Coupling a Fluctuating Fluid with Suspended Structures

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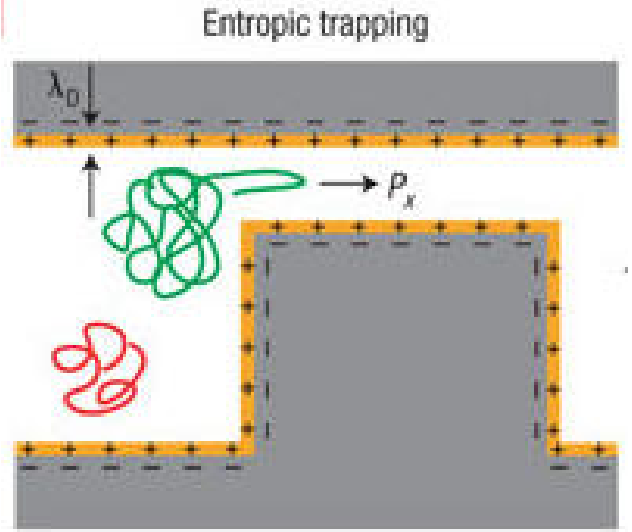
Outline

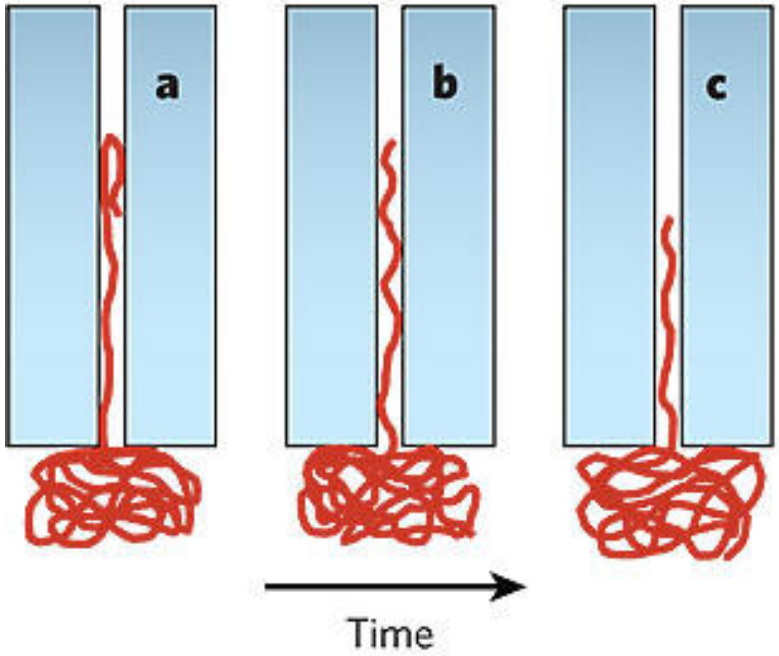
Micro- and nano-hydrodynamics

- 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 focus here not on the technical details of hybrid methods, but rather, on using our method to demonstrate the general conclusion that **fluctuations should be taken into account at the continuum level**.

Example: DNA Filtering



Fu et al., Nature Nanotechnology 2 (2007)



H. Craighead, Nature 442 (2006)

How to coarse grain the fluid (solvent) and couple it to the suspended microstructure (e.g., polymer chain)?

