Multiscale Methods for Hydrodynamics of Complex Fluids

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John Bell, *LBL*

Applied Math Seminar, November 2008

[1]This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-PRES-408395).

Outline

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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).**

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- Essential distinguishing feature from "ordinary" CFD: **thermal fluctuations**!

Example: DNA Filtering

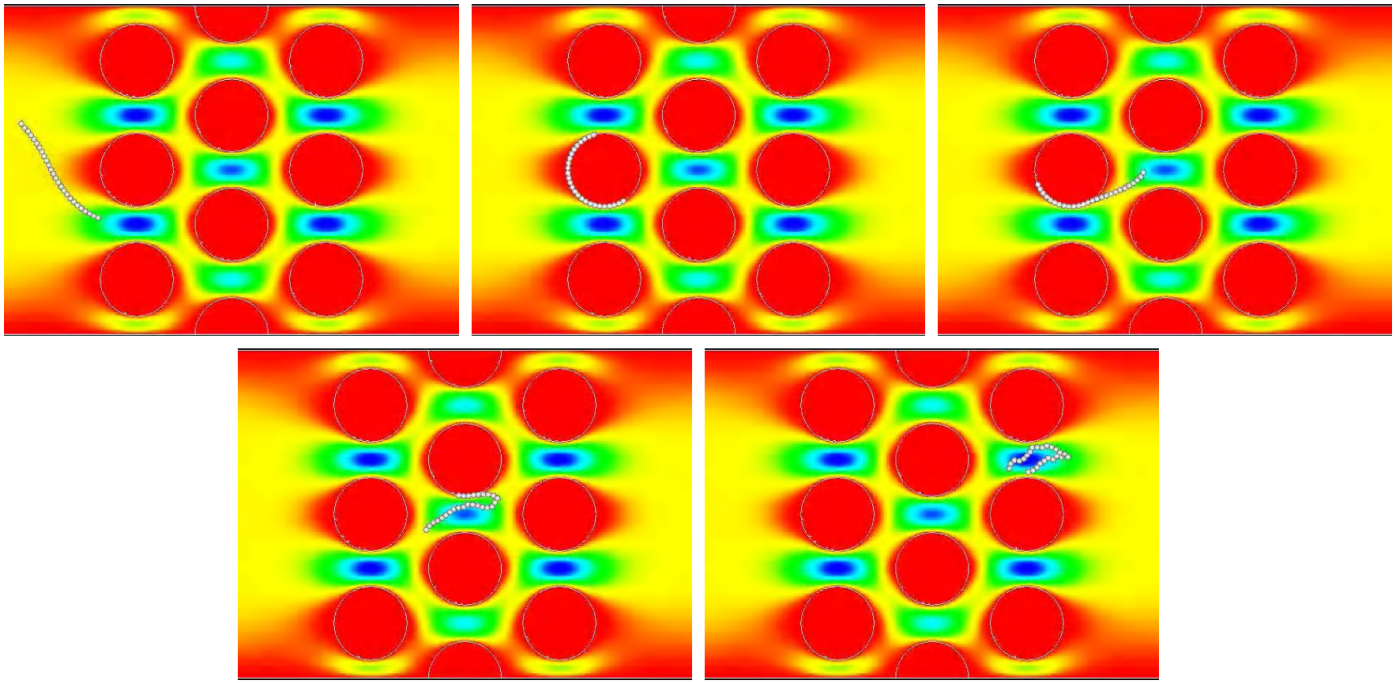


Figure: From the work of David Trebotich (LLNL)

Example: Droplet Formation

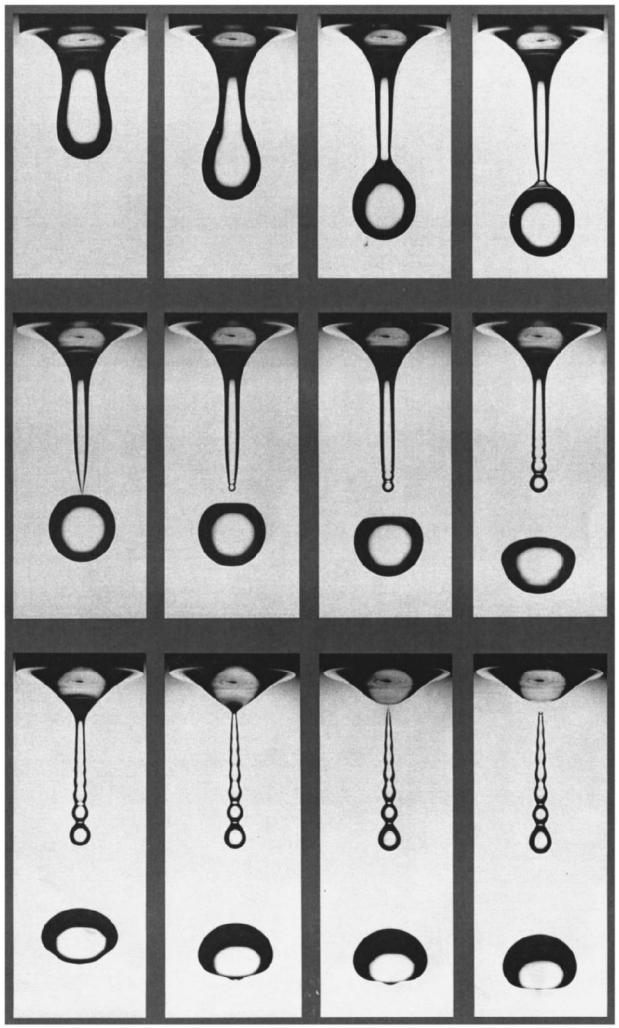
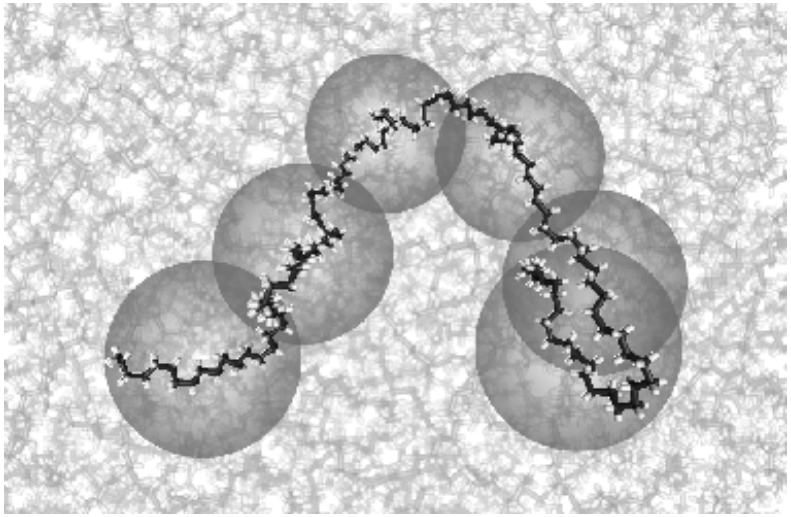


Figure: From Jens Eggers, Reviews of Modern Physics, 69, 1997

Polymer chains



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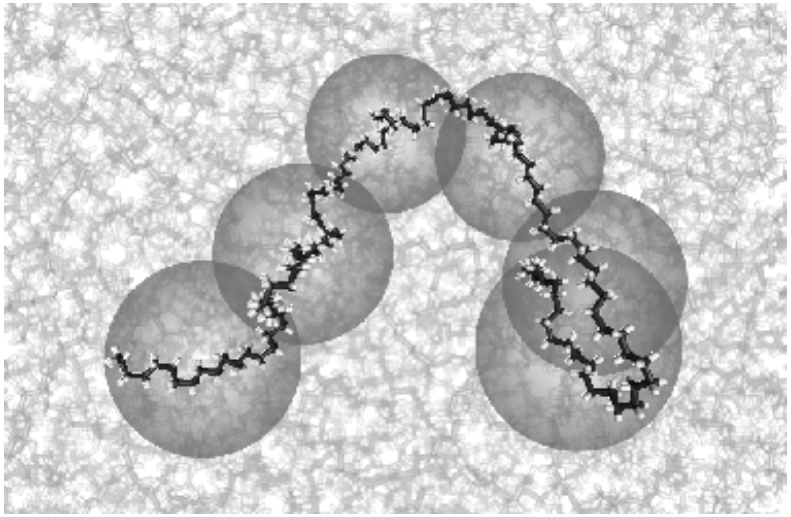

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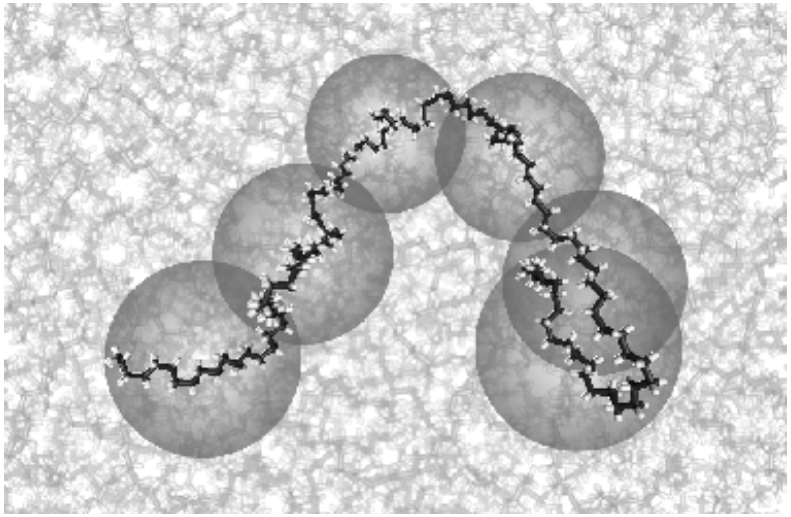

