Stochastic Simulation of Complex Fluid Flows

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Outline

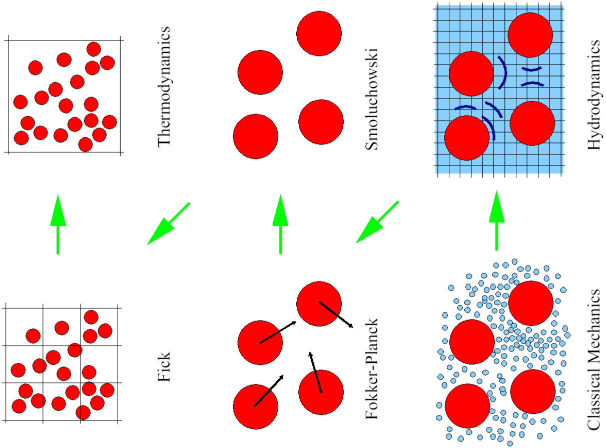


Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

Continuum Models of Fluid Dynamics

- Formally, we consider the continuum field of **conserved quantities**

$$\mathbf{U}(\mathbf{r},t)=\begin{bmatrix}\rho\\ \mathbf{j}\\ e\end{bmatrix}\cong\widetilde{\mathbf{U}}(\mathbf{r},t)=\sum_i\begin{bmatrix}m_i\\ m_i\boldsymbol{\upsilon}_i\\ m_i\upsilon_i^2/2\end{bmatrix}\delta\left[\mathbf{r}-\mathbf{r}_i(t)\right],$$

  where the symbol $\cong$ means that $\mathbf{U}(\mathbf{r},t)$ approximates the true atomistic configuration $\widetilde{\mathbf{U}}(\mathbf{r},t)$ 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.

Compressible Fluctuating Hydrodynamics

$$
\begin{aligned}
D_t\rho &= -\rho\boldsymbol{\nabla}\cdot\mathbf{v} \\
\rho\left(D_t\mathbf{v}\right) &= -\boldsymbol{\nabla}P + \boldsymbol{\nabla}\cdot\left(\eta\overline{\boldsymbol{\nabla}}\mathbf{v} + \boldsymbol{\Sigma}\right) \\
\rho c_p\left(D_t T\right) &= D_t P + \boldsymbol{\nabla}\cdot\left(\mu\boldsymbol{\nabla}T + \boldsymbol{\Xi}\right) + \left(\eta\overline{\boldsymbol{\nabla}}\mathbf{v} + \boldsymbol{\Sigma}\right) : \boldsymbol{\nabla}\mathbf{v},
\end{aligned}
$$

where the variables are the **density** ρ, **velocity** $\mathbf{v}$, and **temperature** T fields,

$$
\begin{aligned}
D_t\square &= \partial_t\square + \mathbf{v}\cdot\boldsymbol{\nabla}\left(\square\right) \\
\overline{\boldsymbol{\nabla}}\mathbf{v} &= \left(\boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}\mathbf{v}^T\right) - 2\left(\boldsymbol{\nabla}\cdot\mathbf{v}\right)\mathbf{I}/3
\end{aligned}
$$

and capital Greek letters denote stochastic fluxes:

$$
\boldsymbol{\Sigma} = \sqrt{2\eta k_B T}\,\mathcal{W}.
$$

$$
\langle\mathcal{W}_{ij}(\mathbf{r},t)\mathcal{W}^{\star}_{kl}(\mathbf{r}',t')\rangle = \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - 2\delta_{ij}\delta_{kl}/3\right)\delta(t-t')\delta(\mathbf{r}-\mathbf{r}').
$$

Incompressible Fluctuating Navier-Stokes

- 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

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

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

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.,

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

Fluctuating Navier-Stokes 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,

$$\mathbf{U} = \langle \mathbf{U} \rangle + \delta \mathbf{U} = \mathbf{U}_0 + \delta \mathbf{U}.$$

- 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].

Finite-Volume Schemes

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

- Generic **finite-volume spatial discretization**

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

  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 $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$,

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

Weak Accuracy

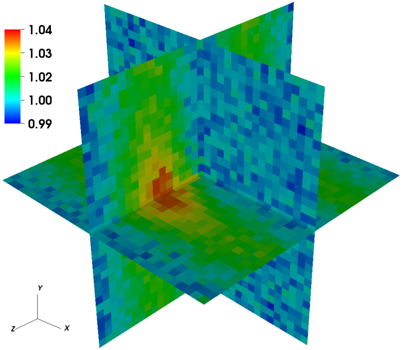


Figure: Spectral power of the first solenoidal mode for an incompressible fluid as a function of the wavenumber. The left panel is for a (normalized) time step $\alpha = 0.5$, and the right for $\alpha = 0.25$.

