Fluctuating Hydrodynamics of Complex Fluid Mixtures

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- A number of postdocs and graduate students at Courant and LBL
- A number of experimentalists (Italy, France).

Fluctuating Hydrodynamics

- **Fluctuating hydrodynamics (FHD)** is a formalism for accounting for thermal fluctuations in traditional fluid equations.
- The key idea, due to Landau & Lifshitz, is to add a **stochastic (momentum, heat, diffusive) flux** corresponding to every dissipative flux.
- The stochastic fluxes are modeled as **space-time white-noise fields** with an amplitude set by **fluctuation-dissipation balance**.
- FHD can be justified using the **theory of coarse-graining** (Mori-Zwanzig formalism), as most clearly explained in works of Pep Espanol [1] (review article by two of us is currently in preparation).
- In this talk I will give some examples of FHD equations that we have studied numerically using traditional CFD methods with fluctuations added in a way to obey **discrete fluctuation-dissipation balance**.

Hydrodynamic Interactions via FHD

- The thermal velocity fluctuations are described by the (unsteady) **fluctuating Stokes equation**,

$$\rho\partial_t \mathbf{v} + \boldsymbol{\nabla}\pi = \eta\boldsymbol{\nabla}^2\mathbf{v} + \sqrt{2\eta k_B T}\,\boldsymbol{\nabla}\cdot\left(\boldsymbol{\sigma}\star\boldsymbol{\mathcal{W}}\right), \quad \text{and } \boldsymbol{\nabla}\cdot\mathbf{v} = 0. \quad (1)$$

  where the **stochastic momentum flux** is spatio-temporal **white noise**,

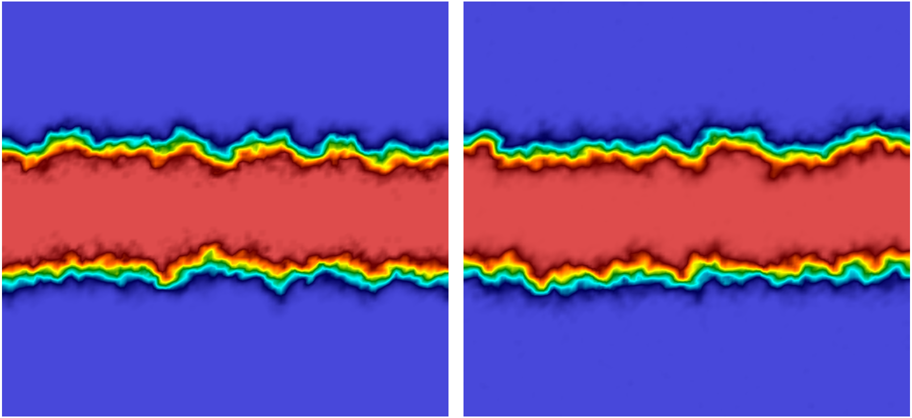
$$\langle \mathcal{W}_{ij}(\mathbf{r},t)\mathcal{W}^{\star}_{kl}(\mathbf{r}',t')\rangle = \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)\delta(t-t')\delta(\mathbf{r}-\mathbf{r}').$$

  and the smoothing kernel $\boldsymbol{\sigma}$ filters out features at scales below a **cutoff scale** σ.

- The **concentration** $c\,(\mathbf{r},t)$ of a **passive tracer** follows an (additive noise) fluctuating advection-diffusion equation,

$$\partial_t c = -\mathbf{u}\cdot\boldsymbol{\nabla}c + \chi_0\boldsymbol{\nabla}^2 c. \quad (2)$$

Giant Fluctuations in Diffusive Mixing



Snapshots of concentration in a miscible mixture showing the development of a *rough* diffusive interface due to the effect of **thermal fluctuations**. These **giant fluctuations** have been studied experimentally and with hard-disk molecular dynamics.

MD vs. Fluct Hydro

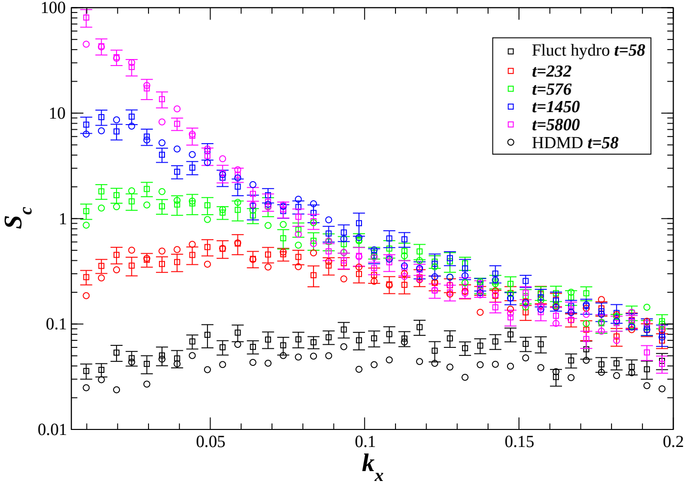


Figure : Discrete spatial spectrum of the interface fluctuations, for fluctuating hydrodynamics (squares) and HD-MD (circles).

