Numerical Methods for Fluctuating Hydrodynamics

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Discrete Simulation of Fluid Dynamics
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Outline

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

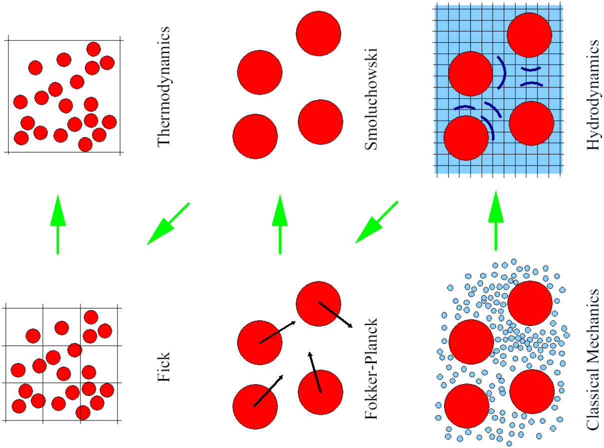


Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

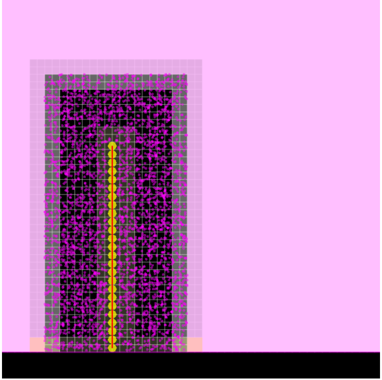
Particle Methods for Complex Fluids

- 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)**

$$m\ddot{\mathbf{r}}_i = \sum_j \mathbf{f}_{ij}(\mathbf{r}_{ij})$$

- 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**.

Direct Simulation Monte Carlo (DSMC)



(MNG)

Tethered polymer chain in shear flow.

- **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 consisten structure and a **non-ideal equation of state**. [1].

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 [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.

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

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

  where the **kinematic viscosity** $\nu = \eta/\rho$, and $\mathbf{v}\cdot\boldsymbol{\nabla}c = \boldsymbol{\nabla}\cdot(c\mathbf{v})$ and $\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v} = \boldsymbol{\nabla}\cdot\left(\mathbf{v}\mathbf{v}^T\right)$ because of incompressibility, $\boldsymbol{\nabla}\cdot\mathbf{v} = 0$.
- Here $\mathcal{P}$ is the orthogonal projection onto the space of divergence-free velocity fields.

Landau-Lifshitz Navier-Stokes (LLNS) Equations

- 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].

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**

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

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

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

Weak Accuracy

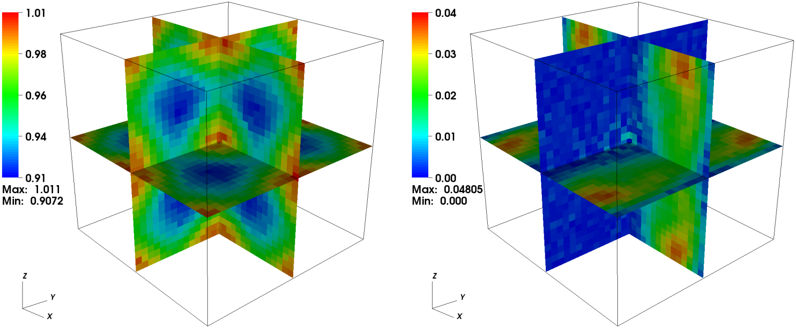


Figure: Equilibrium discrete spectra (static structure factors) $S_{\rho,\rho}(\mathbf{k}) \sim \langle \hat{\rho}\hat{\rho}^{\star} \rangle$ (should be unity for all discrete wavenumbers) and $S_{\rho,\mathbf{v}}(\mathbf{k}) \sim \langle \hat{\rho}\hat{v}_x^{\star} \rangle$ (should be zero) for our RK3 collocated scheme.

Particle/Continuum Hybrid Framework

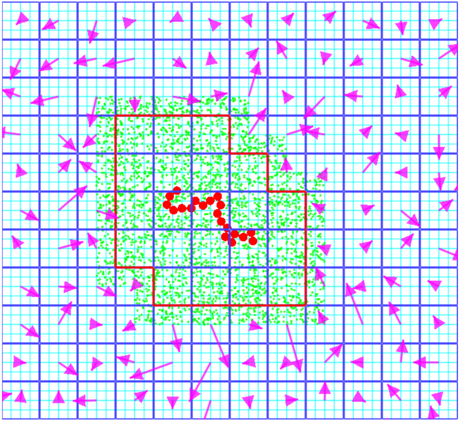


Figure: Hybrid method for a polymer chain.

Fluid-Structure Coupling using Particles

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- 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.

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**.

