APS DFD – 11/24/14

Efficient Modeling of Multicomponent Diffusive Mixing

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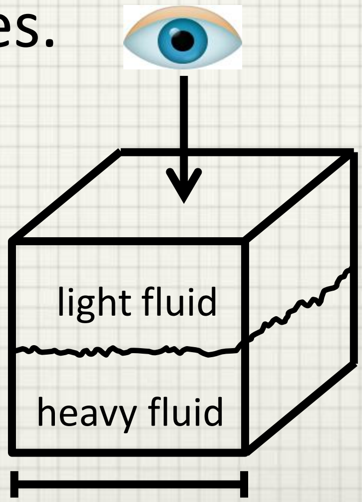
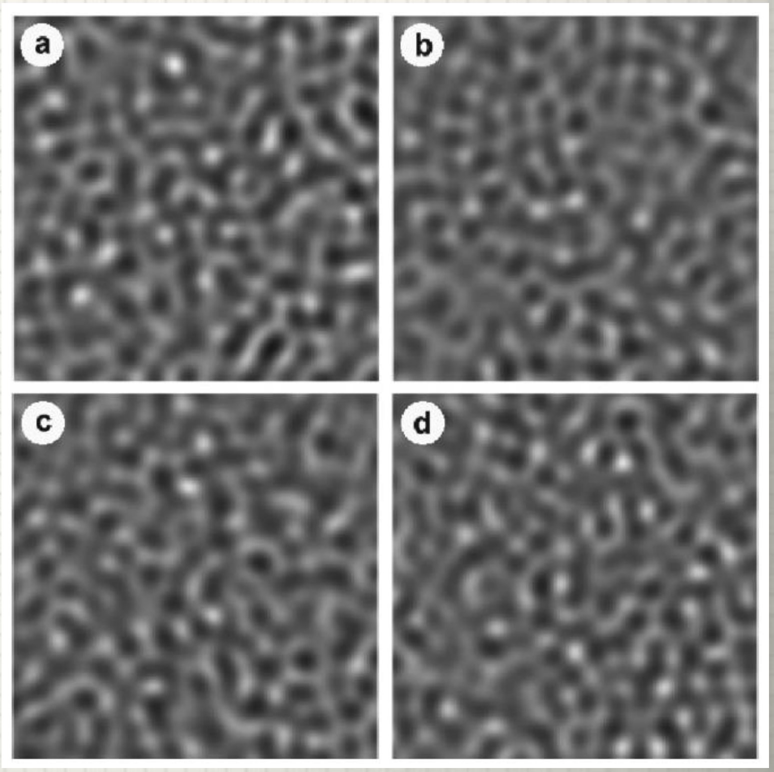
Motivation: Giant Fluctuations

- Experiment: mixing of water and various denser organic compounds ((a) urea, (b) glycerol, (c) polyethylene, (d) lysozyme) with initially flat interface
- Shadowgraph techniques reveal *giant fluctuations* caused by thermal fluctuations develop over several minutes.



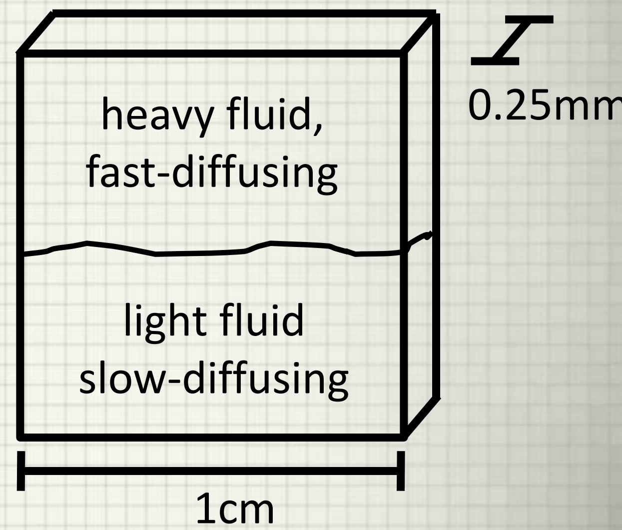
Not an instability!