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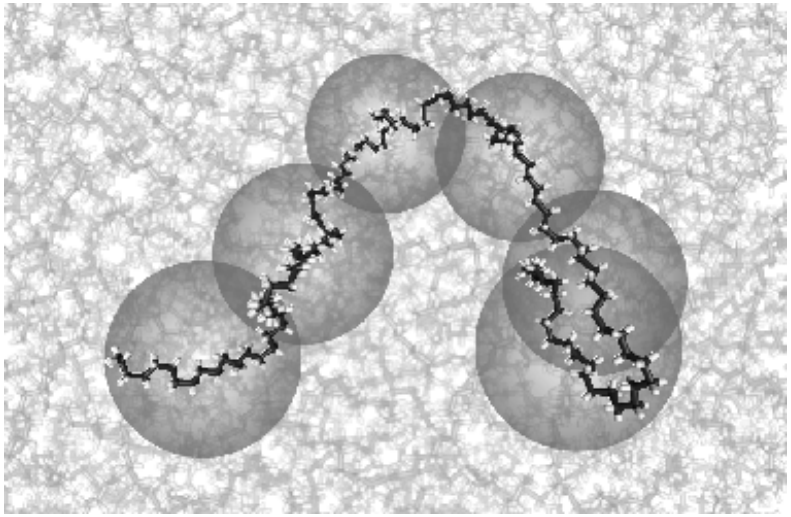

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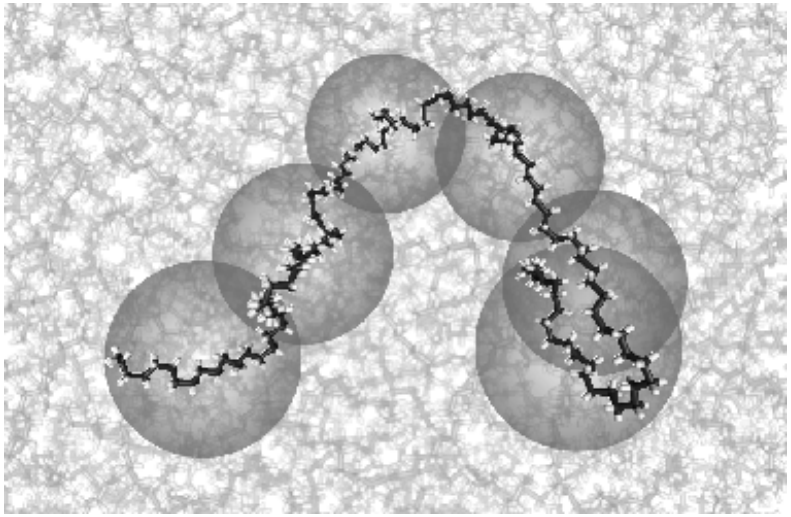

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The issue: **How to couple the polymer model with the surrounding fluid model?**

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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)**

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

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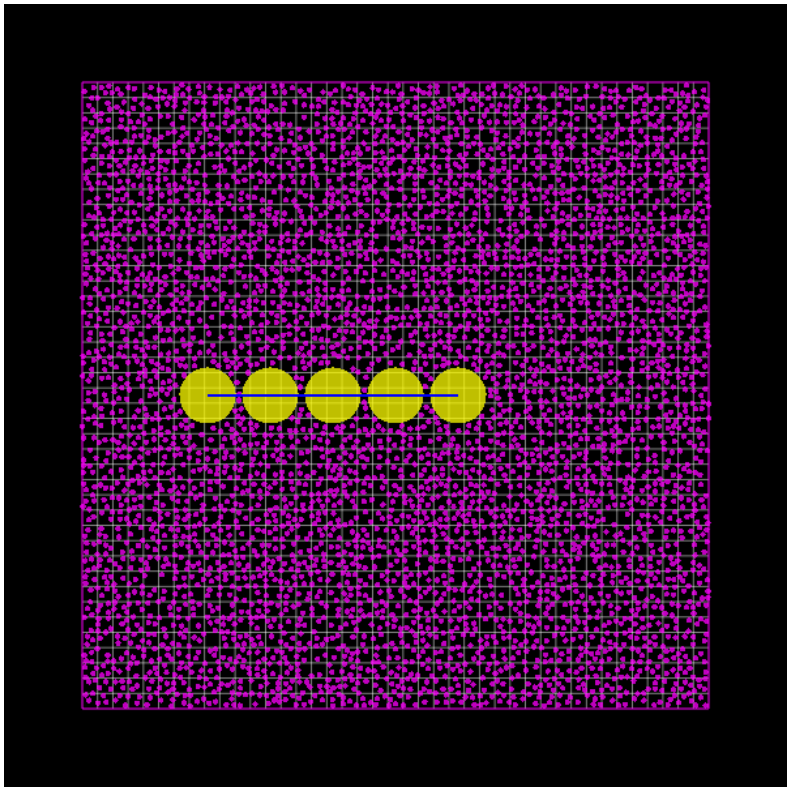
- The stiff repulsion among beads demands small time steps, and chain-chain crossings are a problem.
- For hard spheres, one can use **asynchronous event-driven MD**.
  "*Asynchronous Event-Driven Particle Algorithms*", by A. Donev, to appear in SIMULATION, 2008, **cs.OH/0703096**.

Event-Driven (Hard-Sphere) MD



(MNG)

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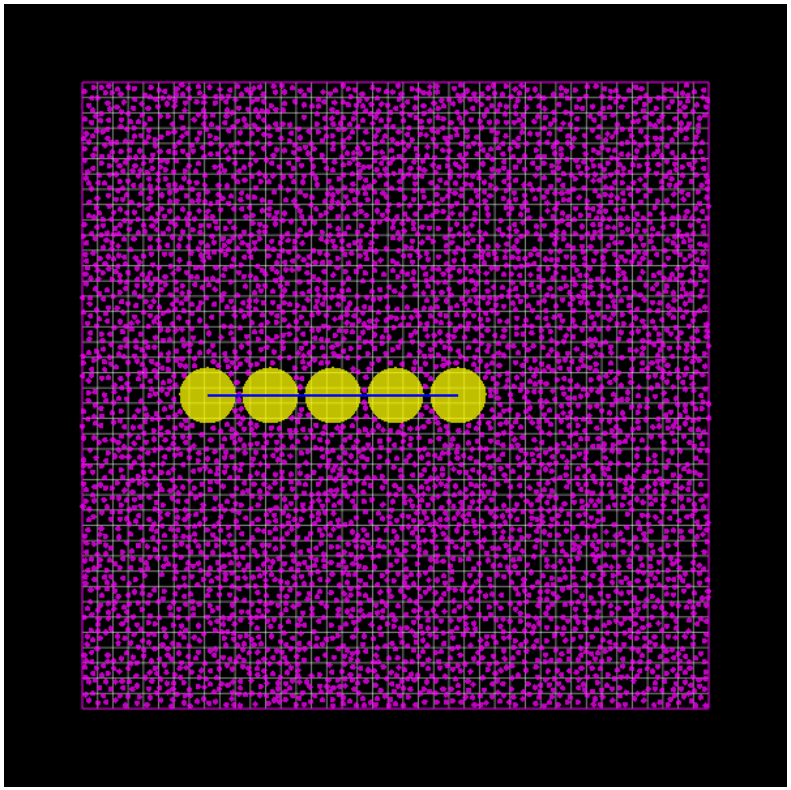

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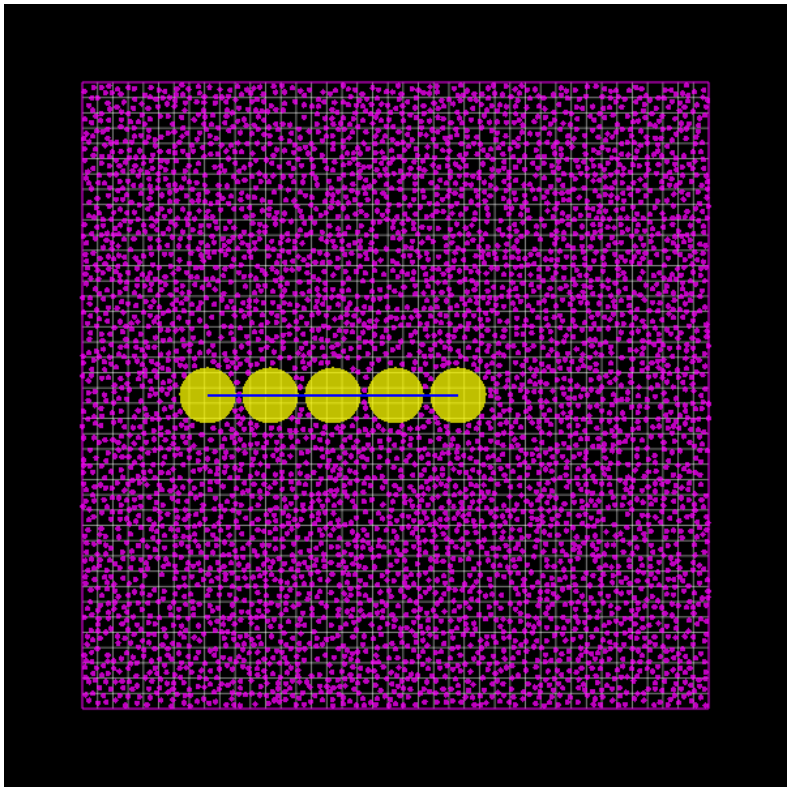

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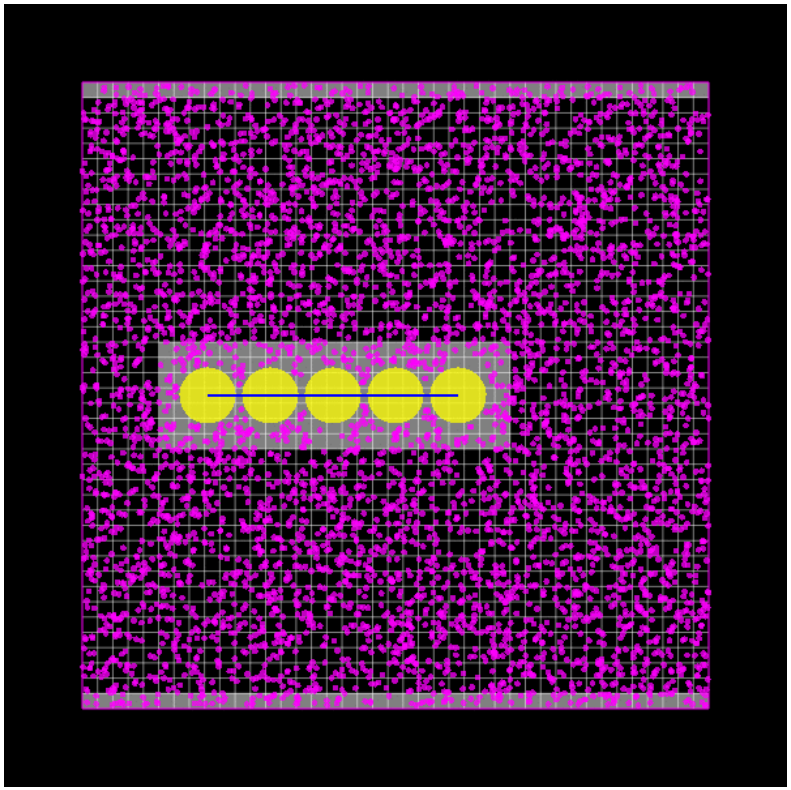
- Most of the computation is "wasted" on the *unimportant solvent particles*!
- Over longer times it is **hydrodynamics** (*local momentum* and energy **conservation**) and **fluctuations** (Brownian motion) that matter.

