Coupling a Fluctuating Fluid with Suspended Structures

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Outline

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- 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)**.

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- Essential distinguishing feature from "ordinary" CFD: **thermal fluctuations**!
- I hope to demonstrate the general conclusion that **fluctuations should be taken into account at all level**.

Levels of Coarse-Graining

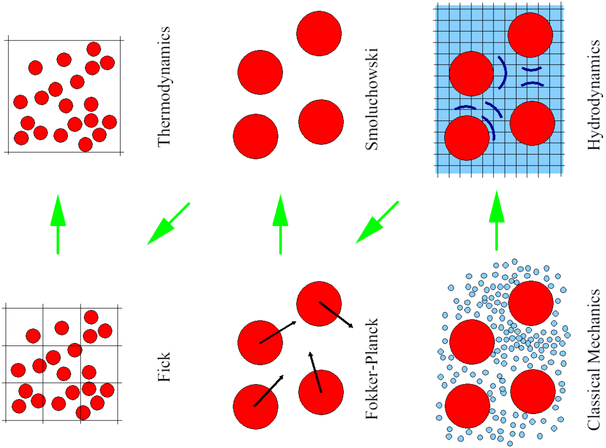

Figure: From Pep Español, “Statistical Mechanics of Coarse-Graining”

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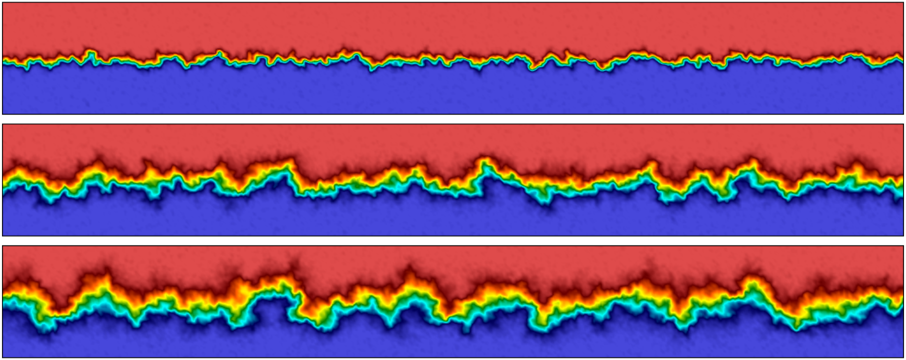
Thermal Fluctuations Matter



Snapshots of concentration in a miscible mixture showing the development of a *rough* diffusive interface between two miscible fluids in zero gravity [1, 2, 3]. A similar pattern is seen over a broad range of Schmidt numbers and is affected strongly by nonzero gravity.

Fluctuating Navier-Stokes Equations

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

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

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

where the **kinematic viscosity** $\nu = \eta/\rho$, and π is determined from incompressibility, $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$.

