Coupling an Incompressible Fluctuating Fluid with Suspended Structures

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Outline

Levels of Coarse-Graining

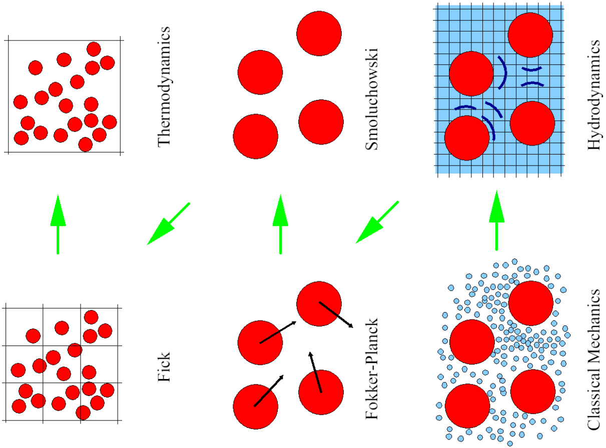


Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

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.
- 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

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

Fluid-Structure Direct Coupling

- The equations of motion in our coupling approach are **postulated** [1] to be

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

  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 [2] **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

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

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 [2], 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 [3] and the **IBM kernel functions** of Charles Peskin [4].
- 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**.

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:

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

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

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

  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**:

$$\alpha = \frac{V \Delta t}{\Delta x}, \quad \beta = \frac{\nu \Delta t}{\Delta x^2}, \tag{3}$$

  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

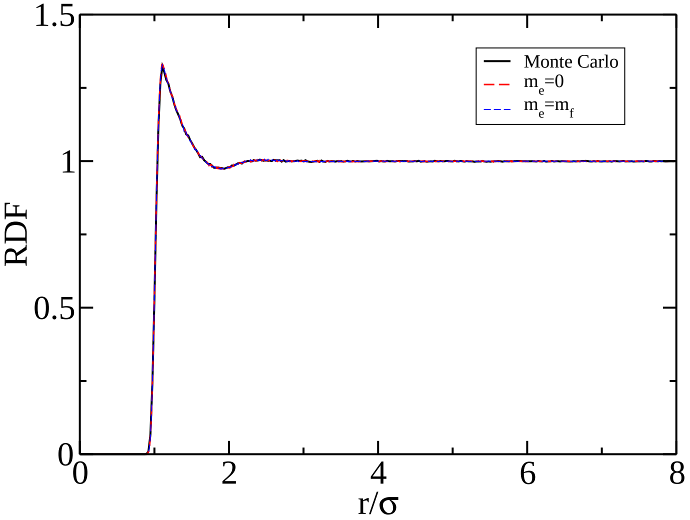


Figure: Equilibrium radial distribution function $g_2(\mathbf{r})$ for a suspension of blobs interacting with a repulsive LJ (WCA) potential.

Hydrodynamic Interactions

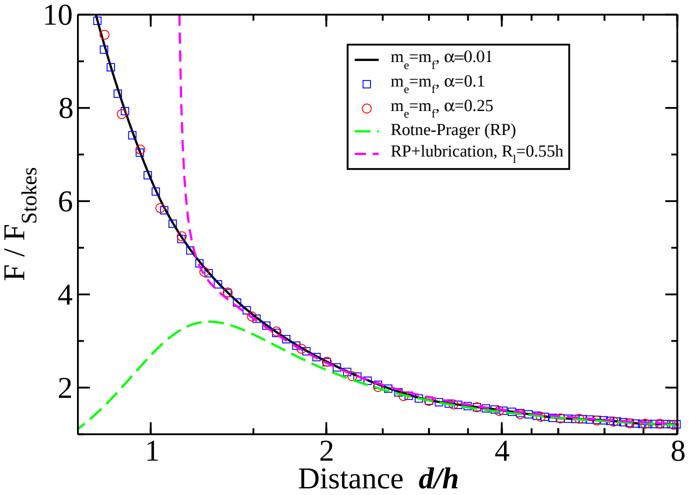


Figure: Effective hydrodynamic force between two approaching blobs at small Reynolds numbers, $\frac{F}{F_{\text{St}}} = -\frac{2F_0}{6\pi\eta R_H v_r}$.

