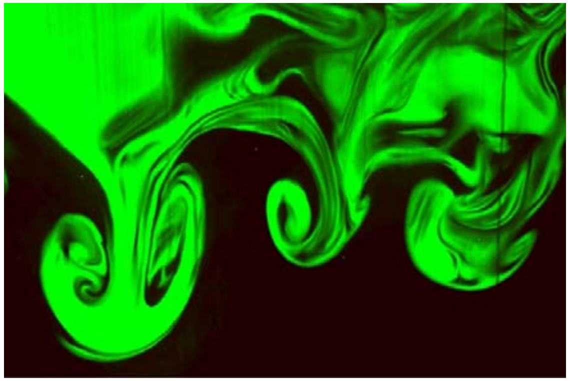
- **Four simulations have been performed:**
  - **Initial density conditions**
    - 2D: 1024^2 (32 × 32 cm)
    - 3D: 256 × 128 × 256 (16 × 10 × 16 cm)
  - **Initial velocity conditions**
    - 2D: 1024^2 (32 × 32 cm) (in progress)
    - 3D: 256 × 128 × 256 (16 × 10 × 32 cm) (in progress)



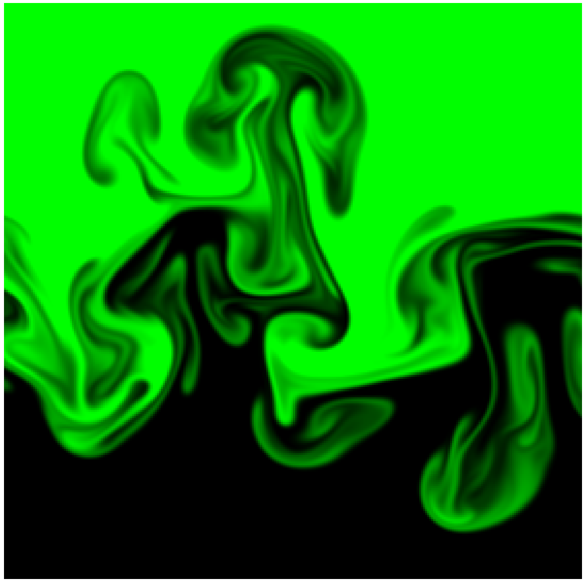
- **Simulation parameters chosen to match experimental conditions**
  - $\rho_1 = 0.9986\ \mathrm{g/cm^3},\ \mu_1 = 0.009\ \mathrm{g/(cm\,s)}$
  - $\rho_2 = 0.9970\ \mathrm{g/cm^3},\ \mu_2 = 0.011\ \mathrm{g/(cm\,s)}$
  - $A = (\rho_1 - \rho_2)/(\rho_1 + \rho_2) = 7.5 \times 10^{-4}$
  - $Sc = \nu/D = 7.0,\ \nu = (\mu_1 + \mu_2)/(\rho_1 + \rho_2)$
  - $g_z = -981\ \mathrm{cm/s^2}$



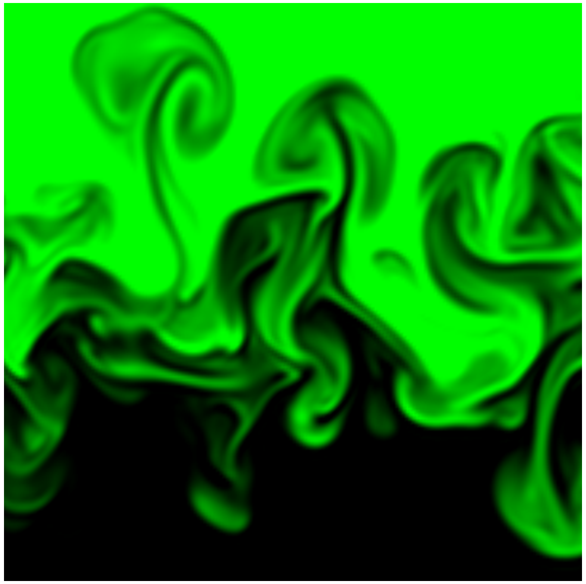
PLIF density images from experiment are qualitatively similar to both 2D and 3D DNS densities