(MNG)
"*Stochastic Event-Driven Molecular Dynamics*" [1],
A. Donev, A. L. Garcia and B. J. Alder,
J. Comp. Phys., 227(4):2644-2665, 2008

Direct Simulation Monte Carlo (DSMC)



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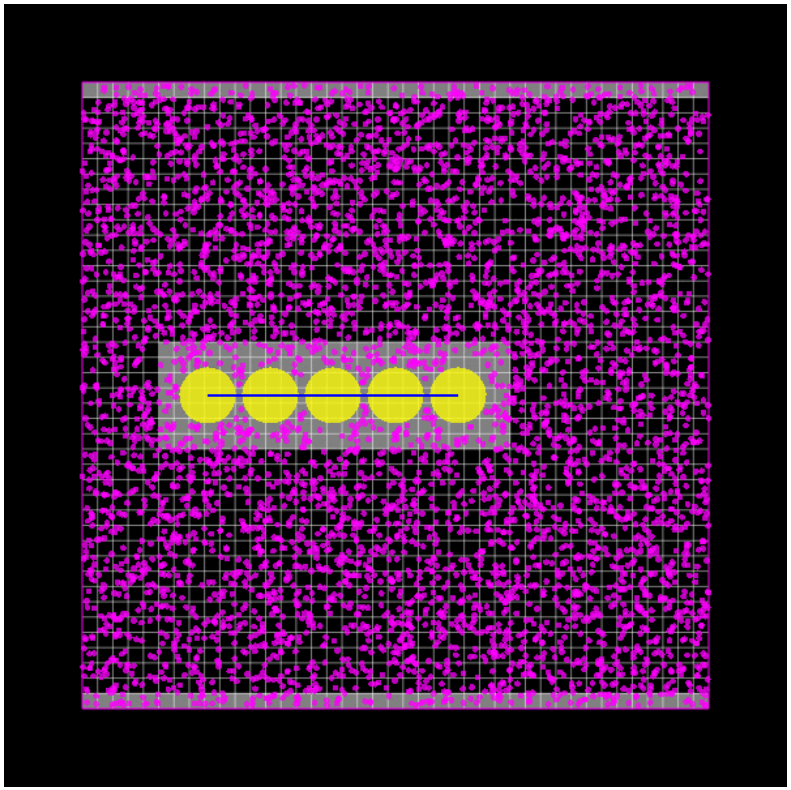

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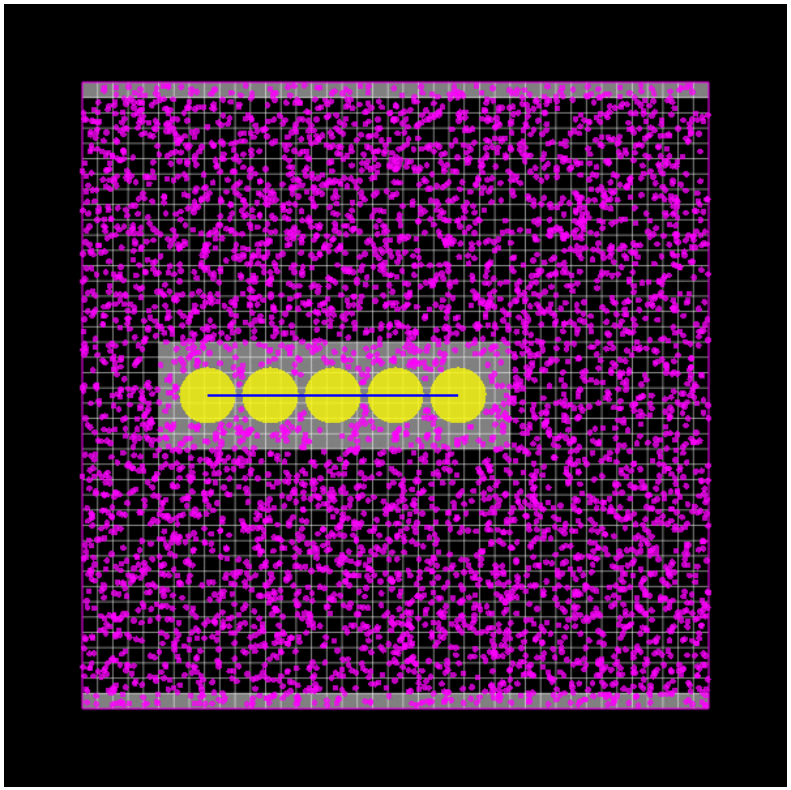

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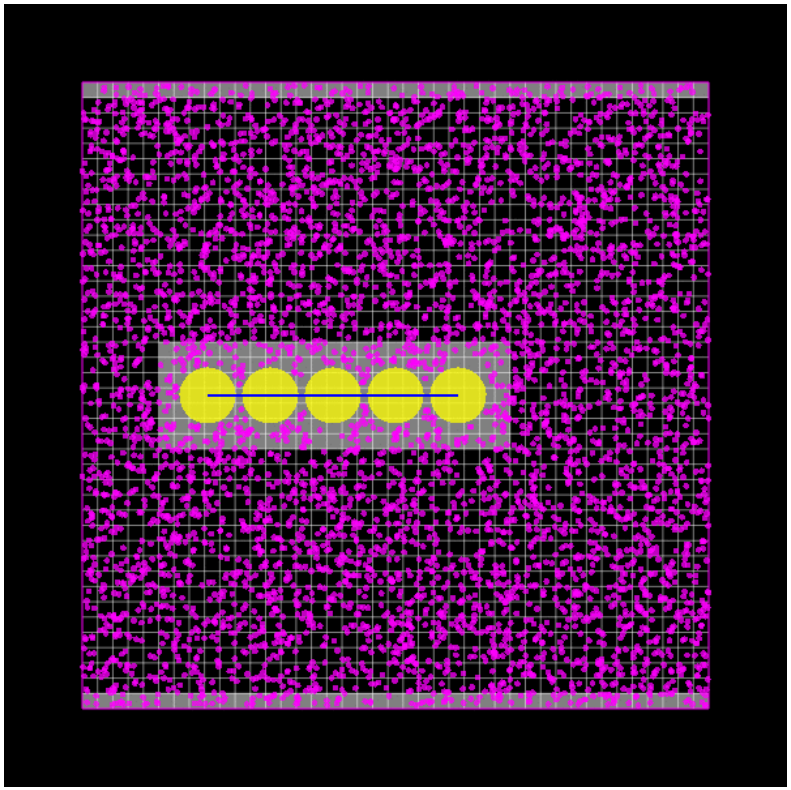

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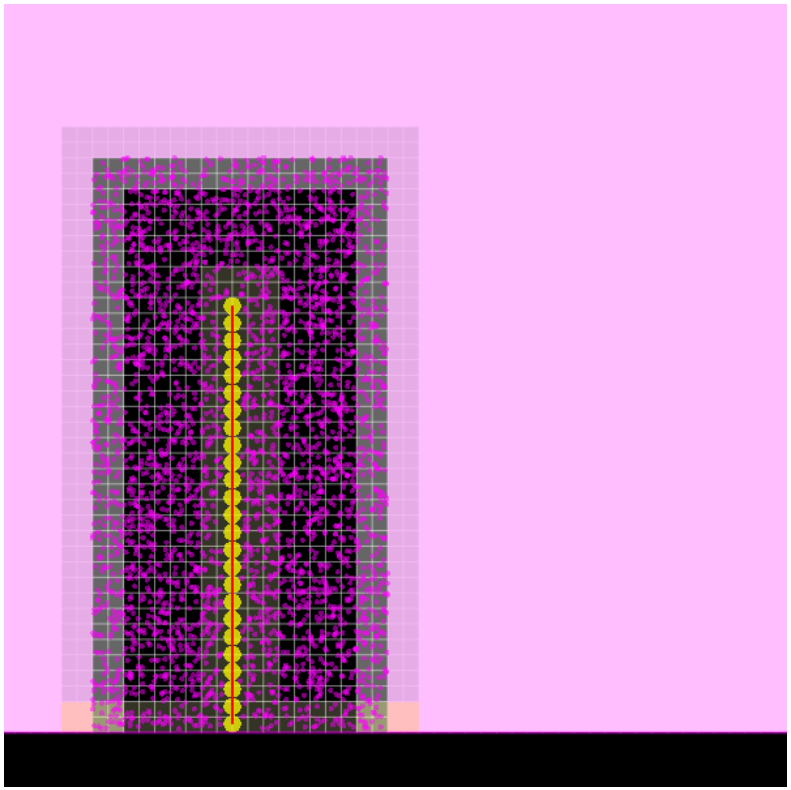
No fluid structure: Viscous fluid that is really an ideal gas! [2]

"*Stochastic Hard-Sphere Dynamics for Hydrodynamics of Non-Ideal Fluids*", by A. Donev, A. L. Garcia and B. J. Alder, **Phys. Rev. Lett. 101:075902 (2008)** [arXiv:0803.0359]

Tethered Polymer in Shear Flow



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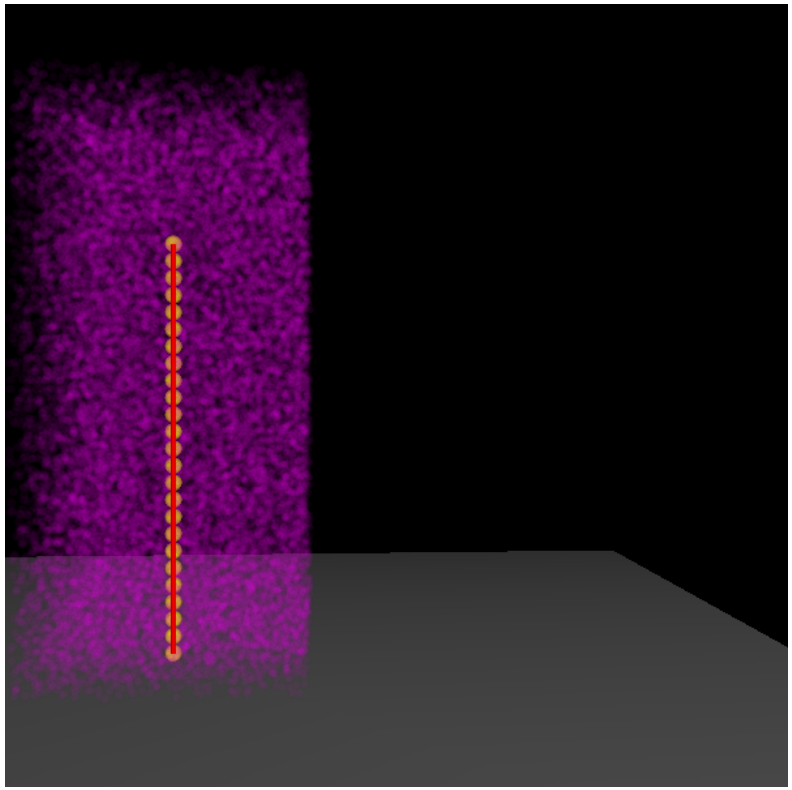

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- We implement **open (stochastic) boundary conditions**: *Reservoir particles* are inserted every timestep in the boundary cells with appropriately biased velocities (local Maxwellian or Chapman-Enskog distributions).

