

Coupling a Fluctuating Fluid with Suspended Structures Part II: Inertial Stochastic Immersed Boundary Method

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Fluid-Bead Coupling

- We want to construct a **bidirectional coupling** between a fluctuating fluid and a bead, which we can think of a small sphere of radius a with position $\mathbf{q}(t)$ and velocity $\mathbf{u} = d\mathbf{q}/dt$.
- Macroscopically, the coupling between flow and suspended structures relies on:
 - **No-stick** boundary condition $\mathbf{v}_{rel} = 0$ at the surface of the bead.
 - Force on the bead is the integral of the stress tensor over the bead 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.
- But the classical models do provide **inspiration** for what is physically reasonable, even if we do not take them literally.

Faxen's Theorem

- Consider the problem of a hard sphere of radius a immersed in an incompressible fluid:

$$\begin{aligned} \rho D_t \mathbf{v} &= \eta \nabla^2 \mathbf{v} - \nabla \pi \text{ with } \nabla \cdot \mathbf{v} = 0 \text{ outside } \|\mathbf{r} - \mathbf{q}(t)\| > a \\ \mathbf{v}(\mathbf{r}, t) &= \mathbf{u}(t) \text{ on the surface } \|\mathbf{r} - \mathbf{q}(t)\| = a \\ \mathbf{v}(\mathbf{r}, t) &= \mathbf{v}_\infty(\mathbf{r}, t) \text{ far away } \|\mathbf{r} - \mathbf{q}(t)\| \gg a, \end{aligned}$$

where $\mathbf{v}_\infty(\mathbf{r}, t)$ is often said to be the “fluid flow in the absence of the particle”, though seems better to call it the “flow at infinity”.

- Faxen derived that for sufficiently small beads, in some appropriate limit (zero Reynolds number), the force on the bead is:

$$\oint_S [-\pi \mathbf{I} + \eta \overline{\nabla \mathbf{v}}] \cdot \mathbf{n} dS = -6\pi a \eta \left[\mathbf{u} - \mathbf{v}_\infty(\mathbf{q}, t) - \frac{a^2}{6} (\nabla^2 \mathbf{v}_\infty) \mathbf{q}(t) \right] \cdot$$

- This is generalization of Stokes's friction law, but note that corrections including inertial effects have since been computed.

Induced Force Method

- An alternative formulation (Bedeaux and Mazur) includes fluid inside the bead but adds an **induced force density** in the fluid equations as an additional Lagrange multiplier:

$$\rho D_t \mathbf{v} = \eta \nabla^2 \mathbf{v} - \nabla \pi + \sqrt{2\eta k_B T} (\nabla \cdot \mathcal{W}) + \mathbf{f}_{ind} \text{ with } \nabla \cdot \mathbf{v} = 0$$

$$\mathbf{v}(\mathbf{r}, t) = \mathbf{u}(t) \text{ and } \pi(\mathbf{r}, t) = 0 \text{ inside } \|\mathbf{r} - \mathbf{q}(t)\| \leq a$$

$$\mathbf{f}_{ind}(\mathbf{r}, t) = 0 \text{ outside } \|\mathbf{r} - \mathbf{q}(t)\| \gg a$$

- Think of the Immersed Boundary method for surfaces, where singular surface force densities are turned into volume force densities.
- The force exerted by the fluid on the bead is:

$$\mathbf{F}_f = - \int_{\mathbf{r}} \mathbf{f}_{ind}(\mathbf{r}, t) d\mathbf{r} = \mathbf{F}_d + \mathbf{F}_s,$$

where we have tried to separate the (dissipative) **viscous friction force** \mathbf{F}_d from the (stochastic) **random force** \mathbf{F}_s due to **thermal fluctuations in the fluid**.

Fluid Equations

- We do not care about the fine details of the flow around a bead, which is nothing like a hard sphere with stick boundaries in reality anyway.
- Therefore, let us take an Immersed Boundary approach and assume

$$\mathbf{f}_{ind} = -\mathbf{F}_f \delta_{\Delta a}(\mathbf{q} - \mathbf{r}),$$

where $\delta_{\Delta a}$ is an **approximate delta function** with support of size Δa (integrates to unity).

- This gives the fluid equations, assuming incompressibility:

$$\rho D_t \mathbf{v} = \eta \nabla^2 \mathbf{v} - \nabla \pi + \sqrt{2\eta k_B T} (\nabla \cdot \mathcal{W}) - (\mathbf{F}_d + \mathbf{F}_s) \delta_{\Delta a}(\mathbf{q} - \mathbf{r}).$$

- One should of course use the full compressible fluctuating equations for better physical fidelity, but that seems much harder.

