Coupling an Incompressible Fluctuating Fluid with Suspended Structures

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Outline

Levels of Coarse-Graining

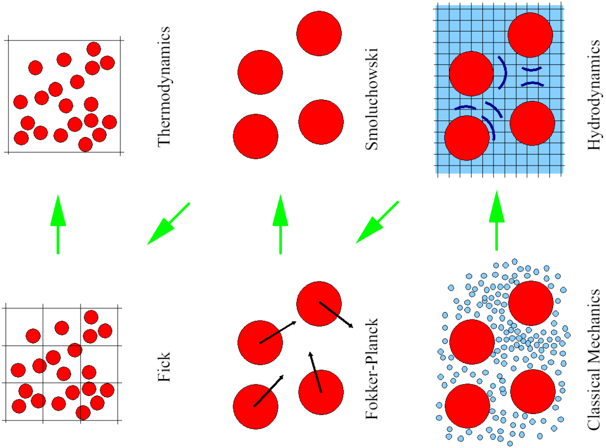


Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

Continuum Models of Fluid Dynamics

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

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

  where the symbol $\cong$ means that $\mathbf{U}(\mathbf{r},t)$ approximates the true atomistic configuration $\widetilde{\mathbf{U}}(\mathbf{r},t)$ 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.
- This leads to **SPDEs of Langevin type** formed by postulating a **white-noise random flux** term in the usual Navier-Stokes-Fourier equations with magnitude determined from the **fluctuation-dissipation balance** condition, following Landau and Lifshitz.

Compressible Fluctuating Hydrodynamics

$$D_t\rho = -\,\rho\boldsymbol{\nabla}\cdot\mathbf{v}$$
$$\rho\left(D_t\mathbf{v}\right) = -\,\boldsymbol{\nabla}P + \boldsymbol{\nabla}\cdot\left(\eta\overline{\boldsymbol{\nabla}}\mathbf{v} + \boldsymbol{\Sigma}\right)$$
$$\rho c_p\left(D_t T\right) = D_t P + \boldsymbol{\nabla}\cdot\left(\mu\boldsymbol{\nabla}T + \boldsymbol{\Xi}\right) + \left(\eta\overline{\boldsymbol{\nabla}}\mathbf{v} + \boldsymbol{\Sigma}\right) : \boldsymbol{\nabla}\mathbf{v},$$

where the variables are the **density** ρ, **velocity** $\mathbf{v}$, and **temperature** T fields,

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

and capital Greek letters denote stochastic fluxes:

$$\boldsymbol{\Sigma} = \sqrt{2\eta k_B T}\,\mathcal{W}.$$
$$\langle\mathcal{W}_{ij}(\mathbf{r},t)\mathcal{W}^{\star}_{kl}(\mathbf{r}',t')\rangle = \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - 2\delta_{ij}\delta_{kl}/3\right)\delta(t-t')\delta(\mathbf{r}-\mathbf{r}').$$

Incompressible Fluctuating Navier-Stokes

- We will consider a binary fluid mixture with mass **concentration** $c = \rho_1/\rho$ for two fluids that are dynamically **identical**, where $\rho = \rho_1 + \rho_2$.
- Ignoring density and temperature fluctuations, equations of **incompressible isothermal fluctuating hydrodynamics** are

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

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

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

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

Fluctuating Navier-Stokes Equations

- Adding stochastic fluxes to the **non-linear** NS equations produces **ill-behaved stochastic PDEs** (solution is too irregular).
- No problem if we **linearize** the equations around a **steady mean state**, to obtain equations for the fluctuations around the mean,

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

- Finite-volume discretizations naturally impose a grid-scale **regularization** (smoothing) of the stochastic forcing.
- A **renormalization** of the transport coefficients is also necessary [1].
- 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) [2, 3].
- Solving these sort of equations numerically requires paying attention to **discrete fluctuation-dissipation balance**, in addition to the usual deterministic difficulties [4, 5].