Separation of Time Scales

- In liquids molecules are caged (trapped) for long periods of time as they collide with neighbors:
  Momentum and heat diffuse much faster than does mass.
- This means that $\chi \ll \nu$, leading to a **Schmidt number**

$$S_c = \frac{\nu}{\chi} \sim 10^3 - 10^4.$$

  This **extreme stiffness** solving the concentration/tracer equation numerically challenging.
- There exists a **limiting (overdamped) dynamics** for c in the limit $S_c \to \infty$ in the scaling

$$\chi\nu = \text{const}.$$

Overdamped Dynamics

- Adiabatic mode elimination gives the following limiting Ito **stochastic advection-diffusion equation**,

$$\partial_t c = \boldsymbol{\nabla} \cdot [\chi(\mathbf{r}) \boldsymbol{\nabla} c] - \mathbf{w} \cdot \boldsymbol{\nabla} c, \tag{3}$$

  which is **exactly the same as** what was derived from **Brownian dynamics**.

- The advection velocity $\mathbf{w}(\mathbf{r}, t)$ is **white in time**, with covariance proportional to a Green-Kubo integral of the velocity auto-correlation function,

$$\begin{aligned}
\langle \mathbf{w}(\mathbf{r}, t) \otimes \mathbf{w}(\mathbf{r}', t') \rangle &= 2\,\delta(t - t') \int_0^\infty \langle \mathbf{u}(\mathbf{r}, t) \otimes \mathbf{u}(\mathbf{r}', t + t') \rangle dt' \\
&= 2\boldsymbol{\mathcal{R}}(\mathbf{r}, \mathbf{r}')\,\delta(t - t') \\
&= \frac{k_B T}{\eta} \int \boldsymbol{\sigma}(\mathbf{r}, \mathbf{q}')\,\mathbf{G}(\mathbf{r}', \mathbf{r}'')\,\boldsymbol{\sigma}^T(\mathbf{r}'', \mathbf{q}'')\,d\mathbf{q}' d\mathbf{q}'',
\end{aligned}$$

  where $\mathbf{G}$ is the Green's function for steady Stokes flow with the appropriate boundary conditions.

Stokes-Einstein Relation

- An explicit calculation for **Stokes flow** gives the explicit result

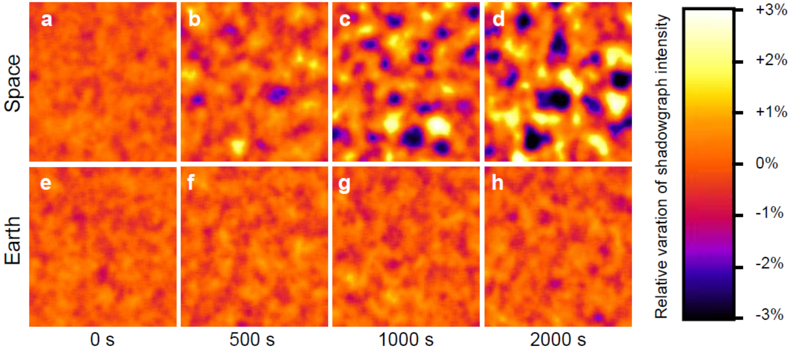
$$\chi(\mathbf{r}) = \chi_0 + \frac{k_B T}{\eta} \int \boldsymbol{\sigma}(\mathbf{r}, \mathbf{r}') \, \mathbf{G}(\mathbf{r}', \mathbf{r}'') \, \boldsymbol{\sigma}^T(\mathbf{r}, \mathbf{r}'') \, d\mathbf{r}' d\mathbf{r}'', \qquad (4)$$

  where **G** is the Green's function for steady Stokes flow.
- For an appropriate filter $\boldsymbol{\sigma}$, this gives **Stokes-Einstein formula** for the diffusion coefficient in a finite domain of length L,

$$\chi = \frac{k_B T}{\eta} \begin{cases} (4\pi)^{-1} \ln \frac{L}{\sigma} & \text{if } d = 2 \\ (6\pi\sigma)^{-1} \left(1 - \frac{\sqrt{2}}{2} \frac{\sigma}{L}\right) & \text{if } d = 3. \end{cases}$$

- The fact that for many liquids Stokes-Einstein holds as a good approximation implies that $\chi_0 \ll \chi$:
  Diffusion in liquids is dominated by advection by thermal velocity fluctuations, and is more similar to eddy diffusion in turbulence than to standard Fickian diffusion.