Bead Equations

- The motion of the bead, whose position is $\mathbf{q}(t)$ is modeled using a Langevin equation:

$$M\dot{\mathbf{u}} = M\ddot{\mathbf{q}} = \mathbf{F}_{ext} + \mathbf{F}_d + \mathbf{F}_s$$

where $\mathbf{F}_{ext} = -\nabla U(\mathbf{q})$ is usually a **conservative force**, but here it is some unspecified external force.

- Note that the total momentum

$$\mathbf{p} = M\mathbf{u} + \int_{\mathbf{r}} \rho \mathbf{v}(\mathbf{r}, t) d\mathbf{r}$$

is conserved when $\mathbf{F}_{ext} = \mathbf{0}$.

- An obvious choice is to assume a **Stokes friction law** for the dissipative coupling,

$$\mathbf{F}_d = -\gamma [\mathbf{u} - \mathbf{v}(\mathbf{q}, t)] \quad \text{where } \gamma \approx 6\pi a\eta$$

which is like Faxen's law *except* that \mathbf{v} is used instead of \mathbf{v}_∞ , which I assume is **not known**.

Dissipative Coupling

- Make the dissipative force more general but still linear,

$$\mathbf{F}_d = -\gamma \left[\mathbf{u} - \int K(\mathbf{q} - \mathbf{r}) \mathbf{v}(\mathbf{r}, t) d\mathbf{r} \right].$$

- In order to also conserve the energy

$$E = \frac{M}{2} \mathbf{u}^2 + \int_{\mathbf{r}} \frac{\rho}{2} v^2(\mathbf{r}, t) d\mathbf{r} + U(\mathbf{q}),$$

it can easily be shown that $K \equiv \delta_{\Delta a}$.

- More generally, the fluid-structure coupling operator must be the adjoint of the structure-fluid coupling operator. See preprint [1]: “*Stochastic Eulerian Lagrangian Methods for Fluid Structure Interactions with Thermal Fluctuations*”, **Paul J. Atzberger**, 2010, <http://arxiv.org/abs/1009.5648>

Stochastic Force

- For every dissipative force there should be a corresponding stochastic forcing, to ensure **fluctuation-dissipation balance** [2, 1].
- For the viscous dissipation this is the stochastic stress term $\sqrt{2\eta k_B T} (\nabla \cdot \mathcal{W})$.
- It is known from Langevin's work that for the viscous damping $-\gamma \mathbf{u}$ one needs a **stochastic force**

$$\mathbf{F}_s = \sqrt{2\gamma k_B T} \widetilde{\mathcal{W}},$$

where $\widetilde{\mathcal{W}}(t)$ is white-noise (derivative of Brownian motion).

- More generally, we want the **equilibrium distribution** of the dynamics to be the **Gibbs distribution**,

$$\Psi(\mathbf{u}, \mathbf{v}) = Z^{-1} \exp\left(-\frac{E}{k_B T}\right).$$

Fluid-Bead Equations

- We finally get the **Inertial Stochastic Immersed Boundary Method (ISIBM)** equations (set $k_B T = 1$)

$$\rho D_t \mathbf{v} = \eta \nabla^2 \mathbf{v} - \nabla \pi + \sqrt{2\eta} (\nabla \cdot \mathcal{W}) - \left(\mathbf{F}_d + \sqrt{2\gamma} \widetilde{\mathcal{W}} \right) \delta_{\Delta a} (\mathbf{q} - \mathbf{r}).$$

$$M \frac{d\mathbf{u}}{dt} = M \frac{d^2 \mathbf{q}}{dt^2} = \mathbf{F}_{ext} + \mathbf{F}_d + \sqrt{2\gamma} \widetilde{\mathcal{W}}$$

$$\mathbf{F}_d = -\gamma \left[\mathbf{u} - \int \delta_{\Delta a} (\mathbf{q} - \mathbf{r}) \mathbf{v}(\mathbf{r}, t) d\mathbf{r} \right]$$

- Dunweg and Ladd [3] ([arXiv:0803.2826v2](https://arxiv.org/abs/0803.2826v2)), and also Atzberger [1], have shown that this system satisfies fluctuation-dissipation balance, that is, the Gibbs distribution is the stationary solution of the Fokker-Planck equation corresponding to the linearized version of the fluid-bead equations.
- One must include the stochastic forcing in the fluid to get the Gibbs-Boltzmann distribution.**

