Coupling a Fluctuating Fluid with Suspended Structures

Aleksandar Donev
Courant Institute, New York University
&
Alejandro L. Garcia, San Jose State University
John B. Bell, Lawrence Berkeley National Laboratory

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Introduction

Particle Methods

Fluctuating Hydrodynamics

Hybrid Particle-Continuum Method

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Conclusions
Flows of fluids (gases and liquids) through micro- (\(\mu m\)) and nano-scale (\(nm\)) structures has become technologically important, e.g., micro-fluidics, microelectromechanical systems (MEMS).

**Biologically-relevant** flows also occur at micro- and nano- scales.

An important feature of small-scale flows, not discussed here, is **surface/boundary effects** (e.g., slip in the contact line problem).

Essential distinguishing feature from “ordinary” CFD: **thermal fluctuations**!

I focus here not on the technical details of hybrid methods, but rather, on using our method to demonstrate the general conclusion that **fluctuations should be taken into account at the continuum level**.
Introduction

Example: DNA Filtering

Fu et al., Nature Nanotechnology 2 (2007)


How to coarse grain the fluid (solvent) and couple it to the suspended microstructure (e.g., polymer chain)?
Figure: From Pep Español, “Statistical Mechanics of Coarse-Graining”
This talk: Particle/Continuum Hybrid

**Figure**: Hybrid method for a polymer chain.
Particle Methods for Complex Fluids

- The most direct and accurate way to simulate the interaction between the **solvent** (fluid) and **solute** (beads, chain) is to use a particle scheme for both: **Molecular Dynamics (MD)**
  \[ m\ddot{r}_i = \sum_j f_{ij}(r_{ij}) \]

- The stiff repulsion among beads demands small time steps, and chain-chain crossings are a problem.

- Most of the computation is “wasted” on the *unimportant solvent particles*!

- Over longer times it is **hydrodynamics** (*local momentum* and *energy conservation*) and **fluctuations** (Brownian motion) that matter.

- We need to coarse grain the fluid model further: *Replace deterministic interactions with stochastic collisions.*
Stochastic conservative collisions of randomly chosen nearby solvent particles, as in DSMC (also related to MPCD/SRD and DPD).

Solute particles still interact with both solvent and other solute particles as hard or soft spheres.

No fluid structure: Viscous ideal gas.

One can introduce biased collision models to give the fluids consistent structure and a non-ideal equation of state. [1].

Tethered polymer chain in shear flow.
Formally, we consider the continuum field of conserved quantities

\[ U(r, t) = \begin{bmatrix} \rho \\ j \\ e \end{bmatrix} \cong \tilde{U}(r, t) = \sum_i \begin{bmatrix} m_i \\ m_i v_i \\ m_i v_i^2 / 2 \end{bmatrix} \delta [r - r_i(t)] , \]

where the symbol \( \cong \) means that \( U(r, t) \) approximates the true atomistic configuration \( \tilde{U}(r, t) \) over long length and time scales.

Formal coarse-graining of the microscopic dynamics has been performed to derive an approximate closure for the macroscopic dynamics [2].

This leads to SPDEs of Langevin type formed by postulating a white-noise random flux term in the usual Navier-Stokes-Fourier equations with magnitude determined from the fluctuation-dissipation balance condition, following Landau and Lifshitz.
\[ D_t \rho = - \rho \nabla \cdot \mathbf{v} \]
\[ \rho (D_t \mathbf{v}) = - \nabla P + \nabla \cdot (\eta \overline{\nabla v} + \Sigma) \]
\[ \rho c_p (D_t T) = D_t P + \nabla \cdot (\mu \nabla T + \Xi) + (\eta \overline{\nabla v} + \Sigma) : \nabla \mathbf{v}, \]

where the variables are the \textbf{density} \( \rho \), \textbf{velocity} \( \mathbf{v} \), and \textbf{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:

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

\[ \langle \mathcal{W}_{ij}(\mathbf{r}, t) \mathcal{W}_{kl}^*(\mathbf{r}', t') \rangle = (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} - 2 \delta_{ij} \delta_{kl} / 3) \delta(t - t') \delta(\mathbf{r} - \mathbf{r'}). \]
The non-linear LLNS equations are ill-behaved stochastic PDEs, and we do not really know how to interpret the nonlinearities precisely.