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The Need for Coarse-Graining

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  A single bead of size a and density ρ' *suspended in a stationary fluid with density* ρ and viscosity η (**Brownian walker**).

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- The real issue is that a wide **separation of timescales occurs**: The *gap between the timescales of microscopic and macroscopic* processes widens as the bead becomes much bigger than the solvent particles (water molecules).
- Typical bead sizes are *nm* (nano-colloids, short polymers) or μm (colloids, DNA), while typical atomistic sizes are $1\mathring{A} = 0.1nm$.

Estimates from Fluid Dynamics

- Classical picture for the following dissipation process: *Push a sphere suspended in a liquid with initial velocity* $V_{th} \sim \sqrt{kT/M}$, $M \approx \rho' a^3$, *and watch how the velocity decays:*

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  - **Thermal fluctuations** get similarly dissipated, but their constant presence pushes the particle diffusively over a **diffusion time** $t_{diff} \approx a^2/D$, where $D \sim kT/(a\eta)$.

Estimates from Molecular Dynamics

- For a typical particle fluid with particle size R, mass m, at temperature kT, and density (volume fraction) ϕ, we have the mean-free path

$$\lambda \approx \frac{R}{c_\lambda \phi},$$

where $c_k = c_k(\phi)$ is about 1 for gases and order 10 or so for liquids. Typical $R \sim 1\mathring{\mathrm{A}} = 0.1nm$, $\lambda \sim 0.1D$.

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- The equation of state (EOS) of the fluid determines how the reduced pressure $p = PV/NkT$ depends on temperature and density. Here $C \sim dp/d\phi$ is a measure of the incompressibility of the liquid (bulk modulus), $C \approx 1$ for gases, $C \sim 10$ for liquids.

Timescale estimates.

- The mean collision time, i.e., the **MD time-scale**, is $t_{coll} \approx \lambda / v_{th}$, where the thermal velocity is $v_{th} \approx \sqrt{\frac{kT}{m}}$, for water

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- The sound speed $c \sim \sqrt{C} \cdot \sqrt{kT/m}$, giving an estimate for the **sound time**

$$t_{sonic} \sim \begin{cases} 1ns \text{ for } a \sim \mu m \\ 1ps \text{ for } a \sim nm \end{cases}, \text{ with gap } \frac{t_{sonic}}{t_{coll}} \sim \frac{a}{\sqrt{C}\lambda} \sim 10^2 - 10^5$$

Estimates contd...

- The viscosity of the particle fluid can be estimated to be

$$\eta \approx c_\eta \frac{\phi\lambda}{R^3}\sqrt{mkT}$$

giving **viscous time** estimates

$$t_{visc} \sim \begin{cases} 1\mu s \text{ for } a \sim \mu m \\ 1ps \text{ for } a \sim nm \end{cases}, \text{ with gap } \frac{t_{visc}}{t_{sonic}} \sim \sqrt{C}\frac{a}{\lambda} \sim 1 - 10^3$$

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- Finally, the **diffusion time** can be estimated to be

$$t_{diff} \sim \begin{cases} 1s \text{ for } a \sim \mu m \\ 1ns \text{ for } a \sim nm \end{cases}, \text{ with gap } \frac{t_{diff}}{t_{visc}} \sim \frac{a}{\phi R} \sim 10^3 - 10^6$$

which can now reach **macroscopic timescales**!

Levels of Coarse-Graining

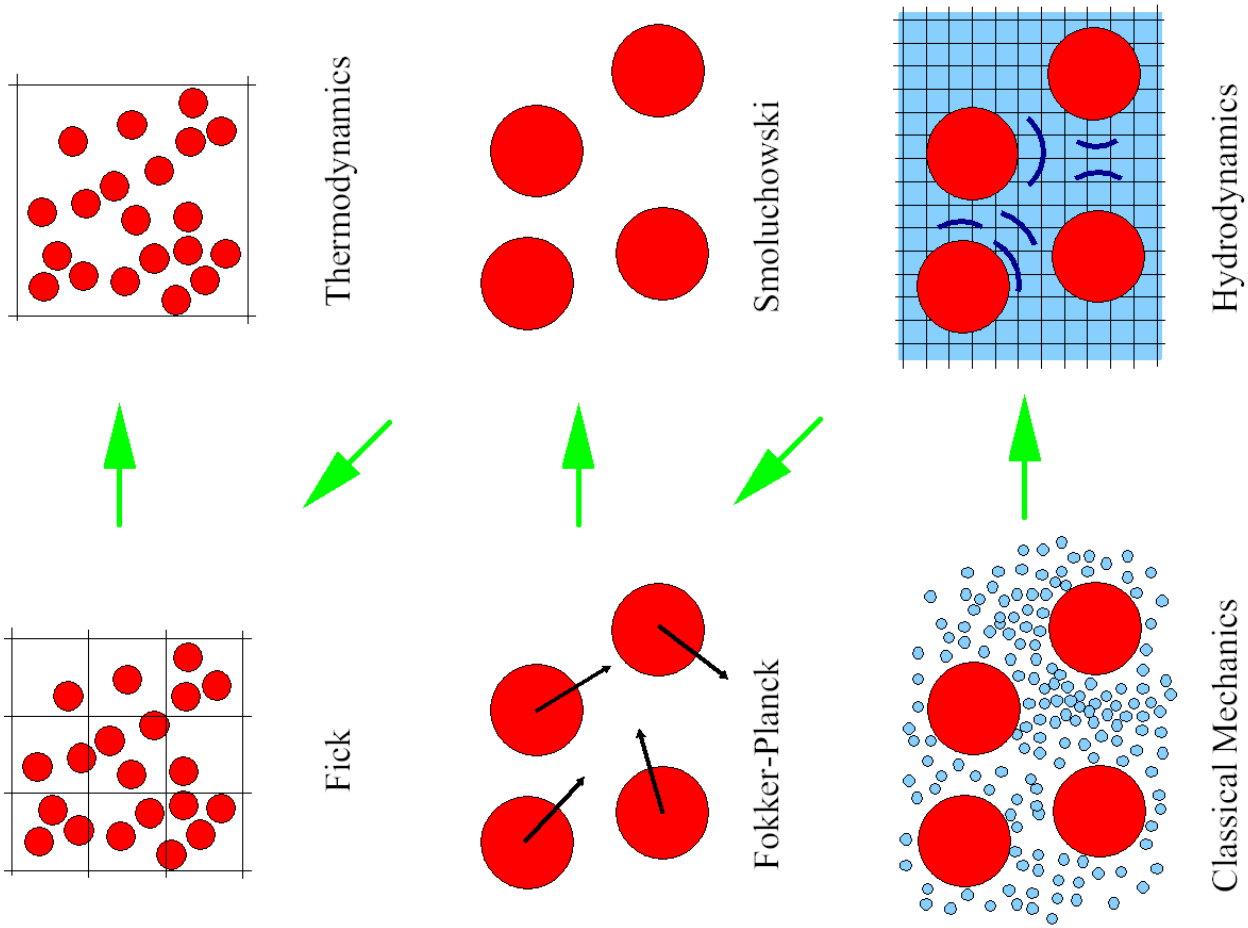

Figure: From Pep Español, "Statistical Mechanics of Coarse-Graining"

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- **Overdamped Brownian dynamics**:

$$d\mathbf{R} = [\mathbf{U} + \frac{\mathbf{D} \cdot \mathbf{F}(\mathbf{R})}{kT} + \frac{\partial}{\partial \mathbf{R}} \cdot \mathbf{D}]dt + \sqrt{2}\mathbf{B} \cdot d\mathbf{W},$$

where $\mathbf{R}$ is the vector containing bead positions, $\mathbf{R} = \{\mathbf{r}_1, ..., \mathbf{r}_N\}$, $\mathbf{U}$ is the unperturbed velocity field at the bead centers, $\mathbf{F}$ are the bead-bead interaction forces, and $dW_i = \sqrt{dt} \cdot \mathcal{N}_i$ are independent Wiener process increments (white noise).

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- Typical assumption for the **diffusion tensor** is that it depends only on the configuration:

$$\mathbf{D} \equiv \mathbf{D}(\mathbf{R}) = \mathbf{B}\cdot\mathbf{B}^T, \text{ usually } \mathbf{D}_{ij} = k_B T[(6\pi\eta a)^{-1}\mathbf{I}\delta_{ij} + \mathbf{\Omega}_{ij}]$$

where $\mathbf{\Omega}_{ij}$ is the **Oseen tensor**, with additional **complex corrections** for flow in bounded domains (channels).

Outline

The equations of hydrodynamics

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

$$\mathbf{u}(\mathbf{r}) = \begin{bmatrix} \rho \\ \mathbf{j} \\ e \end{bmatrix} = \sum_i \begin{bmatrix} 1 \\ \mathbf{v}_i \\ v_i^2/2 \end{bmatrix} m_i \delta_\epsilon(\mathbf{r} - \mathbf{q}_i) = \sum_i \begin{bmatrix} m_i \\ \mathbf{p}_i \\ e_i \end{bmatrix} \delta_\epsilon(\mathbf{r} - \mathbf{q}_i),$$

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- Discrete perspective: We split the physical system into cells, and add the total **conserved quantity** from all of the particles in a given cell. The fluxes represent the transport through the faces between the cells.