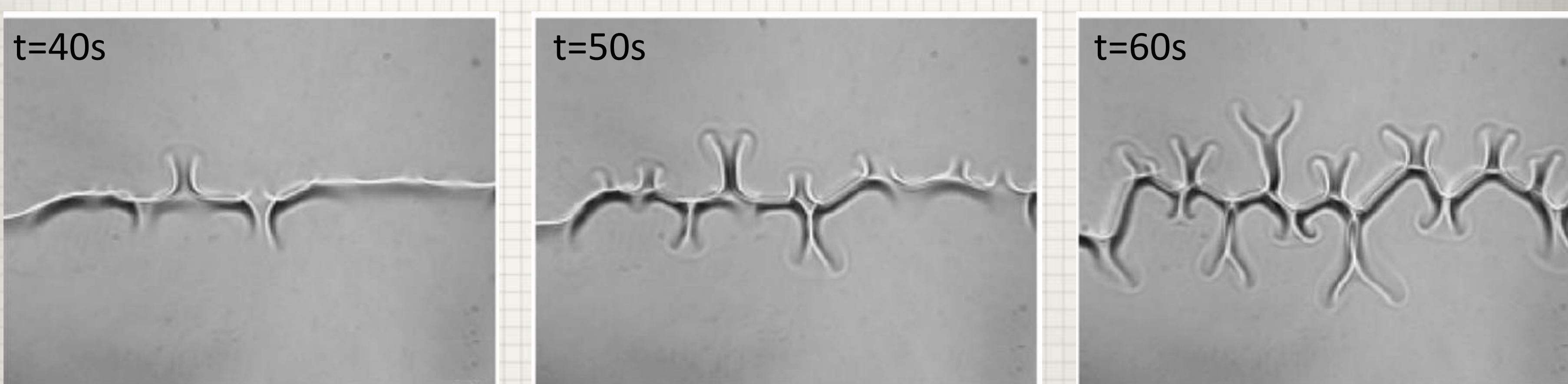


Brogioli et al, Phys. Rev. E., 2000

Motivation: Mixed-Mode Instability

- Experiment: ternary mixture (water, salt, sugar) between two glass plates.
  - Heavy saltwater on top of light sugar water
  - Salt diffuses into water 4x faster than sugar





Carballido-Landeira et al., Physics of Fluids, 2013

Multicomponent Diffusive Mixing

- We are interested in developing a model for multicomponent diffusive mixing at length scales where thermal fluctuations are important.
  - Arbitrary number of fluid components, non-ideal space/time-dependent transport properties, thermal fluctuations.
  - Large Schmidt numbers (momentum diffusion divided by mass diffusion) requires implicit treatment of viscosity
  - Requires long-time integration (minutes to hours). More established particle or compressible methods are not fast enough.

Low Mach Number Fluctuating Hydrodynamics

- We develop a Low Mach number continuum model.
  - Begin with the compressible equations of fluctuating hydrodynamics (Landau & Lifschitz).
  - Make the assumption that acoustic waves are unimportant to the overall solution.
  - Using low Mach number asymptotics, we derive an equation set that mathematically eliminates sound waves and enforces instantaneous acoustic equilibration.
  - Obtain a divergence constraint on velocity (similar to incompressible Navier Stokes) but the divergence is determined by the mixing of fluids.
  - Model allows for larger advective-based time steps.

Low Mach Number Fluctuating Hydrodynamics

- Given an arbitrary number of fluid components with pure densities, $\overline{\rho}_i$
- The total density is the sum of the component densities, $\rho = \sum \rho_i$
- We enforce no volume change upon mixing, $\sum \frac{\rho_i}{\overline{\rho}_i} = 1$
- The resulting low Mach number model is

$$\frac{\partial(\rho \mathbf{v})}{\partial t} = -\nabla \cdot (\rho \mathbf{v}\mathbf{v}^T) - \nabla \pi + \nabla \cdot \boldsymbol{\tau}(\mathbf{v}) + \nabla \cdot \boldsymbol{\Sigma} + \rho \mathbf{g}$$

$$\frac{\partial \rho_i}{\partial t} = -\nabla \cdot (\rho_i \mathbf{v}) + \nabla \cdot \mathbf{F}_i$$

Model for stochastic forcing (Landau, Lifschitz)

Multicomponent non-ideal diffusion (based on works by Kuiken, Giovangigli, Kjelstrup) and stochastic forcing (Ottinger)

Divergence constraint represents "no volume change upon mixing"

