Stochastic Simulation of Complex Fluid Flows

Aleksandar Donev

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

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1. Fluctuating Hydrodynamics

2. Giant Fluctuations in Diffusive Mixing

3. Direct Fluid-Particle Coupling
Levels of Coarse-Graining

Figure: From Pep Español, “Statistical Mechanics of Coarse-Graining”
Formally, we consider the continuum field of conserved quantities

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

where the symbol \( \approx \) means that \( \mathbf{U}(\mathbf{r}, t) \) approximates the true atomistic configuration \( \tilde{\mathbf{U}}(\mathbf{r}, t) \) 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 [1].

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 **density** \( \rho \), **velocity** \( \mathbf{v} \), and **temperature** \( T \) fields,

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

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

$$
\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla \pi + \nu \nabla^2 \mathbf{v} + \nabla \cdot \left( \sqrt{2\nu \rho^{-1} k_B T} \mathcal{W} \right)
$$

$$
\partial_t c + \mathbf{v} \cdot \nabla c = \chi \nabla^2 c + \nabla \cdot \left( \sqrt{2m\chi \rho^{-1} c(1 - c)} \mathcal{W}^{(c)} \right),
$$

where the kinematic viscosity $\nu = \eta/\rho$, and $\pi$ is determined from incompressibility, $\nabla \cdot \mathbf{v} = 0$.

We assume that $\mathcal{W}$ can be modeled as spatio-temporal white noise (a delta-correlated Gaussian random field), e.g.,

$$
\langle \mathcal{W}_{ij}(\mathbf{r}, t) \mathcal{W}_{kl}^*(\mathbf{r}', t') \rangle = (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \delta(t - t') \delta(\mathbf{r} - \mathbf{r}').
$$
- Adding stochastic fluxes to the **non-linear** NS equations produces **ill-behaved stochastic PDEs** (solution is too irregular).
- No problem if we **linearize** the equations around a **steady mean state**, to obtain equations for the fluctuations around the mean,

\[ U = \langle U \rangle + \delta U = U_0 + \delta U. \]

- Finite-volume discretizations naturally impose a grid-scale **regularization** (smoothing) of the stochastic forcing.
- A **renormalization** of the transport coefficients is also necessary [2].
- 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) [3, 4].
- Solving these sort of equations numerically requires paying attention to **discrete fluctuation-dissipation balance**, in addition to the usual deterministic difficulties [3].
$c_t = -v \cdot \nabla c + \chi \nabla^2 c + \nabla \cdot \left( \sqrt{2\chi} \mathcal{W} \right) = \nabla \cdot \left[ -cv + \chi \nabla c + \sqrt{2\chi} \mathcal{W} \right]$ 

- Generic **finite-volume spatial discretization**

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

where $D : \text{faces} \to \text{cells}$ is a **conservative** discrete divergence, $G : \text{cells} \to \text{faces}$ 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 $\nabla \cdot v = 0$,

$$ (DV)^* = - (DV) \text{ if } (DV)1 = 0. $$
Figure: Spectral power of the first solenoidal mode for an incompressible fluid as a function of the wavenumber. The left panel is for a (normalized) time step $\alpha = 0.5$, and the right for $\alpha = 0.25$. 
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 $\mathbf{v}(r, t) = \delta \mathbf{v}(r, t)$, approximately:

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

The velocity fluctuations drive and amplify the concentration fluctuations leading to so-called **giant fluctuations** [5].
Snapshots of concentration in a miscible mixture showing the development of a *rough* diffusive interface between two miscible fluids in zero gravity [2, 5, 4]. A similar pattern is seen over a broad range of Schmidt numbers and is affected strongly by nonzero gravity.
Animation: Changing Schmidt Number
Animation: Diffusive Mixing in Gravity
Experimental results by A. Vailati et al. from a microgravity environment [5] showing the enhancement of concentration fluctuations in space (box scale is **macroscopic**: 5mm on the side, 1mm thick).
Figure: Computer simulations of microgravity experiments.
The linearized equations can be solved in the Fourier domain (ignoring boundaries for now) for any wavenumber $k$, denoting $k_\perp = k \sin \theta$ and $k_\parallel = k \cos \theta$.

One finds giant concentration fluctuations proportional to the square of the applied gradient,

$$S_{c,c}^{\text{neq}} = \langle (\hat{\delta}c)(\hat{\delta}c^*) \rangle = \frac{k_B T}{\rho \chi(\nu + \chi)k^4} (\sin^2 \theta) (\nabla \bar{c})^2,$$

(1)

The finite height of the container $h$ imposes no-slip boundary conditions, which damps the power law at wavenumbers $k \sim 2\pi/h$.

This is difficult to calculate analytically and one has to make drastic approximations, and simulations are ideal to compare to experiments.