Navier-Stokes Equations

The flux expressions assumed in the **compressible Navier-Stokes(-Fourier)** (NS) equations:

$$\mathbf{H} = \begin{bmatrix} \rho\mathbf{v} \\ \rho\mathbf{v}\mathbf{v}^T + P\boldsymbol{\delta} \\ (e+P)\mathbf{v} \end{bmatrix} \text{ and } \mathbf{D} = \begin{bmatrix} 0 \\ \boldsymbol{\tau} \\ \boldsymbol{\tau}\cdot\mathbf{v} + \kappa\boldsymbol{\nabla}T \end{bmatrix}.$$

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Here the **primary variables** are density ρ, velocity $\mathbf{v}$, and temperature T, determined from:

$$\mathbf{j} = \rho\mathbf{v} \text{ and } e = c_v\rho T + \frac{\rho v^2}{2}$$

the **pressure** is determined from the equation of state $P = P(\rho, T)$, and the **viscous stress**

$$\boldsymbol{\tau} = 2\eta\left[\dot{\boldsymbol{\gamma}} - \frac{\mathrm{Tr}(\dot{\boldsymbol{\gamma}})}{3}\right], \text{ where the strain rate } \dot{\boldsymbol{\gamma}} = \frac{1}{2}(\boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}\mathbf{v}^T)$$

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and solved the **linearized NS equations** in Fouier space to obtain the local fluctuations in the density, momentum and energy.

- By comparing to statistical mechanics, they obtained a **fluctuation-dissipation theorem**:

$$\left\langle \boldsymbol{\sigma}_{ij}(\mathbf{r},t)\boldsymbol{\sigma}_{kl}(\mathbf{r}',t') \right\rangle = 2\eta kT\tilde{\boldsymbol{\delta}}_{ijkl}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$$
$$\left\langle \varsigma_i(\mathbf{r},t)\varsigma_i(\mathbf{r}',t') \right\rangle = 2\kappa kT\boldsymbol{\delta}_{ij}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')$$

giving the **Landau-Lifshitz Navier-Stokes** (LLNS) equations.

Incompressible Navier-Stokes

- Under the assumption that the speed of sound is very large, $\delta P(\delta\rho, \delta T) \approx c^2 \delta\rho$, the energy equation decouples from the other two and the density becomes nearly constant, giving the **incompressible Navier-Stokes equations**

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

$$\rho_0 \mathbf{v}_t = -\nabla P - \rho_0 (\mathbf{v} \cdot \nabla)\mathbf{v} + \eta \nabla^2 \mathbf{v},$$

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  where now the pressure $P(\mathbf{r}, t)$ is the Lagrange multipler for the incompressibility constraint.
- Physically, this means that very small changes in the density are sufficient to adjust the pressure arbitrarily and that temperature variations are negligible (isothermal).

When is incompressible OK?

- For stationary flows, the incompressibility assumption is good if $M \ll \min(1, Re)$, where **Mach number** $M = V_{th}/c$ and **Reynolds number** $Re = \rho a V_{th}/\eta$ (see Kramer, Atzberger & Peskin [3]).

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- Both of these conditions require $a \gg \frac{R}{\phi^\alpha} \sim 1nm$

Incompressibility critique contd.

- Mathematically, the sound waves $\sim \exp\left[(ick - \eta k^2/\rho)t\right]$ are *rapidly oscillating* for wavelengths

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- Note however that sound waves persist over timescales *similar* to viscous damping.
- The exact role of sound in propagating hydrodynamic interactions is **still under debate** for concentrated suspensions!

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$$\left(\frac{\delta T}{T}\right)^2 \approx \frac{1}{N_s} = \frac{R^3}{\phi a^3} \ll 1$$

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- Conclusion: **Unless the compressibility is very (unrealistically!) small, an incompressible/isothermal formulation is applicable only when** $a \gg 1nm$.

Problems with the LLNS equations

- Numerically solving the *compressible* LLNS equations via explicit real-space methods has proven to be difficult (work by Alejandro Garcia and John Bell [4], as well as Rafael Delgado-Buscalioni *et al.* [5]): $\Delta t \ll \Delta x/c$.

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- Adding stochastic fluxes to the non-linear NS equations (as derived in the mesoscopic limit by Pep Español [6]) produces **ill-behaved stochastic PDEs**: At small scales one gets **negative densities** and **temperatures**.
- Fluctuations at scales smaller than the atomistic correlation length and time should be renormalized to account for discreteness of matter (recall *ultra-violet catastrophe*).

Hydrodynamics at the nanoscale?

- It is not clear whether the Navier-Stokes equations apply at **nano-scales**. Berni Alder *et al.* have proposed **generalized hydrodynamics** for atomistic scales (wavelength and frequency-dependent viscosity), but this is intractable.

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- Conclusion: **It is necessary to perform systematic coarse graining of particle models to find a non-phenomenological form of the evolution equations for the hydrodynamic fields.**

Outline

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- The **solvent** (fluid, liquid) can be modeled **implicitly** via analytical solutions (Brownian dynamics). But we want **reverse coupling** of the polymer motion on the flow (e.g., *drag reduction*)!

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- The above two conditions are **questionable at nanoscales**, but even worse, they are very hard to implement numerically in an efficient and stable manner, even in the (phenomenological) Lattice-Boltzmann method.

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The Immersed-Structure Method

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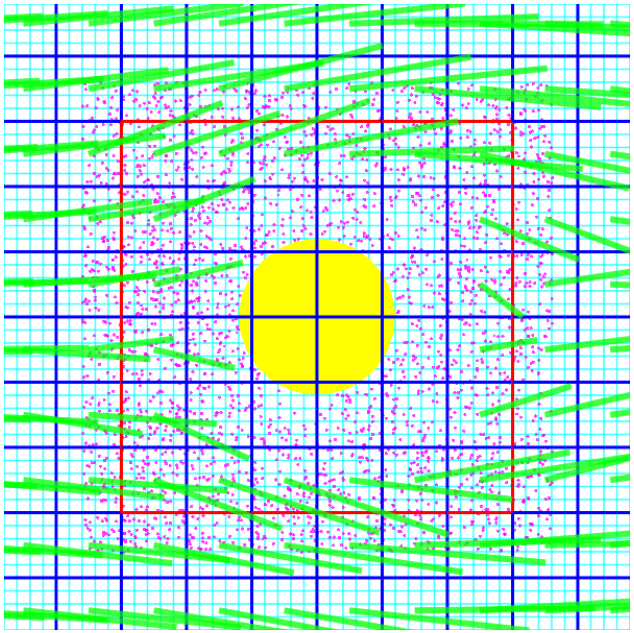
- Approximates the true mass and size into an **effective bead size** to match long-time behavior. This size is often *physically-meaningful*.

Outline

Complex Boundary Conditions using Particles



(MNG)

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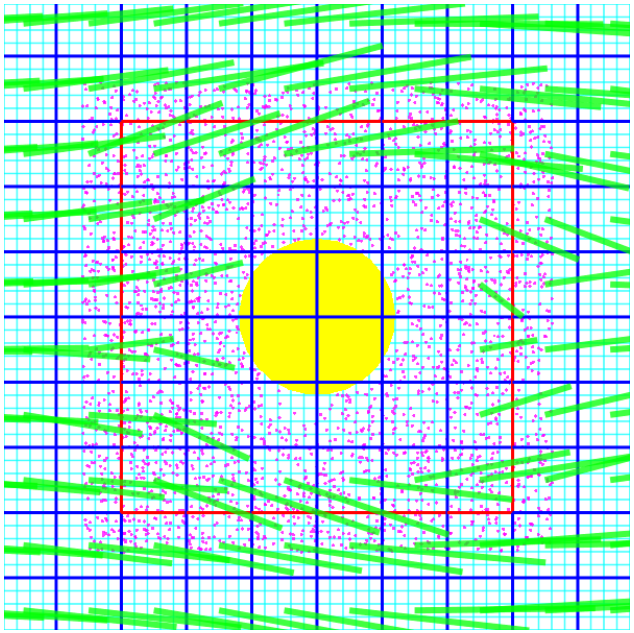

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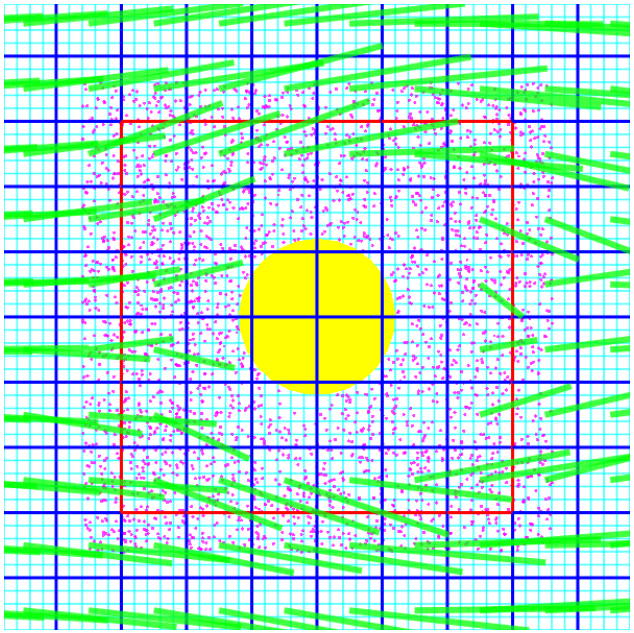

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- Hydro solver is a simple explicit MacCormack **(fluctuating) compressible LLNS** code and is *not aware* of particle patch.
- The method is based on Adaptive Mesh and Algorithm Refinement (AMAR) methodology for conservation laws and ensures **strict conservation** of mass, momentum, *and* energy [7].

