Coupling a Fluctuating Fluid with Suspended Particles

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Outline

1. Introduction
2. Particle-Continuum Hybrid
   - Brownian Bead
3. Direct Fluid-Blob Coupling

Fluid-Structure Coupling

- We want to construct a **bidirectional coupling** between a fluctuating fluid and a small spherical **Brownian particle (blob)**.
- Macroscopically, the coupling between flow and a rigid sphere relies on:
  - **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.
- It is important to point out that **fluctuations should be taken into account at the continuum level**.

Levels of Coarse-Graining

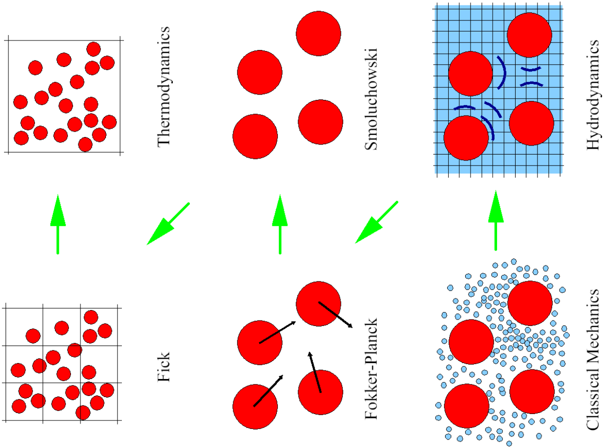

Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

Particle/Continuum Hybrid

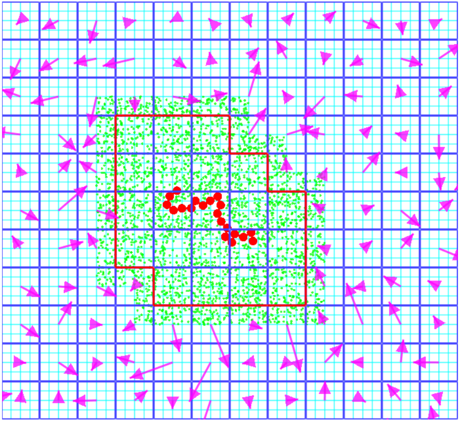

Figure: Hybrid method for a polymer chain.

Particle: Stochastic Collision Dynamics

- The most direct and accurate way to simulate the interaction between the fluid and blob is to use a particle scheme for both, e.g., **Molecular Dynamics** (MD).
- Over longer times it is **hydrodynamics** (local momentum and energy *conservation*) and **fluctuations** (*Brownian motion*) that matter.
- Coarse grain fluid: **Markov Chain Monte Carlo** instead of MD.
- *Replace deterministic interactions with* **conservative stochastic pairwise collisions** *between nearby fluid particles* [1] (based on DSMC, also related to MPCD/SRD and DPD).
- Fluid particles interact with blobs either via deterministic (hard-sphere) or stochastic (MCMC) collisions.

Continuum: Fluctuating Hydrodynamics

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

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

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

and capital Greek letters denote stochastic fluxes:

$$
\boldsymbol{\Sigma} = \sqrt{2\eta k_B T}\,\boldsymbol{\mathcal{W}}.
$$

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

Incompressible Fluctuating Navier-Stokes

- Ignoring density and temperature fluctuations, we obtain the **incompressible approximation**:

$$\rho D_t \mathbf{v} = \eta \boldsymbol{\nabla}^2 \mathbf{v} - \boldsymbol{\nabla} \pi + \sqrt{2\eta k_B T} \left(\boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{W}} \right),$$
$$\boldsymbol{\nabla} \cdot \mathbf{v} = 0$$

where the stochastic stress tensor $\boldsymbol{\mathcal{W}}$ is a white-noise random Gaussian tensor field with covariance

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

- We have developed **numerical schemes** to solve the compressible and incompressible fluctuating equations for simple fluids and miscible binary mixtures on **collocated** [2] and **staggered grids** [3].
- Solving them numerically requires paying attention to **discrete fluctuation-dissipation balance**, in addition to the usual deterministic difficulties.