Finite-Volume Schemes

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

- Generic **finite-volume spatial discretization**

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

  where $\mathbf{D}$: faces $\rightarrow$ cells is a **conservative** discrete divergence, $\mathbf{G}$: cells $\rightarrow$ faces is a discrete gradient.
- Here $\mathbf{W}$ is a collection of random normal numbers representing the (face-centered) stochastic fluxes.
- The **divergence** and **gradient** should be **duals**, $\mathbf{D}^\star = -\mathbf{G}$.
- Advection should be **skew-adjoint** (non-dissipative) if $\boldsymbol{\nabla}\cdot\mathbf{v} = 0$,

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

Temporal Integration

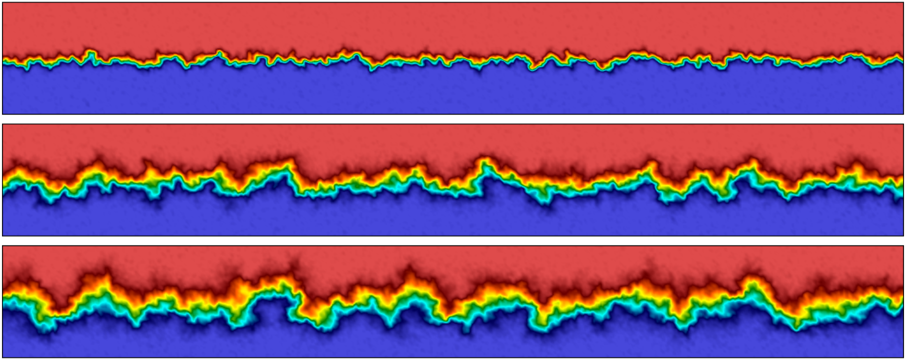
$$\partial_t \mathbf{v} = -\boldsymbol{\nabla}\pi + \nu \boldsymbol{\nabla}^2 \mathbf{v} + \boldsymbol{\nabla} \cdot \left(\sqrt{2\nu\rho^{-1}\, k_B T}\, \boldsymbol{\mathcal{W}} \right)$$

- We use a Crank-Nicolson method for velocity with a Stokes solver for pressure:

$$\begin{aligned} \frac{\mathbf{v}^{n+1} - \mathbf{v}^{n}}{\Delta t} + \mathbf{G}\boldsymbol{\pi}^{n+\frac{1}{2}} &= \nu \mathbf{L}_{\mathbf{v}} \left(\frac{\mathbf{v}^{n} + \mathbf{v}^{n+1}}{2} \right) + (2\nu\Delta t)^{\frac{1}{2}}\, \mathbf{D}_{\mathbf{w}} \mathbf{W}^{n} \\ \mathbf{D}\mathbf{v}^{n+1} &= 0. \end{aligned}$$

- This coupled velocity-pressure *Stokes linear system* can be solved efficiently even in the presence of non-periodic boundaries by using a preconditioned Krylov iterative solver.
- The nonlinear terms such as $\mathbf{v} \cdot \boldsymbol{\nabla} \mathbf{v}$ and $\mathbf{v} \cdot \boldsymbol{\nabla} c$ are handled explicitly using a predictor-corrector approach [5].

Giant Fluctuations in Diffusive Mixing



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.

Fluid-Structure Coupling

- We want to construct a **bidirectional coupling** between a fluctuating fluid and a small spherical **Brownian particle (blob)**.
- Macroscopic coupling between flow and a rigid sphere:
  - **No-slip** boundary condition at the surface of the Brownian particle.
  - Force on the bead is the integral of the (fluctuating) stress tensor over the surface.
- 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 $\mathbf{v}(\mathbf{r}, t)$.
- We do not care about the fine details of the flow around a particle, which is nothing like a hard sphere with stick boundaries in reality anyway.
- Take an **Immersed Boundary Method** (IBM) approach and describe the fluid-blob interaction using a localized smooth **kernel** $\delta_a(\Delta\mathbf{r})$ with compact support of size a (integrates to unity).
- Often presented as an interpolation function for point Lagrangian particles but here a is a **physical size** of the particle (as in the **Force Coupling Method** (FCM) of Maxey *et al*).
- 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,