However, the separation of time scales between the slow diffusion and fast vorticity fluctuations poses a big challenge.
Simulation vs. Experiments

Figure: Giant fluctuations: simulation vs. experiment vs. approximate theory.
We want to construct a bidirectional coupling between a fluctuating fluid and a small spherical Brownian particle (blob).

Macroscopic coupling between flow and a rigid sphere:

- **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.

We saw already that fluctuations should be taken into account at the continuum level.
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 Rafael Delgado-Buscalioni’s talk and paper [6].
Postulate a **no-slip condition** between the particle and local fluid velocities,

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

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 \emph{local averaging operator} \(J(q)\) and the \emph{local spreading operator} \(S(q)\) are **adjoint**, \(S = J^*\).
The equations of motion in our coupling approach are postulated (Pep Español is working on a derivation) to be

\[
\rho (\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = -\nabla \pi + \nu \nabla^2 \mathbf{v} + \nabla \cdot \Sigma - [S (q)] \lambda + \text{corrections}
\]

\[
\dot{u} = F (q) + \lambda
\]

s.t. \( u = [J (q)] \mathbf{v} \) and \( \nabla \cdot \mathbf{v} = 0 \),

where \( \lambda \) is a Lagrange multiplier that enforces the no-slip condition, \( F (q) = -\nabla U (q) \) is the applied force, and \( m_e \) is the excess mass of the particle.

The fluctuationing stress \( \Sigma = \sqrt{2 \nu \rho^{-1} k_B T \mathcal{W}} \) drives the Brownian motion.

In the existing (stochastic) IBM approaches (Paul Atzberger) inertial effects are ignored, \( m_e = 0 \) and thus \( \lambda = -F \).

In the standard approach [7] a frictional (dissipative) force \( \lambda = -\zeta (u - Jv) \) is used instead of a constraint.
Eliminating $\lambda$ we get the particle equation of motion

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

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

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

For the fluid we get the effective equation

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

where the effective mass density matrix (operator) is

$$\rho_{\text{eff}} = \rho + m_e \mathcal{P}SJ \mathcal{P},$$

where $\mathcal{P}$ is the $L_2$ projection operator onto the linear subspace $\nabla \cdot v = 0$. 
One must ensure **fluctuation-dissipation balance** in the coupled fluid-particle system.

This really means that the **stationary** (equilibrium) distribution must be the **Gibbs distribution**

\[
P (v, u, q) = Z^{-1} \exp \left[ -\beta H \right]
\]

where the **Hamiltonian** is postulated to be

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

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

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

The dynamics is **not incompressible in phase space** and so the interpretation of the stochastic terms matters (perhaps Klimontovich?).
Both compressible (explicit) and incompressible schemes have been implemented by Florencio Balboa (UAM) on GPUs.

Spatial discretization is based on previously-developed staggered schemes for fluctuating hydro [4] and the IBM kernel functions of Charles Peskin [8].

Temporal discretization follows a second-order splitting algorithm (move particle + update momenta), and is unconditionally unstable.

The scheme ensures strict conservation of momentum and (almost exactly) enforces the no-slip condition at the end of the time step.

Continuing work on temporal integrators that ensure the correct equilibrium distribution and diffusive (Brownian) dynamics.
We investigate the velocity autocorrelation function (VACF) for the immersed particle

\[ C(t) = \langle u(t_0) \cdot u(t_0 + t) \rangle \]

From equipartition theorem \( C(0) = kT/m \).

However, for an incompressible fluid the kinetic energy of the particle that is less than equipartition,

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

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

Hydrodynamic persistence (conservation) gives a \textbf{long-time power-law tail} \( C(t) \sim (kT/m)(t/t_{\text{visc}})^{-3/2} \) not reproduced in Brownian dynamics.
Figure: (F. Balboa) VACF for a blob with $m_e = m_f = \rho \Delta V$. 
This approach can be extended to immersed rigid bodies (see work by Neelesh Patankar)

\[
\rho \left( \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla \pi + \nu \nabla^2 \mathbf{v} + \nabla \cdot \Sigma - \int_{\Omega} S (q) \lambda (q) \, dq + \, ?
\]

\[
m_e \dot{\mathbf{u}} = F + \int_{\Omega} \lambda (q) \, dq
\]

\[
l_e \dot{\omega} = \tau + \int_{\Omega} [q \times \lambda (q)] \, dq
\]

\[
[J (q)] \mathbf{v} = \mathbf{u} + q \times \omega \quad \text{for all } q \in \Omega
\]

\[
\nabla \cdot \mathbf{v} = 0 \quad \text{everywhere}.
\]

Here \( \omega \) is the immersed body angular velocity, \( \tau \) is the applied torque, and \( l_e \) is the excess moment of inertia of the particle.

The nonlinear advective terms are tricky and need to be carefully thought about, though it may not be a problem at low Reynolds number?
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