Nonequilibrium Fluctuations

- 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 $c_0(\mathbf{r})$:

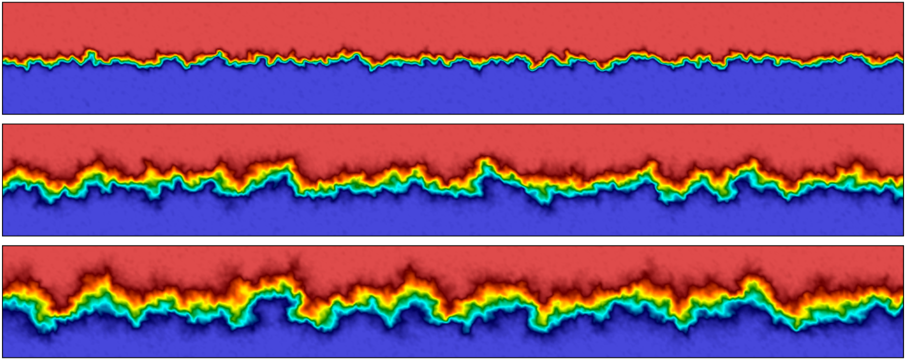
$$c(\mathbf{r}, t) = c_0(\mathbf{r}) + \delta c(\mathbf{r}, t)$$

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

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

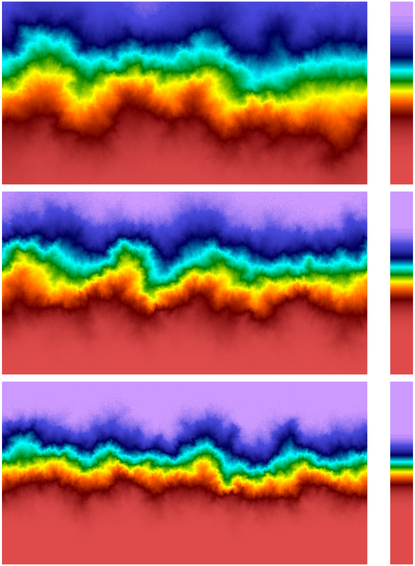
- The velocity fluctuations drive and amplify the concentration fluctuations leading to so-called **giant fluctuations** [5].

Fractal Fronts in Diffusive Mixing

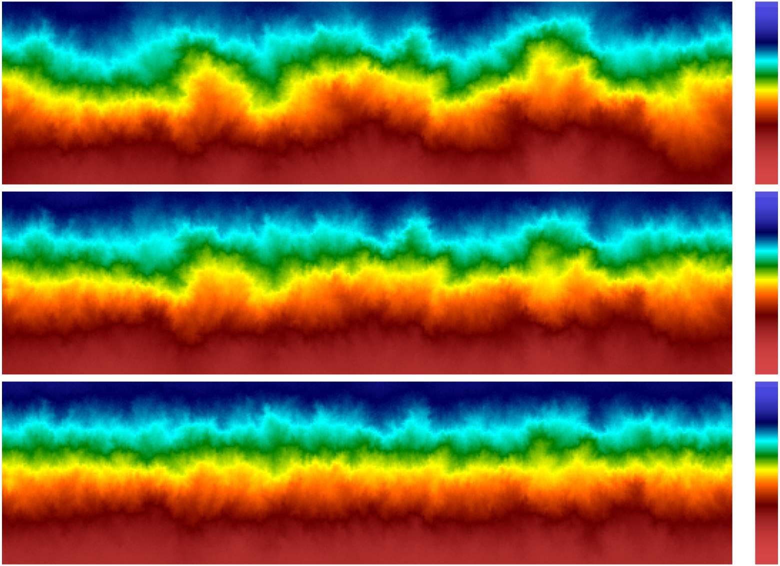


Snapshots of concentration in a miscible mixture showing the development of a *rough* diffusive interface between two miscible fluids in zero gravity [2, 5, 4]. A similar pattern is seen over a broad range of Schmidt numbers and is affected strongly by nonzero gravity.