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

  where the *local averaging* linear operator $\mathbf{J}(\mathbf{q})$ averages the fluid velocity inside the particle to estimate a local fluid velocity.
- The **induced force density** in the fluid because of the particle is:

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

  where the *local spreading* linear operator $\mathbf{S}(\mathbf{q})$ is the reverse (adjoint) of $\mathbf{J}(\mathbf{q})$.
- The physical **volume** of the particle ΔV is related to the shape and width of the kernel function via

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

Fluid-Structure Direct Coupling

- The equations of motion in our coupling approach are **postulated** to be [6]

$$\begin{aligned} \rho\left(\partial_t \mathbf{v} + \mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}\right) &= -\boldsymbol{\nabla}\pi - \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} - \left[\mathbf{S}\left(\mathbf{q}\right)\right]\boldsymbol{\lambda} + \text{'thermal' drift} \\ m_e \dot{\mathbf{u}} &= \mathbf{F}\left(\mathbf{q}\right) + \boldsymbol{\lambda} \\ \text{s.t. } \mathbf{u} &= \left[\mathbf{J}\left(\mathbf{q}\right)\right]\mathbf{v} \text{ and } \boldsymbol{\nabla}\cdot\mathbf{v} = 0, \end{aligned}$$

  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.
- The stress tensor $\boldsymbol{\sigma} = \eta\left(\boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}^T\mathbf{v}\right) + \boldsymbol{\Sigma}$ includes viscous (dissipative) and stochastic contributions. The **stochastic stress**

$$\boldsymbol{\Sigma} = \left(k_B T \eta\right)^{1/2}\left(\boldsymbol{\mathcal{W}} + \boldsymbol{\mathcal{W}}^T\right)$$

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

Momentum Conservation

- In the standard approach a frictional (dissipative) force $\boldsymbol{\lambda} = -\zeta \left(\mathbf{u} - \mathbf{J}\mathbf{v} \right)$ is used instead of a constraint.
- In either coupling the total particle-fluid momentum is conserved,

$$\mathbf{P} = m_e \mathbf{u} + \int \rho \mathbf{v} \left(\mathbf{r}, t \right) d\mathbf{r}, \quad \frac{d\mathbf{P}}{dt} = \mathbf{F}.$$

- Define a *momentum field* as the sum of the fluid momentum and the spreading of the particle momentum,

$$\mathbf{p} \left(\mathbf{r}, t \right) = \rho \mathbf{v} + m_e \mathbf{S}\mathbf{u} = \left(\rho + m_e \mathbf{S}\mathbf{J} \right) \mathbf{v}.$$

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

$$\partial_t \mathbf{p} = -\boldsymbol{\nabla} \pi - \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} - \boldsymbol{\nabla} \cdot \left[\rho \mathbf{v}\mathbf{v}^T + m_e \mathbf{S} \left(\mathbf{u}\mathbf{u}^T \right) \right] + \mathbf{S}\mathbf{F}.$$

Effective Inertia

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

$$m\dot{\mathbf{u}} = \Delta V\, \mathbf{J}\left(\boldsymbol{\nabla}\pi + \boldsymbol{\nabla}\cdot\boldsymbol{\sigma}\right) + \mathbf{F} + \text{blob correction},$$

where the **effective mass** $m = m_e + m_f$ includes the mass of the "excluded" fluid

$$m_f = \rho\Delta V = \rho\left(\mathbf{J}\mathbf{S}\right)^{-1}.$$

- For the fluid we get the effective equation

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

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

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

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

Fluctuation-Dissipation Balance

- One must ensure **fluctuation-dissipation balance** in the coupled fluid-particle system.
- We can eliminate the particle velocity using the no-slip constraint, so only **v** and **q** are independent DOFs.
- This really means that the **stationary** (equilibrium) distribution must be the **Gibbs distribution**

$$P(\mathbf{v},\mathbf{q}) = Z^{-1} \exp\left[-\beta H\right]$$

where the **Hamiltonian** (coarse-grained free energy) is

$$H(\mathbf{v},\mathbf{q}) = U(\mathbf{q}) + m_e \frac{u^2}{2} + \int \rho \frac{v^2}{2}\, d\mathbf{r}.$$
$$= U(\mathbf{q}) + \int \frac{\mathbf{v}^T \rho_{\text{eff}} \mathbf{v}}{2}\, d\mathbf{r}$$

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

contd.

