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A Numerical Scheme for Fluctuating Hydrodynamics of Multispecies Gas Mixtures

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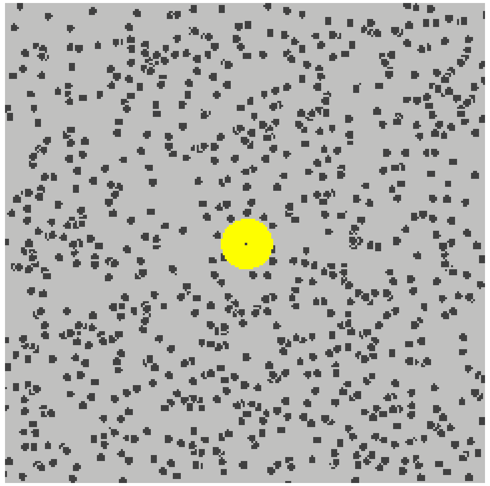
Hydrodynamic Fluctuations

The study of hydrodynamic fluctuations is a seminal topic of statistical mechanics

The topic is of increasing importance given the advances in nanoscale fluid technology, including applications in cellular biology.

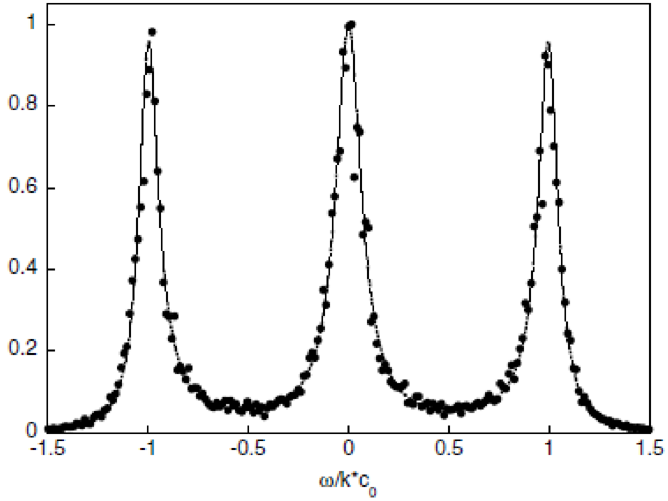
Yet only recently have hydrodynamic fluctuations been incorporated into computational fluid dynamics.

Brownian motion



Blue sky due to Rayleigh scattering from density fluctuations in air

Rayleigh-Brillouin scattering spectrum (dots: DSMC; lines: hydrodynamic theory)



Bruno, et al., Chem. Phys. Lett. 422 517 (2006)

Landau-Lifshitz Stochastic Navier-Stokes

From Landau & Lifshitz, *Statistical Physics*, Part 2

The equations of hydrodynamics…with no specific form of the stress tensor and the heat flux vector simply express the conservation of mass, momentum, and energy. In this form they are therefore ***valid for any motion****, including fluctuational changes…*

The usual expressions for the stress tensor and the heat flux relate them respectively to the velocity gradients and the temperature gradient. When there are fluctuations in a fluid, there are also spontaneous local stresses and heat fluxes unconnected with these gradients; we denote these (as) "random quantities"…

Example: Stochastic Heat Equation (1)

For simple conduction we write the change in energy density in terms of heat flux as

$$\frac{\partial}{\partial t}(\rho E) = -\nabla \cdot \underline{\boldsymbol{Q}}$$

The total heat flux is the sum of two contributions: deterministic and stochastic heat fluxes

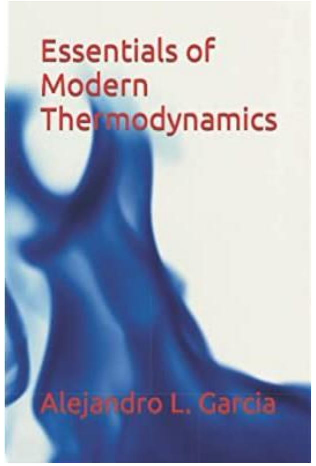
$$\underline{\boldsymbol{Q}} = \boldsymbol{Q} + \widetilde{\boldsymbol{Q}}$$

Write the deterministic heat flux in Onsager form as

$$\boldsymbol{Q} = L\boldsymbol{X}$$

The rate of entropy production in a volume ΔV is

$$\frac{dS}{dt} = \boldsymbol{X} \cdot \boldsymbol{Q}$$ so thermodynamic force is $$\boldsymbol{X} = \Delta V \left(\nabla \frac{1}{T} \right) = -\frac{\Delta V}{T^2} \nabla T$$



8 Euros on Amazon

Example: Stochastic Heat Equation (2)

Comparing this with Fourier law

$$\boldsymbol{Q} = -\lambda\nabla T \qquad \text{tells us that the Onsager coefficient is} \qquad L = \frac{\lambda T^2}{\Delta V}$$

Total heat flux now has the form required for linear response theory

$$\underline{\boldsymbol{Q}} = L\boldsymbol{X} + \widetilde{\boldsymbol{Q}}$$

so by the fluctuation-dissipation theorem the white noise has correlation

$$\left\langle \widetilde{\boldsymbol{Q}}(t)\widetilde{\boldsymbol{Q}}(t')\right\rangle = 2k_{\mathrm{B}}L\,\delta(t-t') \qquad \text{or} \qquad \left\langle \widetilde{\boldsymbol{Q}}(\boldsymbol{r},t)\widetilde{\boldsymbol{Q}}(\boldsymbol{r}',t')\right\rangle = 2\lambda k_{\mathrm{B}}T^2\,\delta(t-t')\,\delta(\boldsymbol{r}-\boldsymbol{r}') \quad \text{as } \Delta V \to 0$$

