Coupling an Incompressible Fluctuating Fluid with Suspended Structures

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Outline

Levels of Coarse-Graining

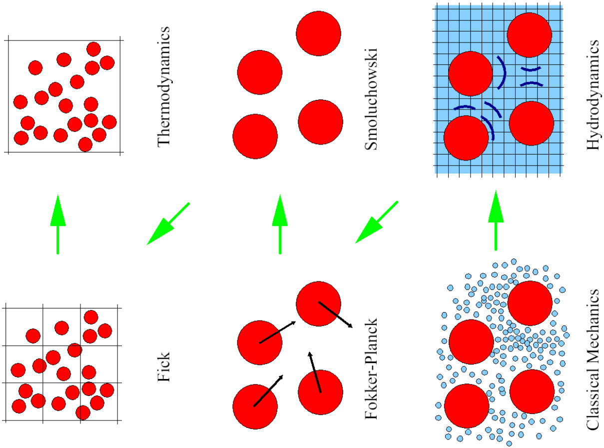


Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

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.

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

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

- Generic **finite-volume spatial discretization**

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

  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

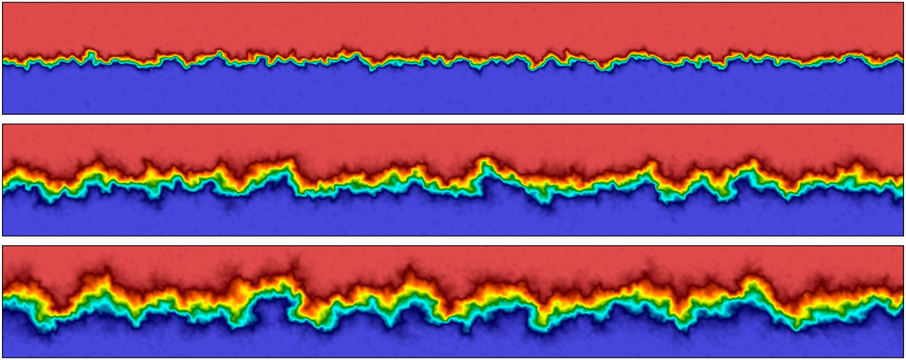
$$\partial_t \mathbf{v} = -\boldsymbol{\nabla}\pi + \nu\boldsymbol{\nabla}^2\mathbf{v} + \boldsymbol{\nabla}\cdot\left(\sqrt{2\nu\rho^{-1}\,k_B T}\,\boldsymbol{\mathcal{W}}\right)$$

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

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

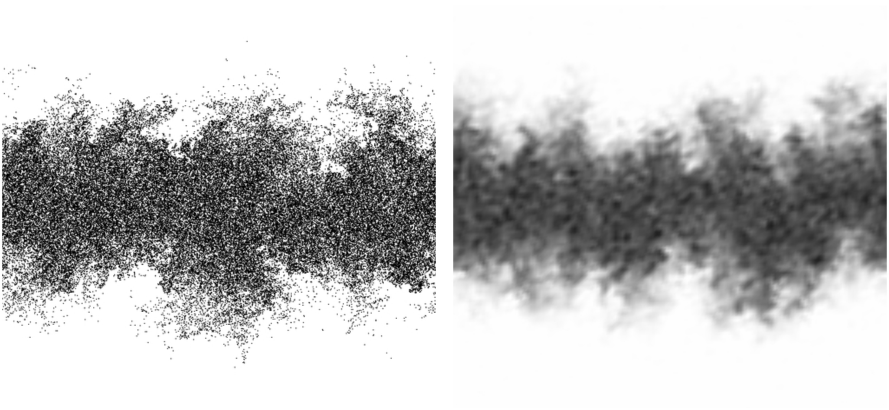
- This coupled velocity-pressure *Stokes linear system* can be solved efficiently even in the presence of non-periodic boundaries by using a preconditioned Krylov iterative solver.
- The nonlinear terms such as $\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}$ and $\mathbf{v}\cdot\boldsymbol{\nabla}c$ are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

Giant Fluctuations in FRAP



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

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

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

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

- For the fluid we get the effective equation

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

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.