Fluid-Structure Coupling using Particles

- Split the domain into a **particle** and a **continuum (hydro) subdomains**, with timesteps $\Delta t_H = K \Delta t_P$.
- Hydro solver is a simple explicit **(fluctuating) compressible** code and is *not aware* of particle patch.
- The method is based on Adaptive Mesh and Algorithm Refinement (AMAR) methodology for conservation laws and ensures **strict conservation** of mass, momentum, *and* energy.

MNG

Continuum-Particle Coupling

- Each macro (hydro) cell is either **particle or continuum**. There is also a **reservoir region** surrounding the particle subdomain.
- The coupling is roughly of the **state-flux** form:
  - The continuum solver provides *state boundary conditions* for the particle subdomain via reservoir particles.
  - The particle subdomain provides *flux boundary conditions* for the continuum subdomain.
- The fluctuating hydro solver is **oblivious** to the particle region: Any conservative explicit finite-volume scheme can trivially be substituted.
- The coupling is greatly simplified because the ideal **particle fluid has no internal structure**.

"*A hybrid particle-continuum method for hydrodynamics of complex fluids*", A. Donev and J. B. Bell and A. L. Garcia and B. J. Alder, **SIAM J. Multiscale Modeling and Simulation 8(3):871-911, 2010**

Our Hybrid Algorithm

1. The hydro solution $\mathbf{u}_H$ is computed everywhere, including the **particle patch**, giving an estimated total flux $\mathbf{\Phi}_H$.
2. **Reservoir particles** are *inserted* at the boundary of the particle patch based on *Chapman-Enskog distribution* from kinetic theory, accounting for *both* collisional and kinetic viscosities.
3. Reservoir particles are *propagated* by Δt and *collisions* are processed, giving the total particle flux $\mathbf{\Phi}_p$.
4. The hydro solution is overwritten in the particle patch based on the particle state $\mathbf{u}_p$.
5. The hydro solution is corrected based on the more accurate flux, $\mathbf{u}_H \leftarrow \mathbf{u}_H - \mathbf{\Phi}_H + \mathbf{\Phi}_p$.

Velocity Autocorrelation Function

- We investigate the **velocity autocorrelation function** (VACF) for a Brownian bead
$$C(t) = \langle \mathbf{v}(t_0) \cdot \mathbf{v}(t_0 + t) \rangle$$
- From equipartition theorem $C(0) = kT/m$.
- For a Brownian particle with density ρ' incompressible hydrodynamic theory gives
$$C(0^+) = \left(1 + \frac{\rho}{2\rho'}\right)^{-1} \frac{kT}{m}$$
because the momentum correlations decay instantly due to sound waves.
- Hydrodynamic persistence (conservation) gives a **long-time power-law tail** $C(t) \sim (kT/m)(t/t_{visc})^{-3/2}$ *not* reproduced in Brownian dynamics.

Large Bead (~1000 particles)

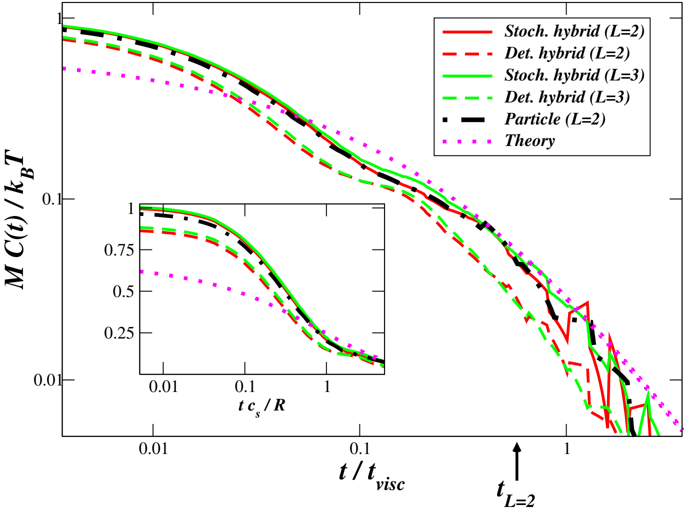

Figure: VACF for a neutrally-buyouant spherical Brownian particle.