Collecting the above and writing $E = \mathrm{c_V}T$ gives the **stochastic heat equation**,

$$\rho\mathrm{c_V}\frac{\partial T}{\partial t} = \lambda\nabla^2 T + \nabla\cdot\sqrt{2\lambda k_{\mathrm{B}}T^2}\,\tilde{\mathbf{Z}} \qquad \text{where } \tilde{\mathbf{Z}} \text{ is Gaussian white noise}$$

Multi-species Compressible FHD

Full multi-species compressible fluctuating hydrodynamic (FHD) equations are

Species flux

Mass (species k)

$$\frac{\partial}{\partial t}(\rho_k) = -\nabla\cdot(\rho_k \mathbf{v}) - \nabla\cdot\left[\boldsymbol{F}_k + \widetilde{\boldsymbol{F}_k}\right]$$

Stress tensor

Momentum

$$\frac{\partial}{\partial t}(\rho\mathbf{v}) = -\nabla\cdot[\rho\mathbf{v}\otimes\mathbf{v} + p\mathbf{I}] - \nabla\cdot\left[\boldsymbol{\Pi} + \widetilde{\boldsymbol{\Pi}}\right] + \rho\boldsymbol{g}$$

Heat flux

Energy

$$\frac{\partial}{\partial t}(\rho E) = -\nabla\cdot[\mathbf{v}(\rho E + p)] - \nabla\cdot\left[\mathbf{Q} + \widetilde{\mathbf{Q}}\right] - \nabla\cdot\left[\left(\boldsymbol{\Pi} + \widetilde{\boldsymbol{\Pi}}\right)\cdot\mathbf{v}\right] + \rho\boldsymbol{g}\cdot\mathbf{v}$$

Summing the mass equation over species gives the continuity equation

Mass (total)

$$\frac{\partial}{\partial t}(\rho) = -\nabla\cdot(\rho\mathbf{v})$$

Dissipative Fluxes – Stress Tensor

Deterministic stress tensor

$$\Pi_{ij} = -\eta\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right) - \delta_{ij}\left(\left(\kappa - \frac{2}{3}\eta\right)\nabla \cdot \mathbf{v}\right)$$

η – shear viscosity
κ – bulk viscosity

Stochastic stress tensor (see Español, *Physica A* **248** 77 (1998)).

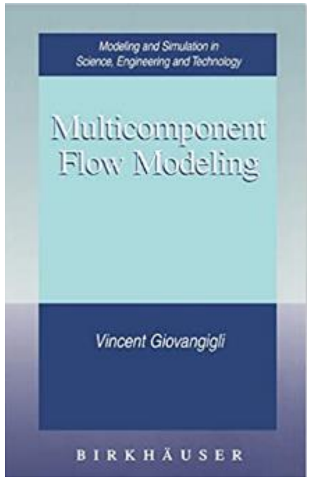
$$\widetilde{\Pi}(\boldsymbol{r}, t) = \sqrt{2k_B T\eta}\tilde{\mathcal{Z}} + \left(\sqrt{\frac{k_B \kappa T}{3}} - \frac{\sqrt{2k_B \eta T}}{3}\right)\mathrm{Tr}\left(\tilde{\mathcal{Z}}\right)I$$

where

$$\tilde{\mathcal{Z}} = \frac{1}{\sqrt{2}}\left(\mathcal{Z} + \mathcal{Z}^{\mathcal{T}}\right)$$

and $\mathcal{Z}$ is an uncorrelated Gaussian tensor field with zero mean and unit variance.

Dissipative Fluxes – Species Flux



Deterministic species flux (see Giovangigli (1999))

$$\boldsymbol{F} = \rho\,\mathrm{Diag}(Y)\,\boldsymbol{D}\left(\nabla X + \frac{(X-Y)}{p}\nabla p + \underset{\text{Soret}}{\frac{X\chi}{T}\nabla T}\right)$$

X – mole fraction
Y – mass fraction

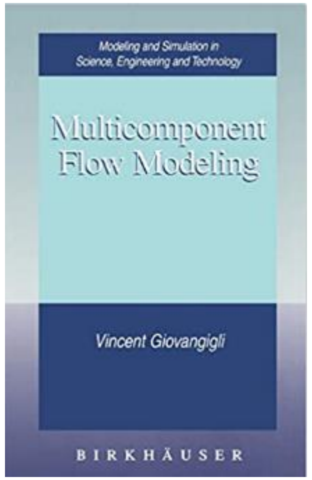
Stochastic species flux (see Balakrishnan, et al., *Phys. Rev. E* **89** 013017 (2014))

$$\widetilde{\boldsymbol{F}} = \boldsymbol{B}\mathcal{Z} \quad \text{where} \quad \boldsymbol{B}\boldsymbol{B}^T = 2k_\mathrm{B}\,\boldsymbol{L} \quad \text{and} \quad \boldsymbol{L} = \frac{\rho\bar{m}}{k_\mathrm{B}}\,\mathrm{Diag}(Y)\,\boldsymbol{D}\,\mathrm{Diag}(Y)$$

The matrix ***B*** is computed from the Cholesky factorization of ***L*** (i.e., "matrix square root").

