Diffusive Transport by Thermal Velocity Fluctuations

Aleksandar Donev
Courant Institute, *New York University*
&
Alejandro L. Garcia, *San Jose State University*
John B. Bell, *Lawrence Berkeley National Laboratory*

University of Rochester
April 15th, 2011

Outline

Micro- and nano-hydrodynamics

- Flows of fluids (gases and liquids) through micro- (μm) and nano-scale (nm) structures has become technologically important, e.g., **micro-fluidics, microelectromechanical systems (MEMS).**
- **Biologically-relevant** flows also occur at micro- and nano- scales.
- Essential distinguishing feature from "ordinary" CFD: **thermal fluctuations**!
- Another important feature of small-scale flows, not discussed here, is **surface/boundary effects** (e.g., slip in the contact line problem).
- Interestingly, **thermal fluctuations can affect the macroscopic transport in fluid mixtures** [1, 2]!

Giant Fluctuations during diffusive mixing

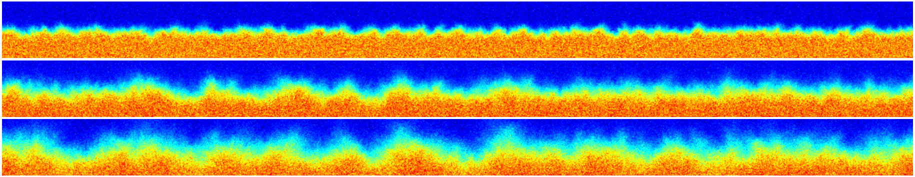


Figure: Snapshots of the concentration during the diffusive mixing of two fluids (red and blue) at $t = 1$ (top), $t = 4$ (middle), and $t = 10$ (bottom), starting from a flat interface (phase-separated system) at $t = 0$.

Giant Fluctuations in Experiments

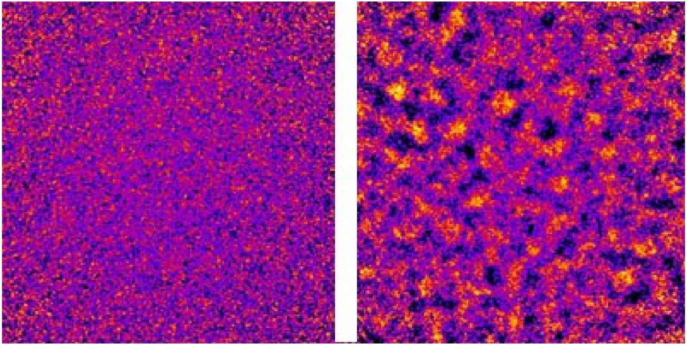


Figure: Experimental snapshots of the steady-state concentration fluctuations in a solution of polystyrene in water with a strong concentration gradient imposed via a stabilizing temperature gradient, in **Earth gravity** (left), and in **microgravity** (right) [private correspondence with Roberto Cerbino]. The strong enhancement of the fluctuations in microgravity is evident.

Coarse-Graining for Fluids

- Assume that we have a **fluid** (liquid or gas) composed of a collection of interacting or colliding **point particles**, each having mass $m_i = m$, position $\mathbf{r}_i(t)$, and velocity $\mathbf{v}_i$.
- Because particle interactions/collisions conserve mass, momentum, and energy, the field

$$\widetilde{\mathbf{U}}(\mathbf{r}, t) = \begin{bmatrix} \tilde{\rho} \\ \tilde{\mathbf{j}} \\ \tilde{e} \end{bmatrix} = \sum_i \begin{bmatrix} m_i \\ m_i \boldsymbol{\upsilon}_i \\ m_i \upsilon_i^2/2 \end{bmatrix} \delta\left[\mathbf{r} - \mathbf{r}_i(t)\right]$$

  captures the slowly-evolving **hydrodynamic modes**, and other modes are assumed to be fast (molecular).
- We want to describe the hydrodynamics at **mesoscopic scales** using a **stochastic continuum approach**.