Levels of Coarse-Graining

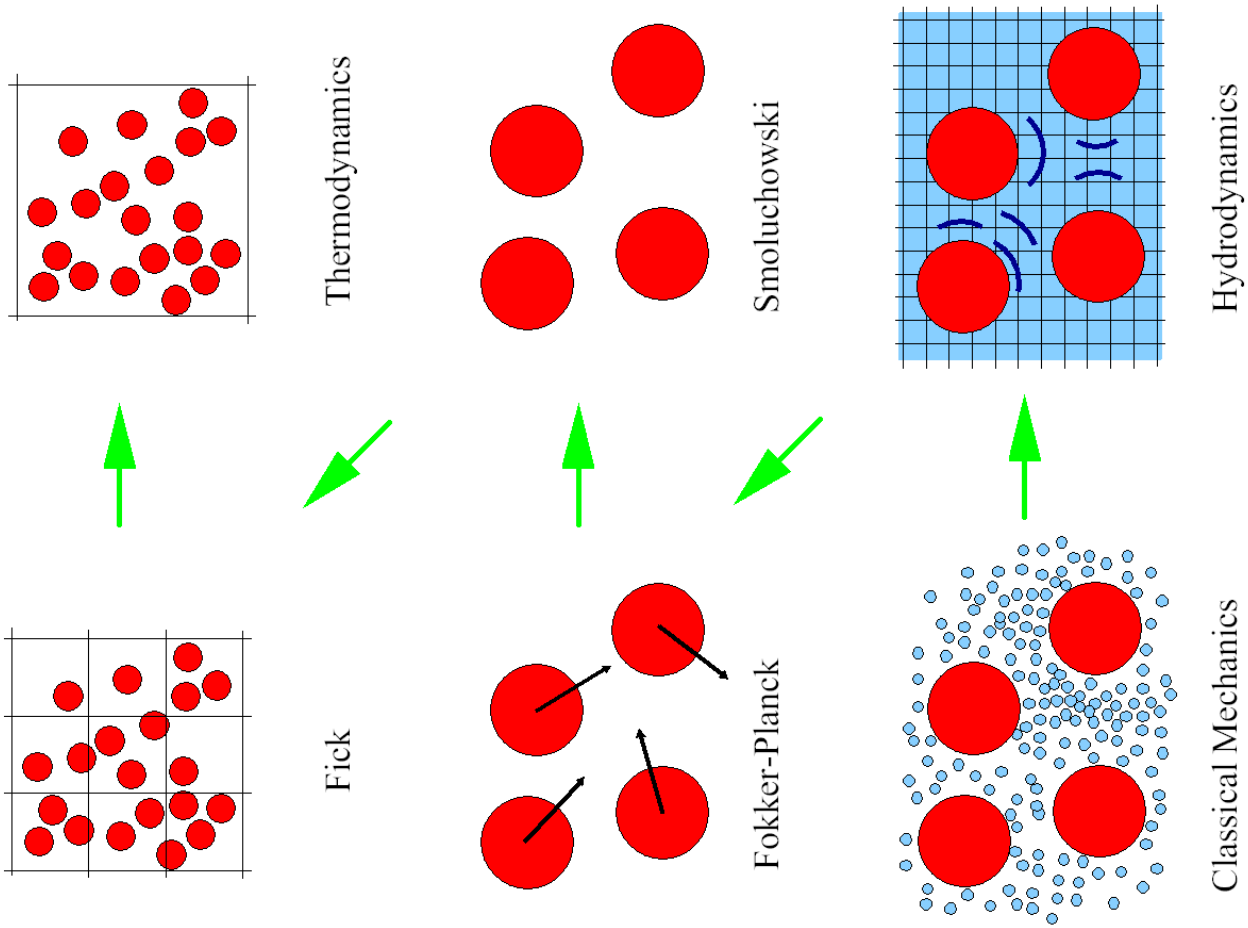


Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

This talk: Particle/Continuum Hybrid

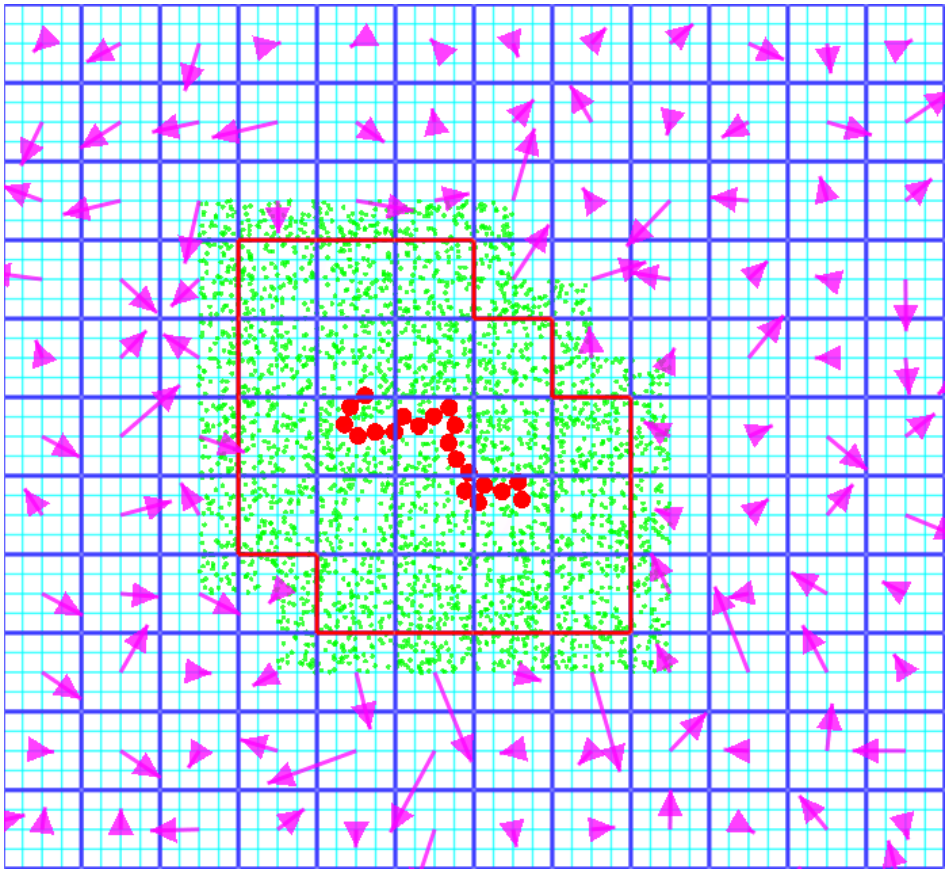