Note: Single species FHD is *much* simpler since continuity equation has no noise term. $\frac{\partial}{\partial t}(\rho) = -\nabla\cdot(\rho\mathbf{v})$

Dissipative Fluxes – Heat Flux



Deterministic heat flux (see Giovangigli (1999))

$$\boldsymbol{Q} = -\lambda \nabla T + (k_B T \chi^T \ \mathrm{Diag}(M)^{-1} + h^T)\ \boldsymbol{F}$$

Dufour

M – molecular mass matrix
h – enthalpy density

Stochastic heat flux

$$\widetilde{\boldsymbol{Q}} = \sqrt{2 k_B T^2 \lambda}\ \boldsymbol{\mathcal{Z}} + (k_B T \chi^T \ \mathrm{Diag}(M)^{-1} + h^T)\widetilde{\boldsymbol{F}}$$

For a full description, see Srivastava, et al., Phys. Rev. E 107 015305 (2023)

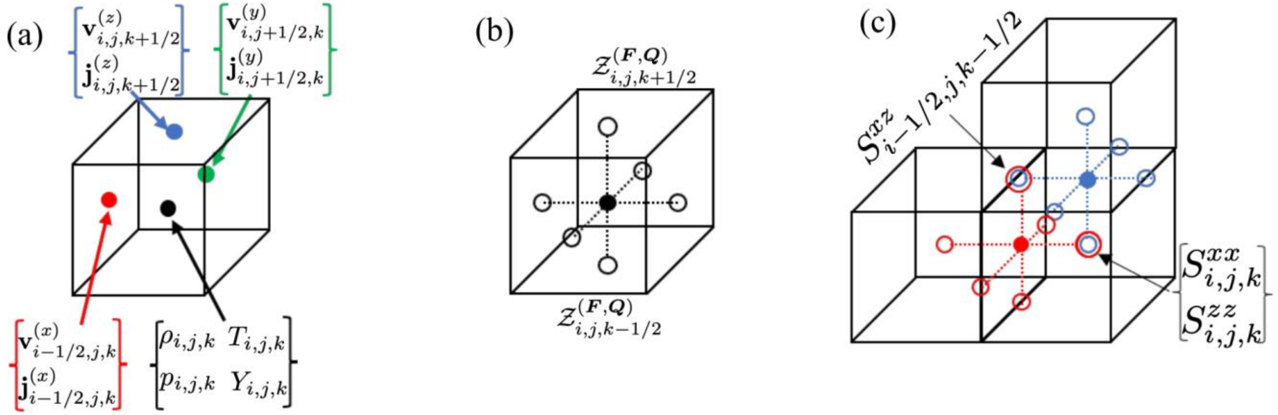
Note: Single species FHD is *much* simpler since $\boldsymbol{F} = \widetilde{\boldsymbol{F}} = 0$

https://github.com/AMReX-FHD/FHDeX

Staggered Grid Formulation

Numerical algorithm described in Srivastava, et al., *Phys. Rev. E* **107** 015305 (2023)

Cell centered –
Density, Energy, Temperature
Face centered –
Velocity, Species and Heat fluxes
Edge & cell centered –
Stress tensor



Temporal integration uses an explicit, three-stage, stochastic Runge-Kutta (RK3) scheme.

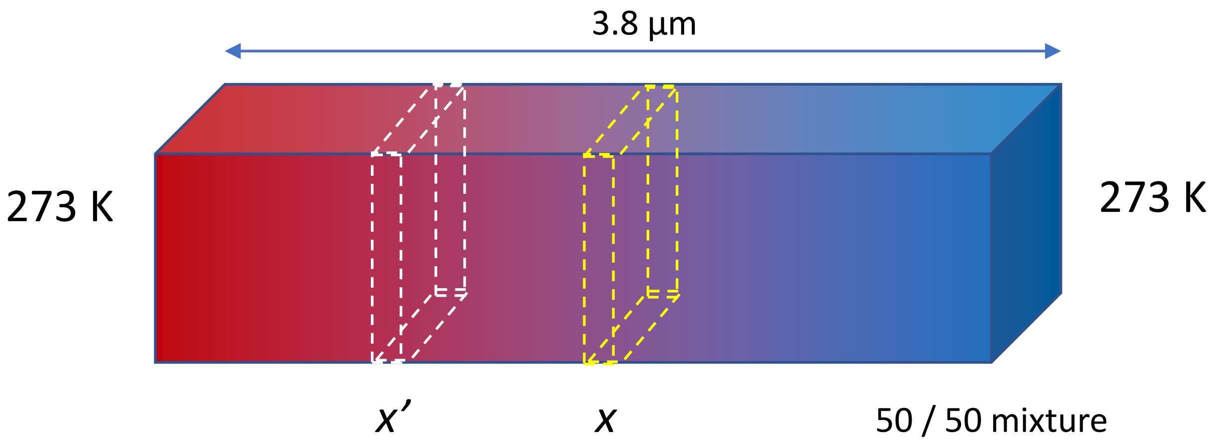
Superior to our previous implementations in Balakrishnan, et al., *Phys. Rev. E* **89** 013017 (2014); Bell et al., *Phys. Rev. E* **76** 016708 (2007); and Garcia et al., *J. Stat. Phys.* **47** 209 (1987).

