Coupling a Fluctuating Fluid with Suspended Particles

Aleksandar Donev

Courant Institute, New York University
&
Alejandro L. Garcia, SJSU
John B. Bell, LBNL
Florencio “Balboa” Usabiaga, UAM
Rafael Delgado-Buscalioni, UAM

ZCAM Workshop
Zaragoza, Spain
October 2011
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”
Figure: Hybrid method for a polymer chain.
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.
\[ D_t \rho = - \rho \nabla \cdot \mathbf{v} \]
\[ \rho (D_t \mathbf{v}) = - \nabla P + \nabla \cdot (\eta \overline{\nabla \mathbf{v}} + \mathbf{\Sigma}) \]
\[ \rho c_p (D_t T) = D_t P + \nabla \cdot (\mu \nabla T + \Xi) + (\eta \overline{\nabla \mathbf{v}} + \mathbf{\Sigma}) : \nabla \mathbf{v}, \]

where the variables are the density \( \rho \), velocity \( \mathbf{v} \), and temperature \( T \) fields,

\[ D_t \square = \partial_t \square + \mathbf{v} \cdot \nabla (\square) \]
\[ \overline{\nabla \mathbf{v}} = (\nabla \mathbf{v} + \nabla \mathbf{v}^T) - 2 (\nabla \cdot \mathbf{v}) \mathbf{I} / 3 \]

and capital Greek letters denote stochastic fluxes:

\[ \mathbf{\Sigma} = \sqrt{2\eta k_B T} \mathbf{\mathcal{W}}. \]

\[ \langle \mathcal{W}_{ij}(\mathbf{r}, t) \mathcal{W}_{kl}^*(\mathbf{r}', t') \rangle = (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - 2\delta_{ij}\delta_{kl} / 3) \delta(t - t') \delta(\mathbf{r} - \mathbf{r}). \]
Ignoring density and temperature fluctuations, we obtain the incompressible approximation:

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

where the stochastic stress tensor \( \mathbf{W} \) is a white-noise random Gaussian tensor field with covariance

\[ \langle \mathbf{W}_{ij}(\mathbf{r}, t) \mathbf{W}_{kl}^*(\mathbf{r}', t') \rangle = (\delta_{ik} \delta_{jl}) \delta(t - t') \delta(\mathbf{r} - \mathbf{r}'). \]

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.
Split the domain into a \textit{particle} and a \textit{continuum (hydro) subdomains}, with timesteps $\Delta t_H = K \Delta t_P$.

Hydro solver is a simple explicit (fluctuating) compressible code and is \textit{not aware} of particle patch.

The method is based on Adaptive Mesh and Algorithm Refinement (AMAR) methodology for conservation laws and ensures \textit{strict conservation} of mass, momentum, \textit{and} energy.
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.

Our Hybrid Algorithm

1. The hydro solution \( u_H \) is computed everywhere, including the particle patch, giving an estimated total flux \( \Phi_H \).

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 \( \Delta t \) and collisions are processed, giving the total particle flux \( \Phi_p \).

4. The hydro solution is overwritten in the particle patch based on the particle state \( u_p \).

5. The hydro solution is corrected based on the more accurate flux, \( u_H \leftarrow u_H - \Phi_H + \Phi_p \).
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 \( \rho' \) 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 \( C(t) \sim (kT/m)(t/t_{\text{visc}})^{-3/2} \) not reproduced in Brownian dynamics.
Figure: VACF for a neutrally-buoyant spherical Brownian particle.
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].
Postulate a **no-slip condition** between the particle and local fluid velocities,

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

enforced by a Lagrange multiplier fluid-blob force \( \lambda \).

The **induced force density** in the fluid because of the particle is:

\[
f = -\lambda \delta_a (q - r) = -[S(q)] \lambda,
\]

which ensures *momentum conservation*.

Crucial for **energy conservation** is that the *local averaging operator* \( J(q) \) and the *local spreading operator* \( S(q) \) are **adjoint**, \( S = J^* \).

I will **ignore the nonlinear advective terms** and simply denote them with ellipses . . .
The equations of motion in our coupling approach are *postulated*

\[
\rho \left( \frac{\partial}{\partial t} \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla \cdot \sigma - S\lambda \\
m_e \ddot{\mathbf{u}} = \mathbf{F} + \lambda \\
s.t. \quad \mathbf{u} = J\mathbf{v},
\]

where \( \lambda \) 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 \( \lambda = -\mathbf{F} \).
- In Lattice-Boltzmann approaches [5] a frictional (dissipative) force \( \lambda = -\zeta (\mathbf{u} - J\mathbf{v}) \) is used instead of a constraint.
Eliminating $\lambda$ we get the particle equation of motion

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

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

$$m_f = \rho (JS)^{-1} = \rho \Delta V = \rho \left[ \int \delta_a^2 (r) \, dr \right]^{-1}.$$

For the fluid we get the effective equation

$$\rho_{\text{eff}} \partial_t \mathbf{v} = -\nabla \cdot \sigma + SF + \ldots$$

where the effective mass density matrix (operator) is

$$\rho_{\text{eff}} = \rho I + m_e SJ.$$
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

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

where the Hamiltonian is postulated to be

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

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

\[ H = U(q) + \int \frac{\mathbf{v}^T \rho_{\text{eff}} \mathbf{v}}{2} dr + \int \epsilon(\rho) dr. \]

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

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

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

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

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

$$
\mathbf{M}(q) = -\mathbf{J} \mathcal{L}^{-1} \mathbf{S}.
$$
For an incompressible fluid the fluid forcing must be projected using the projection operator $\mathcal{P}$, in Fourier space $\hat{\mathcal{P}} = I - k^{-2} (kk^T)$.

Now the effective density matrix for the fluid is

$$\rho_{\text{eff}} = \rho + m_e \mathcal{P} \mathcal{S} \mathcal{J} \mathcal{P}.$$

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

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

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

Incompressible hydro is much harder for non-periodic systems due to additional splitting of pressure terms.
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 $m_e = m_f = \rho \Delta V$. 

$$C(t) = \langle v(t) v(0) \rangle$$

- $c=16$
- $c=8$
- $c=4$
- $c=2$
- $c=1$

HS theory
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)?
References

A Thermodynamically-Consistent Non-Ideal Stochastic Hard-Sphere Fluid.

On the Accuracy of Explicit Finite-Volume Schemes for Fluctuating Hydrodynamics.

Staggered Schemes for Incompressible Fluctuating Hydrodynamics.
Submitted, 2011.

F. Balboa Usabiaga, I. Pagonabarraga, and R. Delgado-Buscalioni.
Inertial coupling for point particle fluctuating hydrodynamics.
In preparation, 2011.

B. Dunweg and A.J.C. Ladd.
Lattice Boltzmann simulations of soft matter systems.

P. J. Atzberger.

C.S. Peskin.
The immersed boundary method.

M. Uhlmann.
An immersed boundary method with direct forcing for the simulation of particulate flows.