Fluid-Structure Coupling

- Consider a blob (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 blob.
- See Florencio Balboa's talk and paper [4].

Local Averaging and Spreading Operators

- Postulate a **no-slip condition** between the particle and local fluid velocities,

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

  enforced by a Lagrange multiplier fluid-blob force $\boldsymbol{\lambda}$.
- The **induced force density** in the fluid because of the particle is:

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

  which ensures **momentum conservation**.
- Crucial for **energy conservation** is that the *local averaging operator* $\mathbf{J}(\mathbf{q})$ and the *local spreading operator* $\mathbf{S}(\mathbf{q})$ are **adjoint**, $\mathbf{S} = \mathbf{J}^{\star}$.
- I will **ignore the nonlinear advective terms** and simply denote them with ellipses ...

Fluid-Structure Direct Coupling

- The equations of motion in our coupling approach are *postulated*

$$\begin{aligned} \rho \left(\partial_t \mathbf{v} + \mathbf{v} \cdot \boldsymbol{\nabla} \mathbf{v} \right) &= -\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} - \mathbf{S} \boldsymbol{\lambda} \\ m_e \dot{\mathbf{u}} &= \mathbf{F} + \boldsymbol{\lambda} \\ \text{s.t. } \mathbf{u} &= \mathbf{J} \mathbf{v}, \end{aligned}$$

  where $\boldsymbol{\lambda}$ is a Lagrange multiplier that enforces the **no-slip condition** and m_e is the **excess mass** of the particle.
- The **fluid fluctuations** drive the Brownian motion: no stochastic forcing of the particle motion.
- In the existing (stochastic) IBM approaches **inertial effects** are ignored, $m_e = 0$ and thus $\boldsymbol{\lambda} = -\mathbf{F}$.
- In Lattice-Boltzmann approaches [5] a frictional (dissipative) force $\boldsymbol{\lambda} = -\zeta \left(\mathbf{u} - \mathbf{J} \mathbf{v} \right)$ is used instead of a constraint.

Effective Inertia

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

$$m\dot{\mathbf{u}} = -\Delta V \left(\mathbf{J} \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} \right) + \mathbf{F} + \cdots ,$$

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

$$m_f = \rho \left(\mathbf{J} \mathbf{S} \right)^{-1} = \rho \Delta V = \rho \left[\int \delta_a^2 \left(\mathbf{r} \right) d\mathbf{r} \right]^{-1} .$$

- For the fluid we get the effective equation

$$\boldsymbol{\rho}_{\text{eff}} \partial_t \mathbf{v} = -\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} + \mathbf{S} \mathbf{F} + \ldots$$

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

$$\boldsymbol{\rho}_{\text{eff}} = \rho \mathbf{I} + m_e \mathbf{S} \mathbf{J}.$$

Fluctuation-Dissipation Balance

- One must ensure fluctuation-dissipation balance in the coupled fluid-particle system. This is work in progress...
- This really means that the **stationary** (equilibrium) distribution must be the **Gibbs distribution**

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

where the **Hamiltonian** is postulated to be

$$H = U(\mathbf{q}) + m_e \frac{u^2}{2} + \int \left[\rho \frac{v^2}{2} + \epsilon(\rho)\right] d\mathbf{r}.$$

- We can eliminate the particle velocity using the no-slip constraint, to obtain the **effective Hamiltonian**

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

- The equations as written do not formally satisfy fluctuation-dissipation balance as the dynamics is **not incompressible in phase space**.

