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An Introduction to Computational Fluctuating Hydrodynamics

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Bringing Science Solutions to the World

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https://ccse.lbl.gov/Research/MuMSS/

Outline

- What is Fluctuating Hydrodynamics (FHD)?
  Origin story and a simple diffusion example

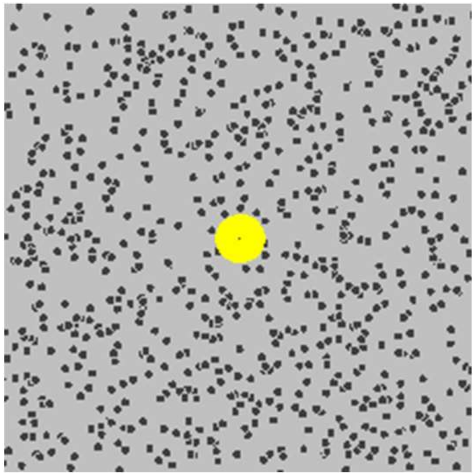
- Introduction to Computational FHD
  A simple numerical program for you to play with

- Advanced Computational FHD modeling
  Examples of mesoscopic systems modeled using FHD

Thermal Fluctuations

The study of stochastic fluctuations at the microscopic scale is a seminal topic of statistical mechanics

Brownian motion



Blue sky due to Rayleigh scattering from density fluctuations in air

Entropy & Probability

A fundamental principle of thermodynamics is that entropy is maximum at thermodynamic equilibrium.

This led Einstein to make the following conjecture regarding entropy and probability:

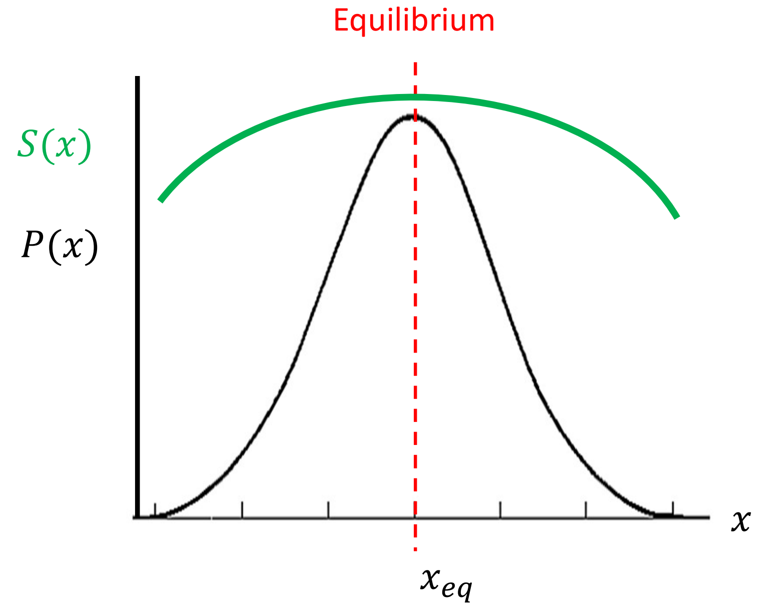
$$P(x) = C\,\exp(-\Delta S(x)/k_B)$$

where $P(x)$ is the probability of a state and

$$\Delta S(x) = S(x_{eq}) - S(x)$$

is the difference in entropy between the equilibrium state and the state x.

k_B: Boltzmann constant
C: Normalization constant



The variable x could be any thermodynamic quantity such as temperature, pressure, density, etc.

Entropy & Probability (cont.)

Remember
$P(x) = C\ \exp(-\Delta S(x)/k_B)$
$\Delta S(x) = S(x_{eq}) - S(x)$

By Taylor expansion about $x = x_{eq}$

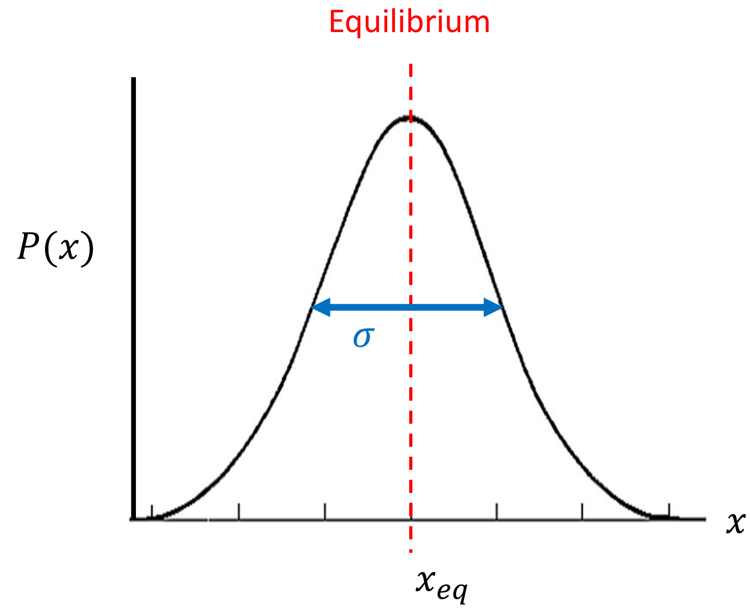
$$\Delta S(x) = \underbrace{\Delta S(x_{eq})}_{\text{zero}} - \underbrace{\left[\frac{dS}{dx}\right]_{x_{eq}}}_{\text{zero}} (x - x_{eq}) - \frac{1}{2}\left[\frac{d^2S}{dx^2}\right]_{x_{eq}} (x - x_{eq})^2$$

The probability of a state is

$$P(x) = C\ \exp(-(x - x_{eq})^2/2\sigma^2)$$

which is a **Gaussian** probability distribution with variance

$$\sigma^2 = \langle \delta x^2 \rangle = \langle (x - x_{eq})^2 \rangle = {-k_B} \Big/ \left[\frac{d^2S}{dx^2}\right]_{x_{eq}}$$



Temperature Fluctuations

Remember

$$\sigma^2 = \langle \delta x^2 \rangle = {-k_B} \Big/ \left[\frac{d^2S}{dx^2}\right]_{x_{eq}}$$

Let's work this out for temperature fluctuations, that is take x to be T.

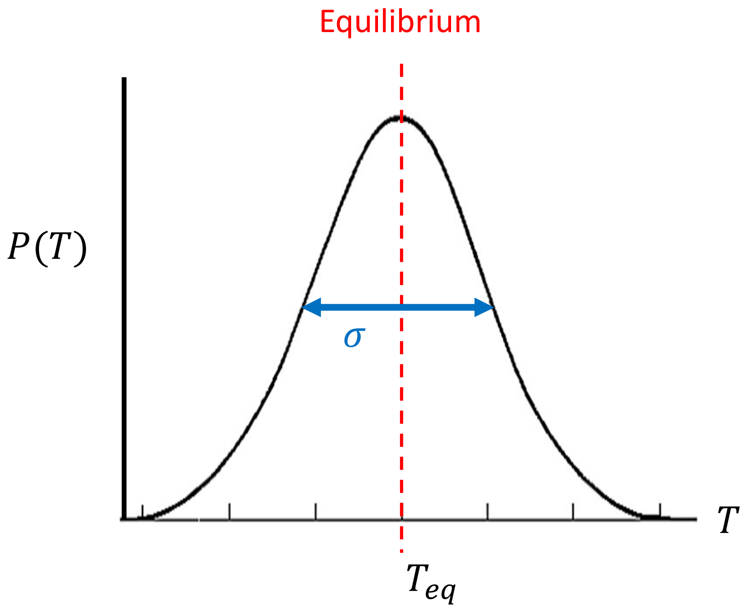
Start with the thermodynamic relation $dE = T\,dS$
and definition of heat capacity, $C_V = dE/dT$ so

$$\frac{dS}{dT} = \frac{C_V}{T} \qquad \text{and} \qquad \frac{d^2S}{dT^2} = -\frac{C_V}{T^2}$$

The variance of temperature fluctuations is

$$\sigma^2 = \langle \delta T^2 \rangle = \left\langle (T - T_{eq})^2 \right\rangle = {k_B T_{eq}^2} \Big/ {C_V}$$

For water, $C_V \approx 9 k_B N$ where N is the number of molecules.
In a cubic micron of water $N \approx 10^{10}$ so $\sigma \approx 10^{-6}$ degrees (tiny!).



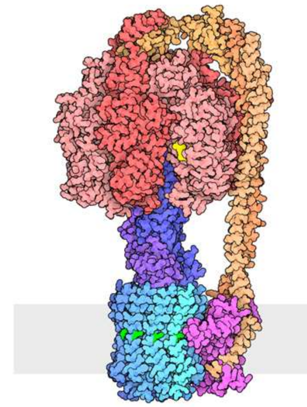
Significance of Thermal Fluctuations

Thermal fluctuations are tiny so why study them?
Two reasons:

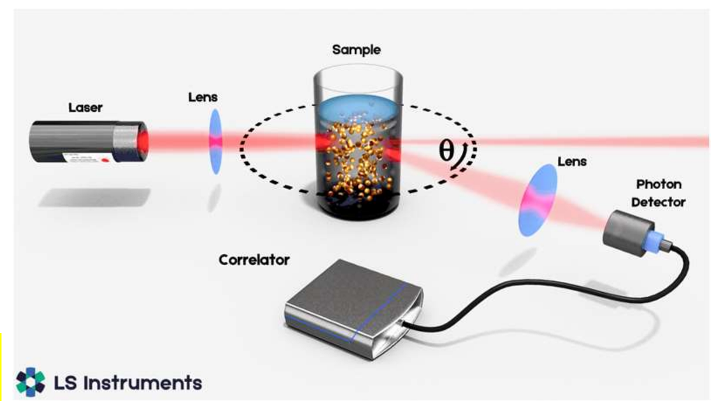
* The understanding of thermal fluctuations is of increasing importance given advances in nanoscale technology, including applications in cellular biology.

* Theoretical models of thermal fluctuations can be *experimentally tested*, leading to improved stochastic hydrodynamic models for other applications (e.g., stochastic climate modelling).

But how can we model the *dynamics* of these fluctuations?



ATP synthase is a molecular motor and ion pump



Origins of Fluctuating Hydrodynamics

In 1957, Landau and Lifshitz formulated the basic equations of fluctuating hydrodynamics in this 2-page paper. A slightly expanded form appears in their textbook.

Soviet Physics JETP 5, Part 3, 512 (1957)

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Hydrodynamic fluctuations

L. D. LANDAU AND E. M. LIFSHITZ

Translated by R. T. Beyer

A general theory of hydrodynamic fluctuations can be constructed by introducing 'outside' terms into the equation of motion of the liquid, as was done by Rytov [1] for the fluctuations of an electromagnetic field in continuous media; he introduced corresponding 'outside' fields in Maxwell's equations.