Friction Coefficient

- Consider applying a constant force \mathbf{F}_{ext} on the bead and measuring its **terminal velocity** \mathbf{u}_0 , ignoring fluctuations:

$$\mathbf{F}_{ext} = -\mathbf{F}_d = \gamma \left[\mathbf{u}_0 - \int \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \mathbf{v}(\mathbf{r}, t) d\mathbf{r} \right] = \gamma [\mathbf{u}_0 - \mathbf{u}_f]$$

- The fluid equation is now simply the **Stokes equation**

$$0 = \eta \nabla^2 \mathbf{v} - \nabla \pi + \mathbf{F}_{ext} \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \quad \Rightarrow$$

$$\mathbf{v}(\mathbf{r}, t) = \left[\int d\mathbf{r}' [\mathbf{G}(\mathbf{r}, \mathbf{r}')] \delta_{\Delta a}(\mathbf{q} - \mathbf{r}') \right] \mathbf{F}_{ext},$$

where \mathbf{G} is the **Green's function** for the Stokes equation (**Oseen tensor**).

- Translational invariance (ignoring boundaries) gives:

$$\mathbf{u}_f = \left[\int d\mathbf{r}' \int d\mathbf{r} [\mathbf{G}(\mathbf{r} - \mathbf{r}')] \delta_{\Delta a}(\mathbf{r}') \delta_{\Delta a}(\mathbf{r}) \right] \mathbf{F}_{ext}$$

Friction Renormalization

- Because of spherical symmetry of $\delta_{\Delta a}$, the double integral is a multiple of the identity matrix,

$$\mathbf{u}_f = \frac{\theta_1}{\eta(\Delta a)} \mathbf{F}_{ext}$$

where $\theta_1 \sim 1$ is a constant that comes out of the integration.

- Taking $\gamma = \eta a \theta_2$, where $\theta_2 \sim 1$ is some constant, we get the **renormalization relation**:

$$\mathbf{F}_{ext} = \eta a \theta_2 \left[\mathbf{u}_0 - \frac{\theta_1}{\eta(\Delta a)} \mathbf{F}_{ext} \right] \Rightarrow$$

$$\mathbf{F}_{ext} = \frac{\theta_2}{1 + a \theta_2 \theta_1 / (\Delta a)} (\eta a \mathbf{u}_0)$$

- In practice we want to adjust the width of the approximate delta function but keep the **effective hydrodynamic radius** a constant:

$$\mathbf{F}_{ext} = 6\pi (\eta a \mathbf{u}_0) \Rightarrow \theta_2 = \frac{6\pi}{1 - 6\pi\theta_1 \left(\frac{a}{\Delta a}\right)} = \frac{6\pi}{1 - g^{-1} \left(\frac{a}{\Delta a}\right)}$$

Inertial Stochastic Immersed Boundary review

- Atzberger [1] explains why it is better to use not a velocity equation, but rather the **total momentum** of the fluid-bead system:

$$\mathbf{p} = \rho \mathbf{v} + M \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \mathbf{u} \quad \Rightarrow \quad (\text{classical Calculus is OK})$$

$$\mathbf{p}_t = \rho \mathbf{v}_t + M \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \frac{d\mathbf{u}}{dt} + M [\nabla_{\mathbf{q}} \delta(\mathbf{q} - \mathbf{r}) \cdot \mathbf{u}] \mathbf{u}.$$

- We can rewrite the last term as a divergence of a Kirkwood stress tensor, to get the equations in conservation form:

$$\begin{aligned} \mathbf{p}_t = & \eta \nabla^2 \mathbf{v} - \nabla \cdot (\pi \mathbf{I} + \rho \mathbf{v} \mathbf{v}^T) + \sqrt{2\eta k_B T} (\nabla \cdot \mathcal{W}) \\ & + \mathbf{F}_{\text{ext}} \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) - \nabla \cdot [(M \mathbf{u} \mathbf{u}^T) \delta_{\Delta a}(\mathbf{q} - \mathbf{r})] \end{aligned}$$

$$M \frac{d\mathbf{u}}{dt} = M \frac{d^2 \mathbf{q}}{dt^2} = \mathbf{F}_{\text{ext}} + \mathbf{F}_d + \sqrt{2\gamma} \widetilde{\mathcal{W}}$$

$$\mathbf{F}_d = -\gamma \left[\mathbf{u} - \int \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \mathbf{v}(\mathbf{r}, t) d\mathbf{r} \right]$$