- A key ingredient of fluctuation-dissipation balance is that that the fluid-particle **coupling is non-dissipative**, i.e., in the absence of viscous dissipation the kinetic energy H is conserved.
- Crucial for **energy conservation** is that $\mathbf{J}(\mathbf{q})$ and $\mathbf{S}(\mathbf{q})$ are **adjoint**, $\mathbf{S} = \mathbf{J}^{\star}$,

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

- The dynamics is **not incompressible in phase space** and "**thermal drift**" correction terms need to be included [7], but they turn out to **vanish** for incompressible flow (gradient of scalar).
- The spatial discretization should preserve these properties: **discrete fluctuation-dissipation balance (DFDB)**.

Numerical Scheme

- Both compressible (explicit) and incompressible schemes have been implemented by Florencio Balboa (UAM) on GPUs.
- Spatial discretization is based on previously-developed **staggered schemes** for fluctuating hydro [2] and the **IBM kernel functions** of Charles Peskin.
- Temporal discretization follows a second-order **splitting algorithm** (move particle + update momenta), and is limited in **stability** only by **advective CFL**.
- 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**.

Spatial Discretization

- **IBM kernel functions** of Charles Peskin are used to average

$$\mathbf{J}\mathbf{v} \equiv \sum_{\mathbf{k}\in\text{grid}} \left\{ \prod_{\alpha=1}^{d} \phi_a \left[q_\alpha - (r_k)_\alpha \right] \right\} \mathbf{v}_k .$$

- Discrete spreading operator $\mathbf{S} = (\Delta V_f)^{-1} \mathbf{J}^\star$

$$(\mathbf{SF})_k = (\Delta x \Delta y \Delta z)^{-1} \left\{ \prod_{\alpha=1}^{d} \phi_a \left[q_\alpha - (r_k)_\alpha \right] \right\} \mathbf{F}.$$

- The discrete kernel function ϕ_a gives **translational invariance**

$$\begin{aligned} \sum_{\mathbf{k}\in\text{grid}} \phi_a (\mathbf{q} - \mathbf{r}_k) &= 1 \text{ and } \sum_{\mathbf{k}\in\text{grid}} (\mathbf{q} - \mathbf{r}_k) \, \phi_a (\mathbf{q} - \mathbf{r}_k) = 0, \\ \sum_{\mathbf{k}\in\text{grid}} \phi_a^2 (\mathbf{q} - \mathbf{r}_k) &= \Delta V^{-1} = \text{const.}, \end{aligned} \tag{3}$$

independent of the position of the (Lagrangian) particle q relative to the underlying (Eulerian) velocity grid.

Temporal Discretization

- **Predict** particle position at midpoint:

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

- **Solve** the coupled **constrained momentum conservation equations** for $\mathbf{v}^{n+1}$ and $\mathbf{u}^{n+1}$ and the Lagrange multipliers $\pi^{n+\frac{1}{2}}$ and $\boldsymbol{\lambda}^{n+\frac{1}{2}}$ (hard to do efficiently!)

$$\begin{aligned}
\rho\frac{\mathbf{v}^{n+1}-\mathbf{v}^n}{\Delta t} + \boldsymbol{\nabla}\pi^{n+\frac{1}{2}} &= -\boldsymbol{\nabla}\cdot\left(\rho\mathbf{v}\mathbf{v}^T + \boldsymbol{\sigma}\right)^{n+\frac{1}{2}} - \mathbf{S}^{n+\frac{1}{2}}\boldsymbol{\lambda}^{n+\frac{1}{2}} \\
m_e\mathbf{u}^{n+1} &= m_e\mathbf{u}^n + \Delta t\,\mathbf{F}^{n+\frac{1}{2}} + \Delta t\,\boldsymbol{\lambda}^{n+\frac{1}{2}} \\
\boldsymbol{\nabla}\cdot\mathbf{v}^{n+1} &= 0 \\
\mathbf{u}^{n+1} &= \mathbf{J}^{n+\frac{1}{2}}\mathbf{v}^{n+1} + \left(\mathbf{J}^{n+\frac{1}{2}} - \mathbf{J}^n\right)\mathbf{v}^n,
\end{aligned} \tag{4}$$