PLIF Image[†]
$\tau = 1.15–1.30$



2D DNS
$\tau = 2.1$



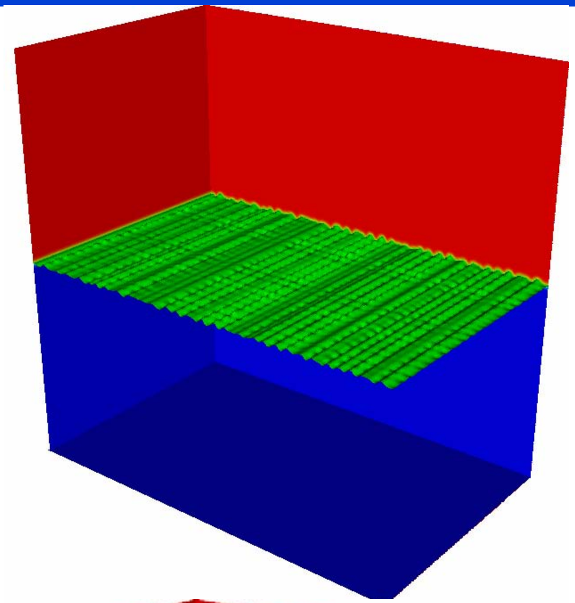
3D DNS
$\tau = 1.95$

- **PLIF images closely resemble DNS, but more resolution is required in 3D to fully resolve all scales present in experiment at later times**
- **Time lag between experiment and simulations with initial density conditions noted with respect to times of similar development**

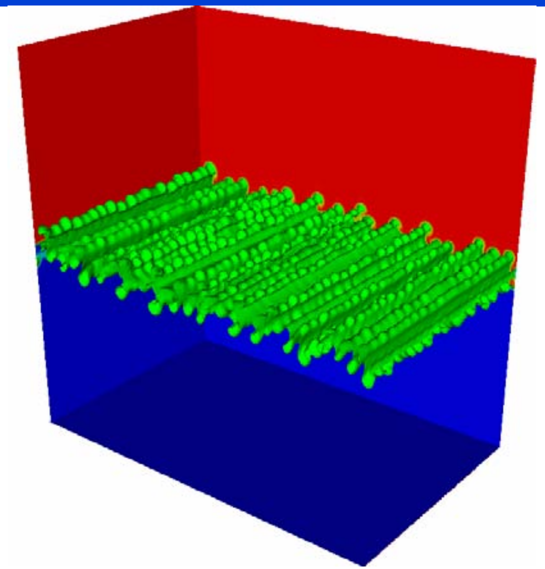
[†] W. Kraft, Texas A&M University

3D DNS visualizations show initially 2D behavior with 3D structure emerging at later times

