Coupling an Incompressible Fluctuating Fluid with Suspended Structures

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Outline

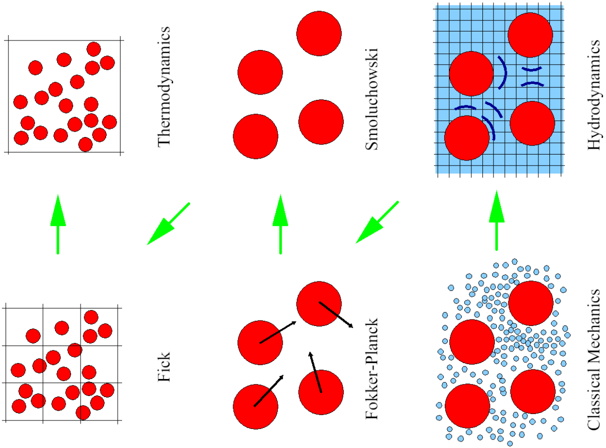

Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

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 (as in the **Force Coupling Method** (FCM) of Maxey *et al* [1]).
- 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 [2]

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

  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. Note **momentum is conserved**.
- In the existing (stochastic) IBM approach [3] **inertial effects** are ignored, $m_e = 0$ and thus $\boldsymbol{\lambda} = -\mathbf{F}$.

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 $\mathbf{v}$ and $\mathbf{q}$ are independent DOFs.
- This really means that the **stationary** (equilibrium) distribution must be the **Gibbs distribution**

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

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 [4], 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 [5] 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

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

- 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**

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

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:

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

where we use the **Adams-Bashforth method** for the advective (kinetic) fluxes, and the discretization of the stochastic flux is described in Ref. [5],

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

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

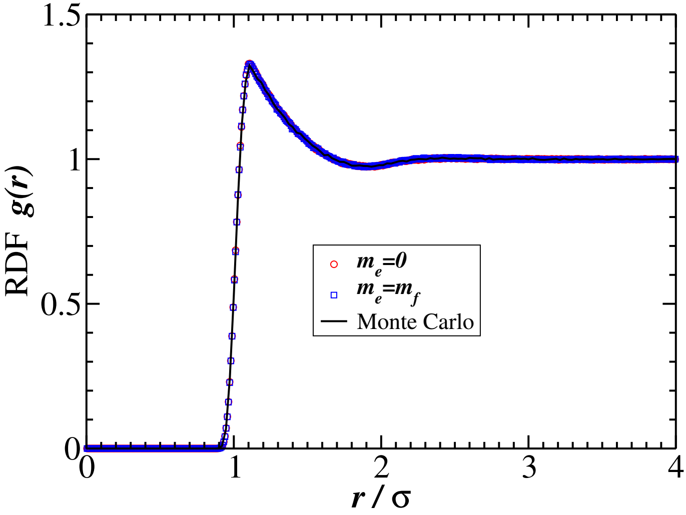

Figure: Equilibrium radial distribution function $g_2(\mathbf{r})$ for a suspension of blobs interacting with a repulsive LJ (WCA) potential.

Hydrodynamic Interactions

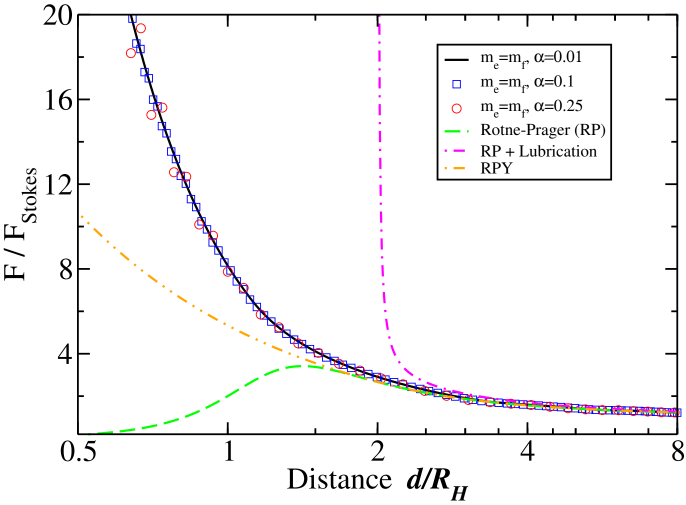

Figure: Effective hydrodynamic force between two approaching blobs at small Reynolds numbers, $\frac{F}{F_{St}} = -\frac{2F_0}{6\pi\eta R_H v_r}$.