The introduction of such additional terms can be accomplished in different equivalent ways. The most advantageous is the form in which the fluctuations of the 'outside quantities' at the various points of the liquid are not correlated with one another. This is accomplished by the introduction of 'outside stress tensor' s_{ik} in the Navier–Stokes equation and the 'outside heat flow' vector $\mathbf{g}$ in the heat conduction equation (the equation of continuity remains unchanged). The system of hydrodynamic equations then takes the form

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0, \tag{1}$$

$$\rho \frac{\partial v_i}{\partial t} + \rho(\mathbf{v}\nabla)v_i = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma'_{ik}}{\partial x_k}, \tag{2}$$

$$\rho T\left(\frac{\partial s}{\partial t} + \mathbf{v}\nabla s\right) = \frac{1}{2}\sigma'_{ik}\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i}\right) - \operatorname{div}\mathbf{q}, \tag{3}$$

$$\sigma'_{ik} = \eta\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \frac{2}{3}\delta_{ik}\frac{\partial v_l}{\partial x_l}\right) + \zeta\frac{\partial v_l}{\partial x_l}\delta_{ik} + s_{ik}, \tag{4}$$

$$\mathbf{q} = -\kappa\nabla T + \mathbf{g} \tag{5}$$

(all the notation agrees with that used in our book [2]). To these equations should be added the relations which define the mean values of the products of components s_{ik} and g_i. We do this by first assuming the fluctuations to be

classical (i.e. their frequencies $\omega \ll kT/\hbar$), while the viscosity and the thermal conductivity of the liquid are non-dispersive.

The rate of change of the total entropy of the liquid S is given by the expression (see ref. 2, §49).

$$\dot{S} = \int\left\{\frac{\sigma'_{ik}}{2T}\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i}\right) - \frac{\mathbf{q}\nabla T}{T^2}\right\}\mathrm{d}V. \tag{6}$$

Following the general rules of fluctuation theory laid down in ref. 3, §§ 117, 120, we select as the values $\dot{x}_a$ figuring in this theory the components of the tensor σ'_{ik} and the vector q †. It is then evident from eq. (6) that the role of the corresponding quantities X_a will be played by

$$-\frac{1}{2T}\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i}\right)\Delta V \quad \text{and} \quad \frac{1}{T^2}\frac{\partial T}{\partial x_i}\Delta V,$$

while eqs (4) and (5) play the role of the relations $\dot{x}_a = -\gamma_{ab}X_b + y_a$ (see ref. 3, §120), where the s_{ik} and g_i correspond to the quantities y_a. The coefficients γ_{ab} in these relations determine directly the mean values

$$\overline{y_a(t_1)y_b(t_2)} = k(\gamma_{ab} + \gamma_{ba})\delta(t_1 - t_2).$$

The final formulas have the form:

$$\begin{aligned}
\overline{s_{ik}(\mathbf{r}_1, t_1)s_{lm}(\mathbf{r}_2, t_2)} &= 2kT[\eta(\delta_{il}\delta_{km} + \delta_{im}\delta_{kl}) \\
&\quad + (\zeta - 2\eta/3)\delta_{ik}\delta_{lm}]\delta(\mathbf{r}_2 - \mathbf{r}_1)\delta(t_2 - t_1), \\
\overline{g_i(\mathbf{r}_1, t_1)g_k(\mathbf{r}_2, t_2)} &= 2kT^2\kappa\delta_{ik}\delta(\mathbf{r}_2 - \mathbf{r}_1)\delta(t_2 - t_1), \\
\overline{g_i(\mathbf{r}_1, t_1)s_{lm}(\mathbf{r}_2, t_2)} &= 0.
\end{aligned} \tag{7}$$

If use is made of the spectral components of the fluctuating quantities, which are defined by

$$x_\omega = \frac{1}{2\pi}\int_{-\infty}^{\infty} x(t)\mathrm{e}^{i\omega t}\,\mathrm{d}t, \quad \overline{x^2} = \iint_{-\infty}^{\infty}\overline{x_\omega x_{\omega'}}\,\mathrm{d}\omega\,\mathrm{d}\omega',$$

then the factor $\delta(t_2 - t_1)$ in eqs (7) is replaced by $\delta(\omega + \omega')/2\pi$.

These results are generalised without difficulty to the case of the presence of dispersion in the coefficients of viscosity or thermal conductivity and the quantum nature of the fluctuations with the aid of the general theory of Callen and others, in the form set forth in ref. 4. There appears only the factor

† An inessential difference, connected with the fact that we are dealing here with a continuous (values at each point of the liquid) as against a discrete set of fluctuating quantities (for which the formulas in ref. 3 were developed), can easily be removed formally by dividing the volume of the liquid into small but finite regions ΔV and carrying out the transition $\Delta V \to 0$ in the final equations.

$(\hbar\omega/2kT)\coth\hbar\omega/2kT$ in the expressions for the average values of the products of the spectral components s_{ik} and g_i, while the quantities η, ζ, κ are to be replaced by their real parts.

References

[1] S. M. Rytov, *Theory of Electrical Fluctuations and Heat Radiation*, Academy of Sciences Press, 1953.
[2] L. D. Landau and E. M. Lifshitz, *Mechanics of Continuous Media*, 2nd edn, Gostekhizdat, 1954.
[3] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, 3rd edn, Gostekhizdat, 1951.
[4] L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media*, Gostekhizdat, in press.

Central Idea of Fluctuating Hydrodynamics

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"…

Stochastic Heat Equation

For simple conduction we write the change in energy density, $\mathcal{E}$, in terms of heat flux, $\boldsymbol{Q}$, as

$$\frac{\partial}{\partial t}\mathcal{E} = -\nabla \cdot \boldsymbol{Q} \qquad \text{where} \qquad \boldsymbol{Q} = \overline{\boldsymbol{Q}} + \widetilde{\boldsymbol{Q}}$$

(Total) = (deterministic) + (stochastic)

Write the deterministic heat flux in Onsager form as

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

(Flux) = (Onsager coefficient) * (Thermodynamic "Force")

From non-equilibrium thermodynamics the rate of entropy change in a volume Ω is

$$\frac{dS}{dt} = \frac{d_{\mathrm{i}}S}{dt} + \frac{d_{\mathrm{e}}S}{dt} = \int_{\Omega} \boldsymbol{X} \cdot \overline{\boldsymbol{Q}} + \left[\frac{\overline{\boldsymbol{Q}}}{T}\right]_{\partial\Omega}$$

(internal dS/dt) + (external dS/dt)

After a few manipulations we find the thermodynamic force

$$\boldsymbol{X} = \boldsymbol{\nabla}\frac{1}{T} = -\frac{1}{T^2}\boldsymbol{\nabla}T \qquad \text{and thus} \qquad \overline{\boldsymbol{Q}} = -\frac{L}{T^2}\boldsymbol{\nabla}T$$

Stochastic Heat Equation (cont.)

Comparing $\overline{\boldsymbol{Q}} = L\boldsymbol{X}$ with Fourier law

$\overline{\boldsymbol{Q}} = -\lambda\boldsymbol{\nabla}T$ tells us that the Onsager coefficient is $L = \lambda T^2$

Total heat flux has the form required for linear response theory

$$\boldsymbol{Q} = \overline{\boldsymbol{Q}} + \widetilde{\boldsymbol{Q}} = \lambda T^2\,\boldsymbol{X} + \widetilde{\boldsymbol{Q}}$$

By the fluctuation-dissipation theorem the white noise has correlation

$$\langle \widetilde{\boldsymbol{Q}}(\boldsymbol{r},t)\widetilde{\boldsymbol{Q}}(\boldsymbol{r}',t')\rangle = 2k_{\mathrm{B}}\,\lambda T^2\,\delta(t-t')\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$

This noise ensures that

$P(x) = C\,\exp(-\Delta S(x)\,/k_B)$

Collecting the above and writing $\mathcal{E} = \rho c_{\mathrm{V}} T$ gives the **stochastic heat equation**,

$$\rho c_{\mathrm{V}}\frac{\partial T}{\partial t} = \lambda\nabla^2 T + \nabla\cdot\sqrt{2\lambda k_{\mathrm{B}} T^2}\,\widetilde{\mathbf{Z}}$$

where $\widetilde{\mathbf{Z}}$ is Gaussian white noise

$$\langle \widetilde{\boldsymbol{Z}}(\boldsymbol{r},t)\widetilde{\boldsymbol{Z}}(\boldsymbol{r}',t')\rangle = \delta(t-t')\,\delta(\boldsymbol{r}-\boldsymbol{r}')$$

Stochastic Species Diffusion Equation

We can derive a similar stochastic diffusion equation for mass diffusion in ideal solutions

$$\partial_t n = \nabla \cdot \left(D \nabla n + \sqrt{2D\,n}\,\widetilde{\boldsymbol{Z}} \right)$$

Dean-Kawasaki equation

where *n* is the number density and *D* is the diffusion coefficient.

Notice the similarity with the stochastic heat equation

$$\partial_t T = \nabla \cdot \left(\kappa \nabla T + \alpha\, T\, \widetilde{\boldsymbol{Z}} \right)$$

where $\kappa = \lambda / \rho c_{\mathrm{V}}$ $\alpha = \sqrt{2 k_B \lambda} / \rho c_{\mathrm{V}}$

The deterministic forms of these two diffusion equations give equivalent solutions however the stochastic noises differ so the stochastic solutions differ.

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Numerics for Stochastic Heat Equation

Write the 1D Stochastic Heat Equation as

white noise

$$\partial_t T = \kappa\, \partial_x^2\, T + \alpha\, \partial_x\, T\, \tilde{Z}$$

where $\kappa = \lambda / \rho c_V$ $\alpha = \sqrt{2 k_B \lambda} / \rho c_V$

Discretize time and space using centered spatial derivatives

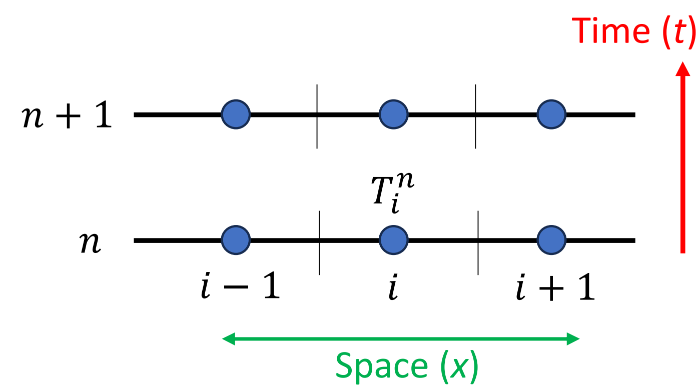
$$\partial_t T = \frac{\partial T}{\partial t} \rightarrow \frac{T_i^{n+1} - T_i^n}{\Delta t} \qquad \partial_x^2\, T = \frac{\partial^2 T}{\partial x^2} \rightarrow \frac{T_{i+1}^n - 2\, T_i^n + T_{i-1}^n}{\Delta x^2}$$

with the stochastic term being

$$\alpha\, \partial_x\, T\, \tilde{Z} \rightarrow \frac{\mathcal{F}_{i+1/2}^n - \mathcal{F}_{i-1/2}^n}{\Delta x}$$

where

$$\mathcal{F}_{i+1/2}^n = \alpha\, T_{i+1/2}^n Z_{i+1/2}^n$$



Numerical Schemes

Forward Euler scheme for $\partial_t T = \kappa\, \partial_x^2\, T + \alpha \partial_x\, T\, \tilde{Z}$

$$T_i^{n+1} = T_i^n + \frac{\kappa \Delta t}{\Delta x^2}\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right) + \frac{\alpha \Delta t}{\Delta x}\left(T_{i+1/2}^n Z_{i+1/2}^n - T_{i-1/2}^n Z_{i-1/2}^n\right)$$