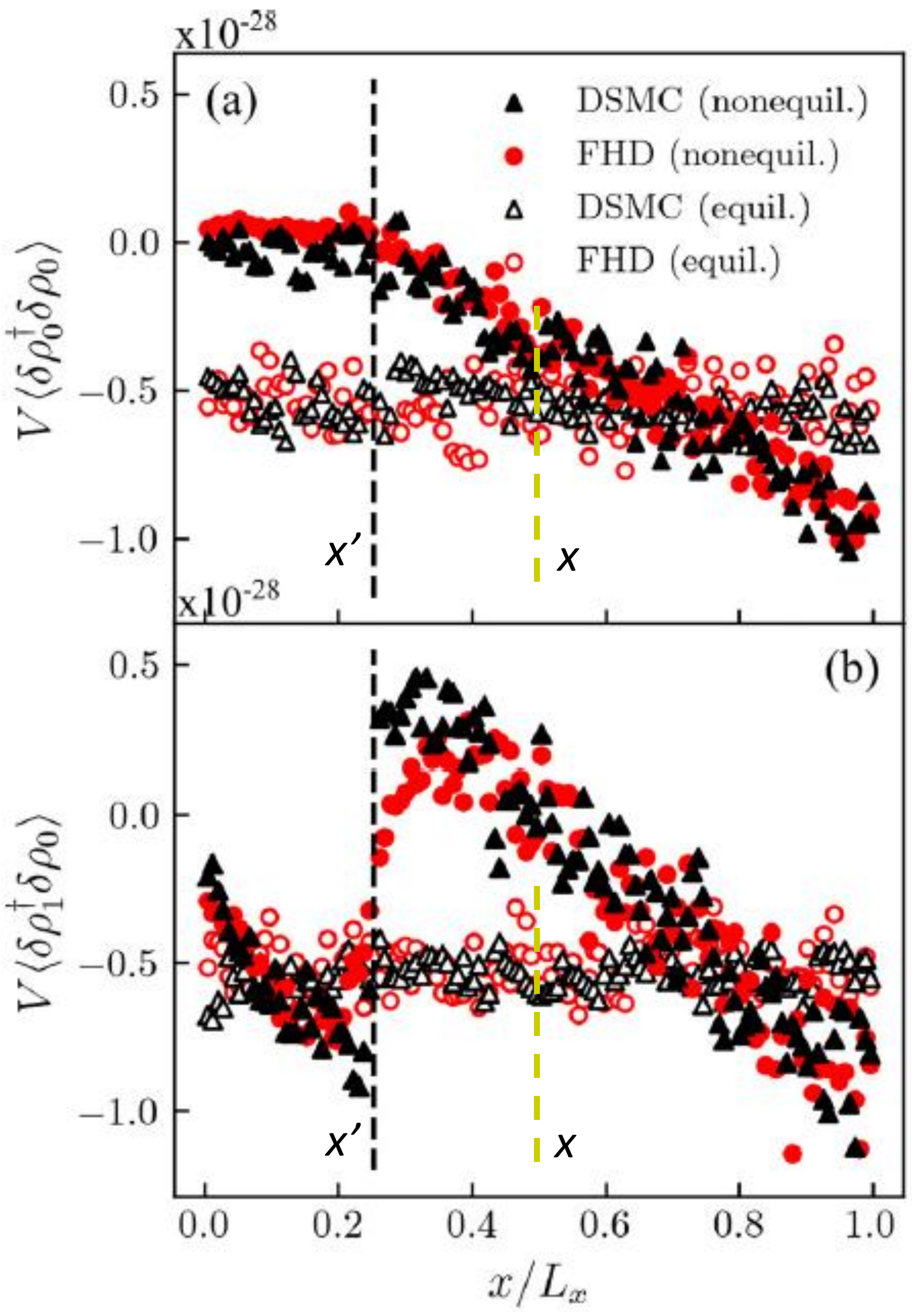
Red/Blue Mixture in ∇c

Spatial correlations of fluctuations for a mixture of “red”/ “ blue” neon gas with a gradient.

(upper) Red – red density correlation
(lower) Blue – red density correlation

FHD and DSMC in excellent agreement for mean values and for all fluctuations.