Figure: Hybrid method for a polymer chain.

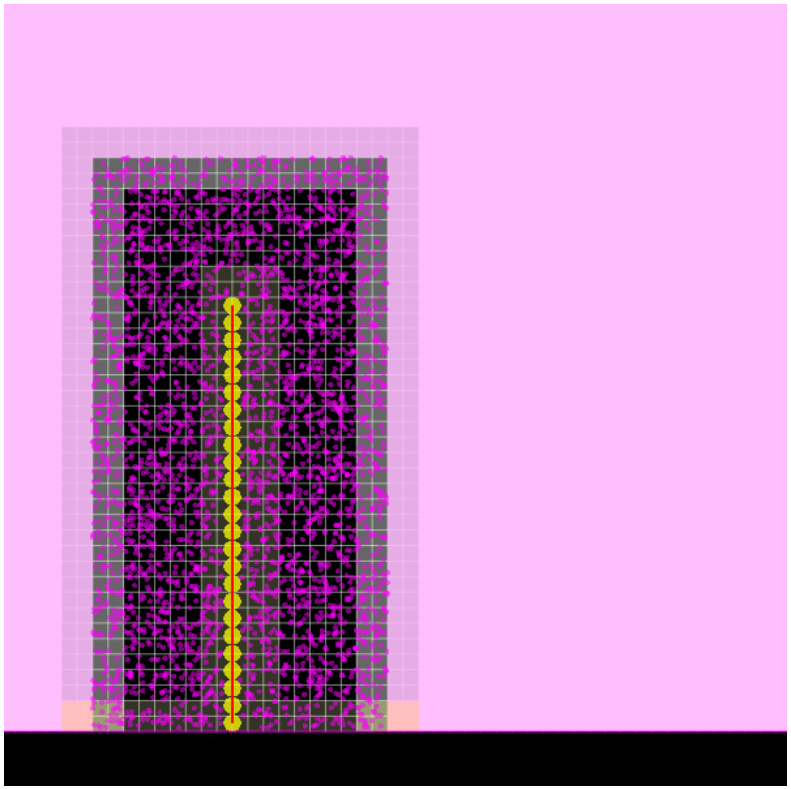
Particle Methods for Complex Fluids

- 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 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**