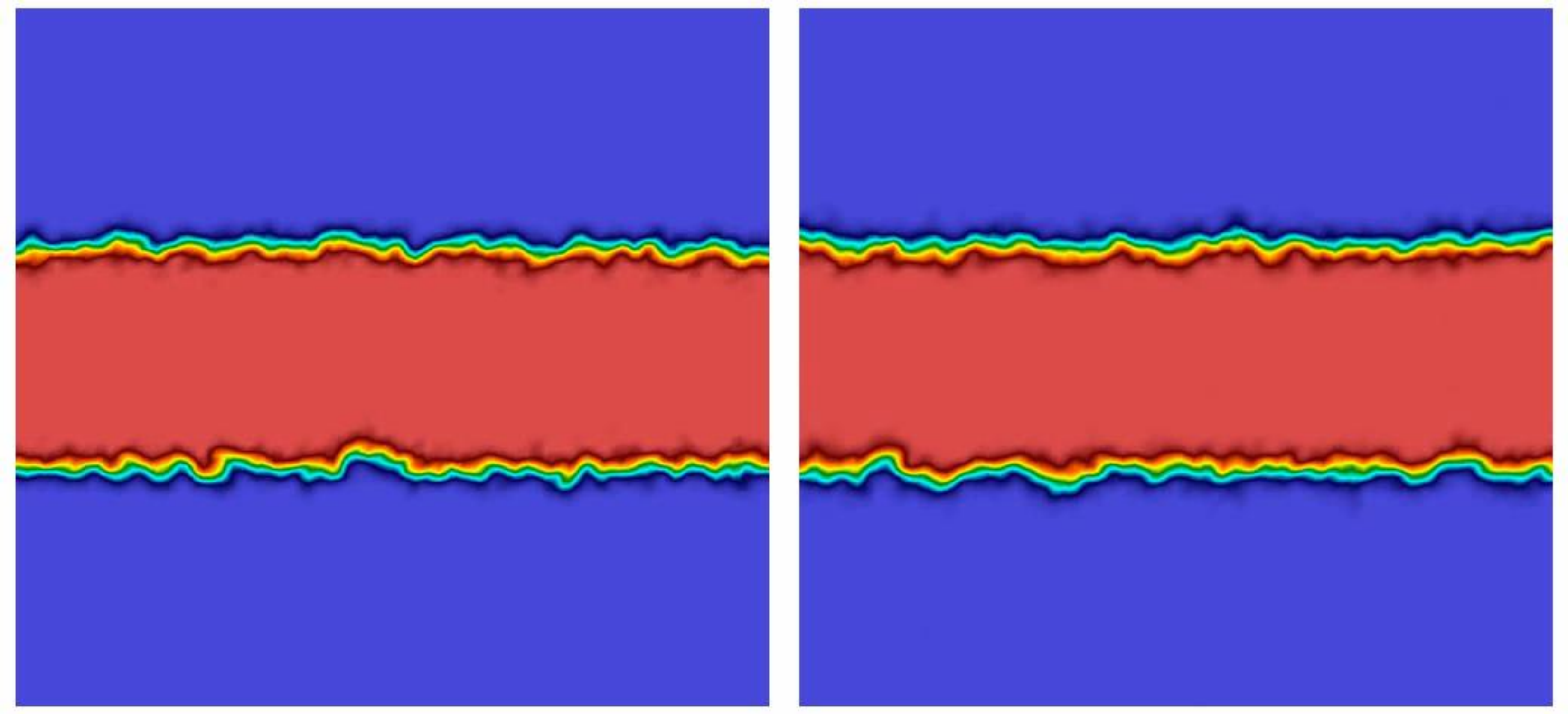
$$\nabla \cdot \mathbf{v} = \nabla \cdot \left(\sum_i \frac{\mathbf{F}_i}{\overline{\rho}_i} \right)$$

Numerical Features

- Staggered grid velocity finite volume formulation
- Arbitrary number of fluid components
- Non-ideal multicomponent diffusion with space/time-varying transport coefficients
- Stokes solver for coupled viscous/projection problem with no loss of accuracy at boundaries
- Projection method preconditioner for Stokes solver; we have demonstrated the overall algorithm is competitive with standard operator split approaches
- Multiple time stepping schemes to support inertial and large Schmidt number (via Stokes approximation) regimes
- Multistage centered scalar advection for stochastic flow; option for higher-order Godunov schemes for deterministic flow
- Implemented in highly scalable BoxLib software framework developed at Berkeley Lab.

