Coupling a Fluctuating Fluid with Suspended Structures

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Applied Math Seminar
NJIT
October 2012

Outline

1. Introduction
2. Fluctuating Hydrodynamics
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4. Numerics
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Micro- and nano-hydrodynamics

- Flows of fluids (gases and liquids) through micro- (μm) 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**.

Levels of Coarse-Graining

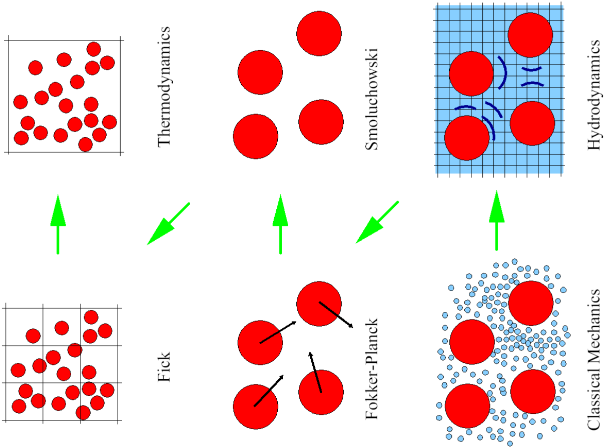
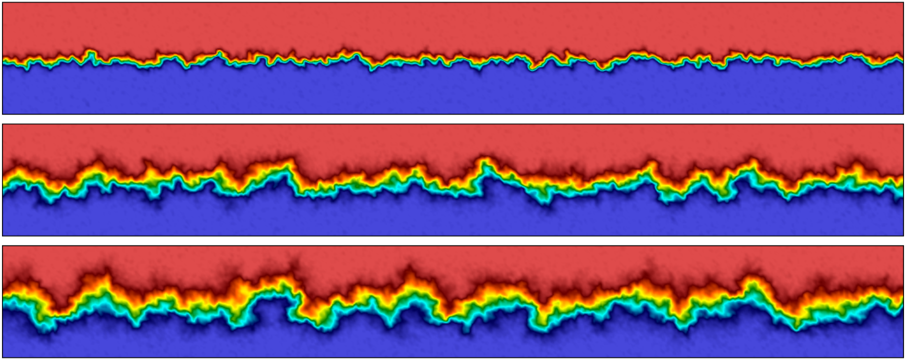


Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

Thermal Fluctuations Matter



Snapshots of concentration in a miscible mixture showing the development of a *rough* diffusive interface between two miscible fluids in zero gravity [1, 2, 3]. A similar pattern is seen over a broad range of Schmidt numbers and is affected strongly by nonzero gravity.

Fluctuating Navier-Stokes Equations

- We will consider a binary fluid mixture with mass **concentration** $c = \rho_1/\rho$ for two fluids that are dynamically **identical**, where $\rho = \rho_1 + \rho_2$ (e.g., **fluorescently-labeled** molecules).
- Ignoring density and temperature fluctuations, equations of **incompressible isothermal fluctuating hydrodynamics** are

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

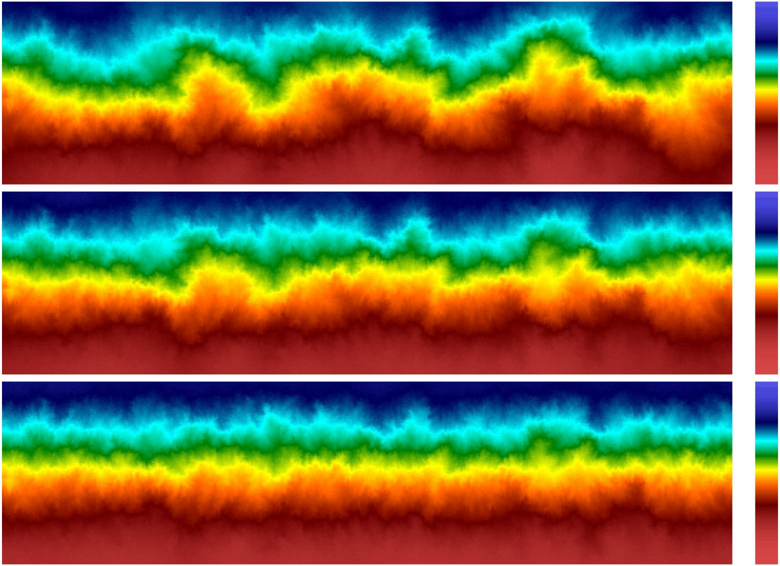
$$\partial_t c + \mathbf{v} \cdot \boldsymbol{\nabla} c = \chi \boldsymbol{\nabla}^2 c + \boldsymbol{\nabla} \cdot \left(\sqrt{2m\chi\rho^{-1} \, c(1-c)} \, \boldsymbol{\mathcal{W}}^{(c)} \right),$$