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

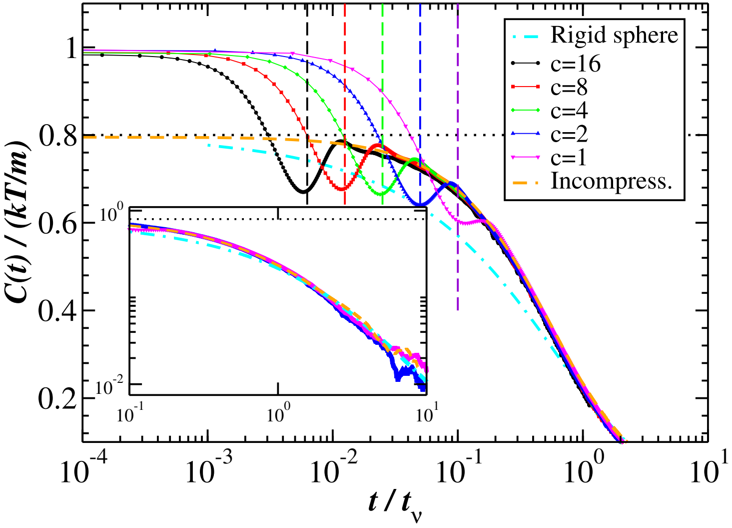

Figure: VACF for a blob with $m_e = m_f = \rho \Delta V$.

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 [6] 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

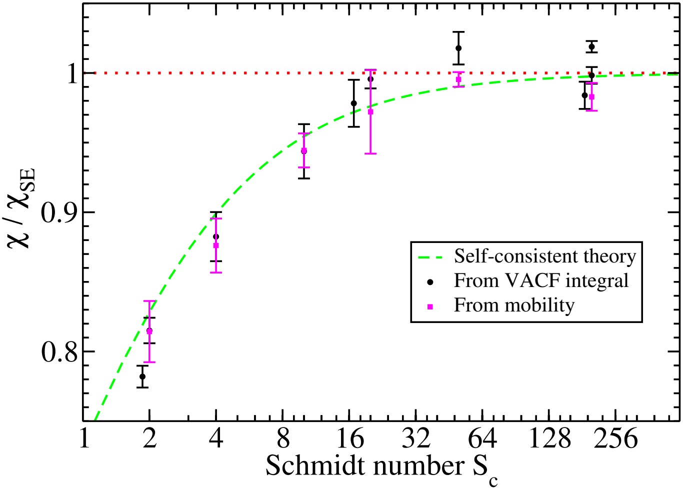

Figure: Corrections to Stokes-Einstein with changing viscosity $\nu = \eta/\rho$, $m_e = m_f = \rho \Delta V$.

Stokes-Einstein Corrections (2D)

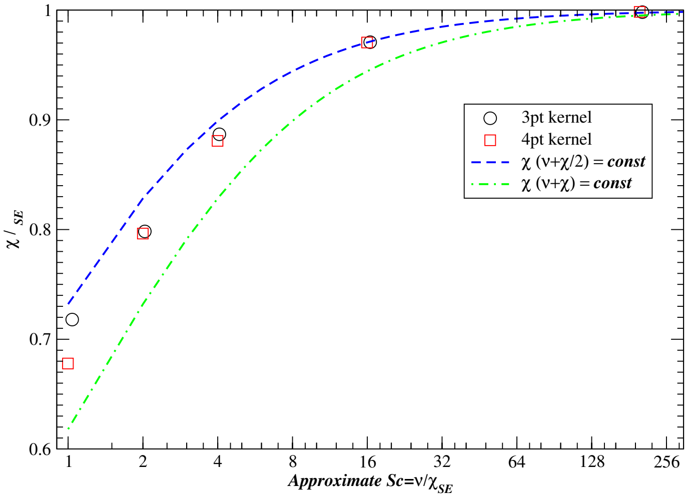

Figure: Corrections to Stokes-Einstein with changing viscosity $\nu = \eta/\rho$, $m_e = m_f = \rho \Delta V$.

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

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

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 $\mathcal{L}^{-1}$,

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

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,

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

Conclusions

- **Fluctuating hydrodynamics** seems to be a very good coarse-grained model for fluids, and can be 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.
- **Particle inertia** can be included in the coupling between blob particles and a fluctuating **incompressible** fluid.
- Stokes-Einstein's relation only holds for **large Schmidt numbers**.
- **Overdamped limit** can be handled just by changing the temporal integrator.
- More **complex particle shapes** can be built out of a collection of blobs.

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