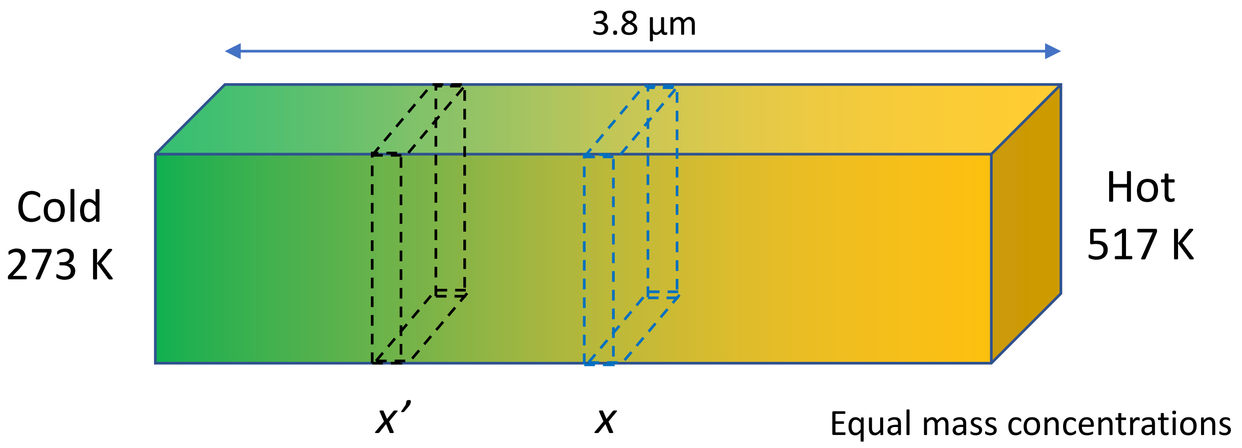


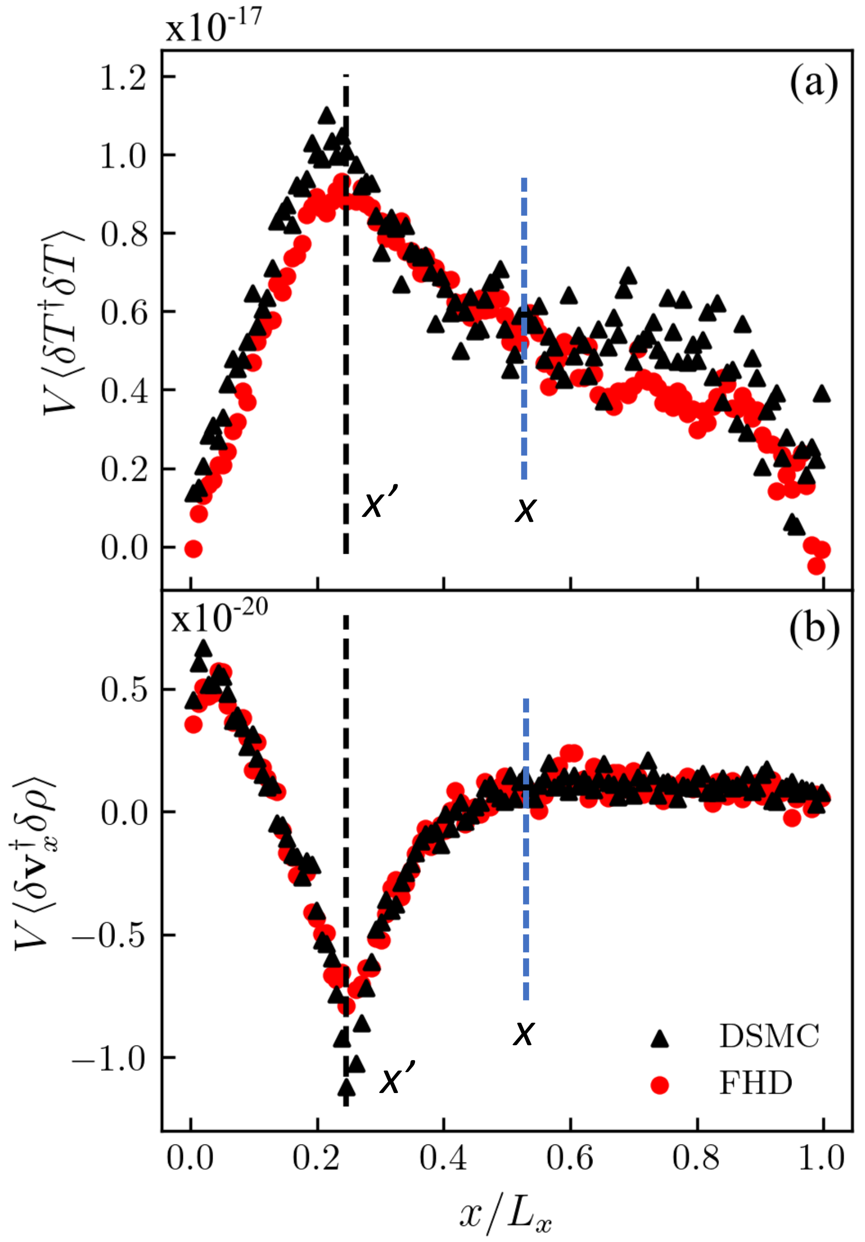
Ne/Kr Mixture in ∇T

Spatial correlations of fluctuations for a neon/krypton mixture in a temperature gradient.

(upper) Temperature – temperature correlation
(lower) Velocity – density correlation

FHD and DSMC are again in excellent agreement; correlations are zero when $\nabla T = 0$