Giant Nonequilibrium Fluctuations



GRADFLEX results by A. Vailati *et al.* from a microgravity environment showing **giant fluctuations** in the concentration of polystyrene in toluene in space (box scale is 5mm on the side, 1mm thick).

Fluctuations become macrosopically large at macroscopic scales!

These come because of **hydrodynamic effects** on diffusion in liquids.

Linearized Fluctuating Hydrodynamics

- When macroscopic gradients are present, steady-state thermal fluctuations become **long-range correlated**.
- Consider a **binary mixture** of fluids and consider **concentration fluctuations** around a macroscopic state $\bar{c}(\mathbf{r}, t)$, $c = \bar{c} + \delta c$.
- The concentration fluctuations are **advected by the random velocities**,

$$\partial_t \bar{c} = \chi \boldsymbol{\nabla}^2 \bar{c}$$

$$\partial_t (\delta c) = -\mathbf{v} \cdot \boldsymbol{\nabla} \bar{c} + \chi \boldsymbol{\nabla}^2 \delta c + \boldsymbol{\nabla} \cdot \left(\sqrt{2\chi \bar{c}}\, \boldsymbol{\mathcal{W}}_c \right)$$

$$\rho \partial_t \mathbf{v} + \boldsymbol{\nabla} \pi = \eta \boldsymbol{\nabla}^2 \mathbf{v} - \beta \rho (\delta c)\, \mathbf{g} + \sqrt{2\eta k_B T}\, \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{W}},$$

  where β is the solutal expansion coefficient. This system of SPDEs can easily be solved numerically once we take the **overdamped limit**.
- Note that here χ is the deterministic (Fickian) diffusion coefficient which is *larger* than the bare χ_0.

Back of the Envelope

- The coupled *linearized velocity*-concentration system in **one dimension**:

$$\begin{aligned} v_t &= \nu v_{xx} + \sqrt{2\rho^{-1}\nu}\, W_x \\ c_t &= \chi c_{xx} - v\bar{c}_x, \end{aligned}$$

  where $\bar{c}_x$ is the imposed background concentration gradient.
- The linearized system can be easily solved in Fourier space to give a **power-law divergence** for the spectrum of the concentration fluctuations as a function of wavenumber k,

$$\langle \hat{c}\hat{c}^{\star} \rangle = \rho \frac{k_B T}{\chi(\chi+\nu)k^4} \left(\bar{c}_x\right)^2 \approx \frac{k_B T}{\chi\eta k^4} \left(\bar{c}_x\right)^2 \text{ for large Sc.}$$

- Concentration fluctuations become **long-ranged** and are **enhanced** as the square of the gradient, to values much larger than equilibrium fluctuations.
- In real life the divergence is **suppressed** by **surface tension**, **gravity**, or **boundaries** (usually in that order).

Simulation versus Theory/Experiment

1. Simulations have the following advantages over analytical theory:
   1. **Numerical linearization** around arbitrary **time-dependent** macroscopic states including **nonlinearities** (e.g., chemistry).
   2. Nontrivial **boundary conditions** can be accounted for relatively easily.
2. Simulations have the following advantages over experiments:
   1. One can easily turn different effects/terms **on and off** to understand what physics is important.
   2. **No measurement noise** or contamination, but still includes thermal fluctuations.
3. Disadvantages of simulations include:
   1. Fluctuations imply **statistical noise**, so long runs needed to compute averages (Monte Carlo).
   2. Cannot easily handle **time and length scale separation**.
   3. Development of computer codes is like developing a new experimental apparatus; it takes time!