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

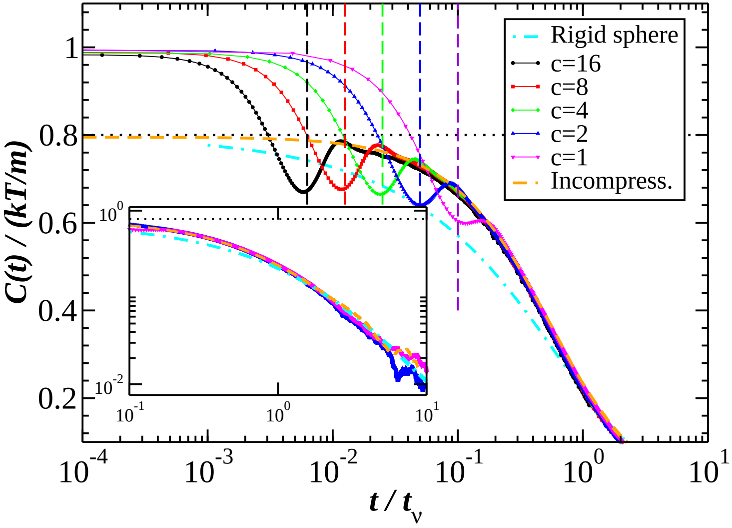


Figure: VACF for a blob with $m_e = m_f = \rho \Delta V$.

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 dimensionless Schmidt number $S_c = \nu/\chi$ controls the separation of time scales between $\mathbf{v}(\mathbf{r}, t)$ and $\mathbf{q}(t)$.
- For $S_c \gg 1$ the Stokes-Einstein relation predicts

$$\chi = \frac{k_B T}{6\pi\eta R_H}, \tag{4}$$

where for our blob with the 3-point kernel function $R_H \approx 0.9\Delta x$.
- Self-consistent theory [6] predicts a correction to Stokes-Einstein's relation,

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

Stokes-Einstein Corrections (preliminary)

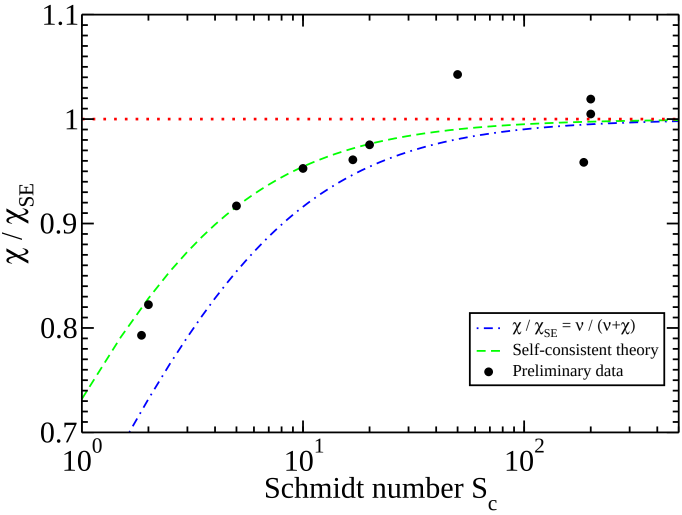
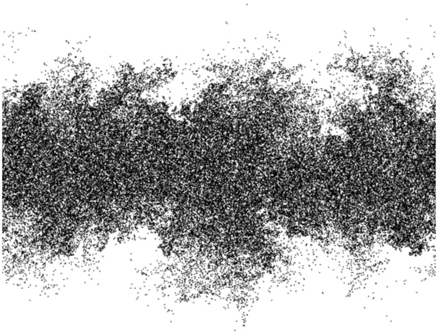
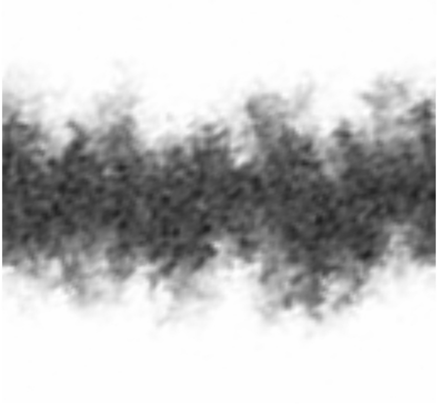


Figure: Corrections to Stokes-Einstein with changing viscosity $\nu = \eta/\rho$, $m_e = m_f = \rho \Delta V$.

Passively-Advected (Fluorescent) Tracers





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 [7] 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.* *[5]* for specialized exponential integrators for $\beta \gg 1$ for $m_e = 0$.

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