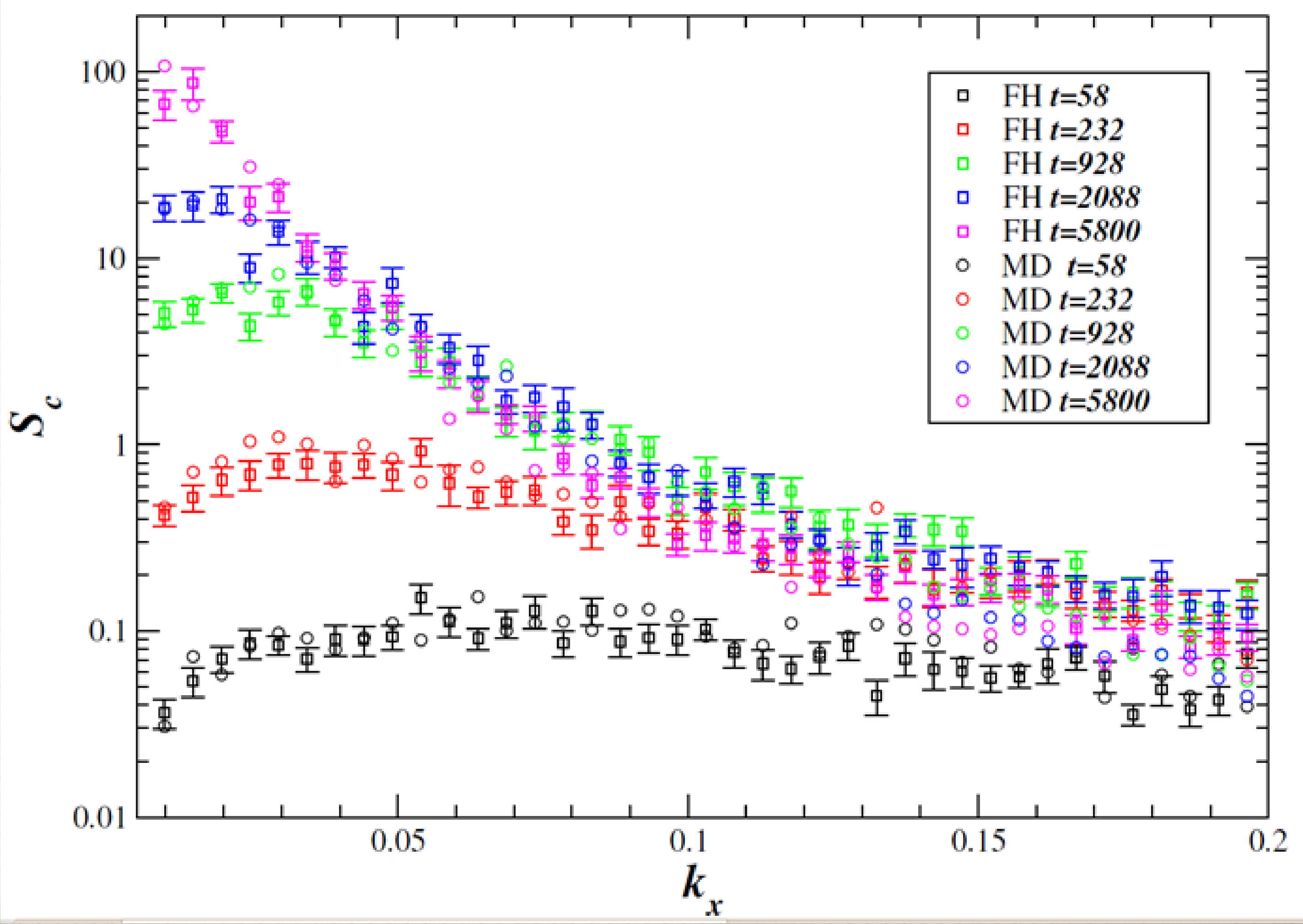
Model Validation

- Diffusive mixing of two fluids with density contrast 4.
  - Left: Molecular dynamics simulation (Skoge 2006, publicly available)
    Right: Low Mach number fluctuating hydrodynamics



