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Hydrodynamics and Flow solver

Requirements and Options

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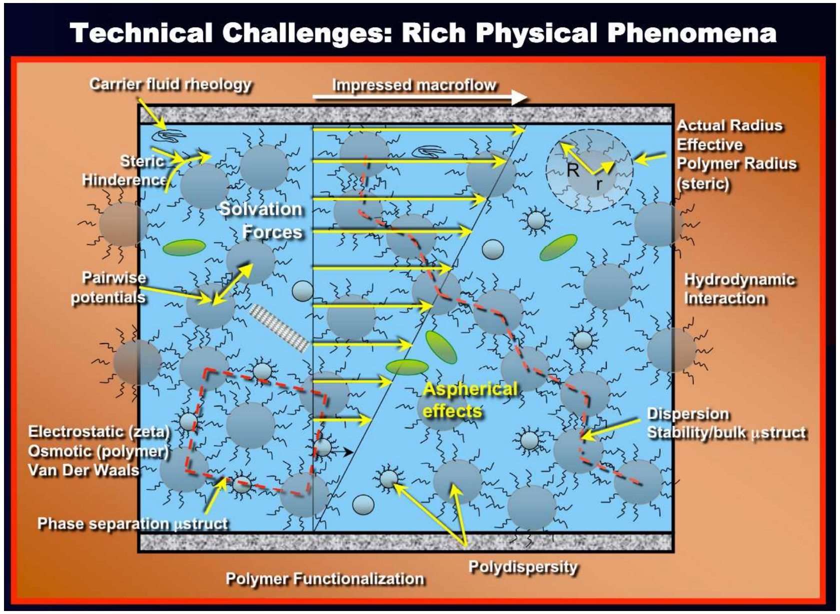
What We Won't Emphasize in this Section

- **MD: effective potential details**
- **Details of fluid-solid coupling strategies**
- **Pe = 0 limit**

Physical System: Total Size and Time

- **High Pe: Rheology of dense, aspherical nanoparticle suspensions**
  - **Length and time scales**
    - **Some rules of thumb**
      - **$O(10^4)$ particles**
      - **Strain O(10) box units**
      - **$\gamma \sim 100\ s^{-1}$**
      - **$2a_{eff} \sim 10 – 1000$ nm**
      - **$\Phi_{sc} \sim 0.5$**
    - **$L \sim O(0.1 – 10\ \mu m)$**
    - **$v_s \sim O(10 – 1000\ \mu m/s)$**
    - **$T \sim O(0.001 – 1\ s)$**



Physical System: Dimensionless Numbers and Timescales

Physical parameters	$a = 10nm$	$a = 1\mu m$
$M \approx \frac{4}{3}\pi a^3 \times 10^{-12}\frac{g}{\mu m^3}$	$4.19 \times 10^{-18} g$	$4.19 \times 10^{-12} g$
$\frac{\xi_E}{\xi_S} \approx 1.6 \times 10^2 a$	≈ 1.6	$\approx 1.6 \times 10^2$
$\xi_S = 6\pi\eta a \approx 1.9 \times 10^{-5} a$	$\approx 1.9 \times 10^{-7} \frac{g}{s}$	$\approx 1.9 \times 10^{-5} \frac{g}{s}$
$D_{col} \approx \frac{k_B T}{6\pi\eta a} \approx \frac{0.2}{a}$	$\approx 20 \frac{\mu m^2}{s}$	$\approx 0.2 \frac{\mu m^2}{s}$

Hydrodynamic numbers	$a = 10nm$	$a = 1\mu m$
$Pe = \frac{v_S a}{D_{col}} \approx 5 v_S a^2$	≈ 0.005	≈ 50
$Re = \frac{v_S a}{\nu} \approx 10^{-6} v_S a$	$\approx 10^{-7}$	$\approx 10^{-5}$
$Kn = \frac{\lambda_{free}}{a} \approx \frac{0.3}{a} \times 10^{-3}$	≈ 0.03	≈ 0.0003
$Ma = \frac{v_S}{c_s} \approx 6.76 \times 10^{-10} v_S$	$\approx 6.8 \times 10^{-10}$	$\approx 6.8 \times 10^{-10}$

Time-scales	$a = 10nm$	$a = 1\mu m$
$\tau_D = \frac{a^2}{D_{col}} \approx 5a^3$	$\approx 5 \times 10^{-6} s$	$\approx 5 s$
$t_S = \frac{a}{v_S} = \frac{\tau_\nu}{Re} = \frac{\tau_D}{Pe}$	$= 0.001 s$	$= 0.1 s$
$\tau_\nu = \frac{a^2}{\nu} \approx 10^{-6} a^2$	$\approx 10^{-10} s$	$\approx 10^{-6} s$
$\tau_B = \frac{M}{\xi_S} = \frac{2}{9}\tau_\nu$	$\approx 2.2 \times 10^{-11} s$	$\approx 2.2 \times 10^{-7} s$
$t_{cs} = \frac{a}{c_s} \approx 6.7 \times 10^{-10} a$	$\approx 6.7 \times 10^{-12} s$	$\approx 6.7 \times 10^{-10} s$

- **Note: Pe, Re, τ_D, t_s**
- **Also, note: τ_ν, timescale for momentum to diffuse in fluid over length a**
  - **Propagation length grows as √t**
    - **SD and the like imply $\tau_\nu = 0$**
- **Low Pe: Suspension Stability/Self Assembly**
  - **$\tau_D = d^2/D_{col} \sim O(0.001 – 1 s)$**
    - **T ~ O(0.1 – 100 s)**
    - **Scales as a^3**