Continuum Models of Fluid Dynamics

- Formally, we consider the continuum field of **conserved quantities**

$$\mathbf{U}(\mathbf{r},t)=\left[\begin{array}{c}\rho\\ \mathbf{j}\\ e\end{array}\right]=\left[\begin{array}{c}\rho\\ \rho\mathbf{v}\\ \rho c_V T+\rho v^2/2\end{array}\right]\cong\widetilde{\mathbf{U}}(\mathbf{r},t),$$

  where the symbol $\cong$ means something like approximates over **long length and time scales**.
- Formal coarse-graining of the microscopic dynamics has been performed to derive an **approximate closure** for the macroscopic dynamics [3].
- This leads to **SPDEs of Langevin type** formed by postulating a random flux term in the usual Navier-Stokes-Fourier equations with magnitude determined from the **fluctuation-dissipation balance** condition, following Landau and Lifshitz.

The SPDEs of Fluctuating Hydrodynamics

- Due to the **microscopic conservation** of mass, momentum and energy,

$$\partial_t \mathbf{U} = -\nabla \cdot [\mathbf{F}(\mathbf{U}) - \mathcal{Z}] = -\nabla \cdot [\mathbf{F}_H(\mathbf{U}) - \mathbf{F}_D(\nabla \mathbf{U}) - \mathbf{B}\mathcal{W}],$$

  where the flux is broken into an **advective** (hyperbolic), **dissipative** (diffusive), and a **stochastic flux**.
- We assume that $\mathcal{W}$ can be modeled as spatio-temporal **white noise**, i.e., a Gaussian random field with covariance

$$\langle \mathcal{W}_i(\mathbf{r}, t) \mathcal{W}_j^\star(\mathbf{r}', t') \rangle = (\delta_{ij})\, \delta(t - t') \delta(\mathbf{r} - \mathbf{r}').$$

- We will consider here binary fluid mixtures of two fluids that are **indistinguishable**, $\rho = \rho_1 + \rho_2$, and define **concentration** $c = \rho_1/\rho$.
- The transport coefficients are the **viscosity** η, thermal conductivity κ, and the **mass diffusion coefficient** χ.

Compressible Fluctuating Navier-Stokes

Neglecting viscous heating, the equations of **compressible fluctuating hydrodynamics** are

$$
\begin{aligned}
D_t\rho &= -\rho\left(\boldsymbol{\nabla}\cdot\mathbf{v}\right)\\
\rho\left(D_t\mathbf{v}\right) &= -\boldsymbol{\nabla}P+\boldsymbol{\nabla}\cdot\left(\eta\overline{\boldsymbol{\nabla}}\mathbf{v}+\boldsymbol{\Sigma}\right)\\
\rho c_v\left(D_t T\right) &= -P\left(\boldsymbol{\nabla}\cdot\mathbf{v}\right)+\boldsymbol{\nabla}\cdot\left(\kappa\boldsymbol{\nabla}T+\boldsymbol{\Xi}\right)\\
\rho\left(D_t c\right) &= \boldsymbol{\nabla}\cdot\left[\rho\chi\left(\boldsymbol{\nabla}c\right)+\boldsymbol{\Psi}\right],
\end{aligned}
$$

where $D_t\square=\partial_t\square+\mathbf{v}\cdot\boldsymbol{\nabla}\left(\square\right)$ is the advective derivative,

$$
\overline{\boldsymbol{\nabla}}\mathbf{v}=\left(\boldsymbol{\nabla}\mathbf{v}+\boldsymbol{\nabla}\mathbf{v}^T\right)-2\left(\boldsymbol{\nabla}\cdot\mathbf{v}\right)\mathbf{I}/3,
$$

the heat capacity $c_v=3k_B/2m$, and the pressure is $P=\rho\left(k_BT/m\right)$.

Incompressible Fluctuating Navier-Stokes

- Ignoring density and temperature fluctuations, equations of **incompressible isothermal fluctuating hydrodynamics** are

$$\partial_t \mathbf{v} = -\boldsymbol{\nabla}\pi - \mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v} + \nu\boldsymbol{\nabla}^2\mathbf{v} + \rho^{-1}\left(\boldsymbol{\nabla}\cdot\boldsymbol{\Sigma}\right), \;\; \boldsymbol{\nabla}\cdot\mathbf{v} = 0$$

$$\partial_t c = -\mathbf{v}\cdot\boldsymbol{\nabla}c + \chi\boldsymbol{\nabla}^2 c + \rho^{-1}\left(\boldsymbol{\nabla}\cdot\boldsymbol{\Psi}\right),$$