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

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

- 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

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

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

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

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

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

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!)

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

- **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:

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

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

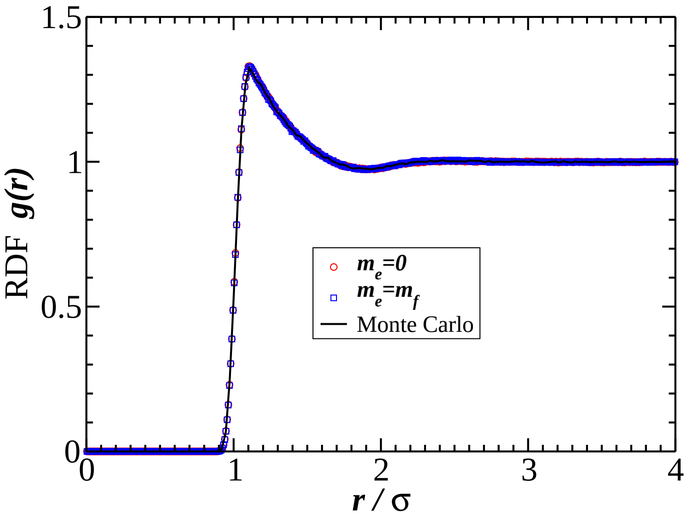


Figure: Equilibrium radial distribution function $g_2(\mathbf{r})$ for a suspension of blobs interacting with a repulsive LJ (WCA) potential.

Hydrodynamic Interactions

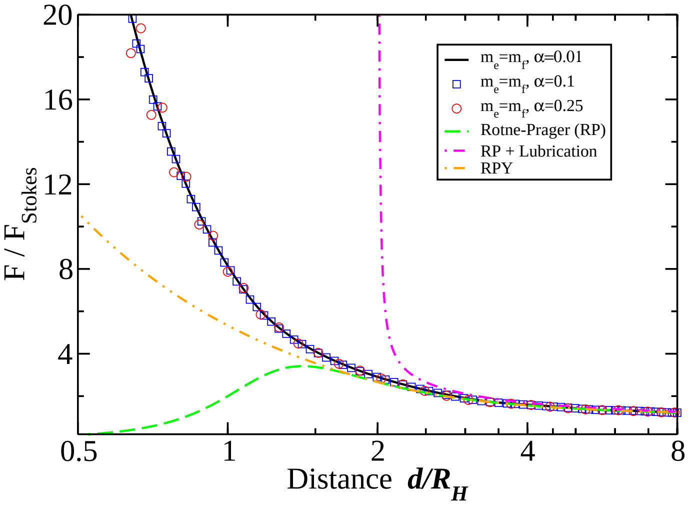


Figure: Effective hydrodynamic force between two approaching blobs at small Reynolds numbers, $\frac{F}{F_{\text{St}}} = -\frac{2F_0}{6\pi\eta R_H v_r}$.

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

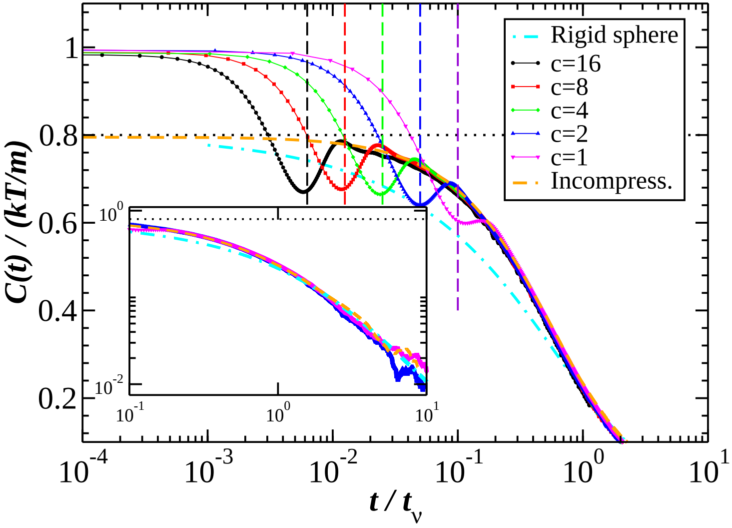


Figure: VACF for a blob with $m_e = m_f = \rho \Delta V$.