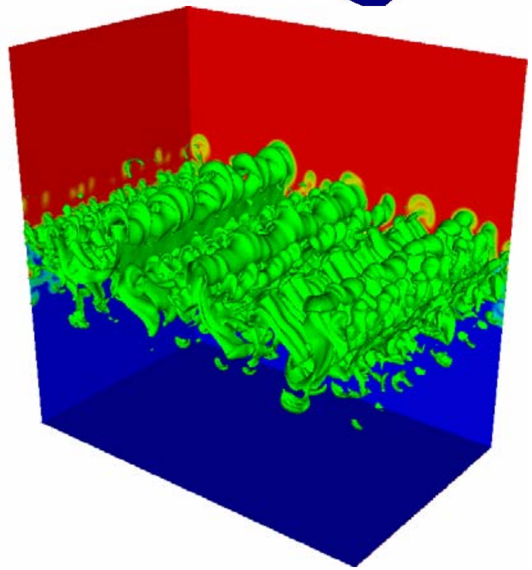
τ = 0.15



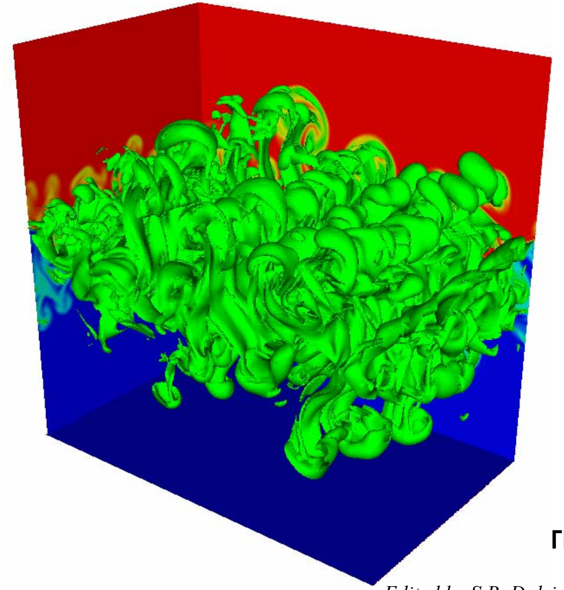
τ = 0.61



τ = 1.06

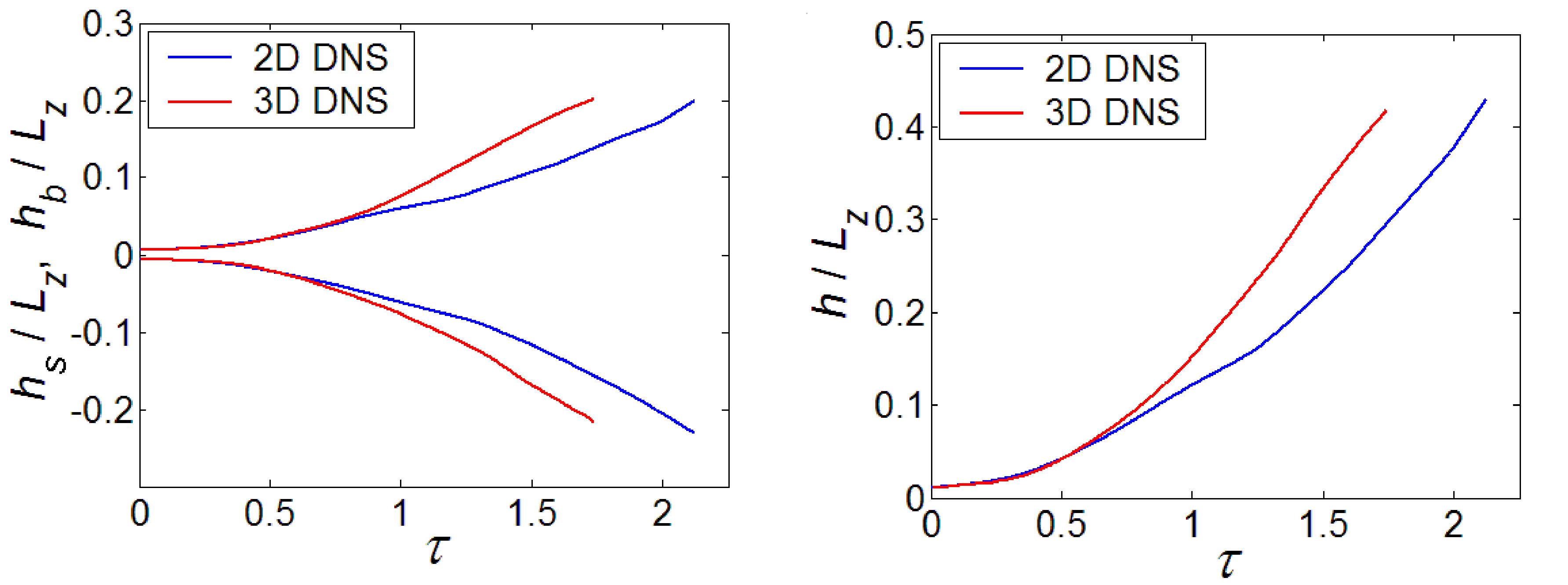


τ = 1.52



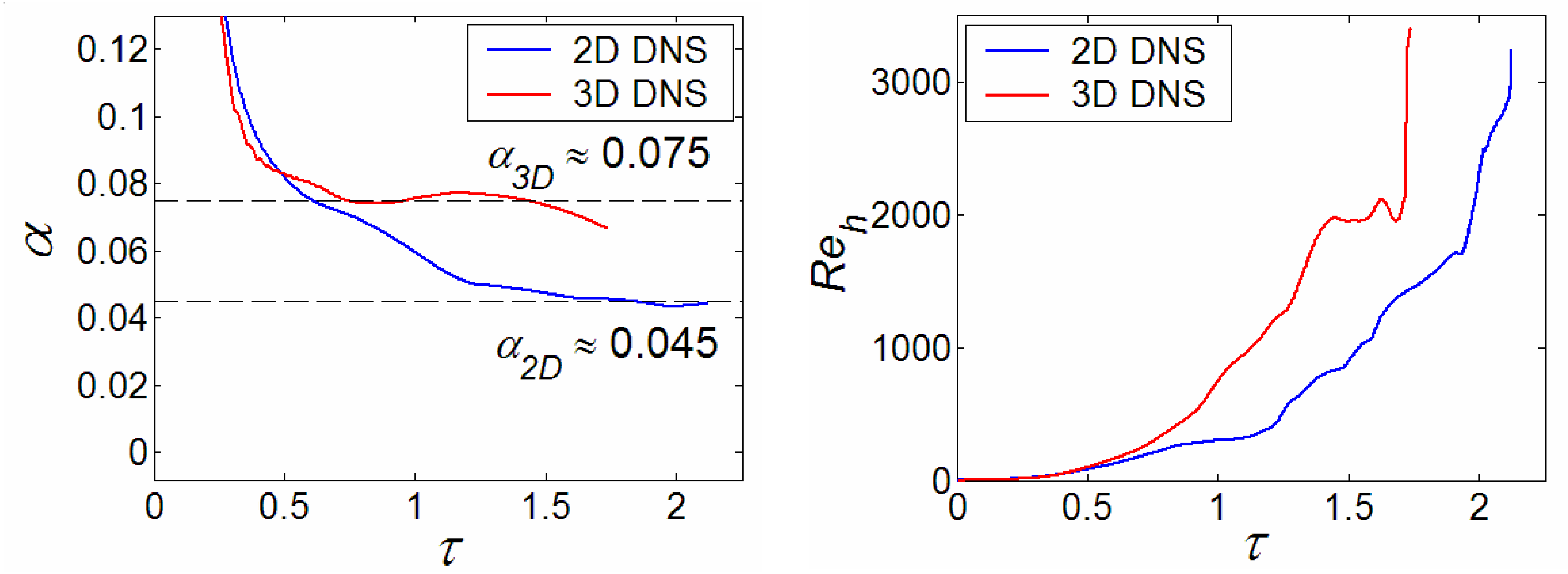
The evolution of the mixing layer width from 2D and 3D DNS show differences, but need to evolve to later times

- **Slopes of front growths are slightly steeper in 3D than in 2D**
- **Unclear whether 3D simulations exhibit a τ^2 growth at late times**