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

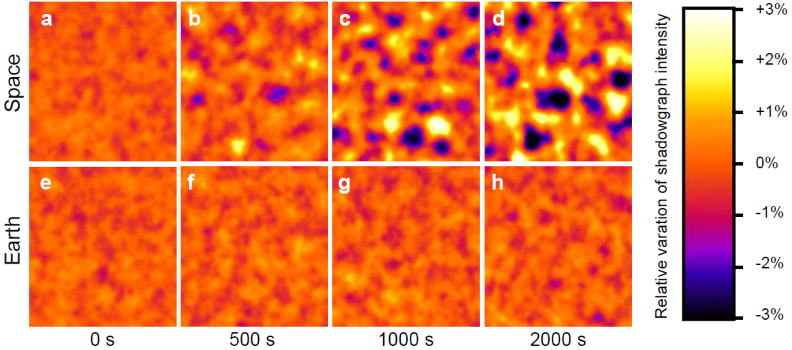
- We assume that $\boldsymbol{\mathcal{W}}$ can be modeled as spatio-temporal **white noise** (a delta-correlated Gaussian random field), e.g.,

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

Fractal Fronts in Diffusive Mixing



Giant Fluctuations in Experiments



Experimental results by A. Vailati *et al.* from a microgravity environment [2] showing the enhancement of concentration fluctuations in space (box scale is **macroscopic**: 5mm on the side, 1mm thick)..

Fluctuating Hydrodynamics Equations

- 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.
- Finite-volume discretizations naturally impose a grid-scale **regularization** (smoothing) of the stochastic forcing.
- A **renormalization** of the transport coefficients is also necessary [1].
- 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, 3].
- Solving these sort of equations numerically requires paying attention to **discrete fluctuation-dissipation balance**, in addition to the usual deterministic difficulties [4].

Finite-Volume Schemes

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

- Generic **finite-volume spatial discretization**

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

  where $\mathbf{D}$: faces $\rightarrow$ cells is a **conservative** discrete divergence, $\mathbf{G}$: cells $\rightarrow$ faces is a discrete gradient.
- Here $\mathbf{W}$ is a collection of random normal numbers representing the (face-centered) stochastic fluxes.
- The **divergence** and **gradient** should be **duals**, $\mathbf{D}^\star = -\mathbf{G}$.
- Advection should be **skew-adjoint** (non-dissipative) if $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$,

$$(\mathbf{DV})^\star = -(\mathbf{DV}) \text{ if } (\mathbf{DV})\,\mathbf{1} = \mathbf{0}.$$