Algorithm Refinement for Fluctuating Hydrodynamics, J. B. Bell and A. L. Garcia and S. A. Williams, SIAM Multiscale Modeling and Simulation, 6, 1256-1280, 2008

Freedom in Bead-Solvent Coupling

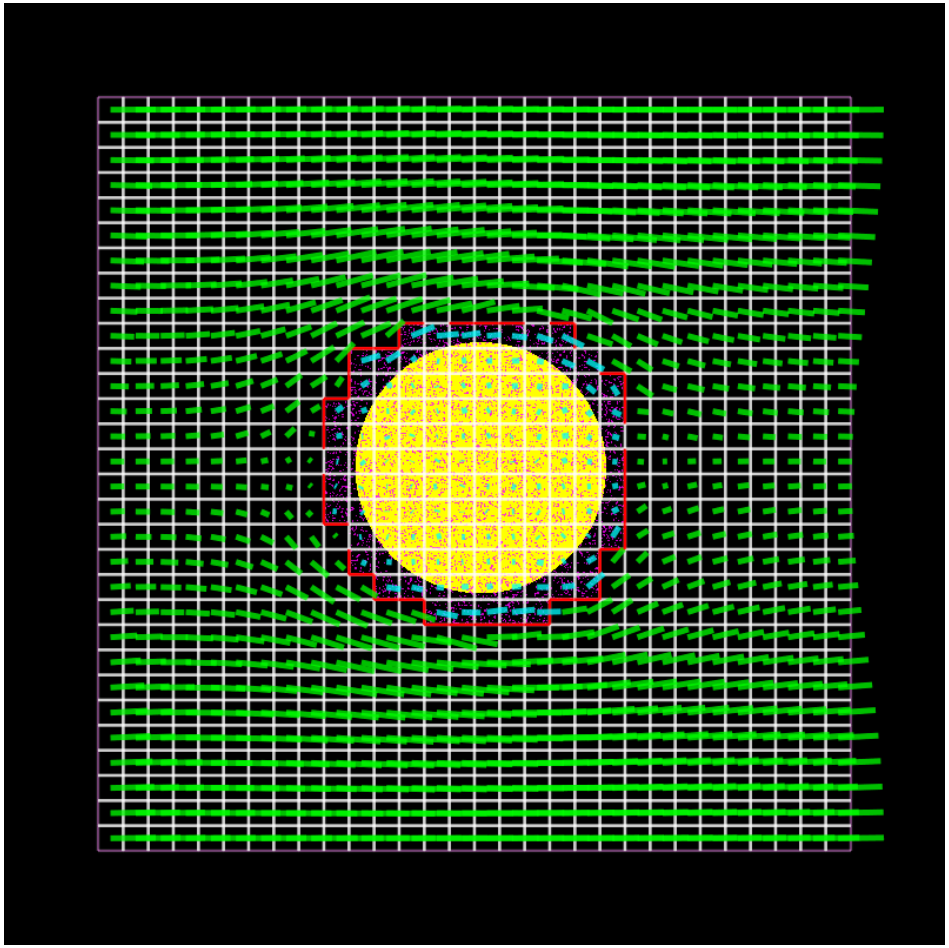

Figure: No event-driven handling at boundaries: **immersed bead**

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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, $\mathbf{u}_H \leftarrow \mathbf{u}_H - \mathbf{\Phi}_H + \mathbf{\Phi}_p$.

Polymer Chains

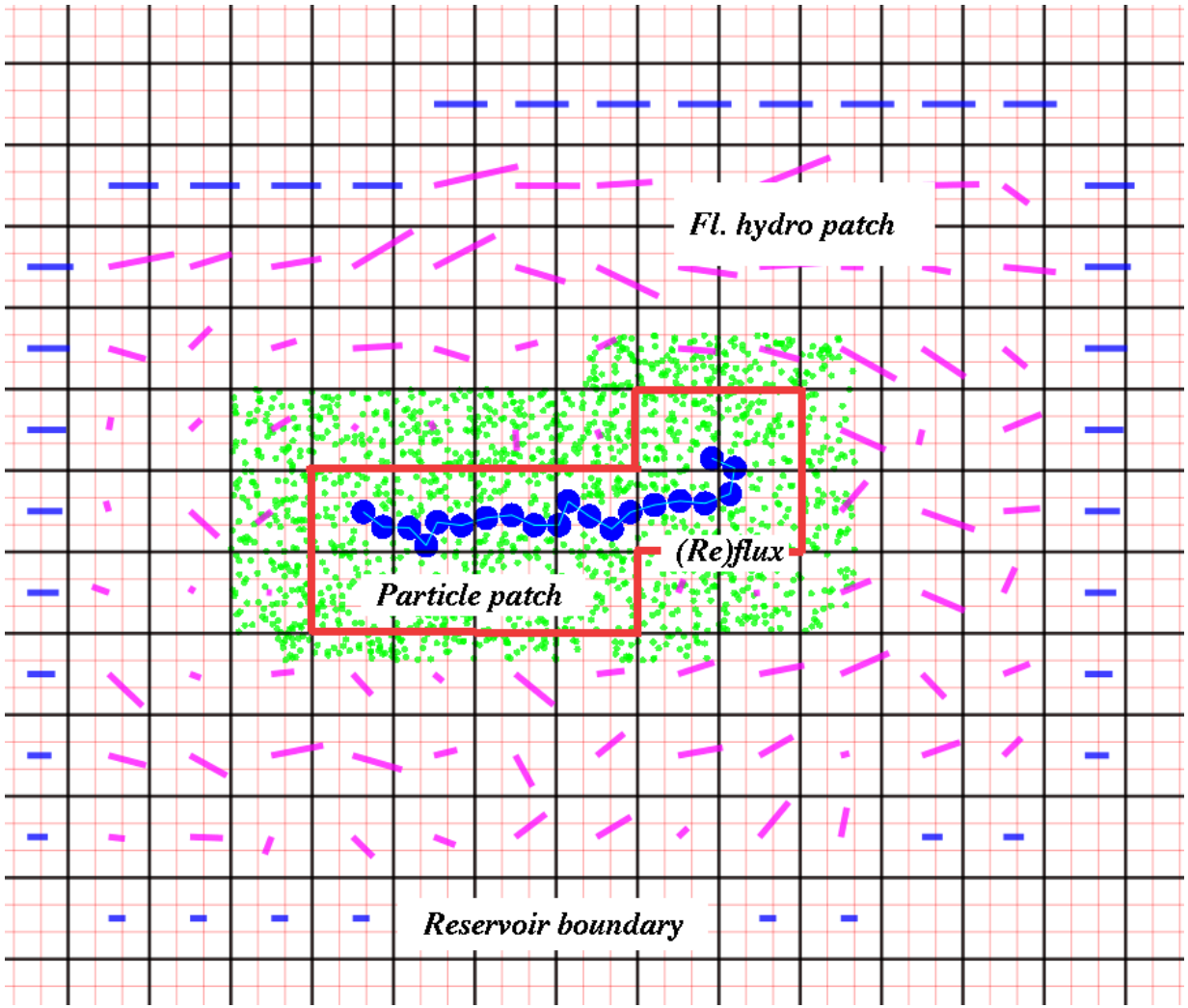
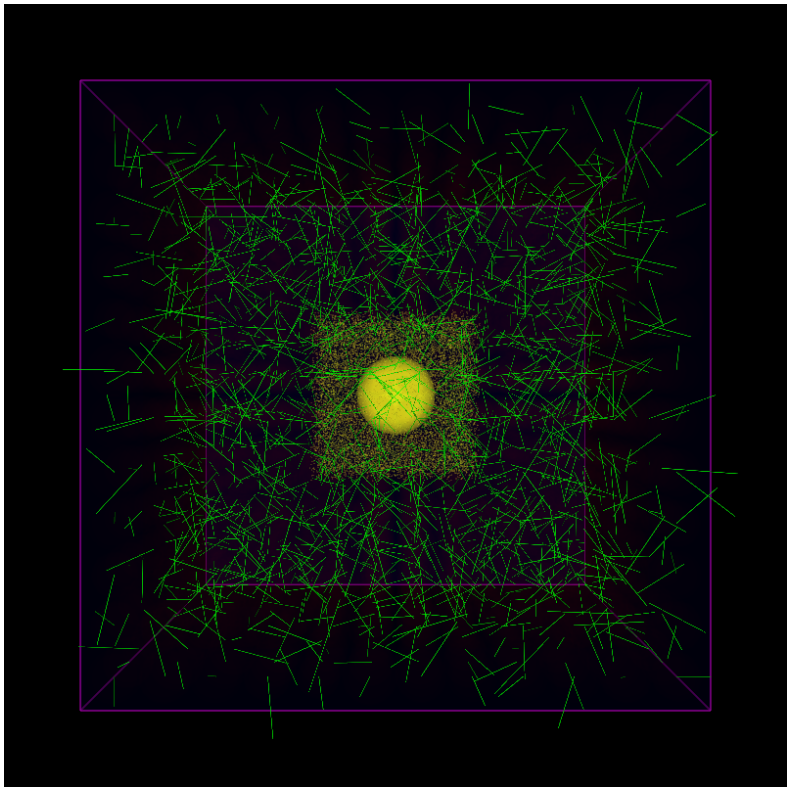
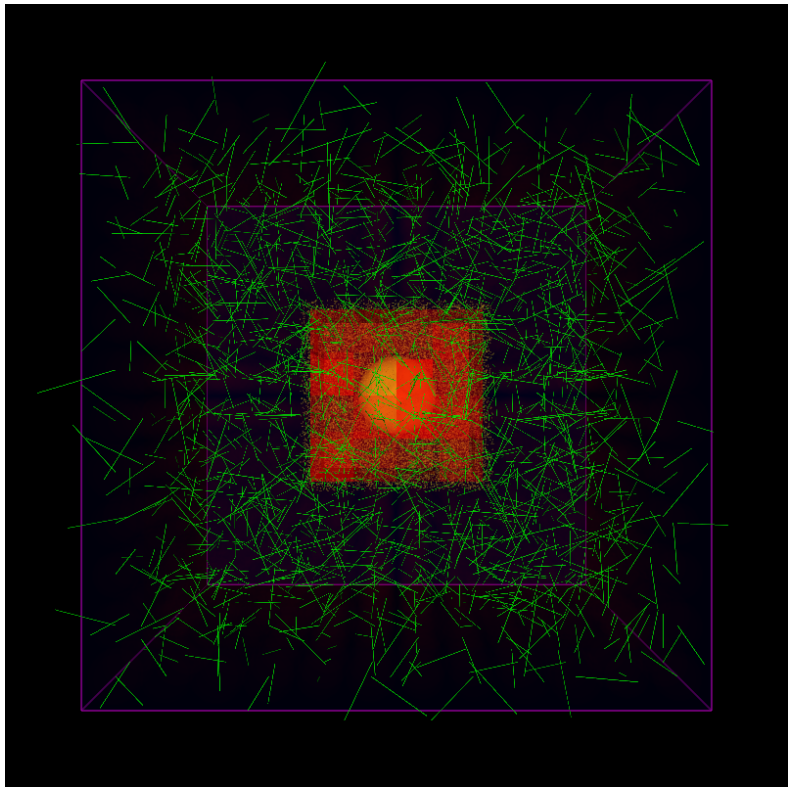


Figure: Hybrid method for a polymer chain.