GRADFLEX transient

1. We numerically solve the equations

$$\rho\partial_t \mathbf{v} + \boldsymbol{\nabla}\pi = \eta\boldsymbol{\nabla}^2\mathbf{v} + \boldsymbol{\nabla}\cdot\left(\sqrt{2\eta k_B T_0}\,\boldsymbol{\mathcal{W}}\right) \quad (5)$$

$$\boldsymbol{\nabla}\cdot\mathbf{v} = 0$$

$$\partial_t c + \mathbf{v}\cdot\boldsymbol{\nabla} c = D\boldsymbol{\nabla}\cdot\left(\boldsymbol{\nabla} c + c\,(1-c)\,S_T\boldsymbol{\nabla} T\right) \quad (6)$$

$$\partial_t T + \mathbf{v}\cdot\boldsymbol{\nabla} T = \kappa\boldsymbol{\nabla}^2 T, \quad (7)$$

2. Our numerical methods perform **numerical linearization** by solving the fully nonlinear equations with weak noise.
3. In the linearized regime **no difference between 2D and 3D** so we sometimes solve 2D equations to speed up computations.
4. Numerically we **separately solve** (5,6) for concentration (overdamped), and we separately solve (5,7) for temperature (inertial) [2].

Comparison to GRADFLEX transient

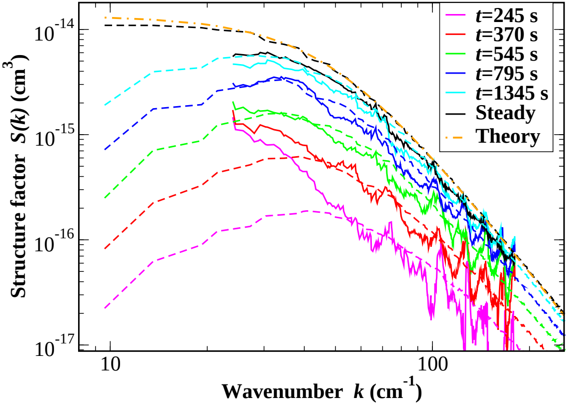


Figure : **Qualitative theory** [3]: $S(k,t) \propto \left[1-\exp(-2Dk^2t)\right]S(k,\infty)$

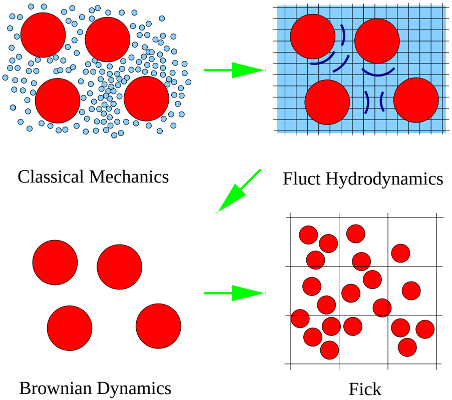
Complex Fluids

We have generalized the models and numerical codes to include more complex fluids:

- **Multispecies mixtures** with complete transport including **thermo and barodiffusion** and boundary conditions and gravity [4]. We have simulated the development of gravity-driven diffusive instabilities and compared to experiments.
- **Chemically-reacting mixtures** [5]. We have studied giant fluctuations in reactive mixtures and found that the nonlinearity of the base (macroscopic) state is crucial and not yet captured in theory.
- **Multiphase liquids** including liquid-vapor coexistence [6]. We have simulated capillary waves, spinodal decomposition, condensation, and the piston effect.
- **Ionic (electrolyte) mixtures** including electrostatic effects at length scales comparable to the Debye length (in preparation).

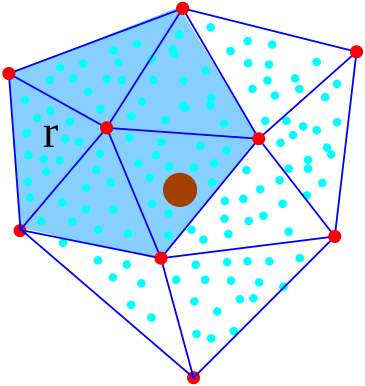
Coarse Graining Brownian Motion

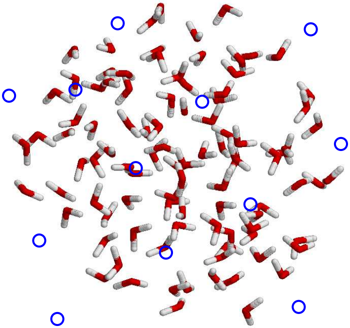
- The proper way to interpret fluctuating hydrodynamics is via the **theory of coarse-graining** (here I follow Pep Espanol) [1].
- The first step is to define a discrete set of **relevant variables**, which are **mesoscopic observables** that **evolve slowly**



Fluctuating Hydrodynamics Level

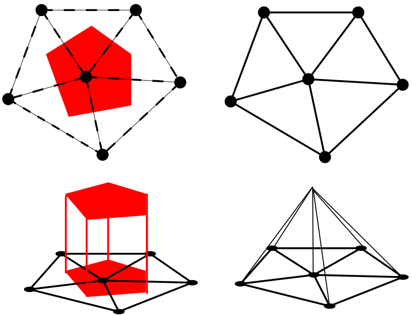
- Relevant variables for **subgrid (nanoscopic) particles** associated to a **grid node** μ are:
    - **discrete mass** $\rho_\mu(t)$ **and momentum density** $\mathbf{g}_\mu(t)$ (including the suspended particle!)
    - **position of the particle** (since momentum of particle is not slow!)