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

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

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

- The dimensionless Schmidt number $S_c = \nu/\chi_{\text{SE}}$ 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

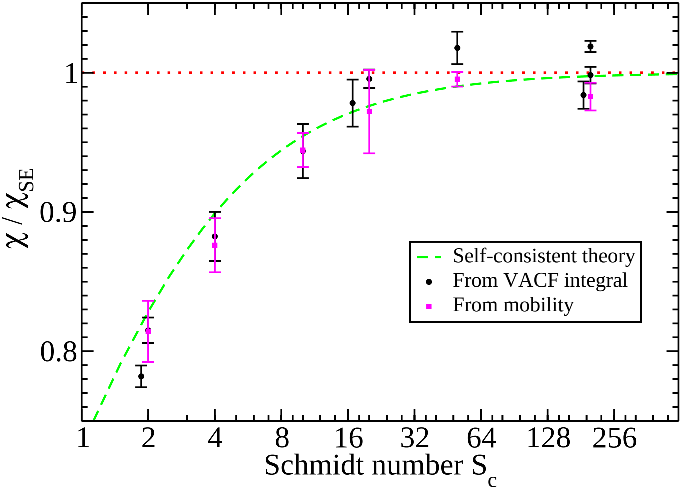


Figure: Corrections to Stokes-Einstein with changing viscosity $\nu = \eta/\rho$, $m_e = m_f = \rho \Delta V$.

Stokes-Einstein Corrections (2D)

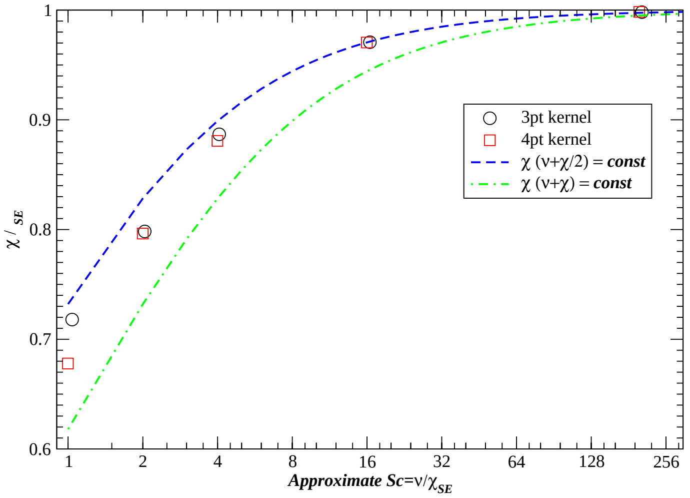
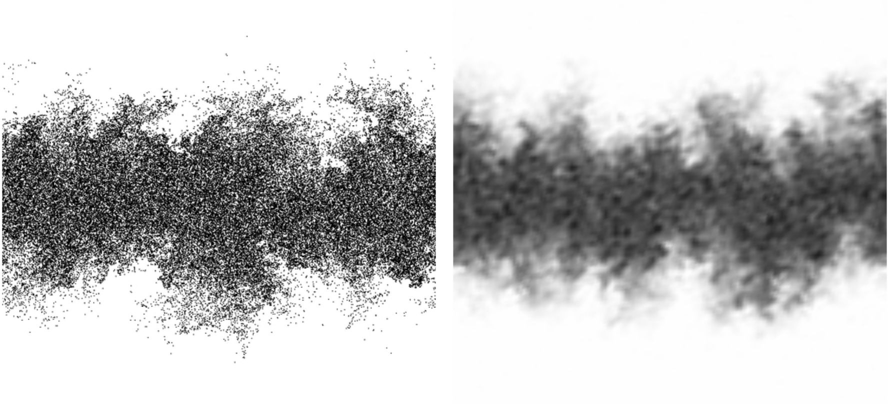


Figure: Corrections to Stokes-Einstein with changing viscosity $\nu = \eta/\rho$, $m_e = m_f = \rho \Delta V$.