- **Correct** particle position,

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

Temporal Integrator (sketch)

- **Predict** particle position at midpoint:

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

- Solve unperturbed fluid equation using **stochastic Crank-Nicolson** for viscous+stochastic:

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

  where we use the **Adams-Bashforth method** for the advective (kinetic) fluxes, and the discretization of the stochastic flux is described in Ref. [2],

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

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

contd.

- Solve for inertial **velocity perturbation** from the particle $\Delta\mathbf{v}$ (too technical to present), and update:

$$\mathbf{v}^{n+1} = \tilde{\mathbf{v}}^{n+1} + \Delta\mathbf{v}.$$

  If neutrally-buyoant $m_e = 0$ this is a non-step, $\Delta\mathbf{v} = \mathbf{0}$.

- Update particle velocity in a **momentum conserving** manner,

$$\mathbf{u}^{n+1} = \mathbf{J}^{n+\frac{1}{2}}\mathbf{v}^{n+1} + \text{slip correction.}$$

- **Correct** particle position,

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

Implementation

- With periodic boundary conditions all required linear solvers (Poisson, Helmholtz) can be done using FFTs only.
- Florencio Balboa has implemented the algorithm on **GPUs using CUDA** in a **public-domain code** (combines compressible and incompressible algorithms):
  `https://code.google.com/p/fluam`
- Our implicit algorithm is able to take a rather large time step size, as measured by the **advective** and **viscous CFL numbers**:

$$\alpha = \frac{V \Delta t}{\Delta x}, \quad \beta = \frac{\nu \Delta t}{\Delta x^2}, \tag{5}$$

  where V is a typical advection speed.
- Note that for compressible flow there is a sonic CFL number $\alpha_s = c\Delta t / \Delta x \gg \alpha$, where c is the speed of sound.
- Our scheme should be used with $\alpha \lesssim 1$. The scheme is stable for any β, but to get the correct thermal dynamics one should use $\beta \lesssim 1$.

Equilibrium Radial Correlation Function

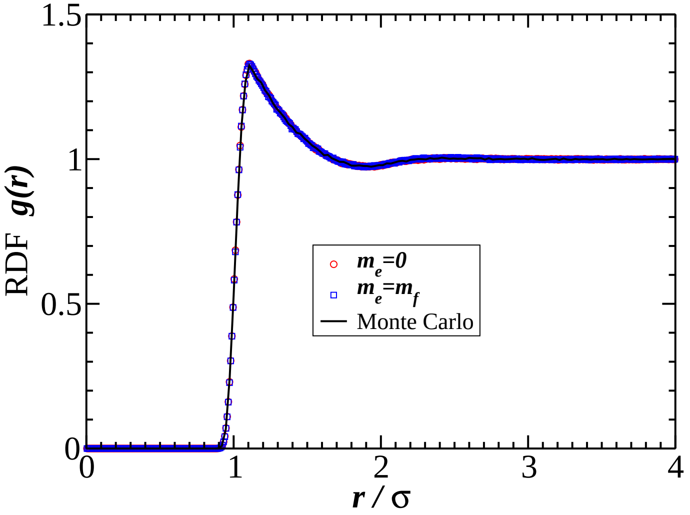


Figure: Equilibrium radial distribution function $g_2(\mathbf{r})$ for a suspension of blobs interacting with a repulsive LJ (WCA) potential.