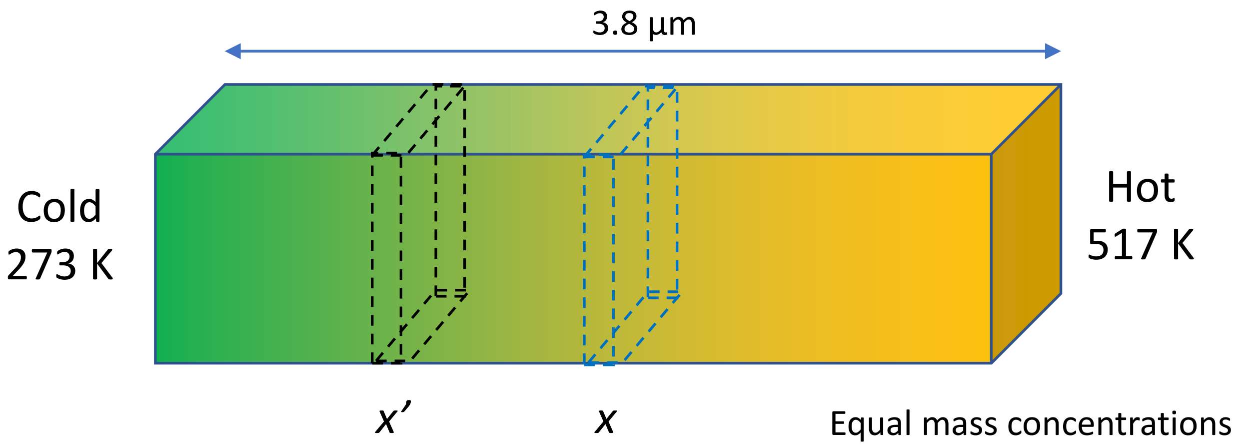


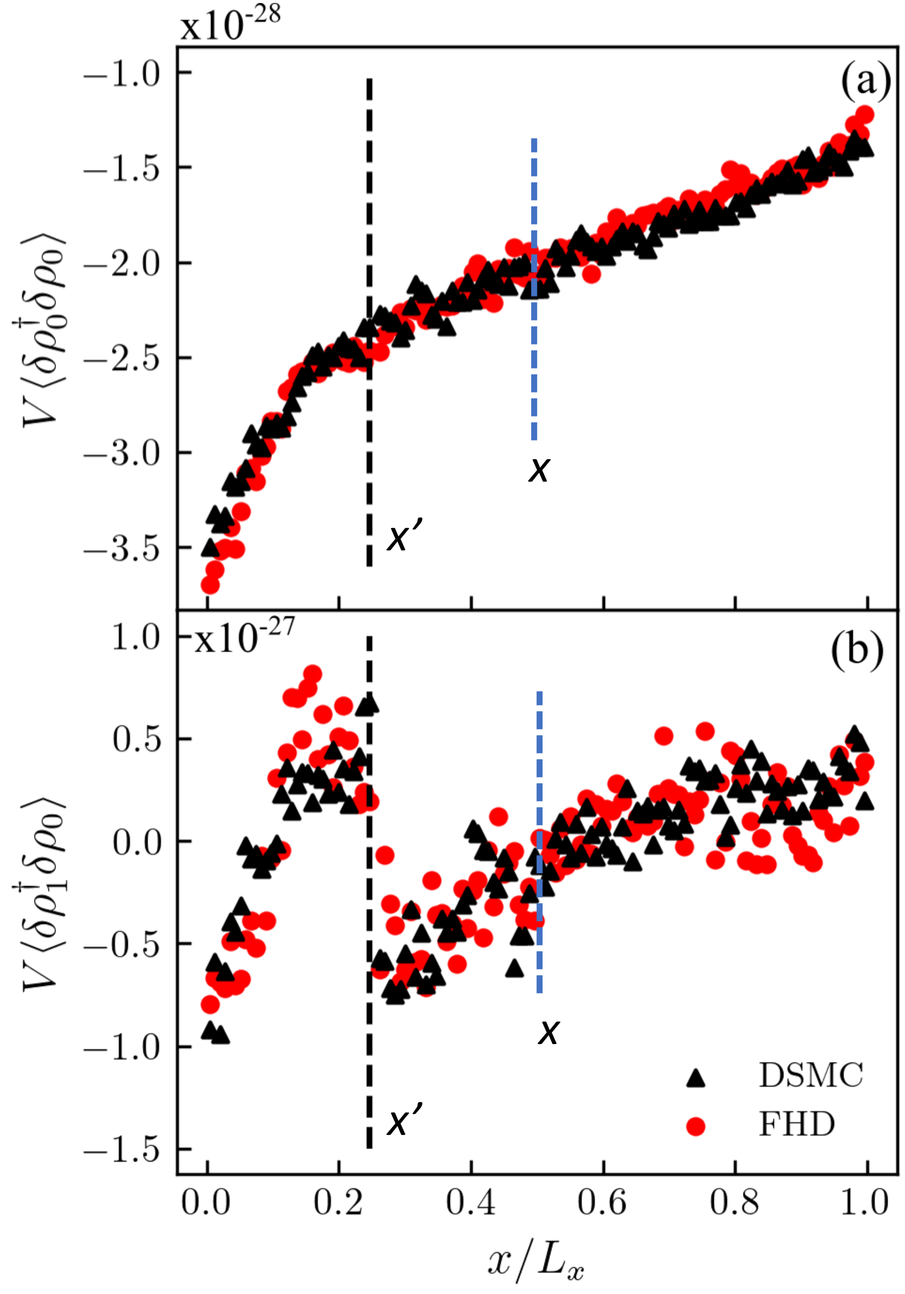
Ne/Kr Mixture in ∇T (cont.)

Spatial correlations of fluctuations for a neon/krypton mixture in a temperature gradient.

Temperature gradient results in a concentration gradient due to the Soret effect.