Weak Accuracy

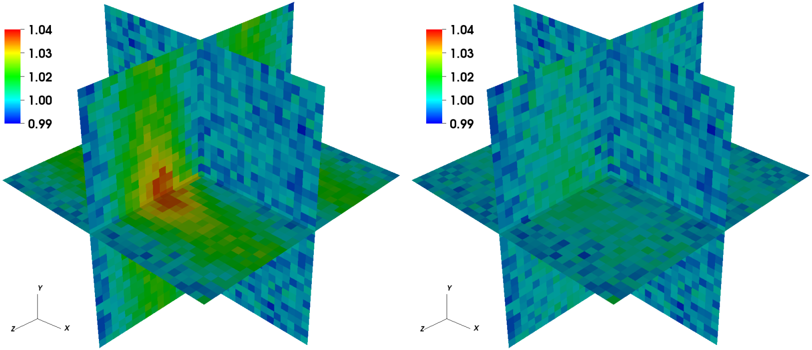


Figure: Spectral power of the first solenoidal mode for an incompressible fluid as a function of the wavenumber. The left panel is for a (normalized) time step $\alpha = 0.5$, and the right for $\alpha = 0.25$.

Fluid-Structure Coupling

- 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**.

Brownian Particle Model

- Consider a **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 particle.
- We will call our particles "**blobs**" since they are not really point particles.

Local Averaging and Spreading Operators

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

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

  where the *local averaging* linear operator $\mathbf{J}(\mathbf{q})$ averages the fluid velocity inside the particle to estimate a local fluid velocity.
- The **induced force density** in the fluid because of the particle is:

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

  where the *local spreading* linear operator $\mathbf{S}(\mathbf{q})$ is the reverse (adjoint) of $\mathbf{J}(\mathbf{q})$.
- The physical **volume** of the particle ΔV is related to the shape and width of the kernel function via

$$\Delta V = (\mathbf{JS})^{-1} = \left[\int \delta_a^2(\mathbf{r})\,d\mathbf{r}\right]^{-1}. \tag{1}$$

Fluid-Structure Direct Coupling

- The equations of motion in our coupling approach are **postulated** [5] to be

$$
\begin{aligned}
\rho\left(\partial_t \mathbf{v}+\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}\right) &= -\boldsymbol{\nabla}\pi-\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}-\left[\mathbf{S}\left(\mathbf{q}\right)\right]\boldsymbol{\lambda}+\text{thermal drift}\\
m_e\dot{\mathbf{u}} &= \mathbf{F}\left(\mathbf{q}\right)+\boldsymbol{\lambda}\\
\text{s.t. }\mathbf{u} &= \left[\mathbf{J}\left(\mathbf{q}\right)\right]\mathbf{v}\text{ and }\boldsymbol{\nabla}\cdot\mathbf{v}=0,
\end{aligned}
$$

  where $\boldsymbol{\lambda}$ is the **fluid-particle force**, $\mathbf{F}\left(\mathbf{q}\right)=-\boldsymbol{\nabla}U\left(\mathbf{q}\right)$ is the externally **applied force**, and m_e is the **excess mass** of the particle.
- The stress tensor $\boldsymbol{\sigma}=\eta\left(\boldsymbol{\nabla}\mathbf{v}+\boldsymbol{\nabla}^T\mathbf{v}\right)+\boldsymbol{\Sigma}$ includes viscous (dissipative) and stochastic contributions. The **stochastic stress**

$$
\boldsymbol{\Sigma}=\left(2k_BT\eta\right)^{1/2}\boldsymbol{\mathcal{W}}
$$

  drives the Brownian motion.
- In the existing (stochastic) IBM approaches [6] **inertial effects** are ignored, $m_e=0$ and thus $\boldsymbol{\lambda}=-\mathbf{F}$.

Momentum Conservation

- In the standard approach a frictional (dissipative) force $\boldsymbol{\lambda} = -\zeta\left(\mathbf{u} - \mathbf{J}\mathbf{v}\right)$ is used instead of a constraint.
- In either coupling the total particle-fluid momentum is conserved,

$$\mathbf{P} = m_e\mathbf{u} + \int \rho\mathbf{v}\left(\mathbf{r}, t\right) d\mathbf{r}, \quad \frac{d\mathbf{P}}{dt} = \mathbf{F}.$$