Relevant Variables

- How to assign the molecules to the **coarse-grained nodes**?
- If one uses a nearest-node assignment, i.e., **Voronoi cells**, one gets divergent Green-Kubo transport coefficients.
- Instead, one can use the dual **Delaunay cells** to construct coarse-grained variables.



$\mathbf{g}_\mu = \sum_{i=0}^{N} m_i \mathbf{v}_0 \delta_\mu(\mathbf{q}_i)$ follows a **conservation law**

Mori-Zwanzig Formalism

- One can use the **(Mori-)Zwanzig formalism** with a **Markovian assumption** (due to separation of timescales) to derive a system of SDEs for the (discrete) coarse-grained variables.
- It turns out that these equations are *exactly* the same as obtained from a Petrov-Galerkin **finite-element discretization** of the fluctuating hydrodynamic SPDEs I wrote earlier, using **the same dual set of basis functions** as used for coarse graining.
  This provides a link between **continuum->discrete** and **discrete->continuum** approaches.
- The TCG gives generalized **Green-Kubo** formulas for the diffusion coefficients.
- A key difference with the phenomenological equations is that the discrete delta function or kernel is **attached to the grid** (artificial!) **rather than to the particle cage** (physical),

$$\boldsymbol{\sigma}\left(\mathbf{r},\mathbf{r}'\right)\rightarrow\Delta\left(\mathbf{r},\mathbf{r}'\right)=\delta_{\mu}\left(\mathbf{r}\right)\delta_{\mu}^{-1}\left(\mathbf{r}'\right).$$

Renormalization of Diffusion

- The **bare diffusion coefficient** concerns **near-field hydrodynamics** and can be computed using MD from

$$\chi_0 = \frac{1}{d} \int_0^{\tau_{MD}} dt \, \langle \delta \hat{\mathbf{V}} \cdot \delta \hat{\mathbf{V}} \rangle_{\text{eq}},$$

where the particle **peculiar velocity** $\delta \hat{\mathbf{V}} = \hat{\mathbf{V}} - \overline{\mathbf{v}}(\hat{\mathbf{R}})$ is the velocity relative to the locally-interpolated fluid velocity.
The bare diffusion coefficient depends on the grid resolution as is not a material constant.

- Observe that χ_0 is different from the macroscopic or **renormalized diffusion coefficient**

$$\chi = \frac{1}{d} \int_0^{\tau \gg \tau_{MD}} dt \, \langle \hat{\mathbf{V}} \cdot \hat{\mathbf{V}} \rangle_{\text{eq}},$$

which is **independent of the grid resolution** but is essentially impossible to compute using MD since it includes **far-field hydrodynamics**.

Chemically-Reactive Mixtures

- The species density equations for a mixture of N_{S} species are given by

$$\frac{\partial}{\partial t}(\rho_s) + \nabla\cdot(\rho_s\mathbf{v} + \mathbf{F}) = m_s\Omega_s, \qquad (s = 1,\dots N_{\mathrm{S}}) \tag{8}$$

- Due to mass conservation $\rho = \sum_s \rho_s$ follows the continuity equation,

$$\frac{\partial}{\partial t}\rho + \nabla\cdot(\rho\mathbf{v}) = 0. \tag{9}$$

- The mass fluxes take the form, excluding barodiffusion and thermodiffusion,

$$\mathbf{F} = \rho\mathbf{W}\left[\chi\boldsymbol{\Gamma}\boldsymbol{\nabla}\mathbf{x} + \sqrt{\frac{2}{n}}\,\chi^{\frac{1}{2}}\boldsymbol{\mathcal{W}}_F(\mathbf{r},t)\right],$$

where n is the number density, x_s is the mole fraction of species s, and $\mathbf{W} = \mathrm{Diag}\{w_s = \rho_s/\rho\}$ contains the mass fractions.