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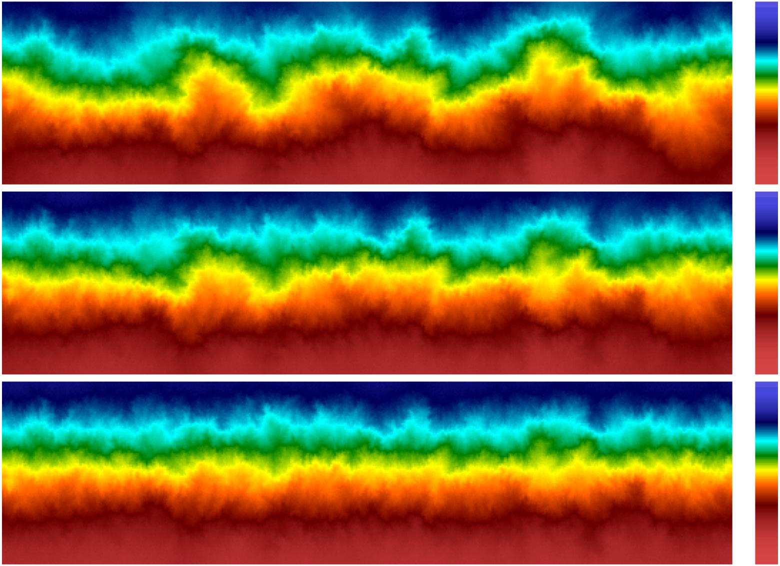
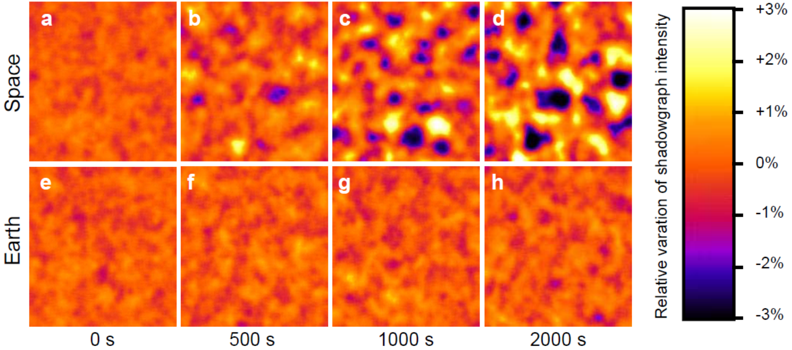
  where the **kinematic viscosity** $\nu = \eta/\rho$, and π is determined from incompressibility, $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$.
- We assume that $\boldsymbol{\mathcal{W}}$ can be modeled as spatio-temporal **white noise** (a delta-correlated Gaussian random field), e.g.,

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

Fractal Fronts in Diffusive Mixing



Giant Fluctuations in Experiments



Experimental results by A. Vailati *et al.* from a microgravity environment [2] showing the enhancement of concentration fluctuations in space (box scale is **macroscopic**: 5mm on the side, 1mm thick)..

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- We have algorithms and codes to solve the compressible equations (**collocated** and **staggered grid**), and recently also the incompressible and **low Mach number** ones (staggered grid) [4, 3].
- Solving these sort of equations numerically requires paying attention to **discrete fluctuation-dissipation balance**, in addition to the usual deterministic difficulties [4].

Finite-Volume Schemes

$$c_t = -\mathbf{v} \cdot \boldsymbol{\nabla} c + \chi \boldsymbol{\nabla}^2 c + \boldsymbol{\nabla} \cdot \left(\sqrt{2\chi} \boldsymbol{\mathcal{W}} \right) = \boldsymbol{\nabla} \cdot \left[-c\mathbf{v} + \chi \boldsymbol{\nabla} c + \sqrt{2\chi} \boldsymbol{\mathcal{W}} \right]$$

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- Generic **finite-volume spatial discretization**

$$\mathbf{c}_t = \mathbf{D} \left[\left(-\mathbf{V}\mathbf{c} + \mathbf{G}\mathbf{c} \right) + \sqrt{2\chi / \left(\Delta t \Delta V \right)} \mathbf{W} \right],$$

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- The **divergence** and **gradient** should be **duals**, $\mathbf{D}^\star = -\mathbf{G}$.
- Advection should be **skew-adjoint** (non-dissipative) if $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$,

$$(\mathbf{D}\mathbf{V})^\star = -(\mathbf{D}\mathbf{V}) \;\text{ if }\; (\mathbf{D}\mathbf{V})\,\mathbf{1} = \mathbf{0}.$$