(upper) Neon – Neon density correlation
(lower) Neon – Krypton density correlation





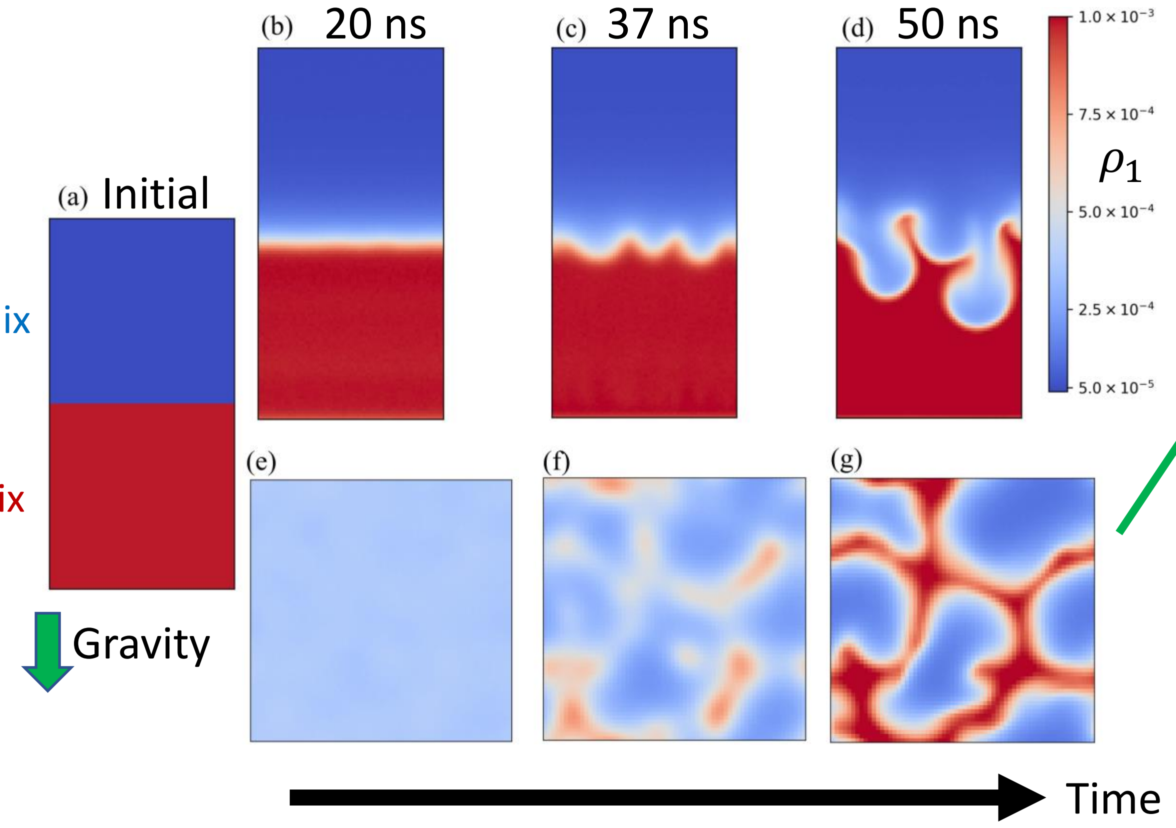
Rayleigh-Taylor Instability

Initial interface is perfectly flat yet hydrodynamic fluctuations naturally trigger the instability.

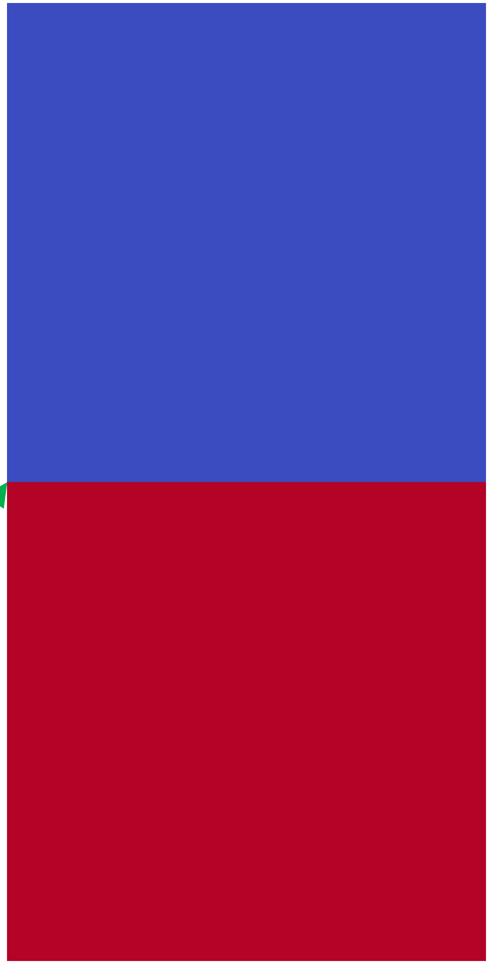
$$\frac{\rho_0 - \rho_1}{\rho_0 + \rho_1} = 0.82$$