Multispecies Mass Diffusion

- $\mathbf{\Gamma}$ is a matrix of thermodynamic factors,

$$\mathbf{\Gamma} = \mathbf{I} + \left(\mathbf{X} - \mathbf{x}\mathbf{x}^T\right) \left(\frac{\partial^2 g_{\text{ex}}}{\partial \mathbf{x}^2}\right),$$

  where $g_{\text{ex}}(\mathbf{x}, T, P)$ is the normalized **excess Gibbs energy density** per particle.

- χ is an **SPD diffusion tensor** that can be related to the **Maxwell-Stefan diffusion coefficients** and Green-Kubo type formulas.

- We, however, do not know values of these for even a single ternary mixture!

  We have studied **ideal mixtures**: hard-sphere **gas mixtures [7]** and **dilute solutions** of salt+sugar in water [4].

Chemical Reactions

- Consider a system with N_{R} **elementary reactions** with reaction r

$$\mathfrak{R}_r : \qquad \sum_{s=1}^{N_{\mathrm{S}}} \nu_{sr}^{+} \mathfrak{M}_s \rightleftarrows \sum_{s=1}^{N_{\mathrm{S}}} \nu_{sr}^{-} \mathfrak{M}_s$$

  The **stoichiometric coefficients** are $\nu_{sr} = \nu_{sr}^{-} - \nu_{sr}^{+}$ and mass conservation requires that $\sum_s \nu_{sr} m_r = 0$.

- Define the dimensionless **chemical affinity**

$$\mathcal{A}_r = \sum_s \nu_{sr}^{+} \hat{\mu}_s - \sum_s \nu_{sr}^{-} \hat{\mu}_s,$$

  where $\hat{\mu}_s = m_s \mu_s / k_B T$ is the dimensionless **chemical potential per particle**.

- Also define the **thermodynamic driving force**

$$\hat{\mathcal{A}}_r = \exp\left(\sum_s \nu_{sr}^{+} \hat{\mu}_s \right) - \exp\left(\sum_s \nu_{sr}^{-} \hat{\mu}_s \right) = \prod_s e^{\nu_{sr}^{+} \hat{\mu}_s} - \prod_s e^{\nu_{sr}^{-} \hat{\mu}_s}$$

Chemical Langevin Equation

- The mass production due to chemistry can be approximated by the chemical Langevin equation (CLE) [5]:

$$\Omega_s = \sum_r \nu_{sr} \left(\frac{P}{\tau_r k_B T} \right) \hat{\mathcal{A}}_r + \sum_r \nu_{sr} \left(\frac{P}{\tau_r k_B T} \prod_s e^{\nu_{sr}^{+} \hat{\mu}_s} \right)^{\frac{1}{2}} \mathcal{Z}(\mathbf{r}, t) \quad (10)$$

- The **CLE** follows from a truncation of the Kramers-Moyal expansion at second order.
  No true thermodynamic equilibrium since it assumes **one-way reactions**.
- The CLE is **not time-reversible** (obeys detailed balance) **at thermodynamic equilibrium** wrt to the Einstein distribution.
  Proper description of chemical reactions requires the use of SDEs driven by **Poisson noise** (not Gaussian).

Nonlinear Chemical Networks

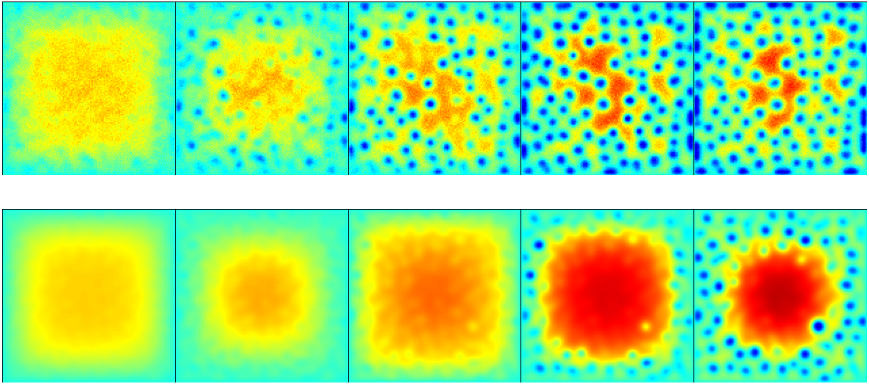
We have studied the Baras-Pearson-Mansour (BPM) model $\mathfrak{M} = (U, V, W, S, U_f, V_f)$,

$$\begin{aligned} \mathfrak{R}_1 : &\quad U + W \leftrightarrows V + W \\ \mathfrak{R}_2 : &\quad V + V \leftrightarrows W + S \\ \mathfrak{R}_3 : &\quad V \leftrightarrows S \\ \mathfrak{R}_4 : &\quad U \leftrightarrows U_f \\ \mathfrak{R}_5 : &\quad V \leftrightarrows V_f \end{aligned} \tag{11}$$

This system can exhibit **limit cycles**, bimodal states (**bistability**), and possibly other nonlinear behavior.