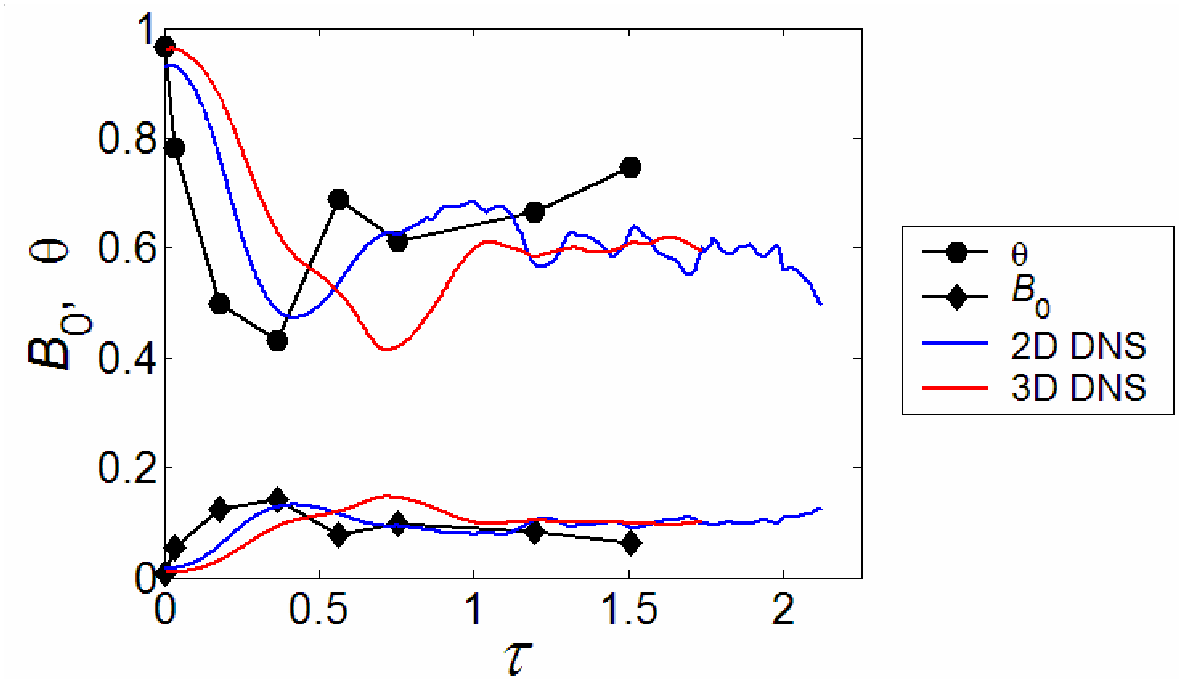
The evolution of α_b and outer-scale Reynolds number from 2D and 3D simulations are quite different

- $\alpha_b = h_b/(A\, g\, t^2)$ **from DNS bracket experimental values 0.06-0.07**
  - **For present initialization,** $\alpha_{3D} > \alpha_{2D}$**, which differs from trend observed using monotone integrated large-eddy simulation (MILES)**
  - **Both simulations seeded with long wavelength perturbations, yet exhibit different late-time** α_b
- **Outer-scale Reynolds number** $Re_h = (h/\nu)\, dh/dt \approx 3{,}500$ **at late times**



The time-evolution of turbulent molecular mixing parameters from 2D and 3D simulations are similar

- **θ quantifies degree of molecular mixing (θ = 1 and 0 represent completely mixed fluids and completely segregated fluids, respectively)**
- **B_0 and B_2 quantify ρ fluctuations for a miscible and immiscible mixture**
- **Values of θ qualitatively agree with experiment, but lag in time**
- **Inclusion of initial velocity data expected to reduce/eliminate time-lag and improve agreement with experimental data**



$$B_0 = \overline{\rho^*}\left(1-\overline{\rho^*}\right) - \overline{\rho^*\left(1-\rho^*\right)}$$

$$B_2 = \overline{\rho^*}\left(1-\overline{\rho^*}\right)$$

$$\theta \equiv \frac{\overline{\rho^*\left(1-\rho^*\right)}}{\overline{\rho^*}\left(1-\overline{\rho^*}\right)} = 1 - \frac{B_0}{B_2}$$