Predictor-Corrector scheme has two steps

$$T_i^{*} = T_i^n + \frac{\kappa \Delta t}{\Delta x^2}\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right) + \frac{\alpha \Delta t}{\Delta x}\left(T_{i+1/2}^n Z_{i+1/2}^n - T_{i-1/2}^n Z_{i-1/2}^n\right)$$

Predictor step

$$T_i^{n+1} = \frac{1}{2}\left[T_i^n + T_i^{*} + \frac{\kappa \Delta t}{\Delta x^2}\left(T_{i+1}^{*} - 2T_i^{*} + T_{i-1}^{*}\right) + \frac{\alpha \Delta t}{\Delta x}\left(T_{i+1/2}^{*} Z_{i+1/2}^n - T_{i-1/2}^{*} Z_{i-1/2}^n\right)\right]$$

Corrector step

There are other explicit schemes (e.g., Runge-Kutta) and implicit schemes (e.g., Crank-Nicolson)

Discretized White Noise

The white noise is discretized as

$$\tilde{Z} \rightarrow Z^n_{i+1/2} = \frac{1}{\sqrt{\Delta t\ \Delta V}}\ \mathbb{N}^n_{i+1/2}$$

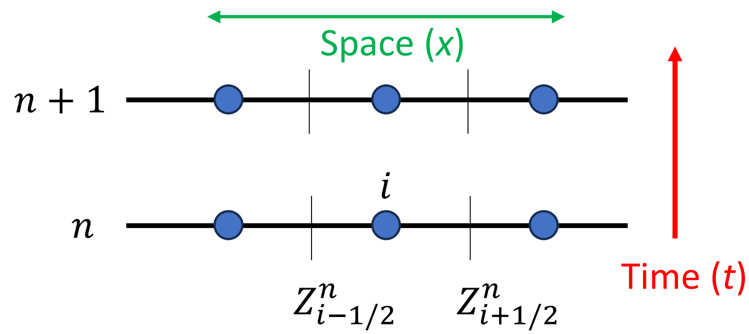
where $\mathbb{N}$ is a normal (Gaussian) distributed random number.

This definition for the discrete noise has a correlation

$$\left\langle Z^n_{i+1/2} Z^{n\prime}_{i\prime+1/2} \right\rangle = \frac{1}{\Delta t\ \Delta V} \left\langle \mathbb{N}^n_{i+1/2}\ \mathbb{N}^{n\prime}_{i\prime+1/2} \right\rangle = \frac{\delta_{n,n\prime}}{\Delta t}\ \frac{\delta_{i,i\prime}}{\Delta V}$$

which is the discretized form of

$$\left\langle \widetilde{\boldsymbol{Z}}(\boldsymbol{r},t) \widetilde{\boldsymbol{Z}}(\boldsymbol{r}',t') \right\rangle = \delta(t-t')\ \delta(\boldsymbol{r}-\boldsymbol{r}')$$



Two Remarks on FHD

Note that in Fluctuating Hydrodynamics:

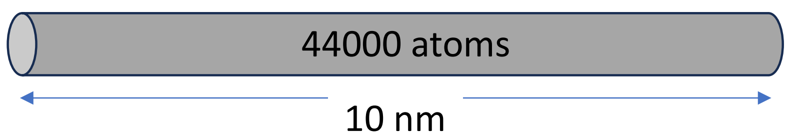
- The stochastic noise terms only appear when there is entropy production (e.g., thermal diffusion). There are **no** noise terms due to reversible forces, such as surface tension, nor due to non-inertial terms, such as the Coriolis force.

- Technically the stochastic fluxes are *additive* noises but in practice we compute them as multiplicative noises.
  For example, we use instantaneous temperature instead of the equilibrium value in the stochastic heat equation. This is justified for our problems of interest (negligible noise-induced drift).

Python Notebook `StochasticHeat`

https://github.com/AlejGarcia/IntroFHD

Demonstration program, `StochasticHeat`, can be downloaded from GitHub.
Written in Python, it computes the Stochastic Heat Equation for temperature fluctuations in an iron rod.



Program options:

- Periodic or Dirichlet boundary conditions
- Forward Euler or Predictor-Corrector schemes
- Equilibrium or Non-equilibrium (∇T) conditions

Runs take only a few minutes on a laptop

QR code for GitHub download

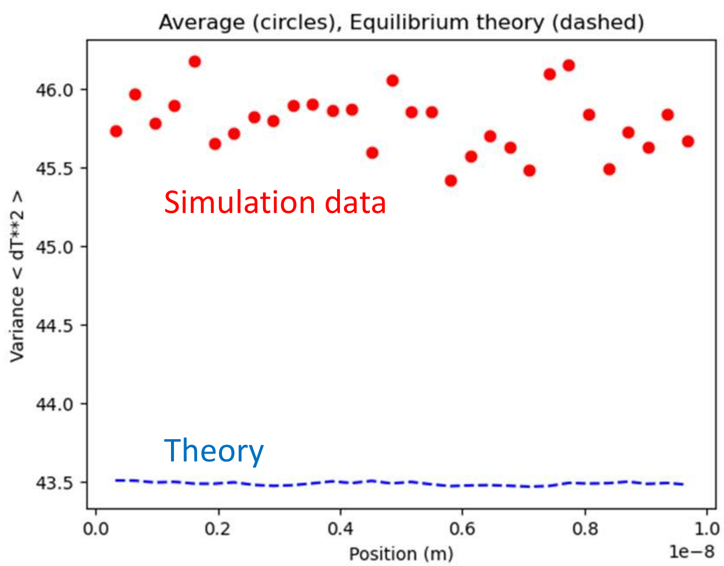
Variance of Temperature Fluctuations

From statistical mechanics, the equilibrium variance of temperature fluctuations is

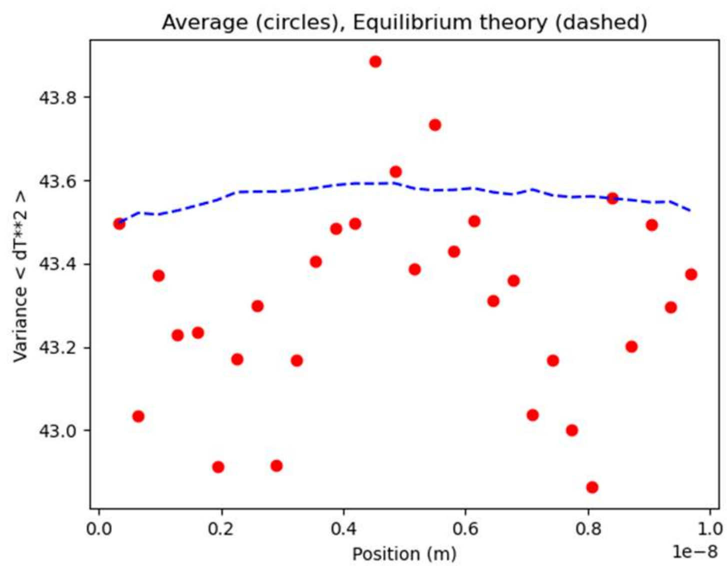
$$\langle \delta T_i^2 \rangle = \frac{k_B \langle T_i \rangle^2}{\rho c_V \Delta V} = \frac{k_B T_{eq}^2}{C_V}$$

2 million steps
N = 32 cells

Forward Euler



Predictor-Corrector



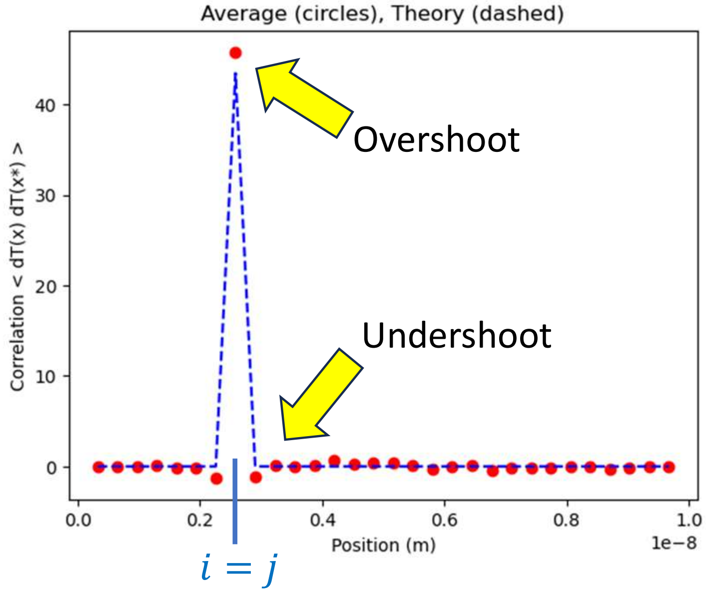
Spatial Correlation of Fluctuations

From statistical mechanics, the equilibrium correlation of temperature fluctuations is

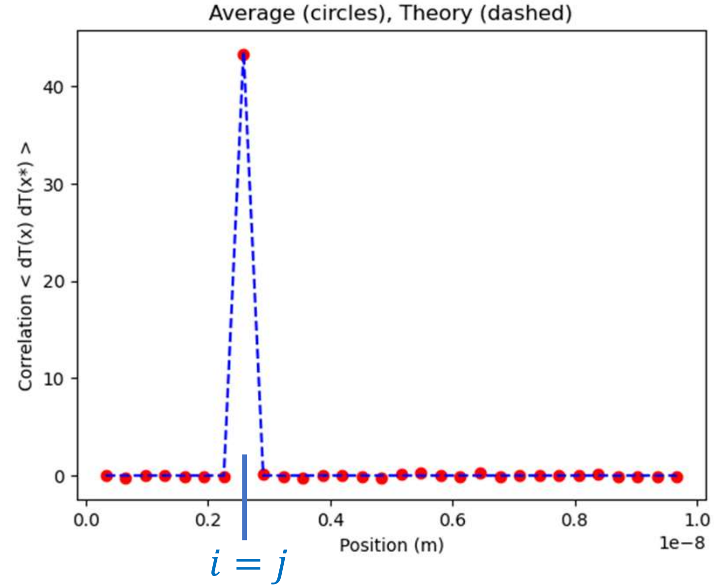
$$\langle \delta T_i \delta T_j \rangle = \langle \delta T_i^2 \rangle \, \delta_{i,j}$$