In principle this system can be simulated using **particle methods**!

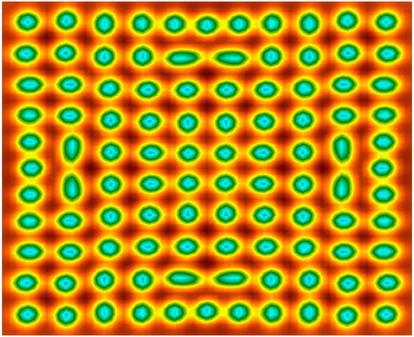
Turing-like Patterns

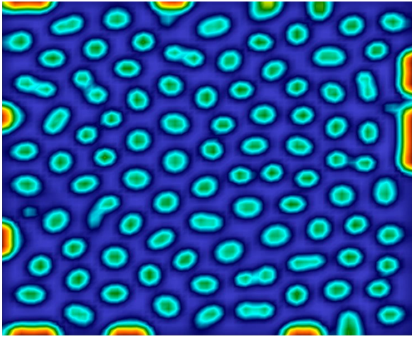


Development of an instability in the BPM model with fluctuations (top) and without (bottom) with complete compressible hydrodynamics (not just reaction-diffusion).

Turing-like Patterns

Fluctuations change the dynamics **qualitatively** in spatially-extended reactive systems! **How do we simulate this?**





Multiphase Systems: Liquid-Vapor

- We will use a **diffusive-interface model** for describing interfaces between two distinct phases such as liquid and vapor of a single species.
- Coarse-grained free energy follows the usual **square-gradient surface tension model**

$$F\left(\rho(\mathbf{r}), \nabla\rho(\mathbf{r}), T(\mathbf{r})\right) = \int \mathrm{d}\mathbf{r}\,\left(f\left(\rho(\mathbf{r}), T(\mathbf{r})\right) + \frac{1}{2}\kappa\left|\nabla\rho(\mathbf{r})\right|^2\right) \quad (12)$$

  The **local free energy density** $f\left(\rho(\mathbf{r}), T(\mathbf{r})\right)$ includes the hard-core repulsions as well as the short-range attractions.
- Assume a **van der Waals** loop for the equation of state,

$$P\left(\rho, T\right) = \frac{nk_B T}{1 - b'n} - a'n^2, \quad (13)$$

$$f = nk_B T \ln\left[\frac{\rho}{1 - b'n}\right] - a'n^2.$$

Fluctuating Hydrodynamics

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{14}$$

$$\partial_t (\rho \mathbf{v}) + \nabla \cdot \left(\rho \mathbf{v}\mathbf{v}^{\mathrm{T}}\right) + \nabla \cdot \boldsymbol{\Pi} = \nabla \cdot (\boldsymbol{\sigma} + \boldsymbol{\Sigma}) \tag{15}$$

$$\partial_t (\rho E) + \nabla \cdot (\rho E \mathbf{v} + \boldsymbol{\Pi} \cdot \mathbf{v}) = \nabla \cdot (\boldsymbol{\psi} + \boldsymbol{\Psi}) + \nabla \cdot ((\boldsymbol{\sigma} + \boldsymbol{\Sigma}) \cdot \mathbf{v}), \tag{16}$$

where the momentum density is $\mathbf{g} = \rho \mathbf{v}$ and
the total local energy density is $\rho E = \frac{1}{2}\rho v^2 + \rho e$.

Momentum Fluxes

- The reversible contribution to the stress tensor is [6]

$$\mathbf{\Pi} = P\mathbf{I} - \left[\left(\kappa\rho\nabla^2\rho + \frac{1}{2}\kappa \left|\nabla\rho\right|^2 \right) \mathbf{I} \right] - (\kappa\nabla\rho \otimes \nabla\rho) + \text{cross term?}$$