Weak Accuracy

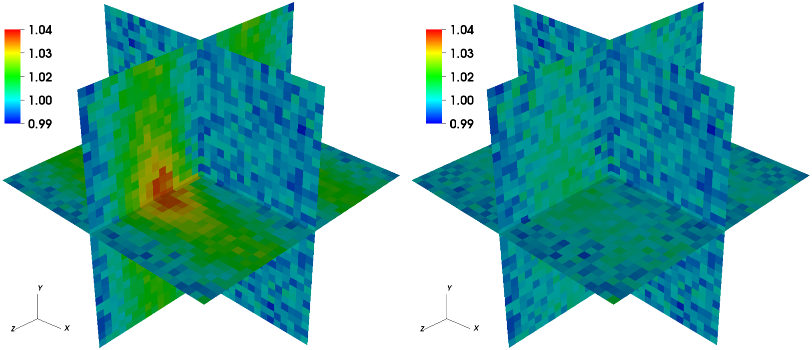

Figure: Spectral power of the first solenoidal mode for an incompressible fluid as a function of the wavenumber. The left panel is for a (normalized) time step $\alpha = 0.5$, and the right for $\alpha = 0.25$.

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- The above two conditions are **questionable at nanoscales**, but even worse, they are very hard to implement numerically in an efficient and stable manner.
- We saw already that **fluctuations should be taken into account at the continuum level**.

Brownian Particle Model

- Consider a **Brownian "particle"** of size a with position $\mathbf{q}(t)$ and velocity $\mathbf{u} = \dot{\mathbf{q}}$, and the velocity field for the fluid is $\mathbf{v}(\mathbf{r}, t)$.

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- Often presented as an interpolation function for point Lagrangian particles but here a is a **physical size** of the particle.
- We will call our particles "**blobs**" since they are not really point particles.

Local Averaging and Spreading Operators

- Postulate a **no-slip condition** between the particle and local fluid velocities,

$$\dot{\mathbf{q}} = \mathbf{u} = [\mathbf{J}(\mathbf{q})]\,\mathbf{v} = \int \delta_a(\mathbf{q} - \mathbf{r})\,\mathbf{v}(\mathbf{r}, t)\,d\mathbf{r},$$

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- The **induced force density** in the fluid because of the particle is:

$$\mathbf{f} = -\boldsymbol{\lambda}\delta_a(\mathbf{q}-\mathbf{r}) = -[\mathbf{S}(\mathbf{q})]\,\boldsymbol{\lambda},$$

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- The physical **volume** of the particle ΔV is related to the shape and width of the kernel function via

$$\Delta V = (\mathbf{JS})^{-1} = \left[\int \delta_a^2(\mathbf{r})\,d\mathbf{r}\right]^{-1}. \tag{1}$$

Fluid-Structure Direct Coupling

- The equations of motion in our coupling approach are **postulated** [5] to be

$$
\begin{aligned}
\rho\left(\partial_t \mathbf{v} + \mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}\right) &= -\boldsymbol{\nabla}\pi - \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} - \left[\mathbf{S}\left(\mathbf{q}\right)\right]\boldsymbol{\lambda} + \text{thermal drift} \\
m_e\dot{\mathbf{u}} &= \mathbf{F}\left(\mathbf{q}\right) + \boldsymbol{\lambda} \\
\text{s.t. } \mathbf{u} &= \left[\mathbf{J}\left(\mathbf{q}\right)\right]\mathbf{v} \text{ and } \boldsymbol{\nabla}\cdot\mathbf{v} = 0,
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where $\boldsymbol{\lambda}$ is the **fluid-particle force**, $\mathbf{F}\left(\mathbf{q}\right) = -\boldsymbol{\nabla}U\left(\mathbf{q}\right)$ is the externally **applied force**, and m_e is the **excess mass** of the particle.

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  drives the Brownian motion.
- In the existing (stochastic) IBM approaches [6] **inertial effects** are ignored, $m_e=0$ and thus $\boldsymbol{\lambda}=-\mathbf{F}$.