Passively-Advected (Fluorescent) Tracers



Larger Reynolds Numbers

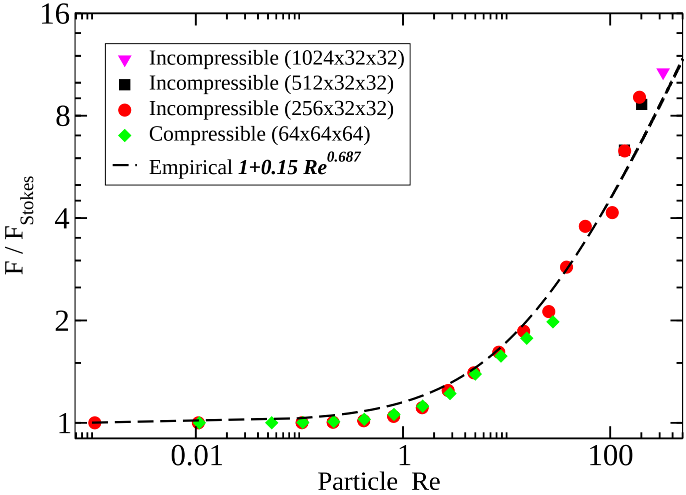


Figure: Drag force on a blob particle in a periodic domain as a function of the particle Reynolds number $\mathrm{Re} = 2R_H \langle u \rangle / \nu$, normalized by the Stokes drag.

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**

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

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

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

Brownian Dynamics (BD)

- 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

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

- 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.

BD without Green's Functions

The following algorithm can be shown to solve the Brownian Dynamics SDE:

- Solve a **steady-state Stokes problem** (here $\delta \ll 1$)

$$\begin{aligned}\mathbf{G}\boldsymbol{\pi}^n &= \eta\boldsymbol{\nabla}^2\mathbf{v}^n + \boldsymbol{\nabla}\cdot\boldsymbol{\Sigma}^n + \mathbf{S}^n\mathbf{F}\left(\mathbf{q}^n\right) \\ &+ \frac{k_B T}{\delta}\left[\mathbf{S}\left(\mathbf{q}^n + \frac{\delta}{2}\widetilde{\mathbf{W}}^n\right) - \mathbf{S}\left(\mathbf{q}^n - \frac{\delta}{2}\widetilde{\mathbf{W}}^n\right)\right]\widetilde{\mathbf{W}}^n \\ \mathbf{D}\mathbf{v}^n &= 0.\end{aligned}$$

- **Predict** particle position:

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

- **Correct** particle position,

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

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, and coupled to immersed particles to model Brownian suspensions.
- The **minimally-resolved blob approach** provides a low-cost but reasonably-accurate representation of rigid particles in flow.
- We have recently successfully extended the blob approach to **reaction-diffusion problems** (with Amneet Bhalla and Neelesh Patankar).
- **Particle inertia** can be included in the coupling between blob particles and a fluctuating **incompressible** fluid.
- More **complex particle shapes** can be built out of a collection of blobs.

Reactive Blobs

- **Continuum**: Diffusion equation for the concentration of the species $c(\mathbf{r}, t)$,

$$\partial_t c = \chi \boldsymbol{\nabla}^2 c + s(\mathbf{r}, t) \text{ in } \Omega \setminus \mathcal{S}, \tag{7}$$
$$\chi(\mathbf{n} \cdot \boldsymbol{\nabla} c) = k\, c \text{ on } \partial\mathcal{S}, \tag{8}$$

where k is the *surface* reaction rate.

- **Reactive-blob** model

$$\partial_t c = \chi \boldsymbol{\nabla}^2 c - \kappa \left[\int \delta_a(\mathbf{q} - \mathbf{r})\, c(\mathbf{r}, t)\, d\mathbf{r} \right] \delta_a(\mathbf{q} - \mathbf{r}) + s,$$

and discretization

$$\partial_t c = \chi \boldsymbol{\nabla}^2 c - \kappa \mathbf{S} \mathbf{J} c + s,$$

where $\kappa = 4\pi k a^2$ is the overall reaction rate.

- Requires specialized linear solvers in the **diffusion-limited regime**.

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