Brownian Dynamics Limit

- For the case of a neutrally-bouyant particle, $m_e = 0$, fluctuation-dissipation balance is restored if one adds an extra drift term to the fluid dynamics:

$$\rho \partial_t \mathbf{v} = -\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} + \mathbf{SF} + (k_B T) \frac{\partial}{\partial \mathbf{q}} \cdot \mathbf{S}.$$

- Paul Atzberger [6] has obtained these equations by carefully taking the limit $m_e \to 0$ and *then* **infinite friction** of the Stokes dissipative fluid-particle coupling [5].
- In the overdamped or Brownian dynamics limit

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

where the **mobility tensor** is related to the Stokes solution operator $\boldsymbol{\mathcal{L}}^{-1}$:

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

Incompressible Approximation

- For an incompressible fluid the fluid forcing must be projected using the **projection operator** $\mathcal{P}$, in Fourier space $\widehat{\mathcal{P}} = \mathbf{I} - k^{-2}\left(\mathbf{k}\mathbf{k}^T\right)$.
- Now the effective density matrix for the fluid is

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

- The modified Gibbs distribution gives a kinetic energy of the particle that is **less than equipartition** suggests,

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

as predicted also for a rigid sphere a long time ago, $m_f/m = \rho'/\rho$.

- Incompressible hydro is much harder for non-periodic systems due to additional splitting of pressure terms.

Numerical Scheme

- Spatial discretization is based on previously-developed **staggered schemes** for fluctuating hydro [3] and the **IBM kernel functions** of Charles Peskin [7].
- Temporal discretization follows a first-order **splitting algorithm** (move particle + update momenta) based on the **Direct Forcing Method** of Uhlmann [8].
- The scheme ensures **strict conservation** of momentum and strictly enforces the no-slip condition using a projection step at the end of the time step.
- Continuing work on **second-order** temporal integrators that reproduce the correct **equilibrium distribution** and **diffusive dynamics**.
- Both compressible (explicit) and incompressible (semi-implicit) methods are work in progress...

Numerical VACF

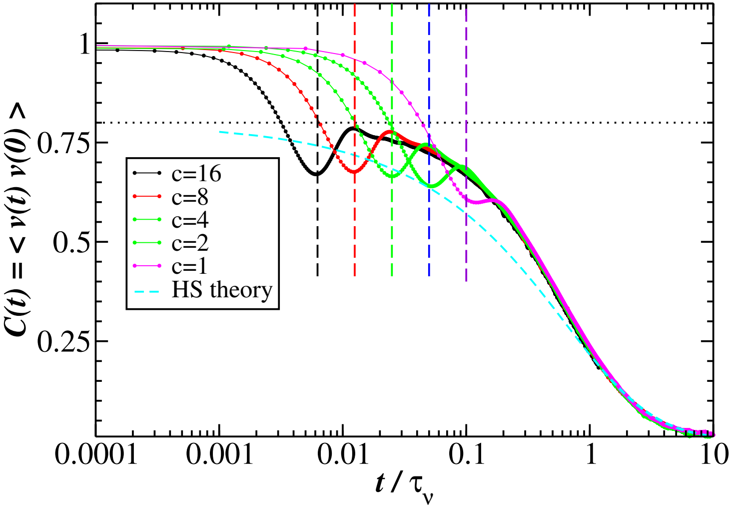

Figure: (F. Balboa) VACF for a blob with $m_e = m_f = \rho \Delta V$.

Conclusions / Discussion

- **Coarse-grained particle methods** can be used to accelerate hydrodynamic calculations at small scales.
- **Hybrid particle continuum methods** closely reproduce purely particle simulations at a fraction of the cost.
- It is **necessary to include fluctuations** in the continuum solver in hybrid methods.
- **Direct fluid-structure coupling** between fluctuating hydrodynamics and microstructure can replace expensive particle methods and complicated hybrid algorithms.
- Ensuring **fluctuation-dissipation balance** is crucial and nontrivial: *How to do it when* $m_e \neq 0$*?*
- Can one derive the proper set of fluid-blob equations, or at least their structure, via **coarse graining** (work with Pep Espanol)?

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