Back to the Brownian Bead



(MNG)



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Velocity Autocorrelation Function

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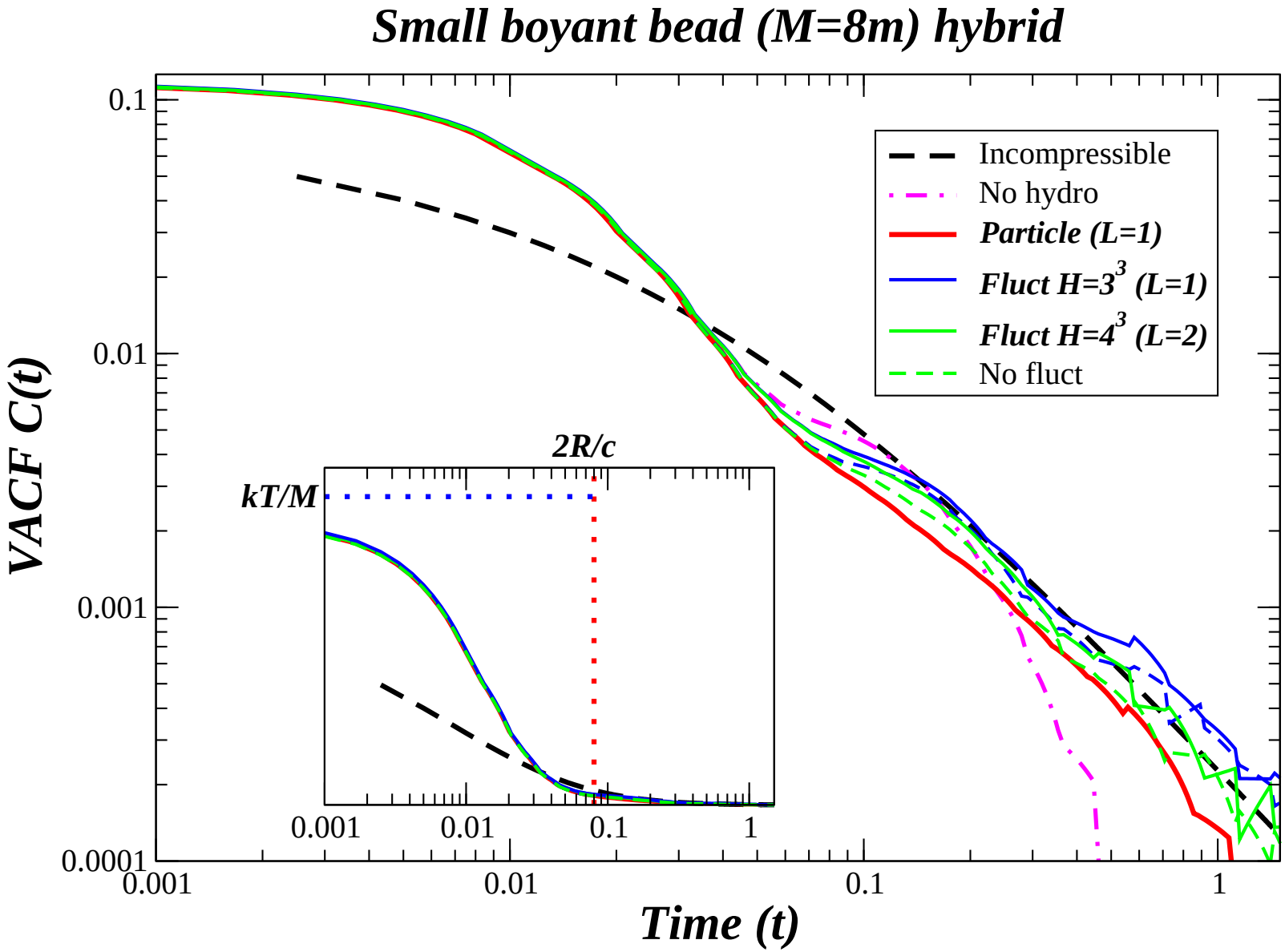
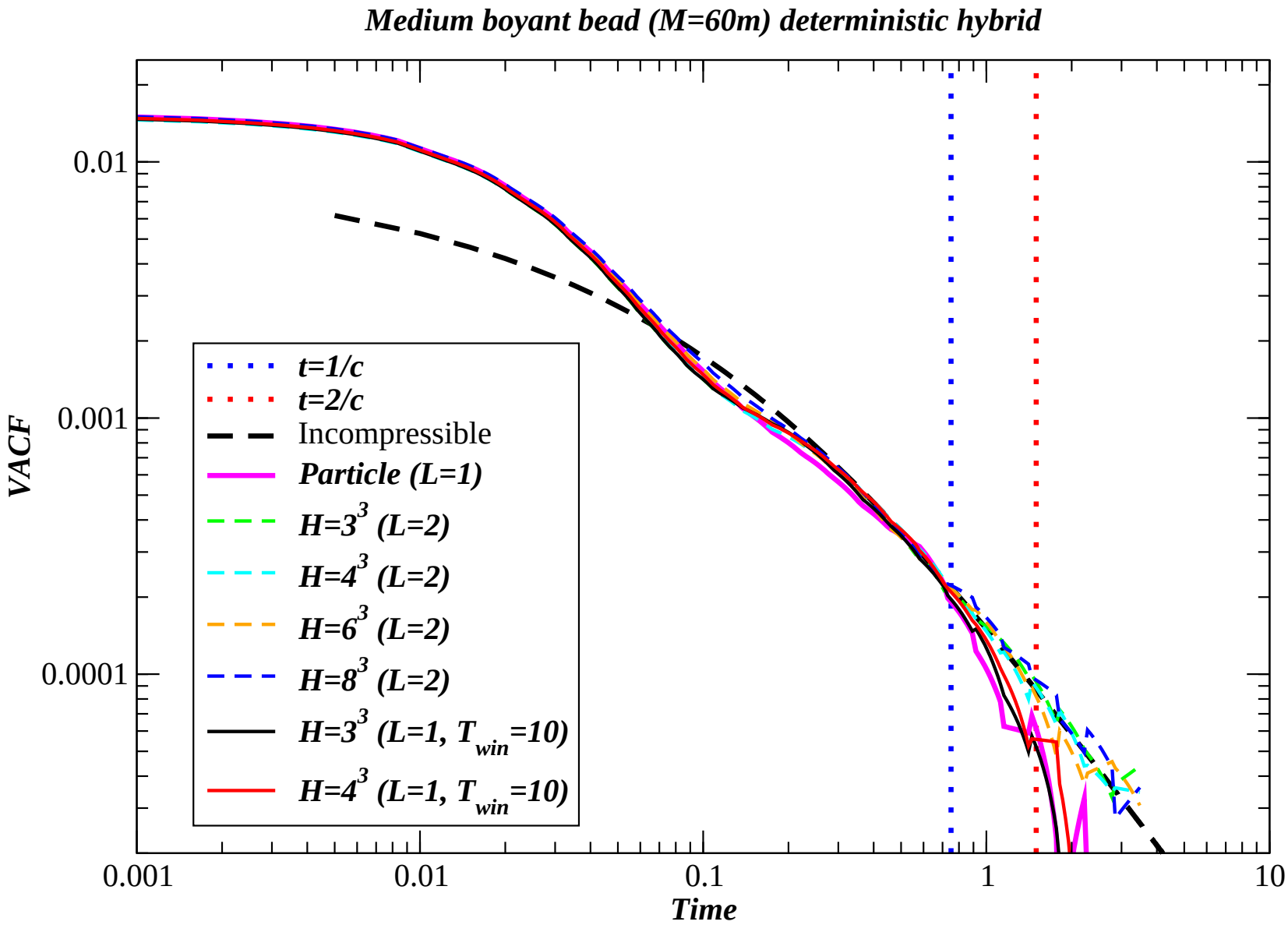
- Hydrodynamic persistence (conservation) gives a **long-time power-law tail** $C(t) \sim (kT/M)(t/t_{visc})^{-3/2}$ *not* reproduced in Brownian dynamics.