2 million steps
N = 32 cells

Forward Euler



Predictor-Corrector



Static Structure Factor

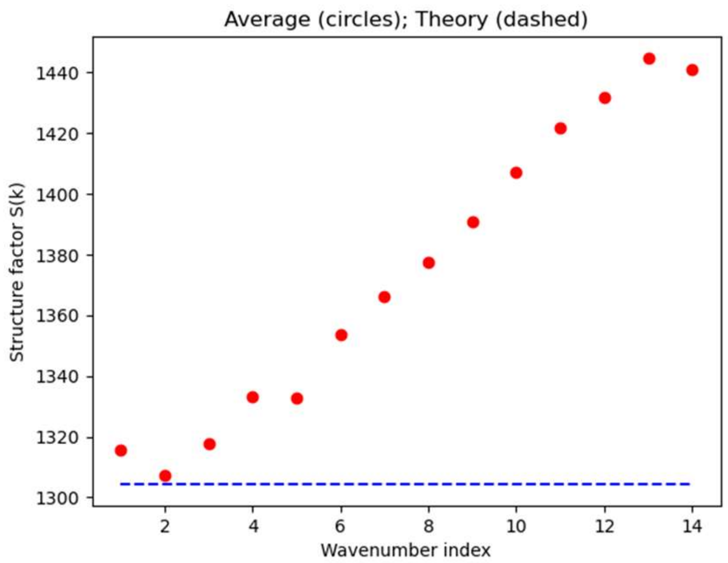
Donev, et al., CAMCOS **5** 149 (2010)

From statistical mechanics, the equilibrium fluctuation power spectrum (structure factor) is

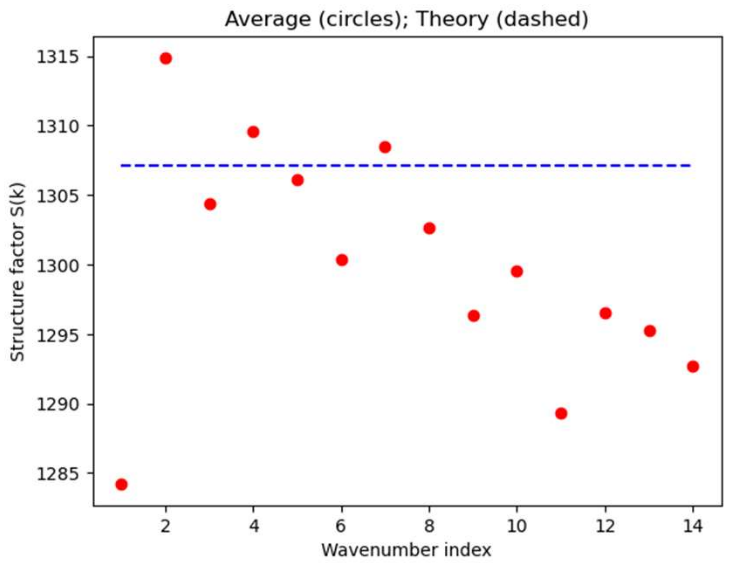
$$S_k = \langle \hat{T}_k \hat{T}_k^{\,*} \rangle = \frac{k_B T_{eq}^2}{\rho c_V} N$$

2 million steps
N = 32 cells

Forward Euler



Predictor-Corrector



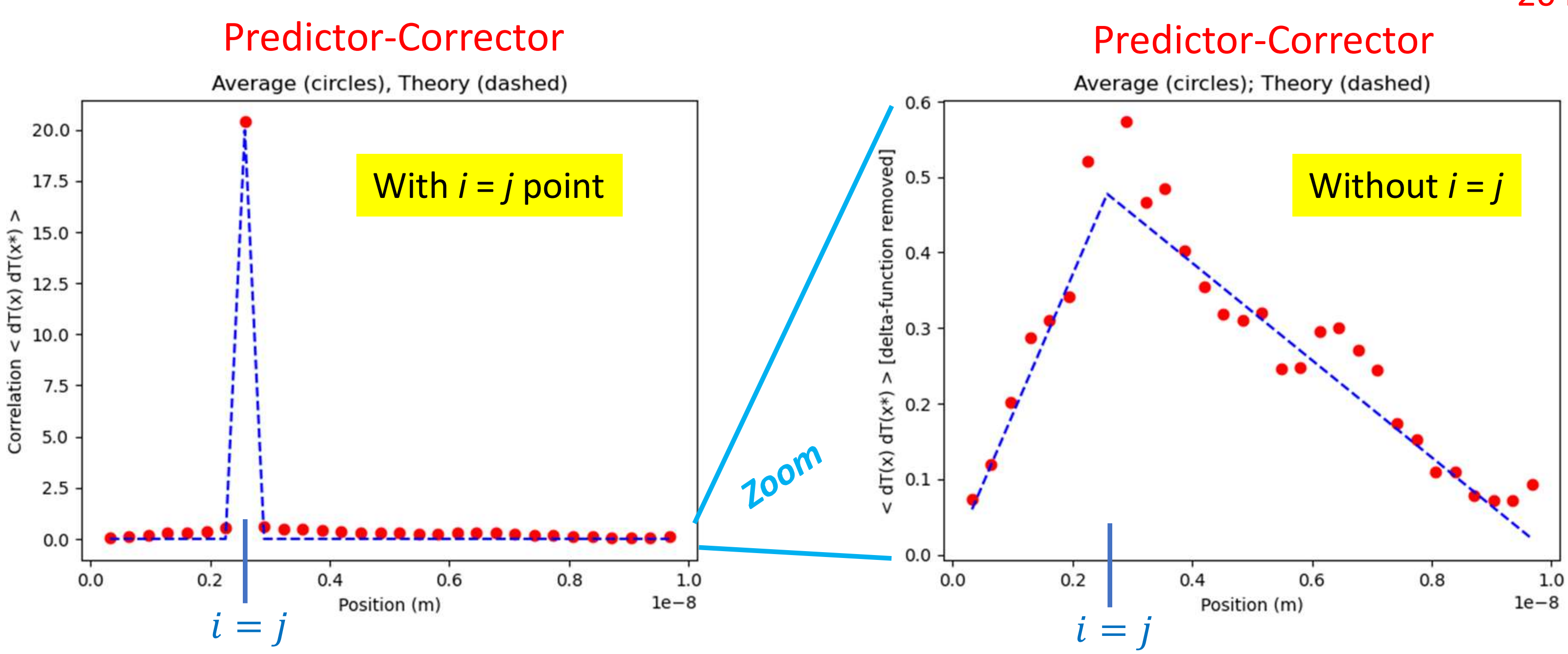
Non-equilibrium Correlation

Garcia, et al., *J. Stat. Phys.*, **47** 209 (1987)

For a non-equilibrium system with a temperature gradient ∇T

$$\langle \delta T_i \delta T_j \rangle = \frac{k_B T_{eq}^2}{\rho c_V \Delta V} \delta_{i,j} + \frac{k_B (\nabla T)^2}{\rho c_V V} \times \begin{cases} x_i\,(\ell - x_j) & (x_i < x_j) \\ x_j\,(\ell - x_i) & \text{otherwise} \end{cases}$$

20 million steps
N = 32 cells



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Multi-species Compressible FHD

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

Species flux

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

Stress tensor

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

Heat flux

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

Summing the mass equation over species gives the continuity equation

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

For incompressible fluids the pressure serves as a Lagrange multiplier that enforces the incompressiblity constraint.
Donev, et al. Phys, Fluids, 27(3), 2015

Dissipative Fluxes – Stress Tensor

Deterministic stress tensor components

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

η – shear viscosity
ζ – bulk viscosity

Stochastic stress tensor

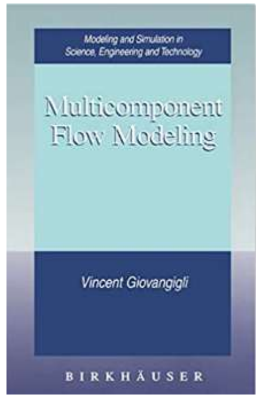
P. Español, *Physica A* 248 77 (1998)

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

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

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

Dissipative Fluxes – Species Flux



Giovangigli (1999)

Deterministic species flux

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

X – mole fraction
Y – mass fraction

Stochastic species flux

Balakrishnan, et al., *Phys. Rev. E* **89** 013017 (2014)

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

The matrix ***B*** is computed from the Cholesky factorization of ***L*** (i.e., “matrix square root”).
Note that by the Second Law of Thermodynamics ***L*** is a positive-semidefinite matrix.

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

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

Dufour

M – molecular mass matrix
h – enthalpy density

Stochastic heat flux

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

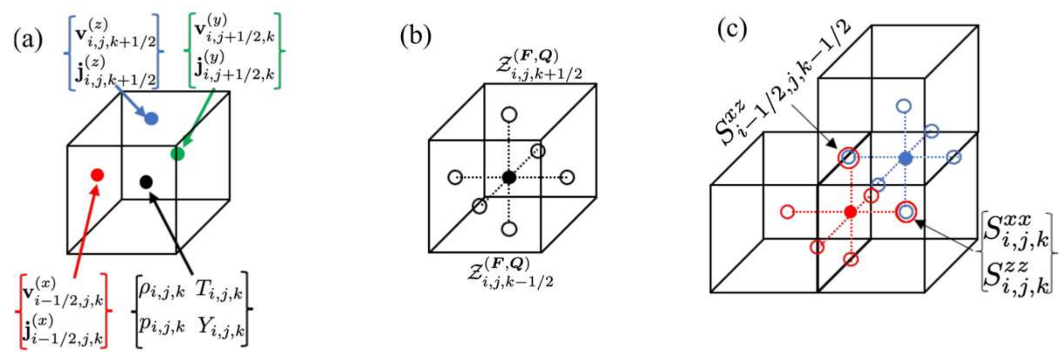
Note: Single species FHD is *much* simpler since $\overline{\boldsymbol{F}} = \widetilde{\boldsymbol{F}} = \boldsymbol{0}$.

Staggered Grid Formulation

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

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).