Heavy mix

Light mix

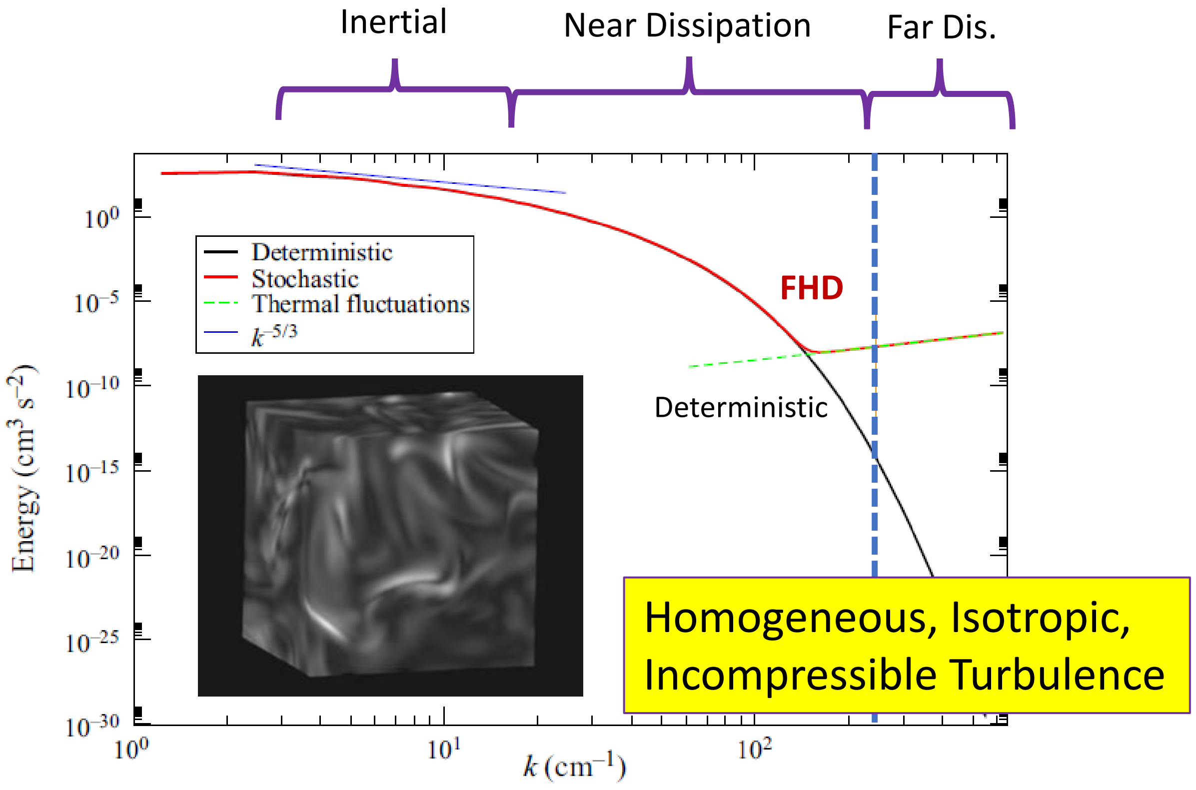


Low Mach (Ma < 0.1)

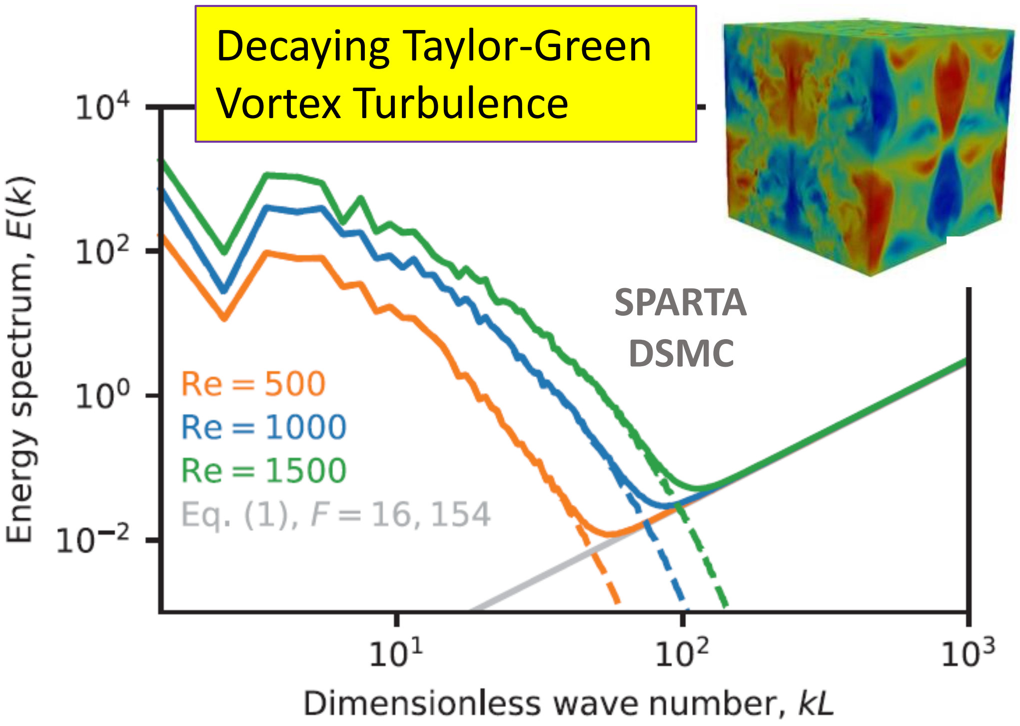


Future Work – Fluctuations & Turbulence

Thermal fluctuations dominate turbulent fluctuations in the near-dissipation range



Bell, et al., *J. Fluid Mech.* **939** A12 (2022)



McMullen, et al., PRL **128**, 114501 (2022)

DSMC23 Workshop

The DSMC23 workshop will be held in Santa Fe, New Mexico, USA, on September 24-27, 2023.

Abstract deadline: April 7th
Abstract acceptance notification: April 14th
Authors need to register by May 12th

https://tinyurl.com/DSMC23

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