  where the **kinematic viscosity** $\nu = \eta/\rho$, and $\mathbf{v}\cdot\boldsymbol{\nabla}c = \boldsymbol{\nabla}\cdot(c\mathbf{v})$ and $\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v} = \boldsymbol{\nabla}\cdot\left(\mathbf{v}\mathbf{v}^T\right)$ because of incompressibility.
- The capital Greek letters denote stochastic fluxes that are modeled as **white-noise** random Gaussian tensor and vector fields,

$$\boldsymbol{\Sigma} = \sqrt{2\eta k_B T}\,\mathcal{W}^{(\mathbf{v})}$$

$$\boldsymbol{\Psi} = \sqrt{2m\chi\rho\, c(1-c)}\,\mathcal{W}^{(c)}.$$

Stochastic Forcing

- The amplitudes of the stochastic forcing is determined from the **fluctuation-dissipation balance principle** of equilibrium statistical mechanics.
- Adding stochastic fluxes to the **non-linear** NS equations produces **ill-behaved stochastic PDEs** (solution is too irregular).
- For now, we will simply **linearize** the equations around a **steady mean state**, to obtain equations for the fluctuations around the mean,

$$\mathbf{U} = \langle \mathbf{U} \rangle + \delta\mathbf{U} = \mathbf{U}_0 + \delta\mathbf{U}.$$

Fluctuations in the presence of gradients

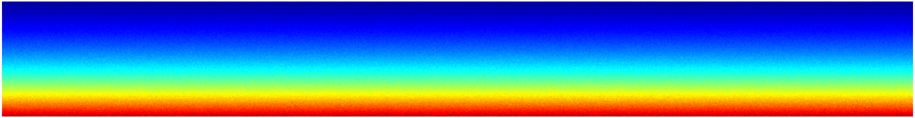
- At **equilibrium**, hydrodynamic fluctuations have non-trivial temporal correlations, but there are no spatial correlations between any variables.
- When macroscopic gradients are present, however, **long-ranged correlated fluctuations** appear.
- Consider a **binary mixture** of fluids and consider **concentration fluctuations** around a non-uniform steady state $c_0(\mathbf{r})$:

$$c(\mathbf{r}, t) = c_0(\mathbf{r}) + \delta c(\mathbf{r}, t)$$

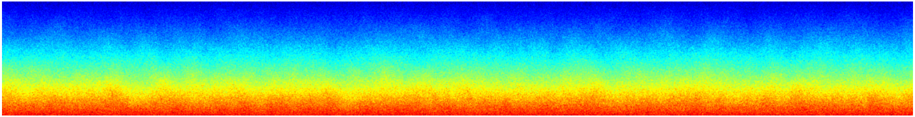
- The velocity fluctuations drive and amplify the concentration fluctuations leading to so-called **giant fluctuations**.

Equilibrium versus Non-Equilibrium

Results obtained using our fluctuating continuum compressible solver.



Concentration for a mixture of two (heavier red and lighter blue) fluids at **equilibrium**, in the presence of gravity.



No gravity but a similar **non-equilibrium** concentration gradient is imposed via the boundary conditions.

Fluctuation-Enhanced Diffusion Coefficient

- Incompressible (isothermal) **linearized** fluctuating hydrodynamics is given by

$$\partial_t (\delta c) + \mathbf{v} \cdot \boldsymbol{\nabla} c_0 = \chi \boldsymbol{\nabla}^2 (\delta c) + \rho^{-1} \boldsymbol{\nabla} \cdot \left[\sqrt{2 m \chi \rho \, c_0 (1 - c_0)} \mathcal{W}^{(c)} \right]$$

$$\mathbf{v}_t + \boldsymbol{\nabla} \pi = \nu \boldsymbol{\nabla}^2 \mathbf{v} + \rho^{-1} \boldsymbol{\nabla} \cdot \left(\sqrt{2 \eta k_B T} \, \mathcal{W}^{(\mathbf{v})} \right), \ \boldsymbol{\nabla} \cdot \mathbf{v} = 0$$

- The **nonlinear** concentration equation includes a contribution to the mass flux due to **advection by the fluctuating velocities** [4, 5],

$$-\mathbf{v} \cdot \boldsymbol{\nabla} (\delta c) + \chi \boldsymbol{\nabla}^2 (\delta c) = \boldsymbol{\nabla} \cdot \left[- (\delta c) (\delta \mathbf{v}) + \chi \boldsymbol{\nabla} (\delta c) \right].$$

- **Does the advective mass flux $-(\delta c) \mathbf{v}$ contribute to the mean (overall) mass transport (mixing rate)?**
  Think about eddy diffusivity in turbulent transport.