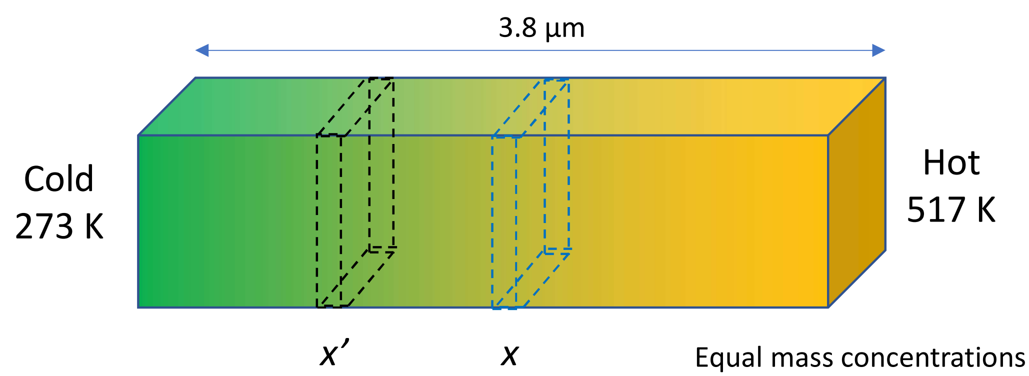
Srivastava, et al., *Phys. Rev. E* 107 015305 (2023)

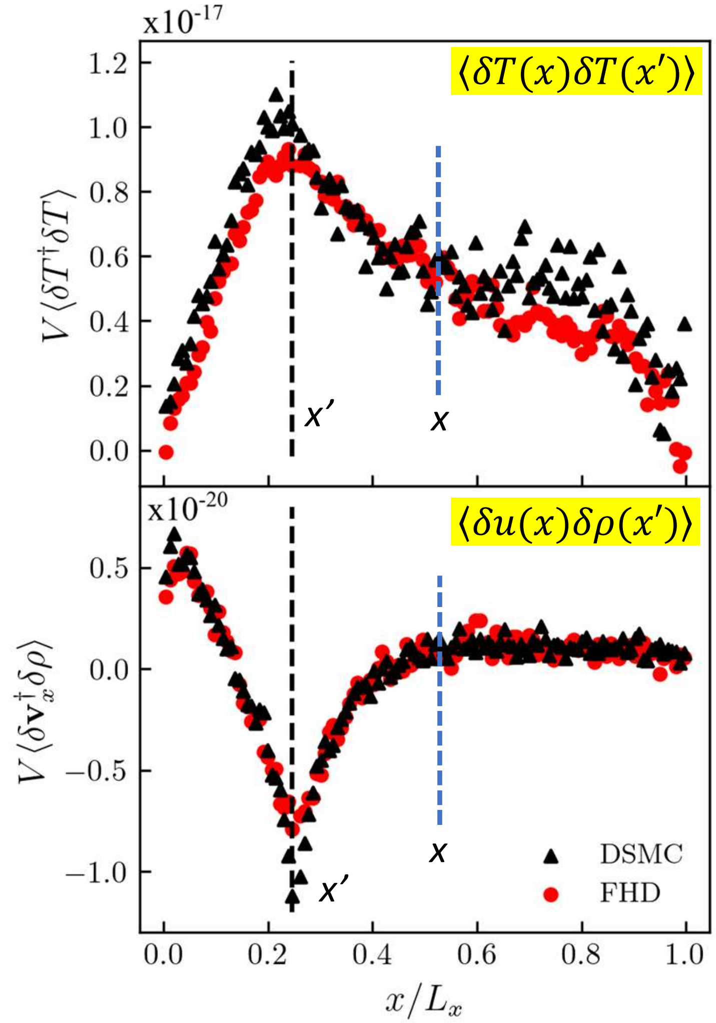
Ne/Kr Mixture in ∇T

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

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

FHD and particle simulations (DSMC) are in excellent agreement; delta correlations when $\nabla T = 0$





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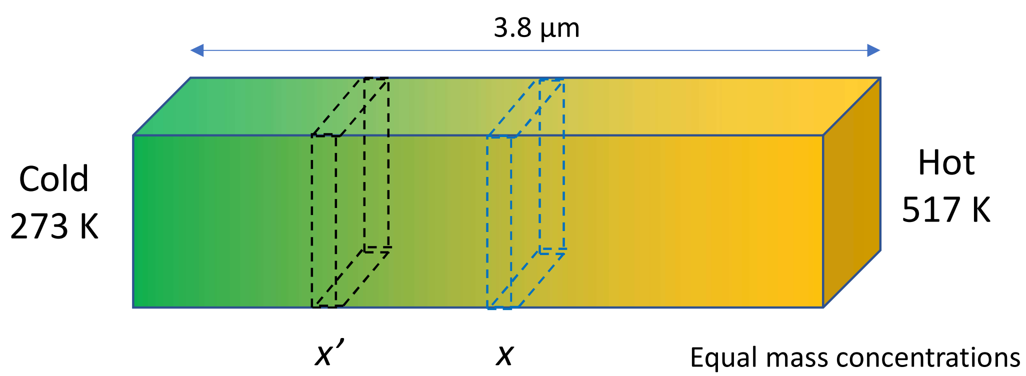
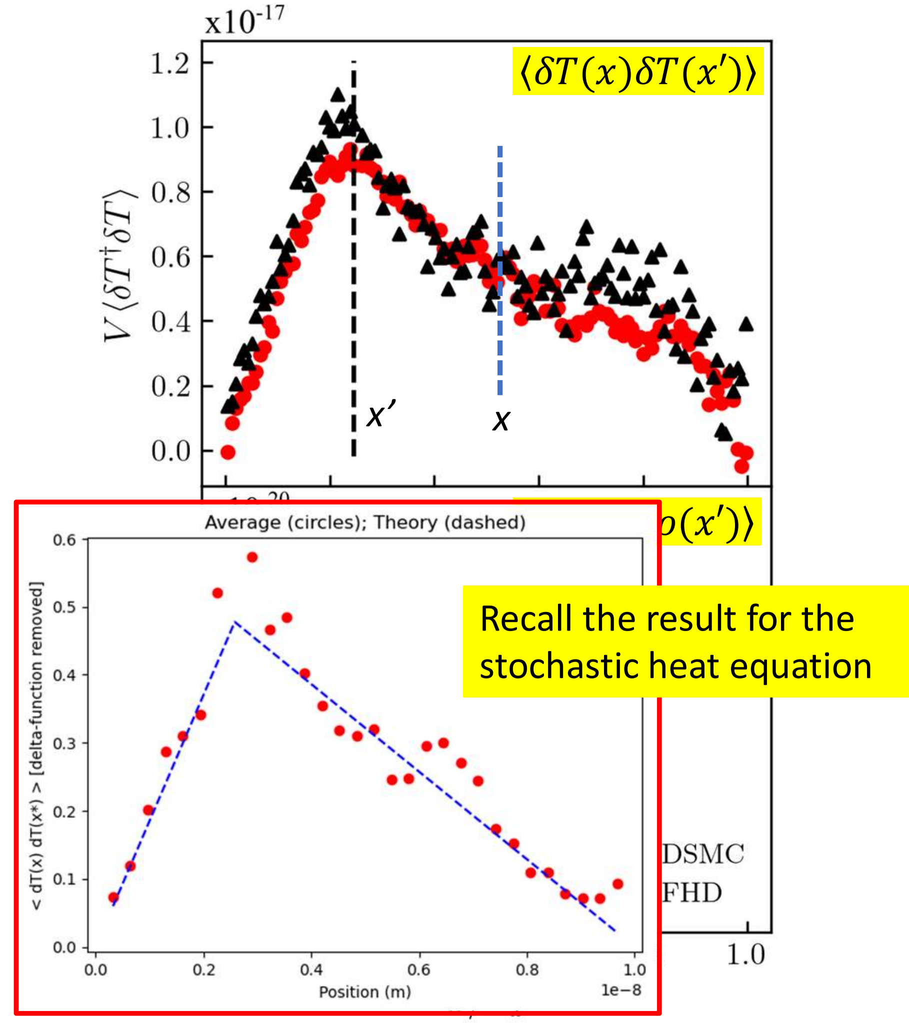
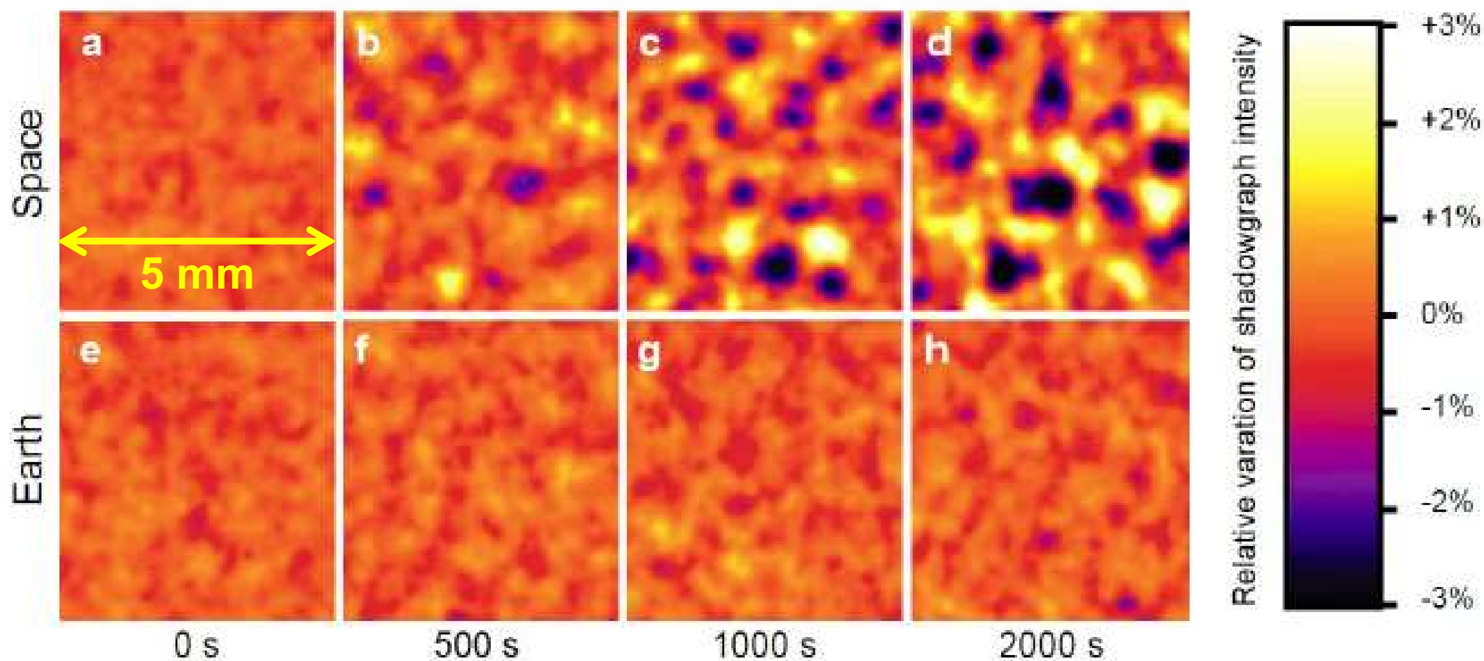
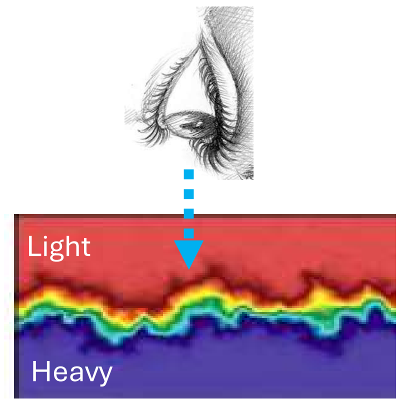




Giant Fluctuation Phenomenon

Vailati, et al., *Nature Comm.*, **2** (2011)