"*A hybrid particle-continuum method for hydrodynamics of complex fluids*", A. Donev and J. B. Bell and A. L. Garcia and B. J. Alder, **SIAM J. Multiscale Modeling and Simulation 8(3):871-911, 2010**

The adiabatic piston problem

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Relaxation Toward Equilibrium

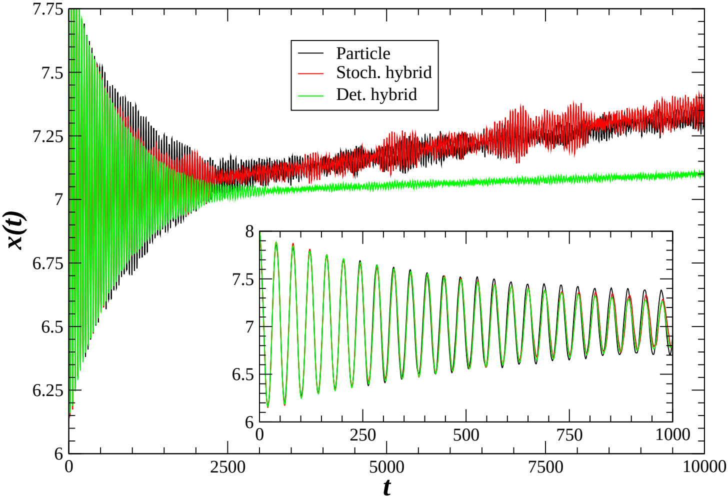


Figure: Massive rigid piston ($M/m = 4000$) not in mechanical equilibrium: **The deterministic hybrid gives the wrong answer!**

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** [7].

Fractal Fronts in Diffusive Mixing

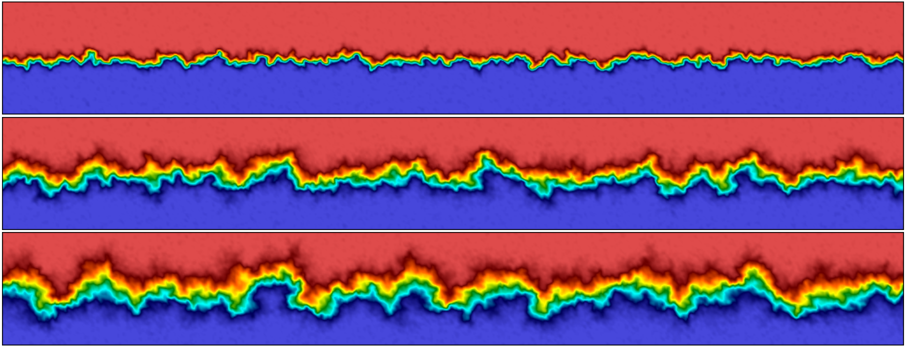


Figure: Snapshots of concentration in a miscible mixture showing the development of a *rough* diffusive interface between two miscible fluids in zero gravity [3, 7, 5].

Giant Fluctuations in Experiments

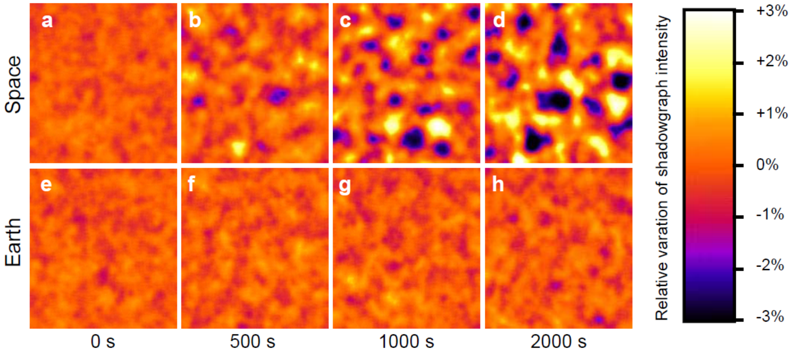


Figure: Experimental results by A. Vailati *et al.* from a microgravity environment [7] showing the enhancement of concentration fluctuations in space (box scale is **macroscopic**: 5mm on the side, 1mm thick).

Fluctuation-Enhanced Diffusion Coefficient

- The **nonlinear** concentration equation includes a contribution to the mass flux due to **advection by the fluctuating velocities**,

$$\partial_t (\delta c) + (\delta \mathbf{v}) \cdot \boldsymbol{\nabla} c_0 = \boldsymbol{\nabla} \cdot [-(\delta c)(\delta \mathbf{v}) + \chi \boldsymbol{\nabla} (\delta c)] + \dots$$

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

$$-\langle (\delta c)(\delta \mathbf{v}) \rangle \approx (\Delta \chi) \boldsymbol{\nabla} c_0.$$

- 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**.