- Define a *momentum field* as the sum of the fluid momentum and the spreading of the particle momentum,

$$\mathbf{p}\left(\mathbf{r}, t\right) = \rho\mathbf{v} + m_e\mathbf{S}\mathbf{u} = \left(\rho + m_e\mathbf{S}\mathbf{J}\right)\mathbf{v}.$$

- Adding the fluid and particle equations gives a **local momentum conservation law**

$$\partial_t\mathbf{p} = -\boldsymbol{\nabla}\pi - \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} - \boldsymbol{\nabla}\cdot\left[\rho\mathbf{v}\mathbf{v}^T + m_e\mathbf{S}\left(\mathbf{u}\mathbf{u}^T\right)\right] + \mathbf{S}\mathbf{F}.$$

Effective Inertia

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

$$m\dot{\mathbf{u}} = \Delta V \, \mathbf{J} \left(\boldsymbol{\nabla}\pi + \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} \right) + \mathbf{F} + \text{blob correction},$$

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

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

- For the fluid we get the effective equation

$$\boldsymbol{\rho}_{\text{eff}} \partial_t \mathbf{v} = - \left[\rho \left(\mathbf{v} \cdot \boldsymbol{\nabla} \right) + m_e \mathbf{S} \left(\mathbf{u} \cdot \frac{\partial}{\partial \mathbf{q}} \mathbf{J} \right) \right] \mathbf{v} - \boldsymbol{\nabla}\pi - \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} + \mathbf{SF}$$

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

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

where $\mathcal{P}$ is the L_2 **projection operator** onto the linear subspace $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$, with the appropriate BCs.

Fluctuation-Dissipation Balance

- One must ensure **fluctuation-dissipation balance** in the coupled fluid-particle system.
- We can eliminate the particle velocity using the no-slip constraint, so only $\mathbf{v}$ and $\mathbf{q}$ are independent DOFs.
- This really means that the **stationary** (equilibrium) distribution must be the **Gibbs distribution**

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

where the **Hamiltonian** (coarse-grained free energy) is

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

$$=U\left(\mathbf{q}\right)+\int\frac{\mathbf{v}^T\rho_{\text{eff}}\mathbf{v}}{2}\,d\mathbf{r}$$

- No entropic contribution to the coarse-grained free energy because our formulation is isothermal and the particles do not have internal structure.

contd.

- A key ingredient of fluctuation-dissipation balance is that that the fluid-particle **coupling is non-dissipative**, i.e., in the absence of viscous dissipation the kinetic energy H is conserved.
- Crucial for **energy conservation** is that $\mathbf{J}(\mathbf{q})$ and $\mathbf{S}(\mathbf{q})$ are **adjoint**, $\mathbf{S} = \mathbf{J}^{\star}$,

$$(\mathbf{J}\mathbf{v}) \cdot \mathbf{u} = \int \mathbf{v} \cdot (\mathbf{S}\mathbf{u})\, d\mathbf{r} = \int \delta_a (\mathbf{q} - \mathbf{r}) (\mathbf{v} \cdot \mathbf{u})\, d\mathbf{r}. \tag{2}$$

- The dynamics is **not incompressible in phase space** and "**thermal drift**" correction terms need to be included [6], but they turn out to **vanish** for incompressible flow (gradient of scalar).
- The spatial discretization should preserve these properties: **discrete fluctuation-dissipation balance (DFDB)**.

Numerical Scheme

- 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 [3] and the **IBM kernel functions** of Charles Peskin [7].
- Temporal discretization follows a second-order **splitting algorithm** (move particle + update momenta), and is limited in **stability** only by **advective CFL**.
- 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**.