Model System

We study the following simple **model steady-state system**, mimicking passive scalar transport in a turbulent field:

A mixture of identical but labeled/colored *(as components 1 and 2) fluids is enclosed in a box of lengths* $L_x \times L_y \times L_z$, *without gravity.*

Periodic boundary conditions are applied in the x *(horizontal) and* z *(depth) directions, and impermeable constant-temperature walls are placed at the top and bottom boundaries.*

A weak constant concentration gradient $\boldsymbol{\nabla} c_0 = \mathbf{g}_c = g_c \hat{\mathbf{y}}$ *is imposed along the* y *axes by enforcing constant concentration boundary conditions at the top and bottom walls.*

Static Structure Factors

- Rewrite the equations in Fourier space as a system of linear additive-noise SODEs:

$$\begin{bmatrix} \widehat{\delta c} \\ \widehat{\delta \mathbf{v}} \end{bmatrix} = -\begin{bmatrix} \nu \, k^2 \widehat{\mathcal{P}} & \mathbf{0} \\ \mathbf{g}_c & \chi k^2 \end{bmatrix} \begin{bmatrix} \widehat{\delta c} \\ \widehat{\delta \mathbf{v}} \end{bmatrix}$$

$$+ \begin{bmatrix} 2\rho^{-1} \nu k_B T \, k^2 \widehat{\mathcal{P}} & \mathbf{0} \\ \mathbf{0} & 2\rho^{-1} \chi \, mc(1-c) \, k^2 \end{bmatrix}^{1/2} \begin{bmatrix} \widehat{\mathcal{W}}^{(c)} \\ \widehat{\mathcal{W}}^{(\mathbf{v})} \end{bmatrix}$$

- These can be solved to obtain the steady-state **static structure factor** (spectrum or covariance)

$$\boldsymbol{\mathcal{S}} = \left\langle \begin{bmatrix} (\delta \mathbf{v}) \, (\delta \mathbf{v})^\star & (\delta \mathbf{v}) \, (\delta c)^\star \\ (\delta c) \, (\delta \mathbf{v})^\star & (\delta c) \, (\delta c)^\star \end{bmatrix} \right\rangle,$$

as a solution to a simple linear system.

Long-Ranged Correlations

To first order in the gradient g_c, the equilibrium spectrum is:

$$\boldsymbol{\mathcal{S}} = \begin{bmatrix} \rho^{-1} k_B T \, \widehat{\boldsymbol{\mathcal{P}}} & g_c \Delta \boldsymbol{\mathcal{S}}^{\star}_{c,\mathbf{v}} \\ g_c \Delta \boldsymbol{\mathcal{S}}_{c,\mathbf{v}} & m\rho^{-1} \, c(1-c) \end{bmatrix},$$

where

$$\Delta \boldsymbol{\mathcal{S}}_{c,\mathbf{v}} = -\rho^{-1} (\nu + \chi)^{-1} k_B T \, k^{-4} \left[\hat{g}_c k^2 - k_{\parallel} \mathbf{k} \right],$$

In particular, denoting $k_{\perp} = k \sin\theta$ and $k_{\parallel} = k \cos\theta$, the important result is that **concentration and velocity fluctuations develop long-ranged correlations**:

$$\Delta \mathcal{S}_{c,v_{\parallel}} = \langle (\widehat{\delta c})(\widehat{\delta v}^{\star}_{\parallel}) \rangle = -\frac{k_B T}{\rho(\nu+\chi) k^2} \left(\sin^2\theta \right).$$

Fluctuation-Enhanced Diffusion

Assuming the advective mass flux can be approximated from the linearized solution:

$$\begin{aligned}\Delta \mathbf{j} &= -\langle (\delta c)(\delta \mathbf{v}) \rangle \approx -\langle (\delta c)(\delta \mathbf{v}) \rangle_{lin} =, \\ &= -(2\pi)^{-6} \int_{\mathbf{k}} d\mathbf{k} \int_{\mathbf{k}'} d\mathbf{k}' \, \langle \widehat{\delta c}(\mathbf{k}, t) \, \widehat{\delta \mathbf{v}}^{\star} (\mathbf{k}', t) \rangle e^{i(\mathbf{k}-\mathbf{k}')\cdot \mathbf{r}} \\ &= -(2\pi)^{-3} \int_{\mathbf{k}} \mathcal{S}_{c,\mathbf{v}}(\mathbf{k}) \, d\mathbf{k} = \Delta\chi \, \mathbf{g}_c,\end{aligned}$$