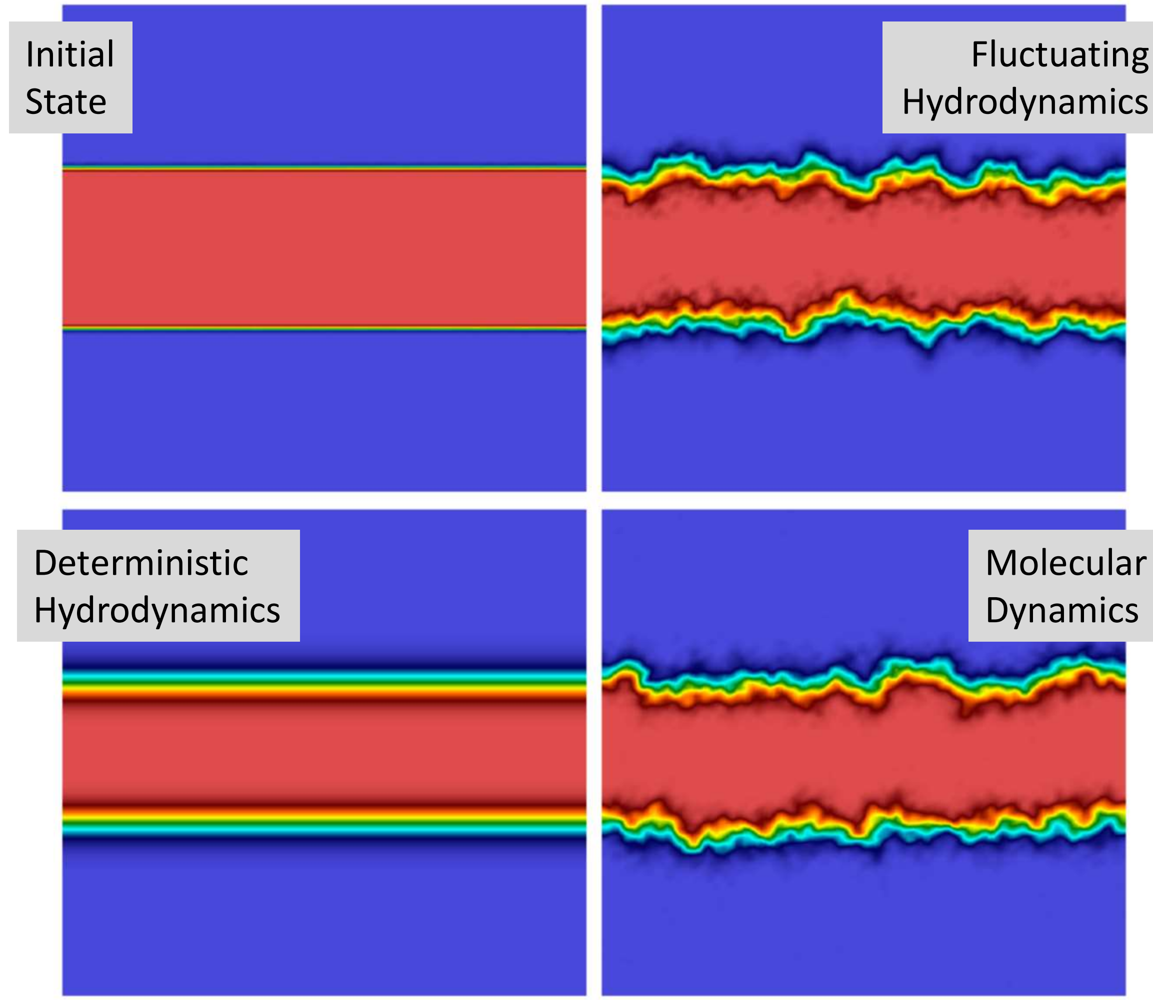


Top-down view of density fluctuations during mixing

Experiments in 2011 found *macroscopic* fluctuations in interface mixing.
Phenomenon due to correlation of concentration-velocity fluctuations.

Giant Fluctuation Simulations

Molecular dynamics simulations of this “giant fluctuation” phenomenon indistinguishable from those using fluctuating hydrodynamics.

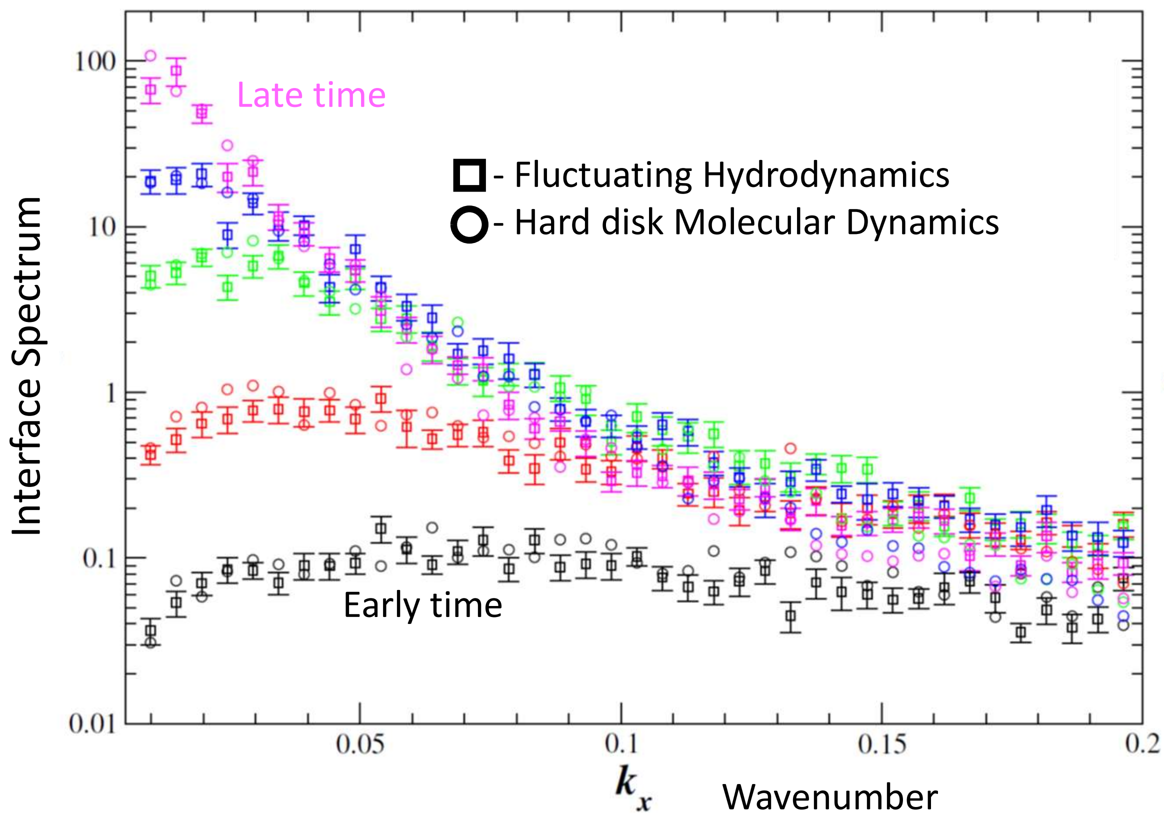


Donev, et al., *CAMCOS,* 9-1:47-105 (2014)

Simulation Results

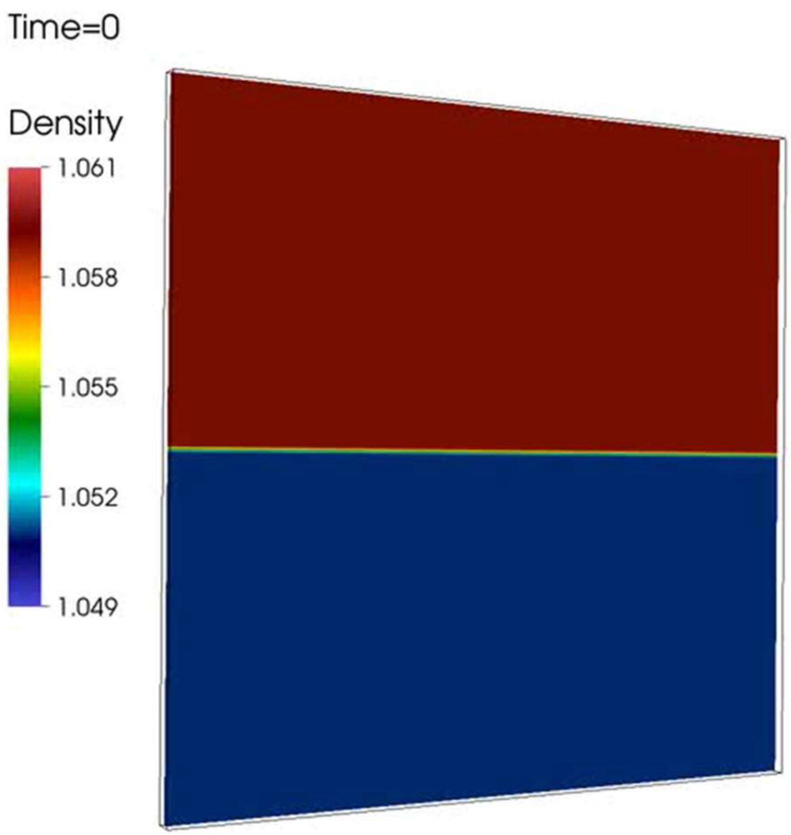
Donev, et al., *CAMCOS,* 9-1:47-105 (2014)

Excellent quantitative agreement between molecular dynamics and FHD for the form and growth rate of the rough mixing interface.

