Numerical Methods for Fluctuating Hydrodynamics

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Discrete Simulation of Fluid Dynamics
Fargo, ND
August 11th, 2011
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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 hope to demonstrate the general conclusion that fluctuations should be taken into account at all level.
Figure: From Pep Español, “Statistical Mechanics of Coarse-Graining”
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.
Particle Methods

Direct Simulation Monte Carlo (DSMC)

- **Stochastic conservative collisions** of randomly chosen **pairs** of 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].

(MNG)

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

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

where the symbol \( \cong \) means that \( \mathbf{U}(r, t) \) approximates the true atomistic configuration \( \tilde{\mathbf{U}}(r, t) \) 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.
\[ D_t \rho = - \rho \nabla \cdot \mathbf{v} \]
\[ \rho (D_t \mathbf{v}) = - \nabla P + \nabla \cdot (\eta \overline{\nabla \mathbf{v}} + \Sigma) \]
\[ \rho c_p (D_t T) = D_t P + \nabla \cdot (\mu \nabla T + \Xi) + (\eta \overline{\nabla \mathbf{v}} + \Sigma) : \nabla \mathbf{v}, \]

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:

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

\[ \langle \mathcal{W}_{ij}(\mathbf{r}, t) \mathcal{W}^*_{kl}(\mathbf{r}', t') \rangle = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - 2\delta_{ij}\delta_{kl}/3) \delta(t - t')\delta(\mathbf{r} - \mathbf{r}') \].
We will consider a binary fluid mixture with mass concentration $c = \rho_1/\rho$ for two fluids that are dynamically identical, where $\rho = \rho_1 + \rho_2$.

Ignoring density and temperature fluctuations, equations of incompressible isothermal fluctuating hydrodynamics are

\[
\partial_t \mathbf{v} = \mathcal{P} \left[ -\mathbf{v} \cdot \nabla \mathbf{v} + \nu \nabla^2 \mathbf{v} + \rho^{-1} (\nabla \cdot \Sigma) \right] \\
\partial_t c = -\mathbf{v} \cdot \nabla c + \chi \nabla^2 c + \rho^{-1} (\nabla \cdot \Psi),
\]

where the kinematic viscosity $\nu = \eta/\rho$, and $\mathbf{v} \cdot \nabla c = \nabla \cdot (c\mathbf{v})$ and $\mathbf{v} \cdot \nabla \mathbf{v} = \nabla \cdot (\mathbf{v}\mathbf{v}^T)$ because of incompressibility, $\nabla \cdot \mathbf{v} = 0$.

Here $\mathcal{P}$ is the orthogonal projection onto the space of divergence-free velocity fields.
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 and low Mach number 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, 6].
Fluctuating Hydrodynamics

Finite-Volume Schemes

\[ c_t = -\mathbf{v} \cdot \nabla c + \chi \nabla^2 c + \nabla \cdot \left( \sqrt{2\chi} \mathcal{W} \right) = \nabla \cdot \left[ -c\mathbf{v} + \chi \nabla c + \sqrt{2\chi} \mathcal{W} \right] \]

- Generic finite-volume spatial discretization

\[ c_t = D \left[ (-Vc + Gc) + \sqrt{2\chi / (\Delta t \Delta V)} \mathcal{W} \right], \]

where \( D : \text{faces} \rightarrow \text{cells} \) is a conservative discrete divergence, \( G : \text{cells} \rightarrow \text{faces} \) is a discrete gradient.

- Here \( \mathcal{W} \) is a collection of random normal numbers representing the (face-centered) stochastic fluxes.

- The divergence and gradient should be duals, \( D^* = -G \).

- Advection should be skew-adjoint (non-dissipative) if \( \nabla \cdot \mathbf{v} = 0 \),

\[ (DV)^* = -(DV) \text{ if } (DV) \mathbf{1} = 0. \]
Figure: Equilibrium discrete spectra (static structure factors) $S_{\rho,\rho}(k) \sim \langle \hat{\rho} \hat{\rho}^* \rangle$ (should be unity for all discrete wavenumbers) and $S_{\rho,v}(k) \sim \langle \hat{\rho} \hat{v}_x^* \rangle$ (should be zero) for our RK3 collocated scheme.
Figure: Hybrid method for a polymer chain.
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.
Hybrid Particle-Continuum Method

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.

The adiabatic piston problem

MNG
Figure: Massive rigid piston ($M/m = 4000$) not in mechanical equilibrium: The deterministic hybrid gives the wrong answer!
When macroscopic gradients are present, steady-state thermal fluctuations become **long-range correlated**.