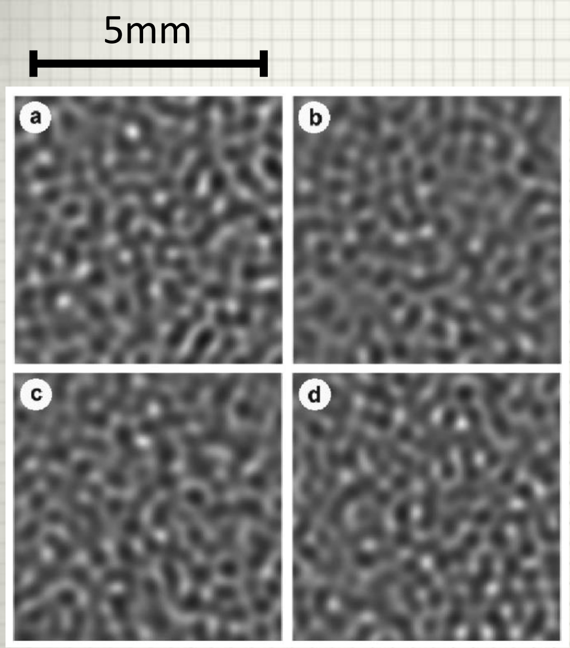
Analysis of Interface Fluctuations

- Discrete spatial spectrum of interface fluctuations shows excellent agreement



Giant Fluctuations

- We are able to reproduce giant fluctuations observed in stable fluid configurations



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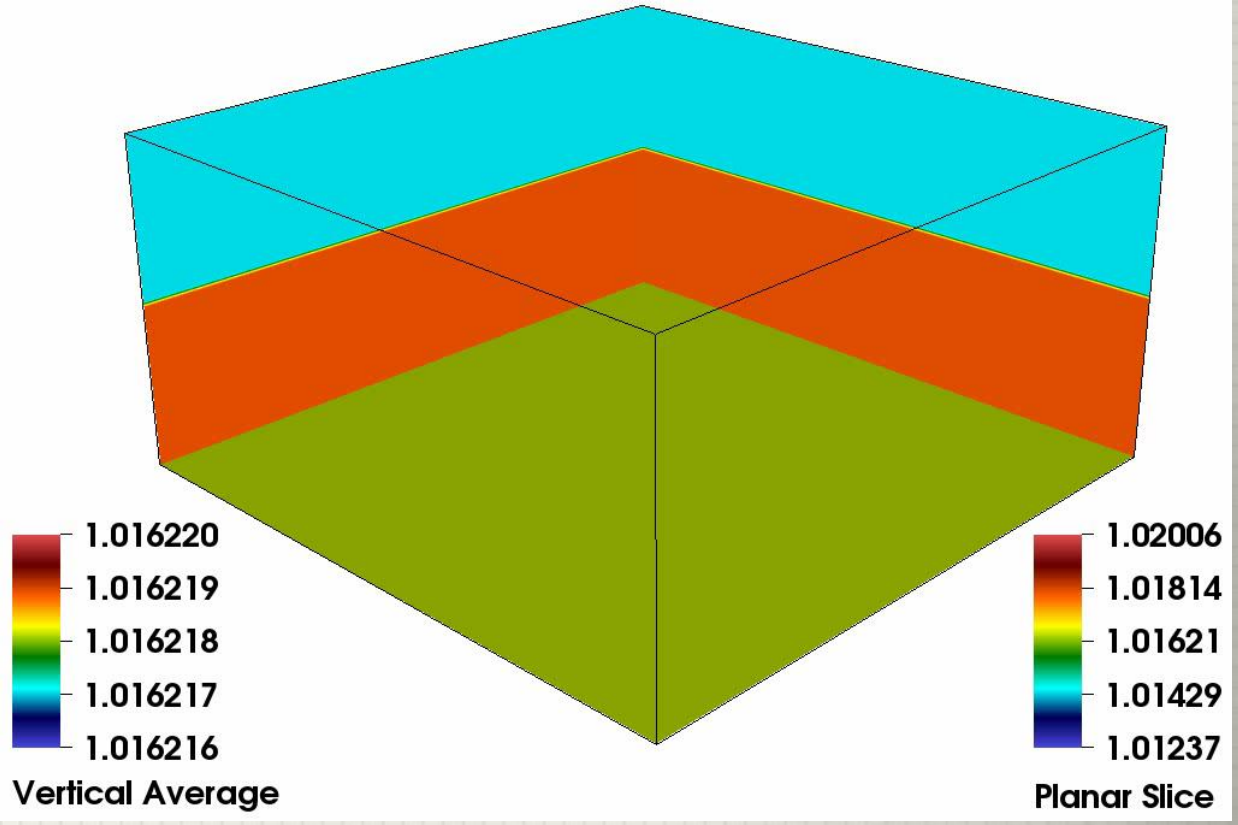
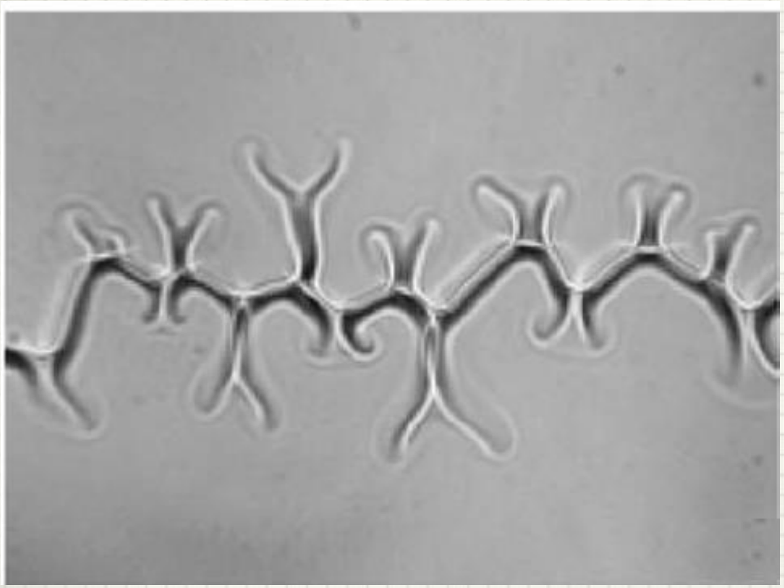