Radius, a = 0.01μm (10nm) and 1μm in water at standard temperature and pressure pressure, moving at a velocity **v_S = 10μm/s**. Colloid assumed neutrally buoyant.
From Padding and Louis (2006) cond-mat/0603391

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Survey of Methods

- Stokes Methods: SD/BEM
  - ASDB/BD-hydro costs ~ O($N^{1.25}$logN) based on Ewald, Fourier sums for long-range terms; ~ O(N) based on PPPM-like method
  - BEM costs ~ O(NlogN) using multipole acceleration
    - no contact and near-contact is expensive
  - Quasi-analytical: aspherical is challenging
    - General form of the near-field terms (subgrid physics)?!
  - Effectively instantaneous hydrodynamics
  - Fluid-particle coupling "built-in"
- FD/FE, LB
  - Solve continuum Navier-Stokes PDE's + B.C.'s and I.C.'s
  - Fluid-particle coupling required
- Particle Based
  - SRD, DPD, SPH, LB

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Continuum Equations for Fluid

- Full Navier-Stokes Equations for Newtonian Fluid

$$\rho \frac{Du_i}{Dt} = \rho F_i + \frac{\partial \sigma_{ij}}{\partial x_j} \qquad \sigma_{ij} = -p\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_i}{\partial x_j}\delta_{ij}\right) + \mu_B \frac{\partial u_i}{\partial x_j}\delta_{ij}$$

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = \rho F_i - \frac{\partial p}{\partial x_i} + \mu\left[\frac{\partial^2 u_i}{\partial x_j \partial x_j} + \frac{1}{3}\frac{\partial}{\partial x_i}\left(\frac{\partial u_j}{\partial x_j}\right)\right] + \mu_B \frac{\partial}{\partial x_i}\left(\frac{\partial u_j}{\partial x_j}\right)$$

- Incompressible fluid

$$\frac{\partial u_i}{\partial x_i} = 0$$

- Small Re, large $Sl = \ell/u_s t$, but $ReSl = \ell^2/\nu\tau = \tau_\nu/\tau$ still small
  - Quasi-static, creeping flow, Stokes Equations are valid with error $O(Re_p^{1/2})$

$$\left.\begin{aligned} &ReSl\frac{\partial \mathbf{u}}{\partial t} + Re\,\mathbf{u}\cdot\nabla\mathbf{u} = \rho\mathbf{F} - \nabla p + \nu\nabla^2\mathbf{u} \\ &\nabla\cdot\mathbf{u} = 0 \end{aligned}\right\} \Rightarrow \begin{aligned} &\nabla p = \rho\mathbf{F}(x,t) + \mu\nabla^2\mathbf{u} \\ &\nabla\cdot\mathbf{u} = 0 \end{aligned}$$

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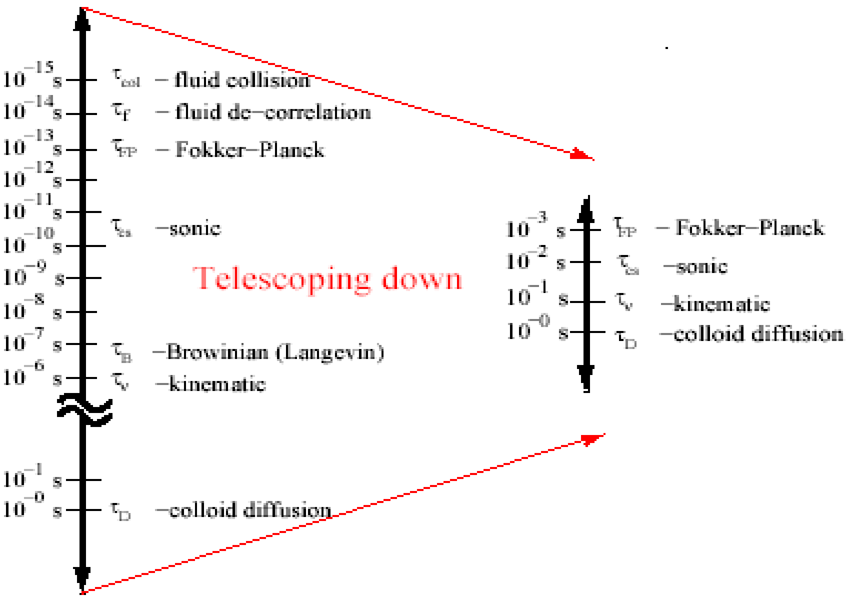
Computational Requirements

- Dense suspensions
  - contact or near contact
- Aspherical
  - general treatment
- Large systems & long times
  - Continuum approaches
    - 2a/dx ~ 10, L ~ 80a
      - $N_{nodes} \sim O(10^7)$
    - $dt/\delta t_{MD} \sim O(10^2 – 10^3)$
      - $T_{MD} \sim O(10^5 – 10^8)$
      - # NS solves ~ $O(10^3 - 10^6)$
- Options?
  - Coarse-grain: "telescope" time scales
  - Explicit algorithms
  - Quasi-implicit/Semi-implicit algorithms
  - SD/BEM



Time scales for 1 μm colloid in water.
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