Temporal Integrator (sketch)

- **Predict** particle position at midpoint:

$$\mathbf{q}^{n+\frac{1}{2}} = \mathbf{q}^{n} + \frac{\Delta t}{2} \mathbf{J}^{n} \mathbf{v}^{n}.$$

- Solve unperturbed fluid equation using **stochastic Crank-Nicolson** for viscous+stochastic:

$$\begin{aligned} \rho \frac{\tilde{\mathbf{v}}^{n+1} - \mathbf{v}^{n}}{\Delta t} + \boldsymbol{\nabla} \tilde{\pi} &= \frac{\eta}{2} \mathbf{L} \left(\tilde{\mathbf{v}}^{n+1} + \mathbf{v}^{n} \right) + \boldsymbol{\nabla} \cdot \boldsymbol{\Sigma}^{n} + \mathbf{S}^{n+\frac{1}{2}} \mathbf{F}^{n+\frac{1}{2}} + \text{adv.}, \\ \boldsymbol{\nabla} \cdot \tilde{\mathbf{v}}^{n+1} &= 0, \end{aligned}$$

  where we use the **Adams-Bashforth method** for the advective (kinetic) fluxes, and the discretization of the stochastic flux is described in Ref. [3],

$$\boldsymbol{\Sigma}^{n} = \left(\frac{2 k_B T \eta}{\Delta V \, \Delta t} \right)^{1/2} \mathbf{W}^{n},$$

  where $\mathbf{W}^{n}$ is a (symmetrized) collection of i.i.d. unit normal variates.

contd.

- Solve for inertial **velocity perturbation** from the particle $\Delta\mathbf{v}$ (too technical to present), and update:

$$\mathbf{v}^{n+1} = \tilde{\mathbf{v}}^{n+1} + \Delta\mathbf{v}.$$

If neutrally-buyoant $m_e = 0$ this is a non-step, $\Delta\mathbf{v} = \mathbf{0}$.

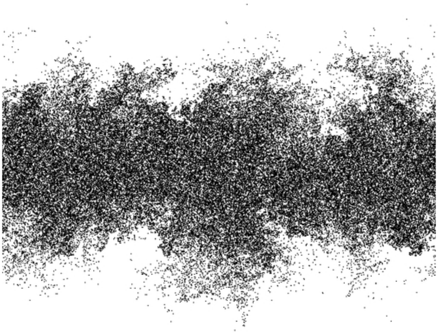
- Update particle velocity in a momentum conserving manner,

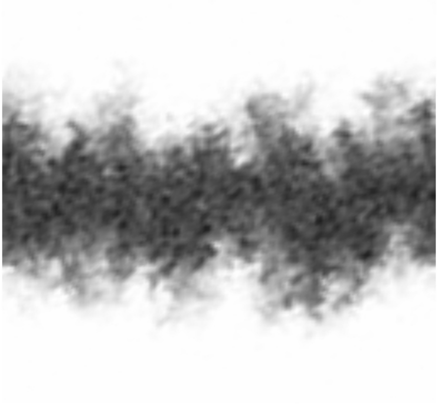
$$\mathbf{u}^{n+1} = \mathbf{J}^{n+\frac{1}{2}}\mathbf{v}^{n+1} + \text{conservation correction}.$$

- **Correct** particle position,

$$\mathbf{q}^{n+1} = \mathbf{q}^{n} + \frac{\Delta t}{2}\mathbf{J}^{n+\frac{1}{2}}\left(\mathbf{v}^{n+1} + \mathbf{v}^{n}\right).$$

Passively-Advected (Fluorescent) Tracers





Velocity Autocorrelation Function

- We investigate the **velocity autocorrelation function** (VACF) for the immersed particle

$$C(t) = \langle \mathbf{u}(t_0) \cdot \mathbf{u}(t_0 + t) \rangle$$

- 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 **long-time power-law tail** $C(t) \sim (kT/m)(t/t_{\text{visc}})^{-3/2}$ *not* reproduced in Brownian dynamics.