Hydrodynamic Interactions

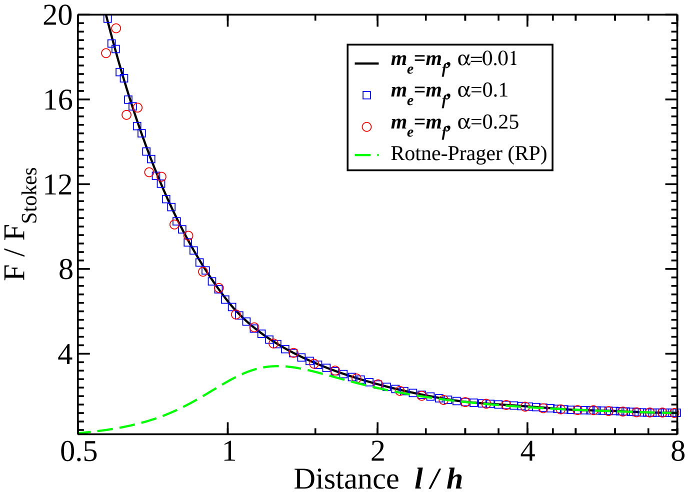


Figure: Effective hydrodynamic force between two approaching blobs at small Reynolds numbers, $\frac{F}{F_{St}} = -\frac{2F_0}{6\pi\eta R_H v_r}$.

Velocity Autocorrelation Function

- We investigate the **velocity autocorrelation function** (VACF) for the immersed particle

$$C(t) = \langle \mathbf{u}(t_0) \cdot \mathbf{u}(t_0 + t) \rangle$$

- From equipartition theorem $C(0) = \langle u^2 \rangle = d\frac{k_B T}{m}$.
- However, for an incompressible fluid the kinetic energy of the particle that is **less than equipartition**,

$$\langle u^2 \rangle = \left[1 + \frac{m_f}{(d-1)m} \right]^{-1} \left(d\frac{k_B T}{m} \right),$$

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** $C(t) \sim (kT/m)(t/t_{\text{visc}})^{-3/2}$ *not* reproduced in Brownian dynamics.

Numerical VACF

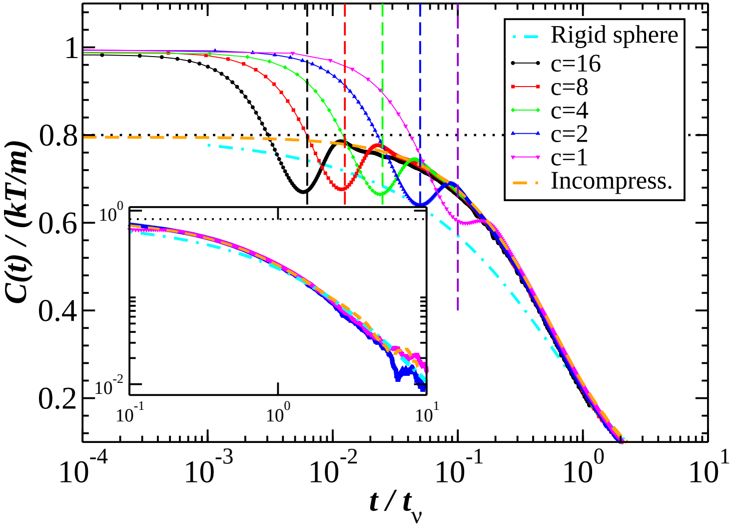


Figure: VACF for a blob with $m_e = m_f = \rho \Delta V$.

Diffusive Dynamics

- At long times, the motion of the particle is diffusive with a diffusion coefficient $\chi = \lim_{t\to\infty} \chi(t) = \int_{t=0}^{\infty} C(t)dt$, where

$$\chi(t) = \frac{\Delta q^2(t)}{2t} = \frac{1}{2dt}\langle[\mathbf{q}(t) - \mathbf{q}(0)]^2\rangle.$$

- The Stokes-Einstein relation predicts

$$\chi = \frac{k_B T}{\mu} \text{ (Einstein) and } \chi_{SE} = \frac{k_B T}{6\pi\eta R_H} \text{ (Stokes)}, \tag{6}$$

where for our blob with the 3-point kernel function $R_H \approx 0.9\Delta x$.