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- Adding the fluid and particle equations gives a **local momentum conservation law**

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$$m_f = \rho \left(\mathbf{JS} \right)^{-1} = \rho \Delta V = \rho \left[\int \delta_a^2 \left(\mathbf{r} \right) d\mathbf{r} \right]^{-1}.$$

- For the fluid we get the effective equation

$$\boldsymbol{\rho}_{\text{eff}} \partial_t \mathbf{v} = - \left[\rho \left(\mathbf{v} \cdot \boldsymbol{\nabla} \right) + m_e \mathbf{S} \left(\mathbf{u} \cdot \frac{\partial}{\partial \mathbf{q}} \mathbf{J} \right) \right] \mathbf{v} - \boldsymbol{\nabla}\pi - \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} + \mathbf{SF}$$

Effective Inertia

- Eliminating $\boldsymbol{\lambda}$ we get the particle equation of motion

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where the effective **mass density matrix** (operator) is

$$\boldsymbol{\rho}_{\text{eff}} = \rho + m_e \mathcal{P} \mathbf{SJ} \mathcal{P},$$

where $\mathcal{P}$ is the L_2 **projection operator** onto the linear subspace $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$, with the appropriate BCs.

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- No entropic contribution to the coarse-grained free energy because our formulation is isothermal and the particles do not have internal structure.

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- Crucial for **energy conservation** is that $\mathbf{J}(\mathbf{q})$ and $\mathbf{S}(\mathbf{q})$ are **adjoint**, $\mathbf{S} = \mathbf{J}^{\star}$,

$$(\mathbf{J}\mathbf{v}) \cdot \mathbf{u} = \int \mathbf{v} \cdot (\mathbf{S}\mathbf{u})\, d\mathbf{r} = \int \delta_a(\mathbf{q} - \mathbf{r})\,(\mathbf{v} \cdot \mathbf{u})\, d\mathbf{r}. \tag{2}$$

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- The dynamics is **not incompressible in phase space** and "**thermal drift**" correction terms need to be included [6], but they turn out to **vanish** for incompressible flow (gradient of scalar).
- The spatial discretization should preserve these properties: **discrete fluctuation-dissipation balance (DFDB)**.

Outline

Numerical Scheme

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- The scheme ensures **strict conservation** of momentum and (almost exactly) enforces the no-slip condition at the end of the time step.
- Continuing work on temporal integrators that ensure the correct **equilibrium distribution** and **diffusive (Brownian) dynamics**.

Temporal Integrator (sketch)

- **Predict** particle position at midpoint:

$$\mathbf{q}^{n+\frac{1}{2}} = \mathbf{q}^n + \frac{\Delta t}{2} \mathbf{J}^n \mathbf{v}^n.$$

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$$\begin{aligned} \rho \frac{\tilde{\mathbf{v}}^{n+1} - \mathbf{v}^{n}}{\Delta t} + \boldsymbol{\nabla} \tilde{\pi} &= \frac{\eta}{2} \mathbf{L} \left(\tilde{\mathbf{v}}^{n+1} + \mathbf{v}^{n} \right) + \boldsymbol{\nabla} \cdot \boldsymbol{\Sigma}^{n} + \mathbf{S}^{n+\frac{1}{2}} \mathbf{F}^{n+\frac{1}{2}} + \text{adv.}, \\ \boldsymbol{\nabla} \cdot \tilde{\mathbf{v}}^{n+1} &= 0, \end{aligned}$$

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where we use the **Adams-Bashforth method** for the advective (kinetic) fluxes, and the discretization of the stochastic flux is described in Ref. [3],

$$\boldsymbol{\Sigma}^n = \left(\frac{2 k_B T \eta}{\Delta V \, \Delta t} \right)^{1/2} \mathbf{W}^n,$$

where $\mathbf{W}^n$ is a (symmetrized) collection of i.i.d. unit normal variates.

contd.