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

  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:

$$
\begin{aligned}
\boldsymbol{\Sigma} &= \sqrt{2\eta k_B T}\,\boldsymbol{\mathcal{W}}. \\
\left\langle \mathcal{W}_{ij}(\mathbf{r},t)\mathcal{W}^{\star}_{kl}(\mathbf{r}',t')\right\rangle &= \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - 2\delta_{ij}\delta_{kl}/3\right)\delta(t-t')\delta(\mathbf{r}-\mathbf{r}').
\end{aligned}
$$

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 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].

Fluid-Structure Coupling

- We want to construct a **bidirectional coupling** between a fluctuating fluid and a small sphere of radius a with position $\mathbf{q}(t)$ and velocity $\mathbf{u} = d\mathbf{q}/dt$ (aka **bead**).
- Macroscopically, the coupling between flow and suspended structures relies on:
  - **No-slip** boundary condition $\mathbf{v}_{rel} = 0$ at the surface of the bead.
  - Force on the bead is the integral of the (fluctuating) stress tensor over the bead 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.

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**

Our Hybrid Algorithm

1. The hydro solution $\mathbf{u}_H$ is computed everywhere, including the **particle patch**, giving an estimated total flux $\mathbf{\Phi}_H$.
2. **Reservoir particles** are *inserted* at the boundary of the particle patch based on *Chapman-Enskog distribution* from kinetic theory, accounting for *both* collisional and kinetic viscosities.
3. Reservoir particles are *propagated* by Δt and *collisions* are processed, giving the total particle flux $\mathbf{\Phi}_p$.
4. The hydro solution is overwritten in the particle patch based on the particle state $\mathbf{u}_p$.
5. The hydro solution is corrected based on the more accurate flux, $\mathbf{u}_H \leftarrow \mathbf{u}_H - \mathbf{\Phi}_H + \mathbf{\Phi}_p$.

Other Hybrid Algorithms

- For molecular dynamics (non-ideal particle fluids) the insertion of reservoir particles is greatly complicated by the need to account for the **internal structure** of the fluid and requires an **overlap region**.
- A hybrid method based on a flux-flux coupling between molecular dynamics and isothermal compressible fluctuating hydrodynamics has been developed by Coveney, De Fabritiis, Delgado-Buscalioni and co-workers [6].
- Some comparisons between different forms of coupling (state-state, state-flux, flux-state, flux-flux) has been performed by Ren [7].
- Reaching relevant time scales ultimately requires a **stochastic immersed structure** approach coupling immersed structures directly to a fluctuating solver (work in progresss).

The adiabatic piston problem

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Relaxation Toward Equilibrium