where the *enhancement* $\Delta\chi$ due to thermal velocity fluctuations is

$$\Delta\chi = -(2\pi)^{-3} \int_{\mathbf{k}} \Delta\mathcal{S}_{c,v_{\parallel}}(\mathbf{k}) \, d\mathbf{k} = \frac{k_B T}{(2\pi)^3 \rho (\chi + \nu)} \int_{\mathbf{k}} \left(\sin^2\theta\right) k^{-2} \, d\mathbf{k}.$$

System-Size Dependence

- The **fluctuation-renormalized diffusion coefficient** is $\chi + \Delta\chi$, and we call χ the **bare diffusion coefficient**.
- Because of the k^{-2}-like divergence, the integral over all $\mathbf{k}$ above diverges unless one imposes a lower bound $k_{min} \sim 2\pi/L$ *and* a **phenomenological cutoff** $k_{max} \sim \pi/L_{mol}$ [6] for the upper bound, where L_{mol} is a **"molecular" length scale**.
- More importantly, the fluctuation enhancement $\Delta\chi$ **depends on** the small wavenumber cutoff $k_{min} \sim 2\pi/L$, where L is the **system size**.
- For simplicity, I will use integrals over k_x and k_z, but one must remember that these ought to be replaced by discrete sums (done numerically).

Two Dimensions

- Assuming a quasi two-dimensional system, $L_z \ll L_x \ll L_y$, we obtain $\Delta\chi\left(L_x\right) \approx$

$$\frac{k_B T}{(2\pi)^3 \rho\left(\chi+\nu\right)} \frac{2\pi}{L_z} 2 \int_{k_x=2\pi/L_x}^{\pi/L_{mol}} dk_x \int dk_y \frac{k_x^2}{\left(k_x^2+k_y^2\right)^2},$$

$$= \frac{k_B T}{4\pi\rho(\chi+\nu)L_z} \ln \frac{L_x}{2L_{mol}}$$

- Notice that L_{mol} is **arbitrary**, since ultimately all we can do is compare a given width L_x to some reference system L_0:

$$\chi_{eff}^{(2D)} \approx \chi + \frac{k_B T}{4\pi\rho(\chi+\nu)L_z} \ln \frac{L_x}{L_0}.$$

- When the system width becomes comparable to the height, **boundaries will intervene** and for $L_x \gg L_y$ the effective diffusion coefficient must become a constant.

Three Dimensions

- For a three dimensional system with fixed height, $L_x = L_z = L \ll L_y$, we get $\Delta\chi\,(L) \approx$

$$\frac{k_B T}{(2\pi)^3 \rho\,(\chi+\nu)}\,4 \int\int_{(k_x,k_z)\geq 2\pi/L}^{(k_x,k_z)\leq \pi/L_{mol}} dk_z dk_x \int dk_y\, \frac{k_x^2+k_z^2}{\left(k_x^2+k_y^2+k_z^2\right)^2}$$

$$= \frac{\ln\left(1+\sqrt{2}\right)\,k_B T}{2\pi\rho(\chi+\nu)}\left(\frac{1}{L_{mol}}-\frac{2}{L}\right)$$

- Unlike in two dimensions, the renormalized diffusion coefficient converges as $L \to \infty$ as L^{-1}:

$$\chi_{eff}^{(3D)} \approx \chi + \frac{\alpha\, k_B T}{\rho(\chi+\nu)}\left(\frac{1}{L_0}-\frac{1}{L}\right).$$

Particle Simulations

- We use the **Direct Simulation Monte Carlo** particle algorithm to simulate a miscible mixture.
- The same results could be obtained from molecular dynamics also (more expensive).
- In particle simulations, a uniform concentration gradient along the vertical (y) direction is implemented by randomly changing the label of particles that collide with the top and bottom walls.
- The **mass flux can be measured** by counting the number of color flips at the top/bottom wall over a long time.
- An alternative is to calculate the average momentum of *all* particles belonging to the first component.