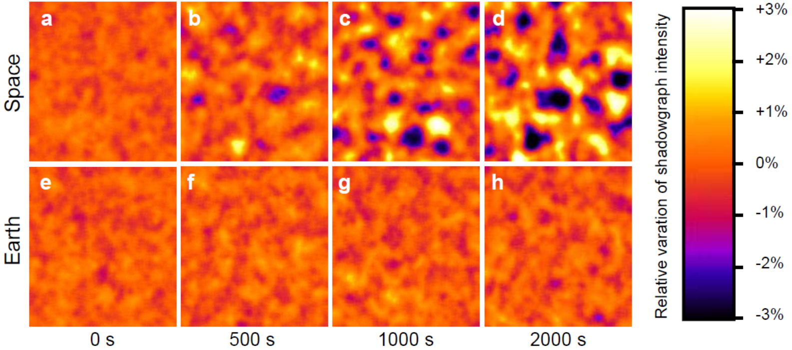
Animation: Changing Schmidt Number



Animation: Diffusive Mixing in Gravity



Giant Fluctuations in Experiments



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).

Giant Fluctuations in Simulations

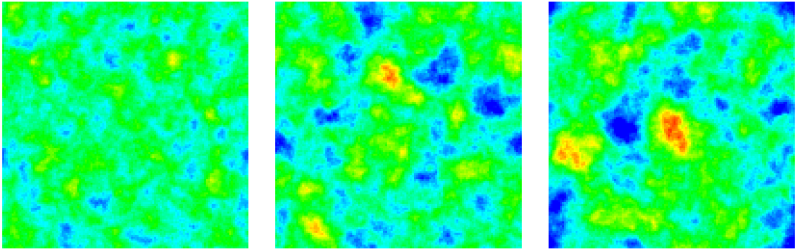


Figure: Computer simulations of microgravity experiments.

Spectrum of Concentration Fluctuations

- 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,

$$S_{c,c}^{\text{neq}} = \langle (\widehat{\delta c})(\widehat{\delta c}^\star) \rangle = \frac{k_B T}{\rho\chi(\nu+\chi)k^4} \left(\sin^2\theta\right) \left(\nabla \bar{c}\right)^2, \tag{1}$$

- 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

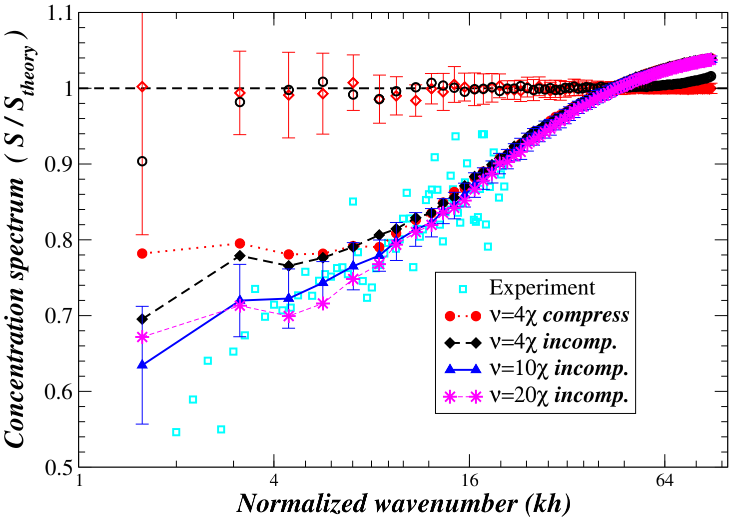


Figure: Giant fluctuations: simulation vs. experiment vs. *approximate* theory.

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**.

Fluid-Structure Coupling

- 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].

Local Averaging and Spreading Operators

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

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

  enforced by a Lagrange multiplier fluid-blob force $\boldsymbol{\lambda}$.
- The **induced force density** in the fluid because of the particle is:

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

  which ensures **momentum conservation**.
- Crucial for **energy conservation** is that the *local averaging operator* $\mathbf{J}(\mathbf{q})$ and the *local spreading operator* $\mathbf{S}(\mathbf{q})$ are **adjoint**, $\mathbf{S} = \mathbf{J}^{\star}$.

Fluid-Structure Direct Coupling

- The equations of motion in our coupling approach are **postulated** (Pep Español is working on a derivation) to be

$$\begin{aligned}\rho\left(\partial_t \mathbf{v}+\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}\right) &= -\boldsymbol{\nabla}\pi+\nu\boldsymbol{\nabla}^2\mathbf{v}+\boldsymbol{\nabla}\cdot\boldsymbol{\Sigma}-\left[\mathbf{S}\left(\mathbf{q}\right)\right]\boldsymbol{\lambda}+\text{corrections}\\ m_e\dot{\mathbf{u}} &= \mathbf{F}\left(\mathbf{q}\right)+\boldsymbol{\lambda}\\ \text{s.t. }\mathbf{u} &= \left[\mathbf{J}\left(\mathbf{q}\right)\right]\mathbf{v}\text{ and }\boldsymbol{\nabla}\cdot\mathbf{v}=0,\end{aligned}$$