- Irreversible contribution to the stress is the viscous stress tensor

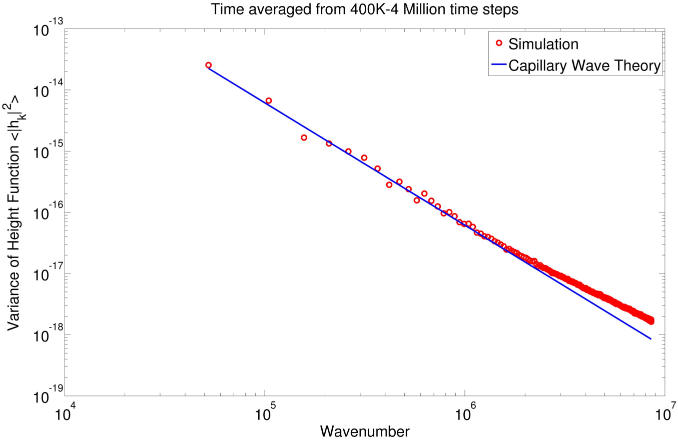
$$\boldsymbol{\sigma} = \eta \left(\nabla\mathbf{v} + (\nabla\mathbf{v})^{\mathrm{T}} \right) + \left(\zeta - \frac{2}{3}\eta \right) (\nabla \cdot \mathbf{v})\,\mathbf{I} \qquad (17)$$

- Stochastic stress tensor obeys fluctuation-dissipation balance

$$\mathbf{\Sigma} = \sqrt{2\eta k_B T}\,\widetilde{\mathcal{W}} + \left(\sqrt{\frac{\zeta k_B T}{3}} - \sqrt{\frac{2\eta k_B T}{3}} \right) \mathrm{Tr}\left(\widetilde{\mathcal{W}} \right) \mathbf{I}, \qquad (18)$$

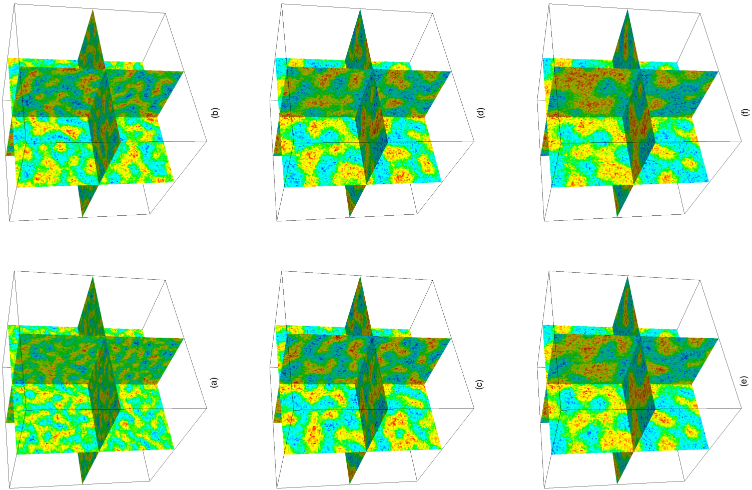
where $\widetilde{\mathcal{W}} = (\mathcal{W} + \mathcal{W}^T)/\sqrt{2}$ is a symmetric white-noise tensor field.

Capillary Waves



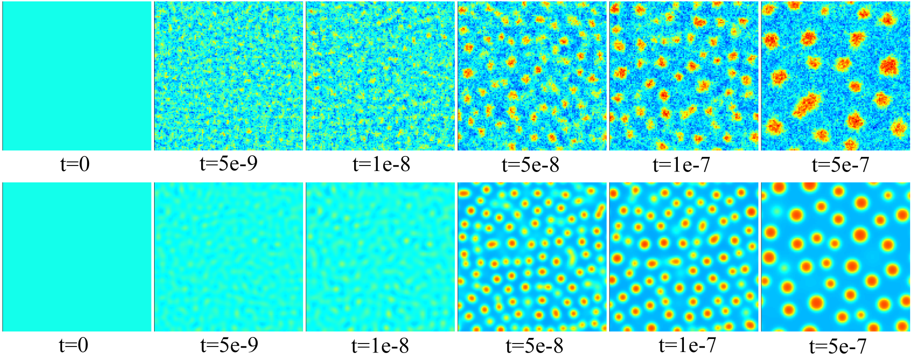
Variance of height fluctuations versus wavenumber comparing 2D simulations (red circles) and **capillary wave theory** (CWT) (black solid line).

Spinodal Decomposition



Spinodal decomposition in a near-critical Argon system at $\rho = 0.416$ g/cc, $T = 145.85$ K leading to a **bicontinuous pattern**.

Condensation



Liquid-vapor spinodal decomposition in a near-critical van der Waals Argon system at $\rho = 0.36$ g/cc, $T = 145.85$ K leading to **droplets** forming in a majority vapor phase.

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