Numerical VACF

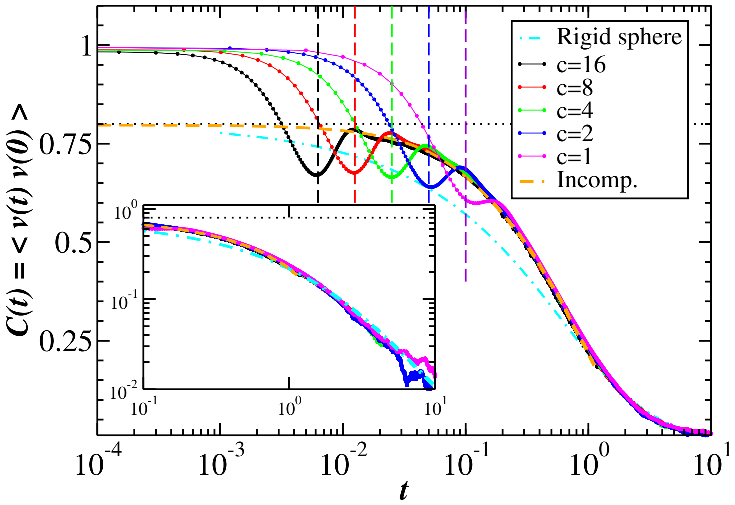


Figure: (F. Balboa) VACF for a blob with $m_e = m_f = \rho \Delta V$.

Immersed Rigid Blobs

- Unlike a **rigid sphere**, a blob particle would not perturb a pure shear flow.
- In the far field our blob particle looks like a force monopole (**stokeset**), and does not exert a force dipole (**stresslet**) on the fluid.
- Similarly, since here we do not include **angular velocity** degrees of freedom, our blob particle does not exert a **torque** on the fluid (rotlet).
- It is possible to include rotlet and stresslet terms, as done in the force coupling method [8] and Stokesian Dynamics in the deterministic setting.
- Proper inclusion of inertial terms and fluctuation-dissipation balance not studied carefully yet...

Immersed Rigid Bodies

- This approach can be extended to immersed rigid bodies (see work by Neelesh Patankar)

$$\begin{aligned}
\rho\left(\partial_t \mathbf{v}+\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}\right) &= -\boldsymbol{\nabla}\pi-\boldsymbol{\nabla}\cdot\boldsymbol{\sigma}-\int_{\Omega}\mathbf{S}\left(\mathbf{q}\right)\boldsymbol{\lambda}\left(\mathbf{q}\right)d\mathbf{q}+\text{th. drift}\\
m_e\dot{\mathbf{u}} &= \mathbf{F}+\int_{\Omega}\boldsymbol{\lambda}\left(\mathbf{q}\right)d\mathbf{q}\\
I_e\dot{\boldsymbol{\omega}} &= \boldsymbol{\tau}+\int_{\Omega}\left[\mathbf{q}\times\boldsymbol{\lambda}\left(\mathbf{q}\right)\right]d\mathbf{q}\\
\left[\mathbf{J}\left(\mathbf{q}\right)\right]\mathbf{v} &= \mathbf{u}+\mathbf{q}\times\boldsymbol{\omega}\text{ for all }\mathbf{q}\in\Omega\\
\boldsymbol{\nabla}\cdot\mathbf{v} &= 0\text{ everywhere.}
\end{aligned}$$

  Here $\boldsymbol{\omega}$ is the immersed body angular velocity, $\boldsymbol{\tau}$ is the applied torque, and I_e is the **excess moment of inertia** of the particle.
- The nonlinear advective terms are tricky, though it may not be a problem at low Reynolds number...
- Fluctuation-dissipation balance needs to be studied carefully...

Conclusions

- Fluctuations are **not just a microscopic phenomenon**: giant fluctuations can reach macroscopic dimensions or certainly dimensions much larger than molecular.
- **Fluctuating hydrodynamics** seems to be a very good coarse-grained model for fluids, despite unresolved issues.
- **Particle inertia** can be included in the coupling between blob particles and a fluctuating incompressible fluid.
- Even coarse-grained methods need to be accelerated due to **large separation of time scales** between advective and diffusive phenomena.
- One can take the **overdamped** (Brownian dynamics) **limit** but it would be much better to construct **many-scale temporal integrators** that are accurate even when they under-resolve the fast fluctuations.

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