The Stochastic Immersed Boundary Method

- Atzberger [1] has studied several limits of the ISBM dynamics, focusing on the limit $M \rightarrow 0$ first ($\mathbf{p} \equiv \mathbf{v}$), and then $\gamma \rightarrow \infty$.
- With this order of limits, the ISBM formulation *essentially* reduces to the **Stochastic Immersed Boundary method** [4]

$$D_t \mathbf{v} = \eta \nabla^2 \mathbf{v} - \nabla \pi + \sqrt{2\eta k_B T} (\nabla \cdot \mathcal{W}) + \mathbf{F}_{ext} \delta_{\Delta a}(\mathbf{q} - \mathbf{r})$$

$$- \nabla [\delta_{\Delta a}(\mathbf{q} - \mathbf{r}) k_B T]$$

$$\frac{d\mathbf{q}}{dt} = \mathbf{u} = \int \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \mathbf{v}(\mathbf{r}, t) d\mathbf{r}$$

Note that there is an additional term (shown in red) coming from the kinetic energy of the bead $\sim k_B T$.

- Note the important difference that now the bead is **advected by the fluid velocity**, as in the classical Immersed Boundary method.
- There is **no inertia** and the average speed of the bead $\langle \mathbf{u} \mathbf{u}^T \rangle = (k_B T / M) \mathbf{I}$ is not reproduced, but the tail of the VACF is [5]!

Brownian Dynamics Limit

- Further also taking the limit $\eta \rightarrow \infty$, that is, the Stokes limit in which the fluid dynamics is much faster than the dynamics of the bead:

$$\mathbf{v}(\mathbf{r}, t) = \left[\int d\mathbf{r}' [\mathbf{G}(\mathbf{r} - \mathbf{r}')] \delta_{\Delta a}(\mathbf{q} - \mathbf{r}') \right] \cdot \mathbf{F}$$

$$\mathbf{F} = \sqrt{2\eta k_B T} (\nabla \cdot \mathcal{W}) + \mathbf{F}_{\text{ext}} \delta_{\Delta a}(\mathbf{q} - \mathbf{r})$$

- The fluid dynamics is now **implicit**, and for the beads we get the traditional **Brownian Dynamics**:

$$\mathbf{u} = \frac{d\mathbf{q}}{dt} = \mathbf{H}\mathbf{F}_{\text{ext}} + \sqrt{2k_B T} \mathbf{H}^{1/2} \widetilde{\mathcal{W}} + (\nabla_{\mathbf{q}} \mathbf{H}) k_B T$$

- This cannot capture the tails of the VACF of the bead, since the fluid dynamics is not resolved!

Brownian Dynamics

- Here the hydrodynamic coupling is captured by the operator

$$\mathbf{H} = \int d\mathbf{r}' \int d\mathbf{r} [\mathbf{G}(\mathbf{r} - \mathbf{r}')] \delta_{\Delta a}(\mathbf{q} - \mathbf{r}') \delta_{\Delta a}(\mathbf{q} - \mathbf{r}).$$

- The hard part, see papers by Atzberger [6], is to not only do the fluid solve to compute $\mathbf{H}\mathbf{F}_{ext}$ but also compute the stochastic forcing $\mathbf{H}^{1/2}\widetilde{\mathcal{W}}$ (he proposed using stochastic multigrid ala Goodman and Sokal).
- Additional care must be payed for (semi)discrete formulations.
- In standard Brownian dynamics $k_B T \mathbf{H}$ is called the **diffusion tensor**, and is usually modeled using some analytical approximations (difficult in complex geometries), e.g., an Oseen tensor with some wall corrections.

Inertial Stochastic Immersed Boundary review

- Recall the full ISIBM conservative formulation:

$$\begin{aligned}
 \mathbf{p}_t &= \eta \nabla^2 \mathbf{v} - \nabla \cdot (\pi \mathbf{I} + \rho \mathbf{v} \mathbf{v}^T) + \sqrt{2\eta k_B T} (\nabla \cdot \mathcal{W}) \\
 &\quad + \mathbf{F}_{ext} \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) - \nabla \cdot [(M \mathbf{u} \mathbf{u}^T) \delta_{\Delta a}(\mathbf{q} - \mathbf{r})] \\
 M \frac{d\mathbf{u}}{dt} &= M \frac{d^2 \mathbf{q}}{dt^2} = \mathbf{F}_{ext} + \mathbf{F}_d + \sqrt{2\gamma} \widetilde{\mathcal{W}} \\
 \mathbf{F}_d &= -\gamma \left[\mathbf{u} - \int \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \mathbf{v}(\mathbf{r}, t) d\mathbf{r} \right] \\
 \mathbf{p} &= \rho \mathbf{v} + M \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \mathbf{u}
 \end{aligned}$$

- The limit $\gamma \rightarrow \infty$ but with **finite** M and η is a sort of “inertial” version of the IBM method, which is of interest but still somewhat elusive.