Finite-volume discretizations naturally impose a grid-scale regularization (smoothing) of the stochastic forcing.

A renormalization of the transport coefficients is also necessary [3].

We have algorithms and codes to solve the compressible equations (collocated and staggered grid), and recently also the incompressible ones (staggered grid) [4, 5].

Solving the LLNS equations numerically requires paying attention to discrete fluctuation-dissipation balance, in addition to the usual deterministic difficulties [4].
We want to construct a bidirectional coupling between a fluctuating fluid and a small sphere of radius $a$ with position $\mathbf{q}(t)$ and velocity $\mathbf{u} = \frac{d\mathbf{q}}{dt}$ (aka bead).

Macroscopically, the coupling between flow and suspended structures relies on:

- **No-slip** boundary condition $\mathbf{v}_{rel} = 0$ at the surface of the bead.
- Force on the bead is the integral of the (fluctuating) 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.
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 LLNS 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.
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, $u_H \leftarrow u_H - \Phi_H + \Phi_p$. 
For molecular dynamics (non-ideal particle fluids) the insertion of reservoir particles is greatly complicated by the need to account for the internal structure of the fluid and requires an overlap region.

A hybrid method based on a flux-flux coupling between molecular dynamics and isothermal compressible fluctuating hydrodynamics has been developed by Coveney, De Fabritiis, Delgado-Buscalioni and co-workers [6].

Some comparisons between different forms of coupling (state-state, state-flux, flux-state, flux-flux) has been performed by Ren [7].

Reaching relevant time scales ultimately requires a stochastic immersed structure approach coupling immersed structures directly to a fluctuating solver (work in progress).
The Importance of Thermal Fluctuations

The adiabatic piston problem

MNG
**Figure:** Massive rigid piston ($M/m = 4000$) not in mechanical equilibrium: The deterministic hybrid gives the wrong answer!
Consider a particle with position $q(t)$ and its velocity $u = \dot{q}$, and the velocity field for the fluid is $v(r, t)$.

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.

The fluid fluctuations drive the Brownian motion: no stochastic forcing of the particle motion.

Take an Immersed Boundary approach and assume the force density induced in the fluid because of the particle is:

$$f_{\text{ind}} = -\lambda \delta_{\Delta a} (q - r) = -S\lambda,$$

where $\delta_{\Delta a}$ is an approximate delta function with support of size $a$ (integrates to unity).
The equations of motion of the Direct Forcing method are postulated to be

\[ \rho \left( \partial_t v + v \cdot \nabla v \right) = \nabla \cdot \sigma - S\lambda \]  

(1)

\[ m\dot{u} = F + \lambda \]  

(2)

subject to \( u = Jv = \int \delta_a (q - r) v(r, t) \, dr \),

(3)

where \( \lambda \) is a Lagrange multiplier that enforces the no-slip condition.

Here \( m \) is the excess mass of the particle over the “dragged fluid”, and the effective mass is

\[ M = m + \Delta m = m + \rho (JS)^{-1} = m + \rho \Delta V \]

The Lagrange multipliers can be eliminated formally to get a fluid equation with effective mass density matrix

\[ \rho_{\text{eff}} = \rho + \Delta m S J. \]
Conclusions

- **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 (work with Rafael Delgado-Buscailioni).
- One must ensure fluctuation-dissipation balance in the coupled fluid-particle system, with effective Hamiltonian

\[ H = \frac{1}{2} \left[ \int \rho v^2 \, dr + m u^2 \right] + U(q), \]

and implement a discrete scheme.
Stochastic Hard-Sphere Dynamics for Hydrodynamics of Non-Ideal Fluids.

P. Español.
Stochastic differential equations for non-linear hydrodynamics.

Diffusive Transport Enhanced by Thermal Velocity Fluctuations.

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

Staggered Schemes for Incompressible Fluctuating Hydrodynamics.
Submitted, 2011.

G. De Fabritiis, M. Serrano, R. Delgado-Buscalioni, and P. V. Coveney.
Fluctuating hydrodynamic modeling of fluids at the nanoscale.

W. Ren.
Analytical and numerical study of coupled atomistic-continuum methods for fluids.