Sampling Cells

- To look at spatial dependence of hydrodynamic variables, we must put a **grid of sampling or (hydrodynamic) cells**.
- Red particles start moving upward, on average, while blue particles move downward. *If color blind there is no movement*!
- In each sampling cell we measure the instantaneous **mass** and **momentum density** of particles of species 1,

$$j_y = \rho_1 v_{1,y}.$$

- We also define an average (macroscopic) concentration

$$\bar{c} = \frac{\langle \rho_1 \rangle}{\langle \rho_1 + \rho_2 \rangle} \neq \langle c \rangle = \left\langle \frac{\rho_1}{\rho_1 + \rho_2} \right\rangle,$$

since $\langle c \rangle$ is a potentially **biased estimator** of the average concentration.

Effective Diffusion

- Because particle collisions preserve color and the only sinks are at the top and bottom walls, the average momentum along the concentration gradient,

$$\langle j_y \rangle = \langle \rho_1 v_{1,y} \rangle = \langle \rho_1 \rangle \langle v_{1,y} \rangle + \langle (\delta \rho_1)(\delta v_{1,y}) \rangle,$$

  does not depend on the position or shape of the sampling cell.
- We therefore define the **effective diffusion coefficient** χ_{eff},

$$\langle j_y \rangle = \langle \rho_1 v_{1,y} \rangle = \rho_0 \chi_{eff} \, g_c,$$

  where the background concentration gradient is defined as

$$g_c = \frac{\bar{c}_T - \bar{c}_B}{L_y - \Delta y}.$$

Locally-Renormalized Diffusion

- The **locally renormalized diffusion coefficient** χ_0 is defined via

$$\langle \rho_1 \rangle \langle v_{1,y} \rangle = \rho_0 \chi_0 \left(\boldsymbol{\nabla}_y \bar{c} \right).$$

- Note that $\boldsymbol{\nabla}_y \bar{c} \neq g_c$ since $\bar{c}(y)$ is somewhat nonlinear (we fit a polynomial to $\bar{c}(y)$).
- Linearized fluctuating hydrodynamics assumes that χ_0 is a materials constant (bare diffusion coefficient).
- Better to think of χ_0 as a parameter that can depend on the shape of the hydrodynamic cell.

Theory for χ_0

$$\rho_0 \chi_{eff} = \chi - (2\pi)^{-3} \int_{\mathbf{k}} \Delta \mathcal{S}_{c,v_{\parallel}}(\mathbf{k})\, d\mathbf{k}$$

$$\rho_0 \chi_0 = \chi - (2\pi)^{-3} \int_{\mathbf{k}} \left[1 - F(\mathbf{k})\right] \Delta \mathcal{S}_{c,v_{\parallel}}(\mathbf{k})\, d\mathbf{k}$$

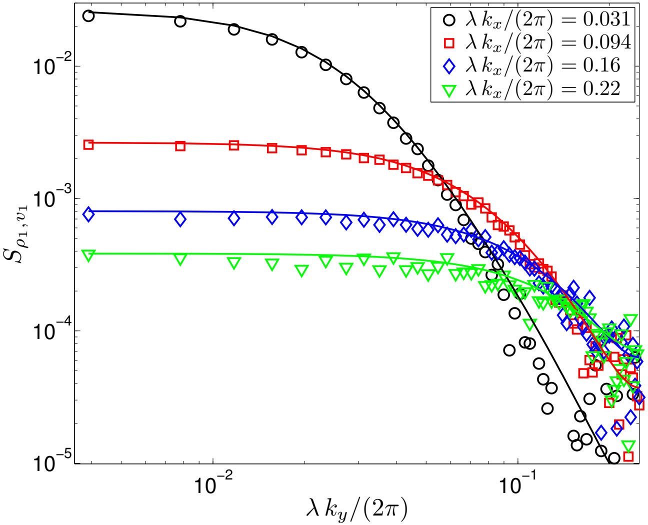
$$\chi_{\text{eff}} = \chi_0 - (2\pi)^{-3} \int_{\mathbf{k}} F(\mathbf{k}) \left[\Delta \mathcal{S}_{c,v_{\parallel}}(\mathbf{k})\right] d\mathbf{k} \text{ (no cutoff needed!)}$$

- Here $F(\mathbf{k})$ is a product of low pass filters, one for each dimension,

$$F_x(k_x) = 2\left[1 - \cos(k_x \Delta x)\right] / (k_x \Delta x)^2 = \text{sinc}^2(k_x \Delta x/2).$$

- The actual (effective) diffusion coefficient χ_{eff} includes contributions from all wavenumbers present in the system.
- The renormalized χ_0 only includes "sub-grid" contributions, from wavenumbers larger than $2\pi/\Delta x$.