Direct Forcing Method

- It turns out this limit has sort of been implemented in the deterministic sense by Uhlmann and is called the **direct forcing method** [7].
- My collaborator Rafael D. Buscallioni and his student Florencio Balboa (visiting Courant in the spring!) have implemented the direct forcing method for beads immersed in an isothermal compressible fluid solver.
- The published formulations seem to all be semi-discrete in time and I could not find a **purely continuum formulation**.
- A quick derivation however shows that the algorithm by Uhlmann is a **projection algorithm** for solving the constrained evolution equations of what I will call the **overdamped ISIBM limit**.

Overdamped ISIBM equations

- Not attempting to do the stochastic terms rigorously, the **overdamped ISIBM** equations are:

$$\begin{aligned} \mathbf{p}_t &= \eta \nabla^2 \mathbf{v} - \nabla \cdot (\pi \mathbf{I} + \rho \mathbf{v} \mathbf{v}^T) + \sqrt{2\eta k_B T} (\nabla \cdot \mathcal{W}) \\ &\quad + \mathbf{F}_{\text{ext}} \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) - \nabla \cdot [(m \mathbf{u} \mathbf{u}^T) \delta_{\Delta a}(\mathbf{q} - \mathbf{r})] + (?) \\ m \frac{d\mathbf{u}}{dt} &= \mathbf{F}_{\text{ext}} + \boldsymbol{\lambda} \\ \text{subject to } \mathbf{u} &= \frac{d\mathbf{q}}{dt} = \int \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \mathbf{v}(\mathbf{r}, t) d\mathbf{r}. \end{aligned}$$

- The force $\boldsymbol{\lambda}$ is a Lagrange multiplier that enforces the constraint that the bead is **advected by the interpolated fluid velocity** (the integral of the “induced force”).
- I purposely changed notation for the mass of the bead from M to m ...

Excess mass

- The equations are written in terms of the momentum field \mathbf{p} :

$$\mathbf{p} = \rho \mathbf{v} + m \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \mathbf{u}.$$

- In practice one uses \mathbf{v} as a variable instead. The bead velocity \mathbf{u} is no longer really an independent variable, and it can formally be eliminated from the continuum description.
- The mass of the bead should be taken to be the **excess mass of the bead** over the “excluded” fluid:

$$m = M - \Delta m = M - \Delta V \int \delta_{\Delta a}(\mathbf{q} - \mathbf{r}) \rho(\mathbf{r}, t) d\mathbf{r} = M - \rho \Delta V,$$

where ΔV is a parameter that represents the **effective volume of the bead**,

$$\Delta V = \left[\int \delta_{\Delta a}^2(\mathbf{q} - \mathbf{r}) d\mathbf{r} \right]^{-1}.$$

Upcoming Implementations

- The ISBM form of coupling has been implemented and is used widely in Lattice-Boltzmann codes, which solve the isothermal *compressible* equations of fluctuating hydrodynamics (density fluctuates as well).
- Dunweg and Ladd [3] report that a three point discrete delta (interpolation) function provides a reasonably translationally-invariant $g \approx 1.2 \pm 0.03$, but the four-point is even better, $g \approx 1.5 \pm 0.01$.
- I have only recently begun working on developing numerical schemes for these types of problems:
 - Paul Atzberger is working on **exponential temporal stochastic integrators** in existing SIBM code: **rigorous** solution to carefully study the model and its limits.
 - Rafael D. Buscallioni and his student have a **direct forcing method** with a compressible fluid solver (almost fluctuating).
 - Some of us are working on **real-space incompressible fluctuating schemes** that satisfy fluctuation-dissipation balance [2], which will be used for the fluid solver in the future.

Open Questions

- Does the proposed ISIBM formulation have the *right physics in the deterministic setting*, for example, does it reproduce terms in generalizations of Faxen's theorem?
- How should compressibility (**sound effects**) and temperature be included in the coupling (e.g., ultrasound or thermal conduction in nano-colloidal suspensions)?
- What do the various formulations give for the **VACF of the bead compared to the particle-continuum hybrid** (the gold standard)?
- The *equipartition theorem* $C(0) = k_B T / M$ should be reproduced (assuming discrete FDB). But...
 - Where does the $2/3$ due to missing sound come in for incompressible formulations?
 - What happens as γ increases? Can we take the limit $\gamma \rightarrow \infty$ directly?

References/Questions?



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