- The dimensionless Schmidt number $S_c = \nu/\chi_{SE}$ controls the separation of time scales between $\mathbf{v}(\mathbf{r}, t)$ and $\mathbf{q}(t)$.
- Self-consistent theory [1] predicts a correction to Stokes-Einstein's relation for small S_c,

$$\chi\left(\nu + \frac{\chi}{2}\right) = \frac{k_B T}{6\pi\rho R_H}.$$

Stokes-Einstein Corrections

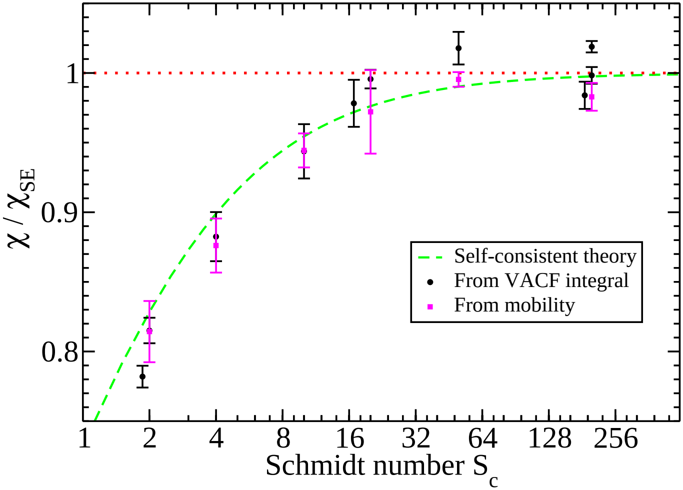
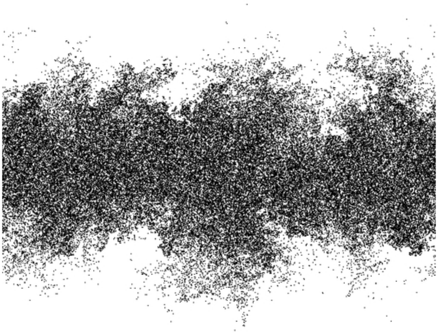
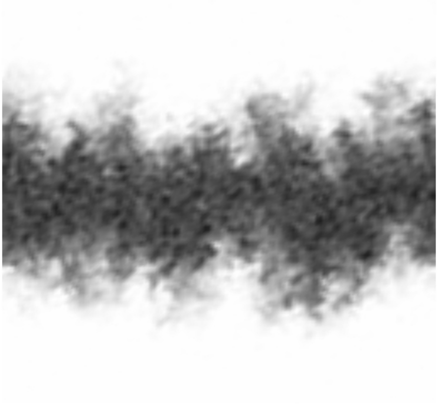


Figure: Corrections to Stokes-Einstein with changing viscosity $\nu = \eta/\rho$, $m_e = m_f = \rho \Delta V$.

Passively-Advected (Fluorescent) Tracers





Larger Reynolds Numbers

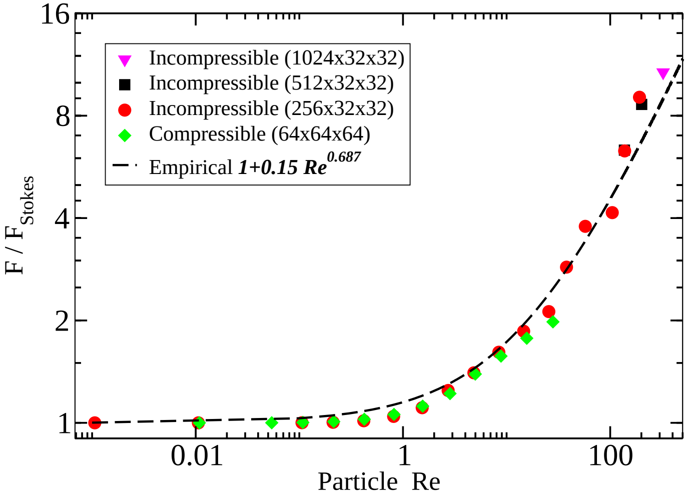


Figure: Drag force on a blob particle in a periodic domain as a function of the particle Reynolds number $\text{Re} = 2R_H \langle u \rangle / \nu$, normalized by the Stokes drag.