Mixed Mode Instability

- Simulation parameters match experimental setup for ternary mixed-mode instability.



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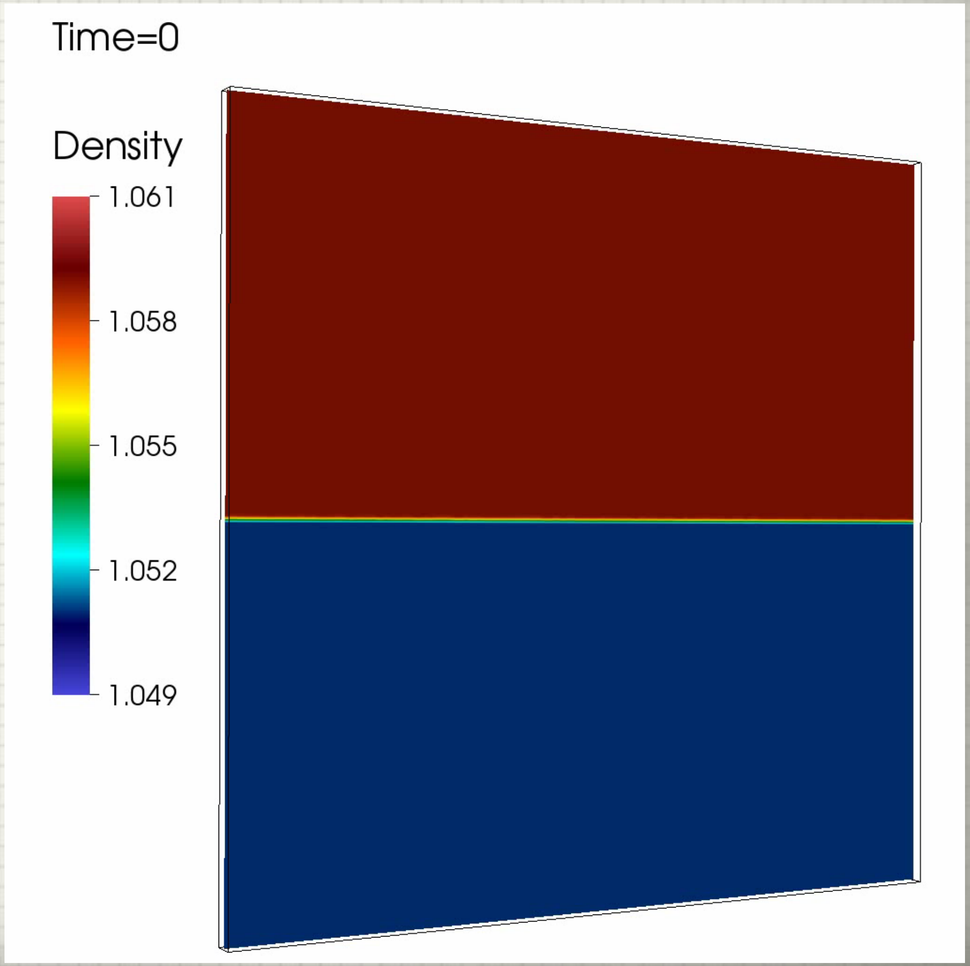

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- A. Donev et al., **"Low Mach Number Fluctuating Hydrodynamics of Multispecies Liquid Mixtures",** *in preparation*