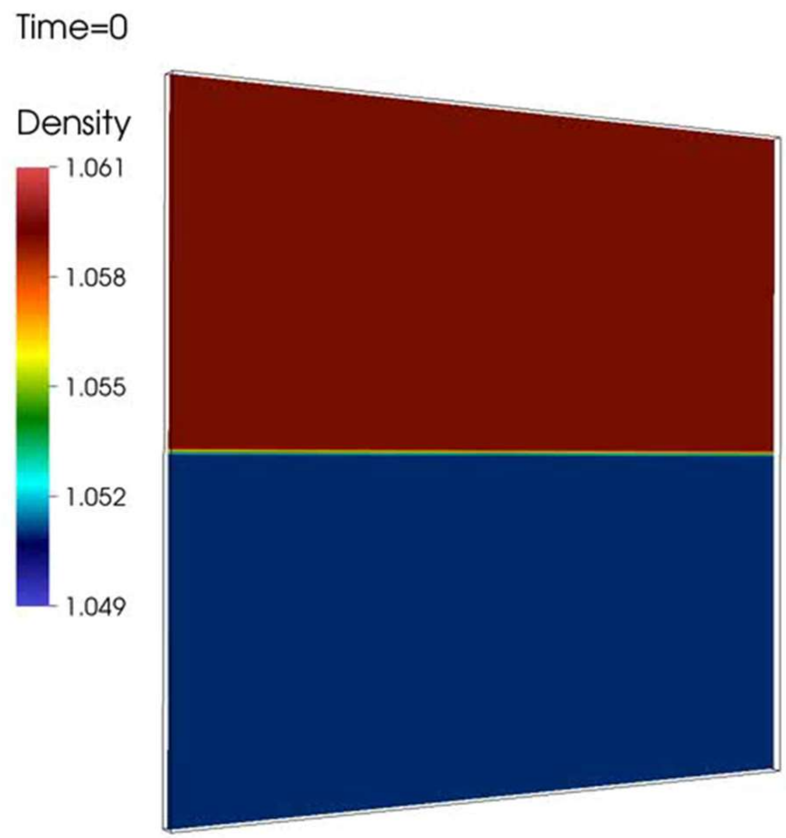


FHD & Instabilities

Donev, et al., *Physics of Fluids*, 27(3):037103 (2015)



Stochastic Hydrodynamics

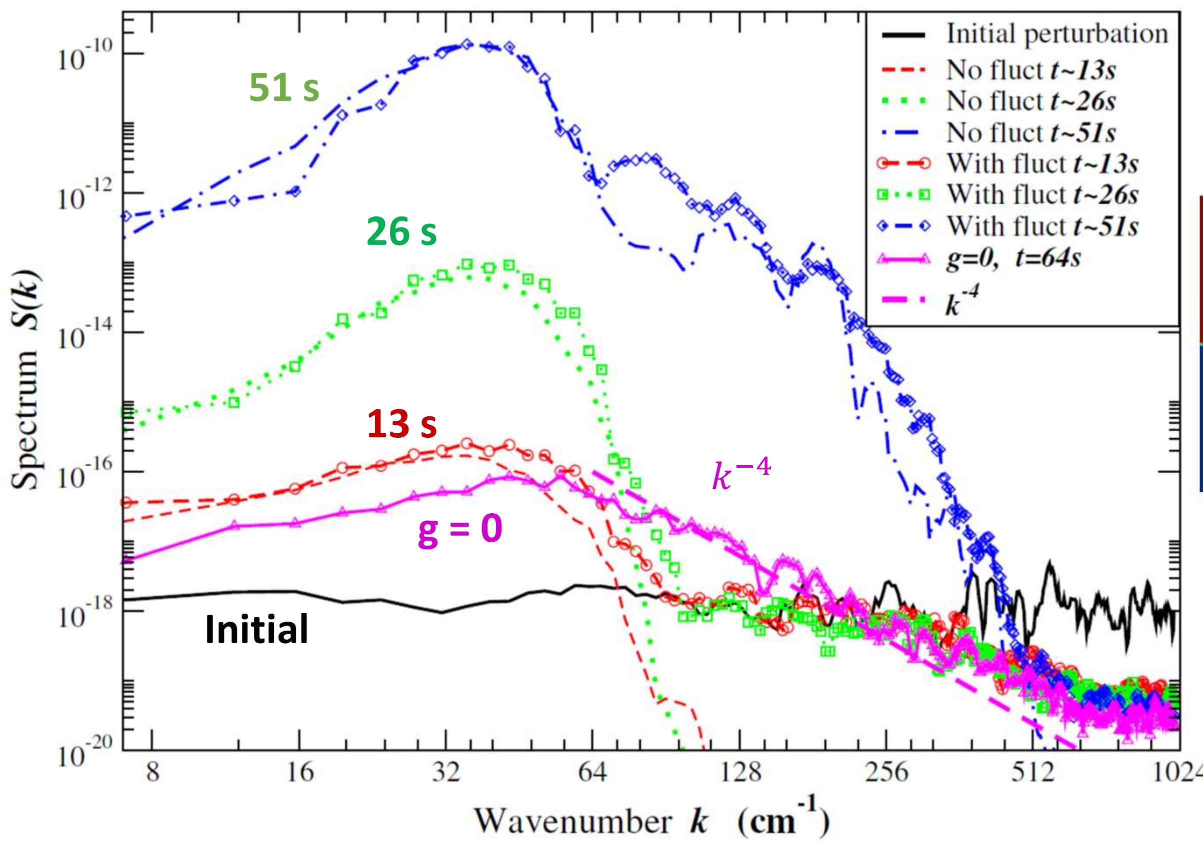


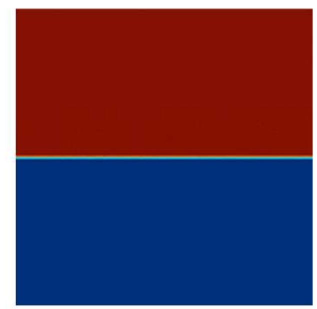
Deterministic Hydrodynamics

Mixed-mode Instability

Donev, et al., *Physics of Fluids*, 27(3):037103 (2015)

The non-equilibrium fluctuation signal is trampled by the large amplitude of the hydrodynamic instability





With gravity

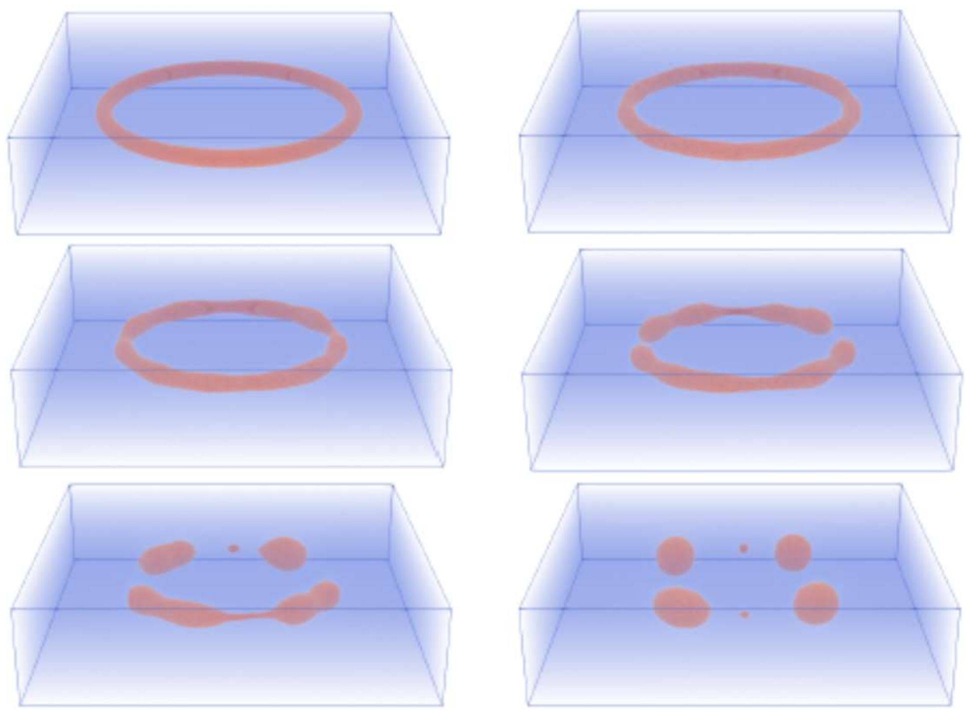
FHD & Multi-phase fluids

Can us diffuse interface models (e.g., Cahn-Hillard) in FHD to study multi-fluid interfaces.

We have simulated the Rayleigh-Plateau instability for liquid cylinders pinching into droplets.

Currently investigating droplets on solid surfaces with contact angle boundary conditions.

Breakup of a liquid torus into droplets



Barker, et al., *Proc. Nat. Acad. Sci.*, **120** e2306088120 (2023)

Kim, et al., *J. Chem. Phys.*, **146**, 124110 (2017)

FHD & Chemistry

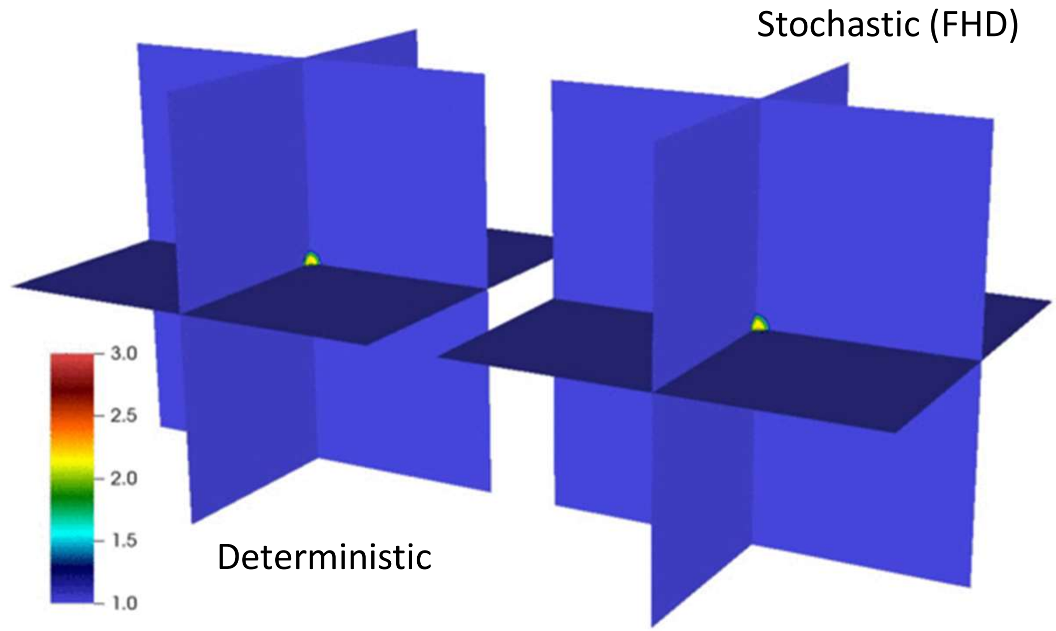
Chemical reactions can be incorporated into FHD by adding source terms to the species equation.