Consider a **binary mixture** of fluids and consider **concentration fluctuations** around a steady state $c_0(r)$:

$$c(r, t) = c_0(r) + \delta c(r, t)$$

The concentration fluctuations are **advected by the random velocities** $v(r, t) = \delta v(r, t)$, approximately:

$$\partial_t (\delta c) + (\delta v) \cdot \nabla c_0 = \chi \nabla^2 (\delta c) + \sqrt{2\chi k_B T} (\nabla \cdot \mathcal{W}_c)$$

The velocity fluctuations drive and amplify the concentration fluctuations leading to so-called **giant fluctuations** [7].
Figure: Snapshots of concentration in a miscible mixture showing the development of a *rough* diffusive interface between two miscible fluids in zero gravity [3, 7, 5].
Figure: Experimental results by A. Vailati et al. from a microgravity environment [7] showing the enhancement of concentration fluctuations in space (box scale is macroscopic: 5mm on the side, 1mm thick).
The nonlinear concentration equation includes a contribution to the mass flux due to advection by the fluctuating velocities,

\[ \partial_t (\delta c) + (\delta v) \cdot \nabla c_0 = \nabla \cdot \left[ - (\delta c) (\delta v) + \chi \nabla (\delta c) \right] + \ldots \]

Simple (quasi-linear) perturbative theory suggests that concentration and velocity fluctuations become correlated and

\[ -\langle (\delta c) (\delta v) \rangle \approx (\Delta \chi) \nabla c_0. \]

The fluctuation-renormalized diffusion coefficient is \( \chi + \Delta \chi \) (think of eddy diffusivity in turbulent transport).

Because fluctuations are affected by boundaries, \( \Delta \chi \) is system-size dependent.
Consider the effective diffusion coefficient in a system of dimensions $L_x \times L_y \times L_z$ with a concentration gradient imposed along the $y$ axis.

In two dimensions, $L_z \ll L_x \ll L_y$, linearized fluctuating hydrodynamics predicts a logarithmic divergence

$$\chi_{\text{eff}}^{(2D)} \approx \chi + \frac{k_B T}{4\pi \rho(\chi + \nu)L_z} \ln \frac{L_x}{L_0}$$

In three dimensions, $L_x = L_z = L \ll L_y$, $\chi_{\text{eff}}$ converges as $L \to \infty$ to the macroscopic diffusion coefficient,

$$\chi_{\text{eff}}^{(3D)} \approx \chi + \frac{\alpha k_B T}{\rho(\chi + \nu)} \left( \frac{1}{L_0} - \frac{1}{L} \right)$$

We have verified these predictions using particle (DSMC) simulations at hydrodynamic scales [3].
Fluctuation-Enhanced Diffusive Mixing

Particle Simulations

Figure: Divergence of diffusion coefficient in two dimensions.

- **Kinetic theory**: $\chi_{\text{eff}}$ (System A)
- $\chi_0$ (System A)
- $\chi_{\text{eff}}$ (System B)
- $\chi_0$ (System B)
- $\chi_{\text{eff}}$ (SPDE, A)

Theory $\chi_0$ (A)
Theory $\chi_0$ (B)
Theory $\chi_{\text{eff}}$
Consider a particle of diameter $a$ with position $\mathbf{q}(t)$ and its 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.

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:

$$ f_{\text{ind}} = -\lambda \delta_a (\mathbf{q} - \mathbf{r}) = -S\lambda, $$

where $\delta_a$ 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

$$\rho \left( \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \nabla \cdot \sigma - S \lambda$$  \hspace{1cm} (1)

$$m_e \dot{u} = F + \lambda$$  \hspace{1cm} (2)

subject to

$$u = J\mathbf{v} = \int \delta_a (\mathbf{q} - \mathbf{r}) \mathbf{v} (\mathbf{r}, t) \, d\mathbf{r},$$  \hspace{1cm} (3)

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

Here $m_e$ is the **excess mass** of the particle over the “dragged fluid”, and the **effective mass** is

$$m = m_e + m_f = m + \rho \left( JS \right)^{-1} = m + \rho \Delta V$$

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

$$\rho_{\text{eff}} = \rho + \Delta m S J.$$
One must ensure fluctuation-dissipation balance in the coupled fluid-particle system, with effective Hamiltonian

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

and implement a discrete scheme.

We investigate the **velocity autocorrelation function** (VACF) for a Brownian bead

\[ C(t) = 2d^{-1} \langle \mathbf{v}(t_0) \cdot \mathbf{v}(t_0 + t) \rangle \]

Hydrodynamic persistence (conservation) gives a **long-time power-law tail** \( C(t) \sim (t/t_\nu)^{-3/2} \) that can be quantified using fluctuating hydrodynamics.

From equipartition theorem \( C(0) = k_B T/m \), but incompressible hydrodynamic theory gives \( C(t > t_c) = 2/3 \left( k_B T/m \right) \) for a neutrally-boyant particle.
Figure: (Work with Florencio Balboa and Rafael Delgado-Buscallioni) Normalized VACF \( C(t) = \langle v_x(0)v_x(t) \rangle \) for different fluid compressibilities (speeds of sound).
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 continuum hydrodynamics and in compressible, incompressible, and low Mach number finite-volume solvers.

Instead of an ill-defined “molecular” or “bare” diffusivity, one should define a locally renormalized diffusion coefficient $\chi_0$ that depends on the length-scale of observation.

Direct fluid-structure coupling between fluctuating hydrodynamics and microstructure.
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.

Fluctuating Lattice Boltzmann.

Fractal fronts of diffusion in microgravity.
*Nature Communications*, 2:290, 2011.