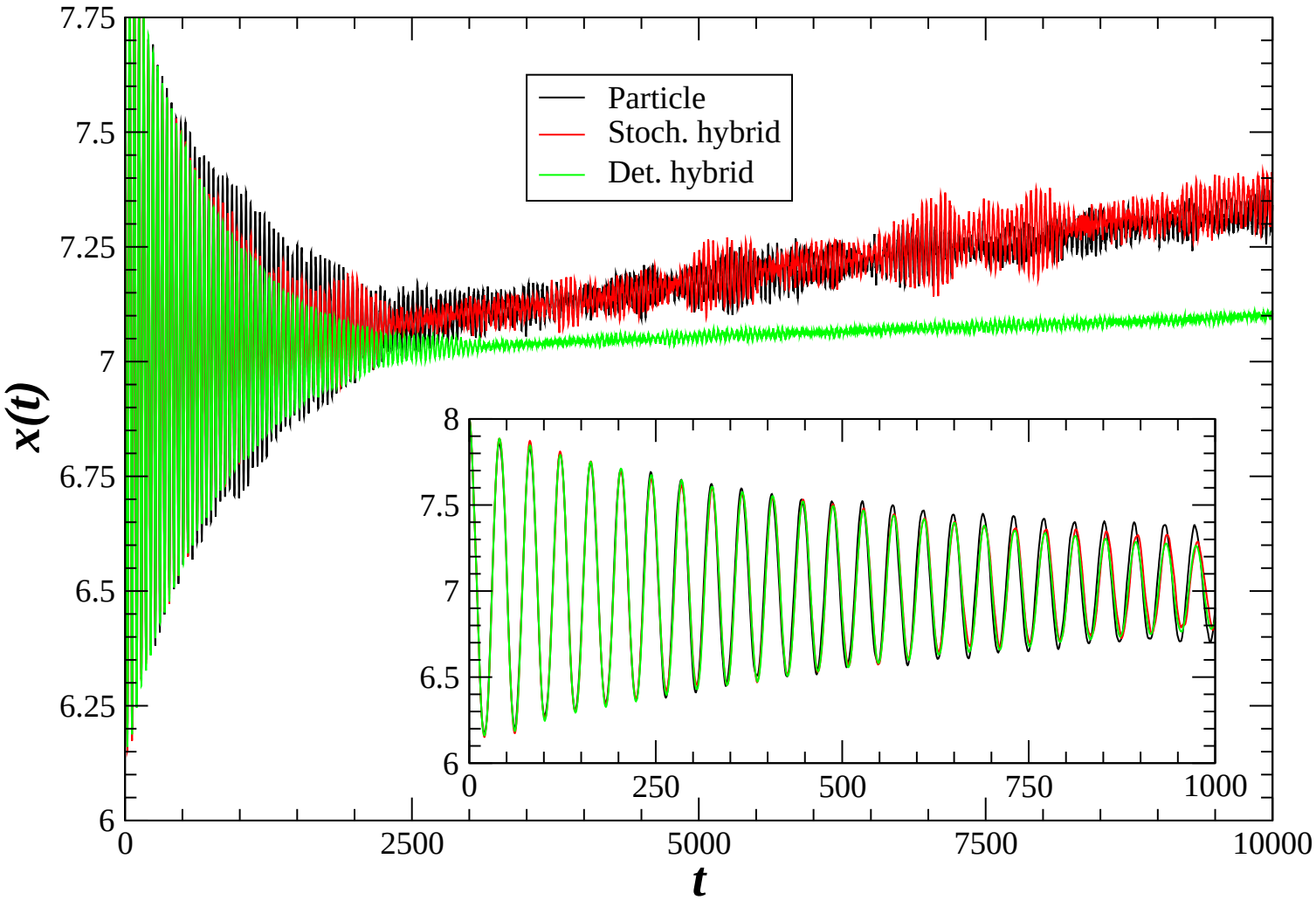

Figure: Massive rigid piston ($M/m = 4000$) not in mechanical equilibrium: **The deterministic hybrid gives the wrong answer!**

Fluid-Structure Direct Coupling

- Consider a particle 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:

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

where $\delta_{\Delta a}$ 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

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

$$m\dot{\mathbf{u}} = \mathbf{F} + \boldsymbol{\lambda} \quad (2)$$

$$\text{s.t.} \quad \mathbf{u} = \mathbf{J}\mathbf{v} = \int \delta_a\left(\mathbf{q}-\mathbf{r}\right)\mathbf{v}\left(\mathbf{r},t\right)d\mathbf{r}, \quad (3)$$

  where $\boldsymbol{\lambda}$ is a Lagrange multiplier that enforces the no-slip condition.
- Here m is the **excess mass** of the particle over the "dragged fluid", and the **effective mass** is

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

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

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

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 the continuum solver in hybrid methods.
- **Direct fluid-structure coupling** between fluctuating hydrodynamics and microstructure (work with Rafael Delgado-Buscallioni).
- One must ensure fluctuation-dissipation balance in the coupled fluid-particle system, with effective Hamiltonian

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

and implement a discrete scheme.

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