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

From the chemical Langevin equation

$$\bar{\Omega}_k = \sum_{r}^{\text{reactions}} \nu_{k,r}\, a_k(\{\rho_i\})$$

$$\widetilde{\Omega_k} = \sum_{r}^{\text{reactions}} \nu_{k,r} \sqrt{a_k(\{\rho_i\})}\; \mathcal{Z}_r$$



$\nu_{k,r}$ - Stochiometric coefficients

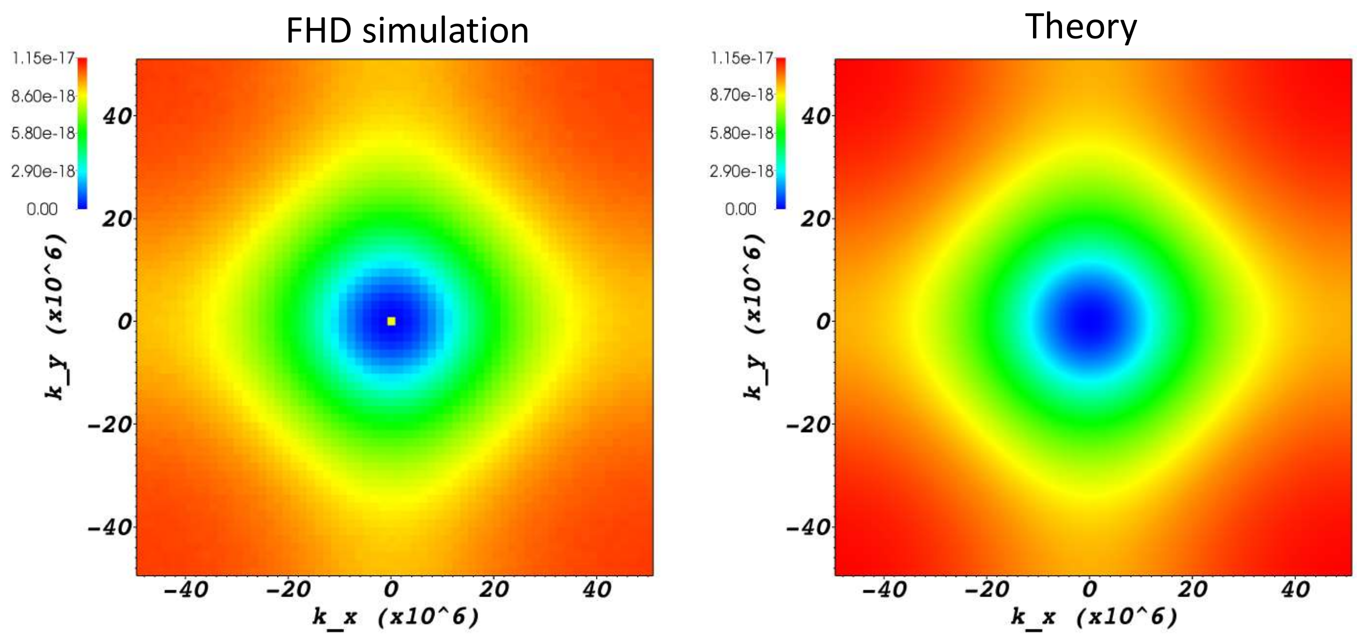
$a_k(\{\rho_i\})$ - Propensity (rate) function

FHD & Electrolytes

Peraud, et al., Phys. Rev. F, 1(7):074103 (2016)

By replacing chemical potential with electrochemical potential we can model charged species, such as ions in electrolyte solutions

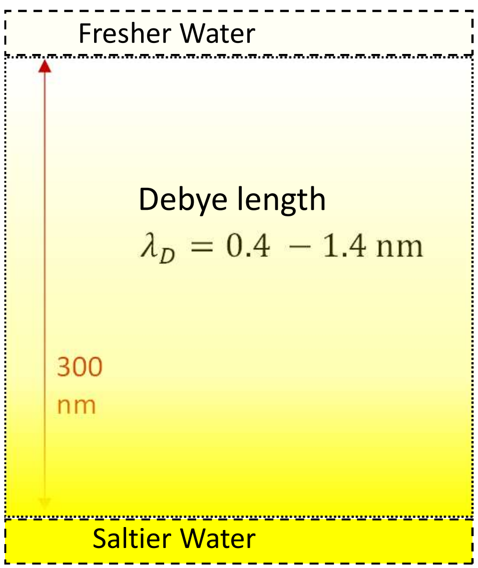
Static structure factor for charge fluctuations has a characteristic length scale, the Debye length.



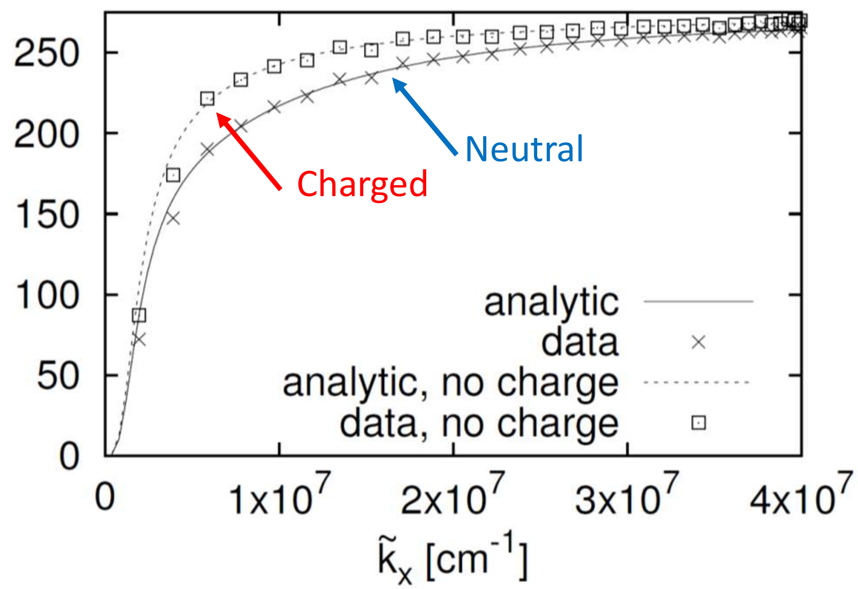
FHD & Electrolytes (cont.)

Peraud, et al., Phys. Rev. F, 1(7):074103 (2016)

Simulation results give the expected "giant fluctuations" spectrum, which is different for charged versus neutral species.



$k_x^4 \times \langle \delta\rho_{\mathrm{Na}}(k_x)\delta\rho_{\mathrm{Na}}(k_x)^* \rangle$

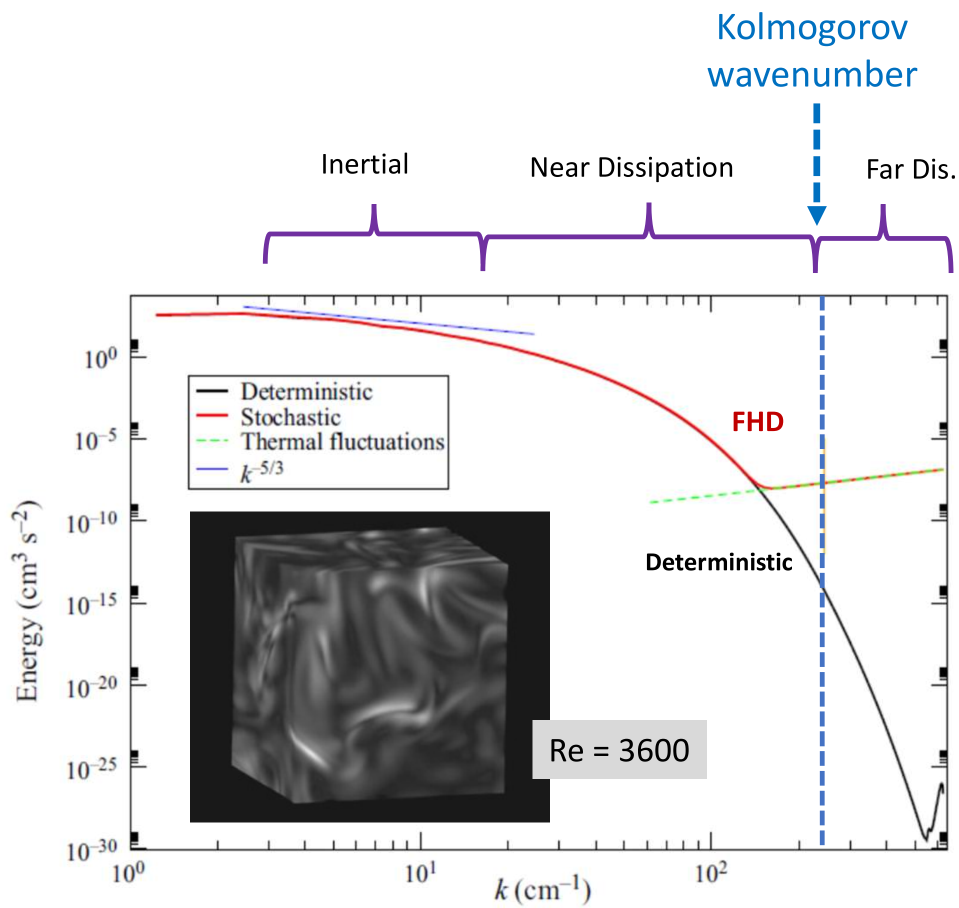


FHD & Turbulence

Thermal fluctuations dominate turbulent fluctuations in the near-dissipation range, that is, for length scales *larger* than the Kolmogorov length.

This theoretical prediction by Greg Eyink was confirmed by our FHD simulations of homogeneous, isotropic, incompressible turbulence.

Also verified in DSMC particle simulations



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

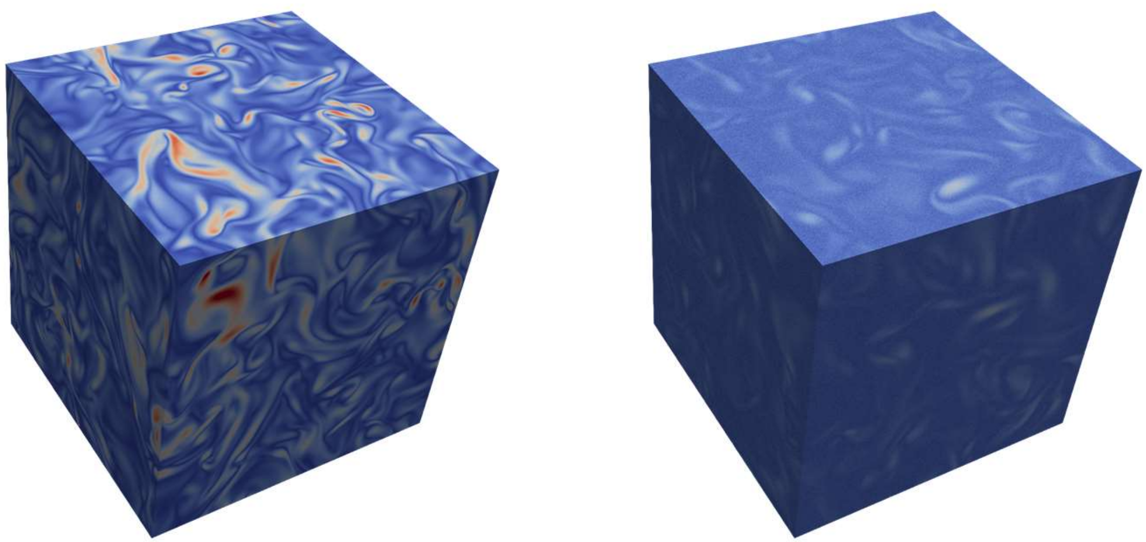
Summary & Remarks

Here are some closing thoughts:

- Thermal fluctuations can produce interesting meso- and macroscopic phenomena (e.g., giant fluctuation effect).
- Fluctuating hydrodynamics is a powerful methodology for the study of these phenomena.
- There are accurate and efficient numerical methods for the fluctuating hydrodynamic equations.
- Simple FHD models, such as the stochastic heat equation, are an accessible introduction suitable for university students.
- Many opportunities exist for applying FHD to problems that are of interest to mathematicians, scientists, and engineers.

Thank you for your attention and participation

Questions?



Vorticity in compressible turbulence simulations
(left) Deterministic | (right) Stochastic

https://github.com/AlejGarcia/IntroFHD

QR code for GitHub download

UNUSED SLIDES