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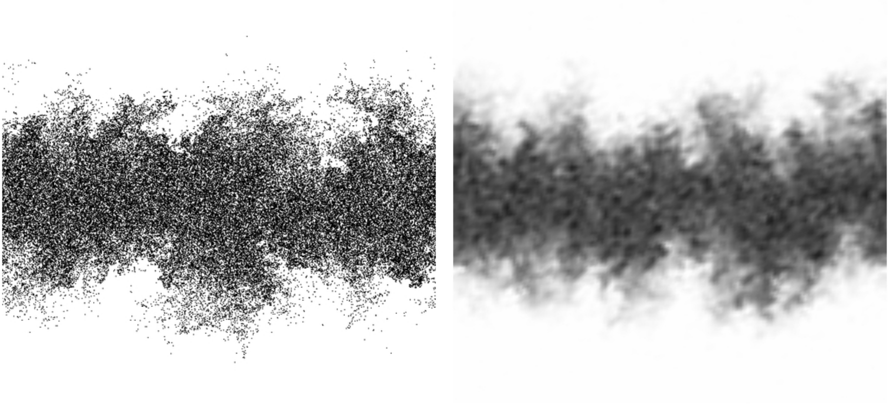
Passively-Advected (Fluorescent) Tracers



Velocity Autocorrelation Function

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as predicted also for a rigid sphere a long time ago, $m_f/m = \rho'/\rho$.

- Hydrodynamic persistence (conservation) gives a **long-time power-law tail** $C(t) \sim (kT/m)(t/t_{visc})^{-3/2}$ *not* reproduced in Brownian dynamics.

Numerical VACF

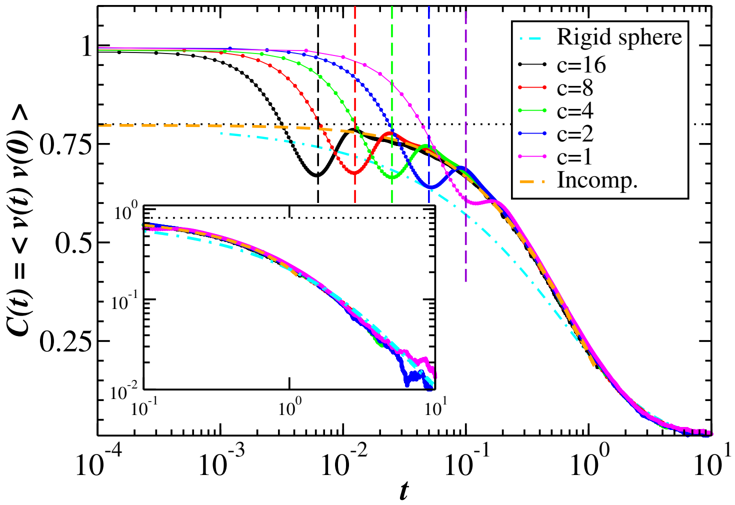

Figure: (F. Balboa) VACF for a blob with $m_e = m_f = \rho \Delta V$.

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- It is possible to include rotlet and stresslet terms, as done in the force coupling method [8] and Stokesian Dynamics in the deterministic setting.
- Proper inclusion of inertial terms and fluctuation-dissipation balance not studied carefully yet...

Immersed Rigid Bodies

- This approach can be extended to immersed rigid bodies (see work by Neelesh Patankar)

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\begin{aligned}
\rho \left(\partial_t \mathbf{v} + \mathbf{v} \cdot \boldsymbol{\nabla} \mathbf{v} \right) &= -\boldsymbol{\nabla} \pi - \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} - \int_{\Omega} \mathbf{S}\left(\mathbf{q}\right) \boldsymbol{\lambda}\left(\mathbf{q}\right) d\mathbf{q} + \text{th. drift} \\
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- Even coarse-grained methods need to be accelerated due to **large separation of time scales** between advective and diffusive phenomena.
- One can take the **overdamped** (Brownian dynamics) **limit** but it would be much better to construct **many-scale temporal integrators** that are accurate even when they under-resolve the fast fluctuations.

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