  where $\boldsymbol{\lambda}$ is a Lagrange multiplier that enforces the **no-slip condition**, $\mathbf{F}\left(\mathbf{q}\right)=-\boldsymbol{\nabla}U\left(\mathbf{q}\right)$ is the applied force, and m_e is the **excess mass** of the particle.
- The **fluctuationing stress** $\boldsymbol{\Sigma}=\sqrt{2\nu\rho^{-1}k_B T}\,\boldsymbol{\mathcal{W}}$ drives the Brownian motion.
- In the existing (stochastic) IBM approaches (Paul Atzberger) **inertial effects** are ignored, $m_e=0$ and thus $\boldsymbol{\lambda}=-\mathbf{F}$.
- In the standard approach [7] a frictional (dissipative) force $\boldsymbol{\lambda}=-\zeta\left(\mathbf{u}-\mathbf{J}\mathbf{v}\right)$ is used instead of a constraint.

Effective Inertia

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

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

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

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

- For the fluid we get the effective equation

$$\boldsymbol{\rho}_{\mathrm{eff}} \partial_t \mathbf{v} = -\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} + \mathbf{S} \mathbf{F} + \ldots$$

  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 $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$.

Fluctuation-Dissipation Balance

- 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**

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

where the **Hamiltonian** is postulated to be

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

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

$$H(\mathbf{v}, \mathbf{q}) = U(\mathbf{q}) + \int \frac{\mathbf{v}^T \boldsymbol{\rho}_{\text{eff}} \mathbf{v}}{2} \, d\mathbf{r}$$

- The dynamics is **not incompressible in phase space** and so the interpretation of the stochastic terms matters (perhaps Klimontovich?).

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 [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**.

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

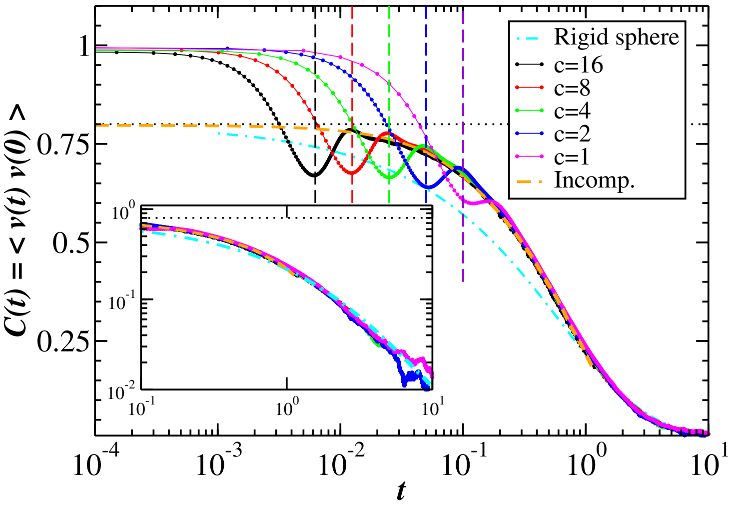


Figure: (F. Balboa) VACF for a blob with $m_e = m_f = \rho \Delta V$.

Extensions to Immersed Rigid Bodies

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

$$\begin{aligned}
\rho\left(\partial_t \mathbf{v} + \mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}\right) &= -\boldsymbol{\nabla}\pi + \nu\boldsymbol{\nabla}^2\mathbf{v} + \boldsymbol{\nabla}\cdot\boldsymbol{\Sigma} - \int_\Omega \mathbf{S}\left(\mathbf{q}\right)\boldsymbol{\lambda}\left(\mathbf{q}\right)d\mathbf{q} + ? \\
m_e\dot{\mathbf{u}} &= \mathbf{F} + \int_\Omega \boldsymbol{\lambda}\left(\mathbf{q}\right)d\mathbf{q} \\
I_e\dot{\boldsymbol{\omega}} &= \boldsymbol{\tau} + \int_\Omega \left[\mathbf{q}\times\boldsymbol{\lambda}\left(\mathbf{q}\right)\right]d\mathbf{q} \\
\left[\mathbf{J}\left(\mathbf{q}\right)\right]\mathbf{v} &= \mathbf{u} + \mathbf{q}\times\boldsymbol{\omega} \text{ for all } \mathbf{q}\in\Omega \\
\boldsymbol{\nabla}\cdot\mathbf{v} &= 0 \text{ everywhere.}
\end{aligned}$$

  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 and need to be carefully thought about, though it may not be a problem at low Reynolds number?

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