Overdamped Limit ($m_e = 0$)

- [With Eric Vanden-Eijnden] In the **overdamped limit**, in which momentum diffuses much faster than the particles, the motion of the blob at the diffusive time scale can be described by the fluid-free **Stratonovich** stochastic differential equation

$$\dot{\mathbf{q}} = \mu \mathbf{F} + \mathbf{J}(\mathbf{q}) \circ \mathbf{v}$$

where the random advection velocity is a **white-in-time** process is the solution of the **steady Stokes equation**

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

and the blob **mobility** is given by the Stokes solution operator $\boldsymbol{\mathcal{L}}^{-1}$,

$$\mu(\mathbf{q}) = -\mathbf{J}(\mathbf{q})\, \boldsymbol{\mathcal{L}}^{-1} \mathbf{S}(\mathbf{q}).$$

Brownian Dynamics

- For multi-particle suspensions the mobility matrix $\mathbf{M}(\mathbf{Q}) = \{\boldsymbol{\mu}_{ij}\}$ depends on the positions of all particles $\mathbf{Q} = \{\mathbf{q}_i\}$, and the limiting equation in the **Ito** formulation is the usual **Brownian dynamics** equation

$$\dot{\mathbf{Q}} = \mathbf{MF} + \sqrt{2k_B T}\,\mathbf{M}^{\frac{1}{2}}\widetilde{\mathcal{W}} + k_B T\left(\frac{\partial}{\partial \mathbf{Q}} \cdot \mathbf{M}\right).$$

- It is possible to construct temporal integrators for the overdamped equations, without ever constructing $\mathbf{M}^{\frac{1}{2}}\widetilde{\mathcal{W}}$ (work in progress).
- The limiting equation when excess **inertia** is included has not been derived though it is believed inertia does not enter in the overdamped equations.

Immersed Rigid Blobs

- Unlike a **rigid sphere**, a blob particle would not perturb a pure shear flow.
- In the far field our blob particle looks like a force monopole (**stokeset**), and does not exert a force dipole (**stresslet**) on the fluid.
- Similarly, since here we do not include **angular velocity** degrees of freedom, our blob particle does not exert a **torque** on the fluid (rotlet).
- 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 (work with Neelesh Patankar)

$$
\begin{aligned}
\rho \left(\partial_t \mathbf{v} + \mathbf{v} \cdot \boldsymbol{\nabla} \mathbf{v} \right) &= -\boldsymbol{\nabla} \pi - \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} - \int_\Omega \mathbf{S}\left(\mathbf{q}\right) \boldsymbol{\lambda}\left(\mathbf{q}\right) d\mathbf{q} + \text{th. drift} \\
m_e \dot{\mathbf{u}} &= \mathbf{F} + \int_\Omega \boldsymbol{\lambda}\left(\mathbf{q}\right) d\mathbf{q} \\
I_e \dot{\boldsymbol{\omega}} &= \boldsymbol{\tau} + \int_\Omega \left[\mathbf{q} \times \boldsymbol{\lambda}\left(\mathbf{q}\right)\right] d\mathbf{q} \\
\left[\mathbf{J}\left(\mathbf{q}\right)\right] \mathbf{v} &= \mathbf{u} + \mathbf{q} \times \boldsymbol{\omega} \text{ for all } \mathbf{q} \in \Omega \\
\boldsymbol{\nabla} \cdot \mathbf{v} &= 0 \text{ everywhere.}
\end{aligned}
$$

  Here $\boldsymbol{\omega}$ is the immersed body angular velocity, $\boldsymbol{\tau}$ is the applied torque, and I_e is the **excess moment of inertia** of the particle.
- The nonlinear advective terms are tricky, though it may not be a problem at low Reynolds number...
- Fluctuation-dissipation balance needs to be studied carefully...

Conclusions

- Fluctuations are **not just a microscopic phenomenon**: giant fluctuations can reach macroscopic dimensions or certainly dimensions much larger than molecular.
- **Fluctuating hydrodynamics** seems to be a very good coarse-grained model for fluids, despite unresolved issues.
- **Particle inertia** can be included in the coupling between blob particles and a fluctuating incompressible fluid.
- 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**: See work by Atzberger *et al.* for specialized exponential integrators for $\beta \gg 1$ for $m_e = 0$.

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