Spectra from Particle Data



Spectra from Particle Data

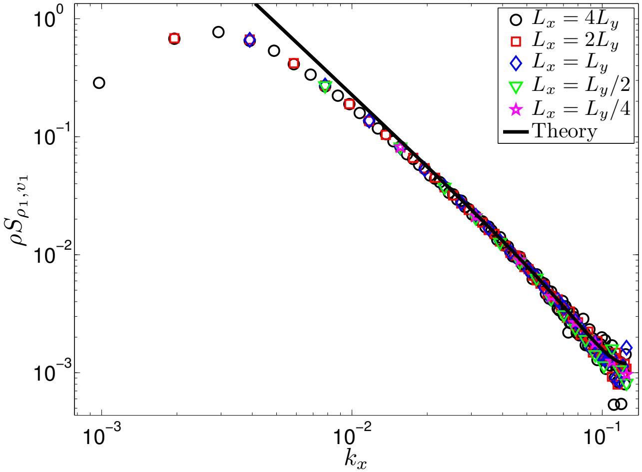


Figure: Comparison of theoretical spectra and particle data for $k_y = 0$.

Two Dimensions

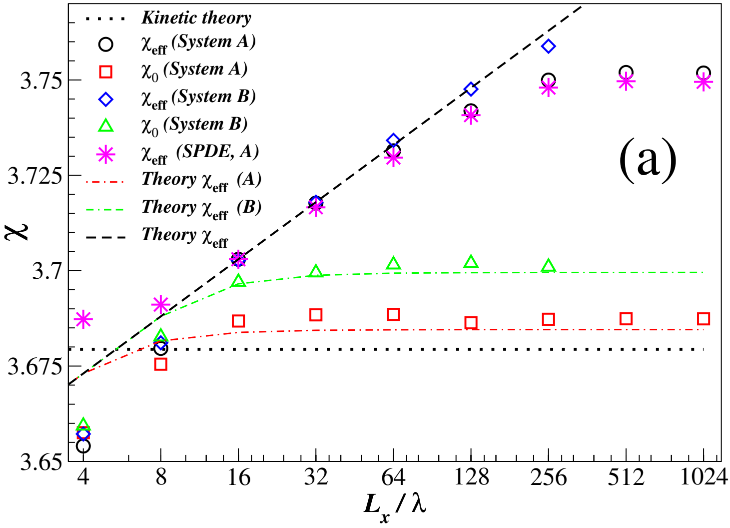


Figure: Diffusion enhancement in two dimensions.

Three Dimensions

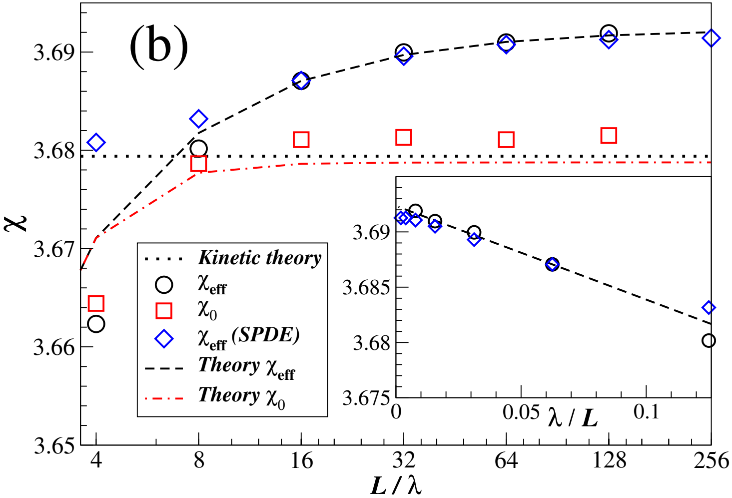


Figure: Diffusion Enhancement in three dimensions.