$$\rho^* \equiv \frac{\rho-\rho_2}{\rho_1-\rho_2} = f_1$$

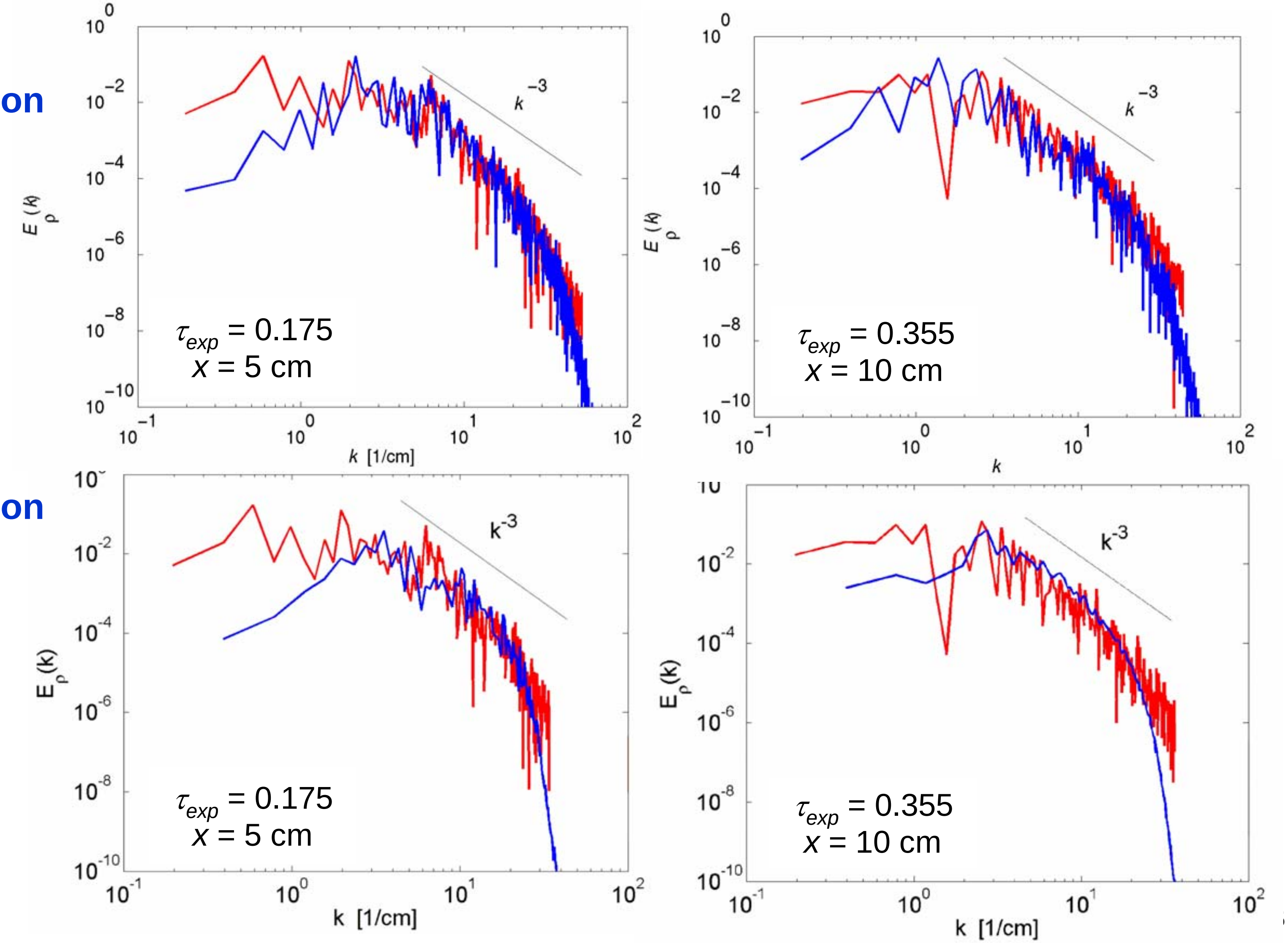
$\overline{f}$ is a spatial average

Density spectra from 2D and 3D DNS show generally good agreement for intermediate *k* at later times

Experiment

2D Simulation

3D Simulation



These are the first DNS of the TAMU Water Channel experiment using experimentally-measured data

- **Similarly-initialized 2D and 3D simulations exhibit different mixing layer growth rates and α_b**
- **Mixing parameters from both 2D and 3D simulations are in good agreement with measured values, but exhibit early-time lag**
- **Late-time density spectra are in generally good agreement with measured spectra, and also exhibit early-time lag**
- **Addition of initial velocity in DNS may be needed to match experimental data**
- **Simulations with *both* initial density and velocity conditions are in progress**