Fluctuation-Enhanced Diffusion Coefficient

- 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**

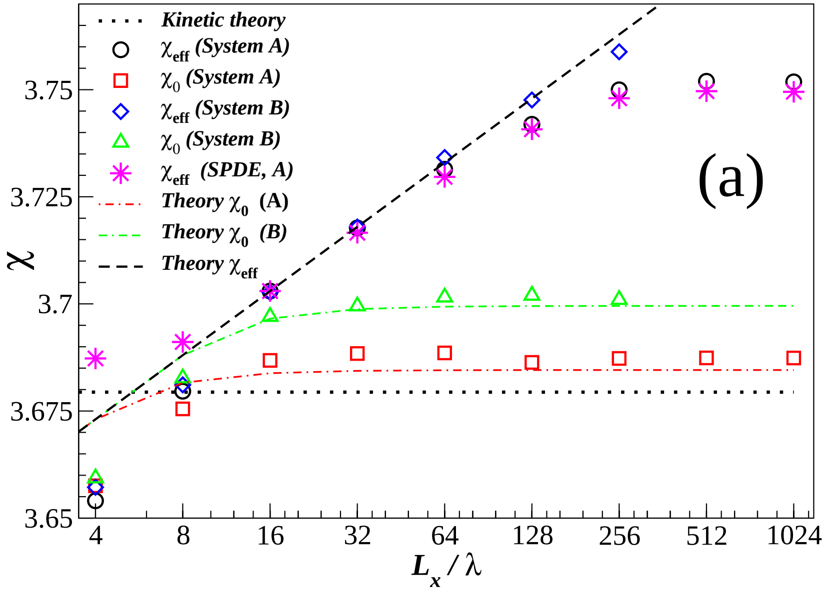
$$\chi_{\text{eff}}^{(2D)} \approx \chi + \frac{k_B T}{4\pi\rho(\chi+\nu)L_z} \ln \frac{L_x}{L_0}$$

- In **three dimensions**, $L_x = L_z = L \ll L_y$, χ_{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].

Particle Simulations



Fluid-Structure Direct Coupling

- 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:

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

where δ_a is an **approximate delta function** with support of size a (integrates to unity).

Fluid-Structure Direct Coupling

- The equations of motion of the Direct Forcing method are *postulated* to be

$$\begin{aligned} \rho\left(\partial_t \mathbf{v} + \mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v}\right) &= \boldsymbol{\nabla}\cdot\boldsymbol{\sigma} - \mathbf{S}\boldsymbol{\lambda} & (1)\\ m_e \dot{\mathbf{u}} &= \mathbf{F} + \boldsymbol{\lambda} & (2)\\ \text{s.t.} \quad \mathbf{u} = & \; \mathbf{J}\mathbf{v} = \int \delta_a\left(\mathbf{q}-\mathbf{r}\right)\mathbf{v}\left(\mathbf{r},t\right) d\mathbf{r}, & (3) \end{aligned}$$

  where $\boldsymbol{\lambda}$ 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

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

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

$$\rho_{\text{eff}} = \rho + \Delta m \mathbf{S}\mathbf{J}.$$

Fluctuation-Dissipation Balance

- One must ensure fluctuation-dissipation balance in the coupled fluid-particle system, with effective Hamiltonian

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

  and implement a discrete scheme.
- We investigate the **velocity autocorrelation function** (VACF) for a Brownian bead

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

- 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 $C(t > t_c) = 2/3\,(k_B T/m)$ for a neutrally-boyant particle.

Velocity Autocorrelation Function

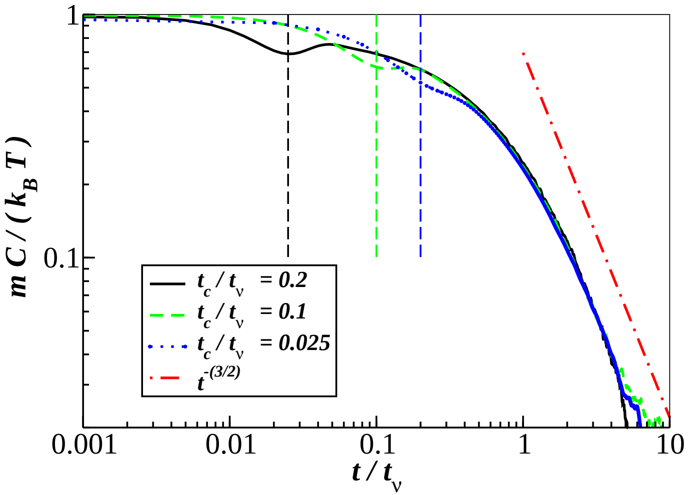


Figure: (Work with Florencio Balboa and Rafael Delgado-Buscallioni) Normalized VACF $C(t) = \langle v_x(0) v_x(t) \rangle$ for different fluid compressibilities (speeds of sound).

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 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** χ_0 that depends on the length-scale of observation.
- **Direct fluid-structure coupling** between fluctuating hydrodynamics and microstructure.

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