Relations to VACF

- In the literature there is a lot of discussion about the effect of the **long-time hydrodynamic tail** on the transport coefficients [7],

$$C(t) = \langle \mathbf{v}(0) \cdot \mathbf{v}(t) \rangle \approx \frac{k_B T}{12\rho \left[\pi \left(D + \nu\right) t\right]^{3/2}} \text{ for } \frac{L_{mol}^2}{(\chi + \nu)} \ll t \ll \frac{L^2}{(\chi + \nu)}$$

- *This is in fact* **the same effect** *as the one we studied!* Ignoring prefactors,

$$\Delta\chi_{VACF} \sim \int_{t=L_{mol}^2/(\chi+\nu)}^{t=L^2/(\chi+\nu)} \frac{k_B T}{\rho \left[(\chi + \nu) t\right]^{3/2}} dt \sim \frac{k_B T}{\rho (\chi + \nu)} \left(\frac{1}{L_{mol}} - \frac{1}{L} \right),$$

which is like what we found (all the prefactors are in fact identical also).

Estimates of Diffusion Enhancement

- The hydrodynamic contribution to the diffusion coefficient for a large **three dimensional system** is

$$\Delta\chi \sim \frac{k_B T}{\rho(\chi+\nu)L_{\text{mol}}},$$

- For both gases and liquids, denoting the number density $n = \rho/m$,

$$\Delta\chi \sim \left(n\sigma^3\right)\chi \sim \phi\chi.$$

- For liquids $\phi \sim 1$ and thus $\Delta\chi \sim \chi$, which is why was the first hydrodynamic correction to kinetic theory to be measured in MD.
- The fluctuation contribution always dominates for sufficiently large (quasi) **two-dimensional systems**,

$$\frac{\Delta\chi}{\chi} \sim \left(n\sigma^3\right)\frac{\sigma}{L_z}\ln\frac{L_x}{\sigma}.$$

Self-Consistent Theory

- A **self-consistent form** in three dimensions may be:

$$\chi_{\text{eff}}^{(3D)} = \chi + \frac{\alpha\, k_B T}{\rho(\chi_{\text{eff}} + \nu_{\text{eff}})} \left(\frac{1}{L_0} - \frac{1}{L} \right)$$

- In two dimensions, it is **postulated** that a self-consistent form shows different asymptotics

$$\chi_{\text{eff}}^{(2D)} \approx \chi \left[1 + \frac{k_B T}{2\pi\rho\chi(\chi_{\text{eff}} + \nu_{\text{eff}}) L_z} \ln \frac{L_x}{L_0} \right]^{1/2}$$

- Concentration **fluctuations become macroscopic** in two dimensions,

$$\frac{\langle (\delta c)(\delta c) \rangle_{\text{neq}}^{(2D)}}{(\Delta c)^2} \sim \left(n\sigma^3 \right) \frac{\sigma}{L_z},$$

which could be measured in thin liquid films and hard-disk MD.

Future Directions

- Transport of other quantities, like momentum and heat.
- Other types of **nonlinearities** in the LLNS equations:
  - Dependence of transport coefficients on fluctuations.
  - Dependence of noise amplitude on fluctuations.
- Implications to **finite-volume solvers** for fluctuating hydrodynamics.
- **Self-consistent theory** in two dimensions?
- **Stochastic homogenization**: *Can we write a nonlinear equation that is well-behaved and correctly captures the flow at scales above some chosen "coarse-graining" scale?*

References

A. Donev, A. L. Garcia, Anton de la Fuente, and J. B. Bell.
Diffusive Transport by Thermal Velocity Fluctuations.
ArXiv e-print 1103.5532, 2011.

A. Donev, A. L. Garcia, Anton de la Fuente, and J. B. Bell.
Enhancement of Diffusive Transport by Nonequilibrium Thermal Fluctuations.
ArXiv e-print 1103.5244, 2011.

P. Español.
Stochastic differential equations for non-linear hydrodynamics.
Physica A, 248(1-2):77–96, 1998.

D. Bedeaux and P. Mazur.
Renormalization of the diffusion coefficient in a fluctuating fluid I.
Physica, 73:431–458, 1974.

P. Mazur and D. Bedeaux.
Renormalization of the diffusion coefficient in a fluctuating fluid II.
Physica, 75:79–99, 1974.

D. Brogioli and A. Vailati.
Diffusive mass transfer by nonequilibrium fluctuations: Fick's law revisited.
Phys. Rev. E, 63(1):12105, 2000.

Y. Pomeau and P. Résibois.
Time dependent correlation functions and mode-mode coupling theories.
Phys. Rep., 19:63–139, June 1975.