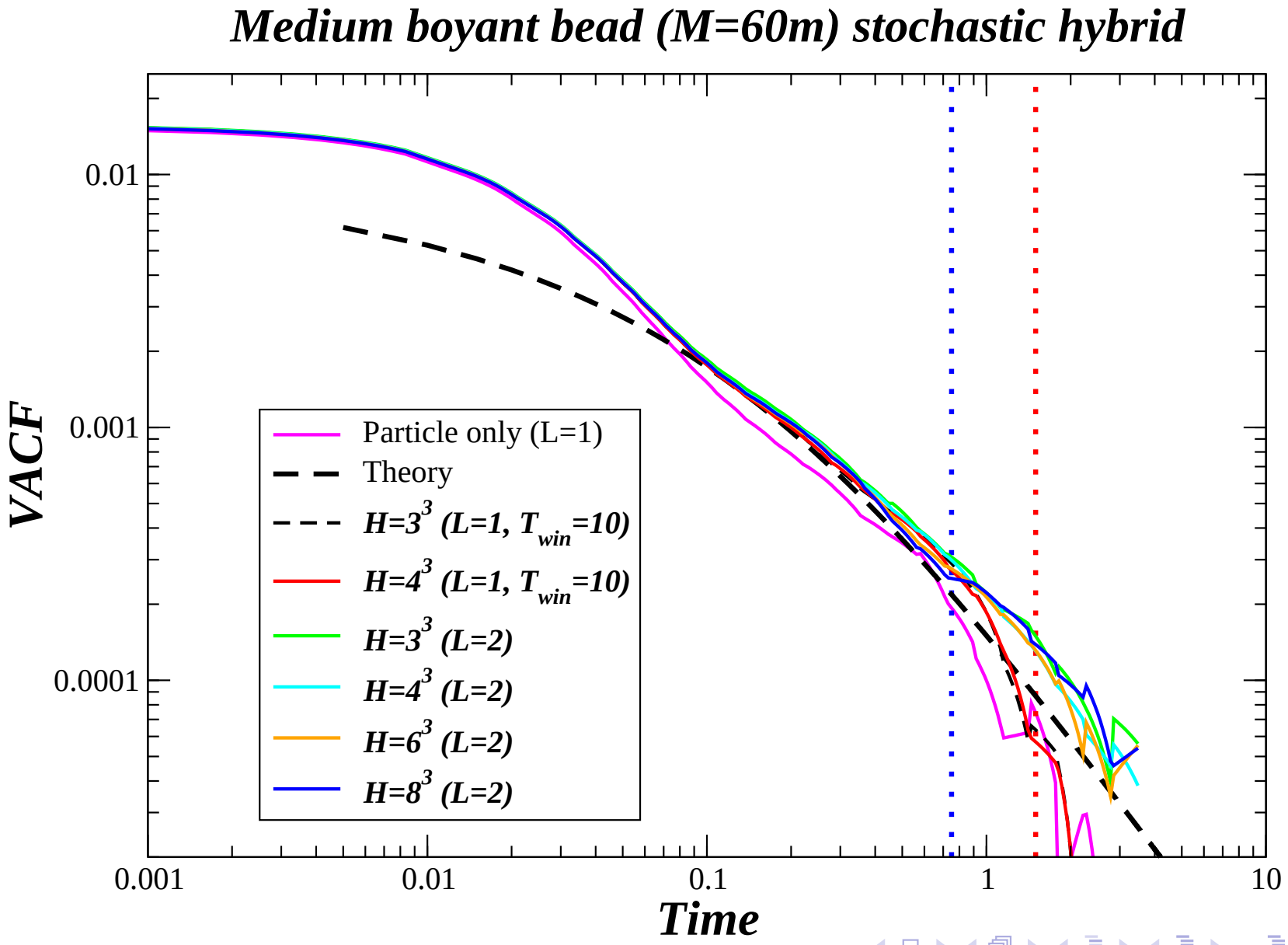
Small Bead (~10 particles)



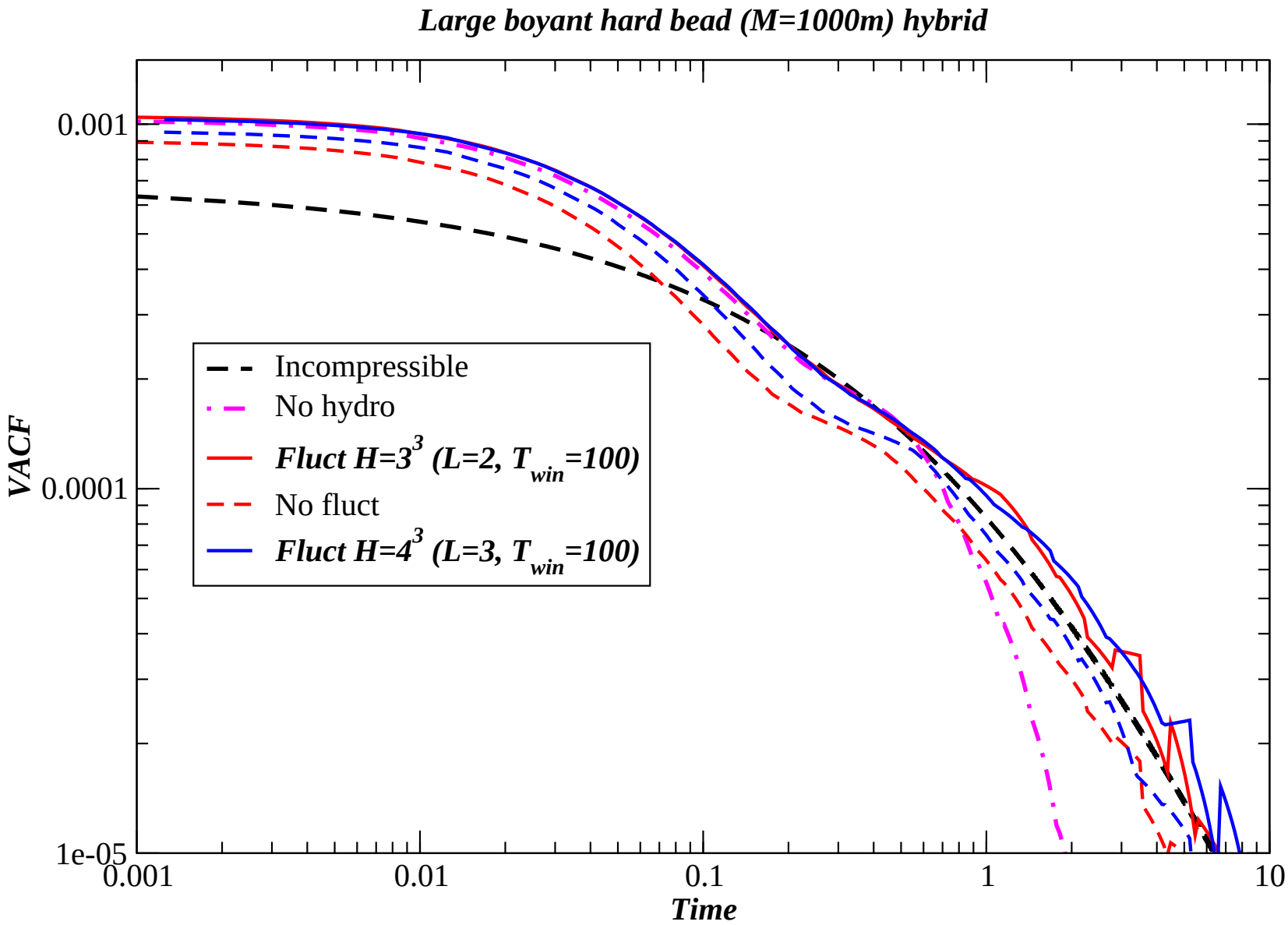
Medium Bead (˜100 particles)



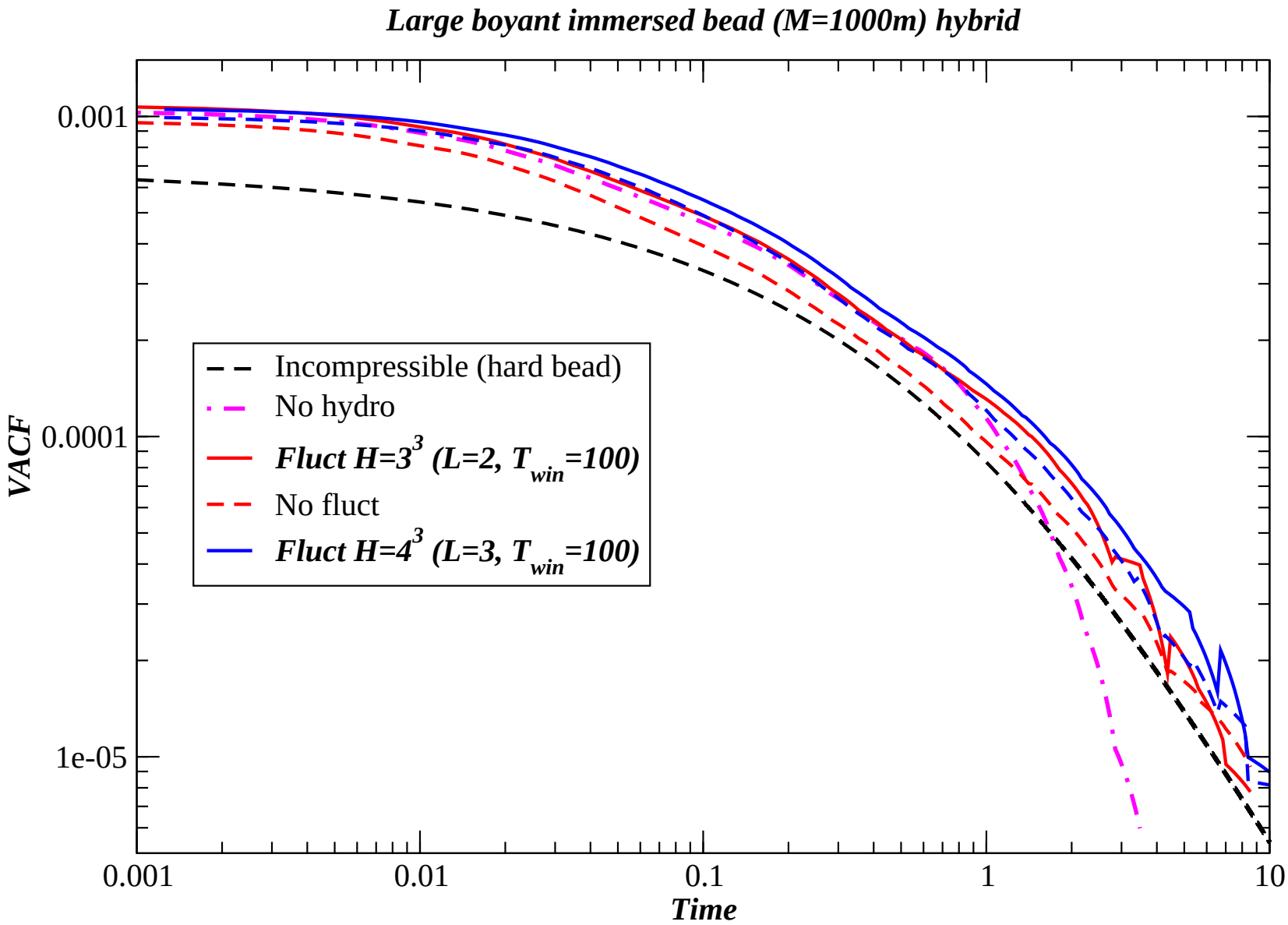
Medium Bead contd.



Large Hard Bead (~1000 particles)



Large Soft Bead (˜1000 particles)



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- Couple our **non-ideal stochastic hard-sphere gas** to continuum hydrodynamics with *microscopic fidelity*.
- Ultimately we require an **Adaptive Mesh and Algorithm Refinement** (AMAR) framework that couples deterministic MD for the polymer chains (**micro**), a stochastic solvent (**micro-meso**), with compressible fluctuating Navier-Stokes (**meso**), and incompressible CFD (**macro**).

References/Questions?

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