

On the derivation of viscoelastic models for rod-like suspensions

Richard Höfer

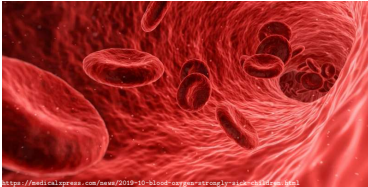
Institut de Mathématiques de Jussieu – Paris Rive Gauche
Université Paris Cité

Conférence Singflows

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Joint work with Marta Leocata (LUISS, Rome)
and Amina Mecherbet (Université Paris Cité)

Suspensions



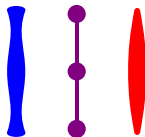
Doi model for viscoelasticity of dilute rigid suspensions

Model for inertialess rod-like Brownian particles with density $f(t, x, \xi)$, $\xi \in S^2$ particle orientation (see e.g. [Doi-Edwards '86]):

$$\begin{aligned} \partial_t f + u \cdot \nabla_x f + \operatorname{div}_\xi (P_{\xi^\perp} (\xi \cdot \nabla u) f) &= D_t \Delta_x f + D_r \Delta_\xi f, \\ -\operatorname{div}(\mu_{\text{eff}}[f] Du) + \nabla p &= h + \operatorname{div} \sigma_e, \quad \operatorname{div} u = 0, \end{aligned}$$

$$\text{Elastic stress: } \sigma_e = \lambda_1 \int_{S^2} (3\xi \otimes \xi - \operatorname{Id}) f \, d\xi,$$

$$\text{Effective viscosity: } \mu_{\text{eff}}[f] = 2 + \lambda_2 \int_{S^2} \xi \otimes \xi \otimes \xi \otimes \xi f \, d\xi$$



Study of the macroscopic system (well-posedness, numerical simulation, ...) [Constantin '05], [Helzel-Otto-Tzavaras '06,'08,'16,'17], [Masmoudi-Lions '07], [Degond-Liu '09], [Bae-Trivisa '12,'13], [La '18].

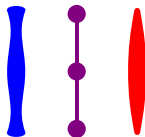
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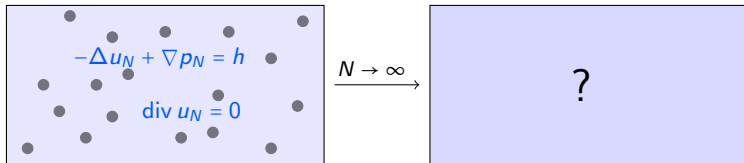


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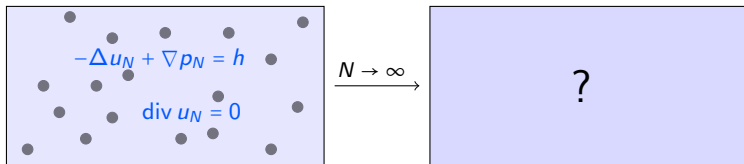
Related models: liquid crystals, elastic polymers, active particles.

Goal: Rigorous derivation of the Doi-model – the elastic stress – from a microscopic fluid-particle-system.

Einstein's effective viscosity formula



Einstein's effective viscosity formula

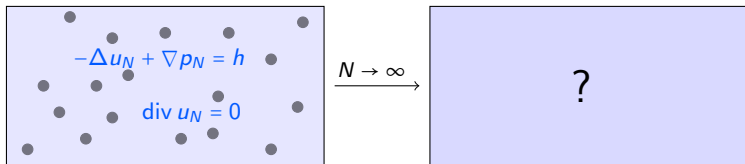


Einstein 1906: For inertialess spherical particles the suspension can be described by an **effective viscosity**

$$\mu_{\text{eff}} = 1 + \frac{5}{2}\phi + o(\phi),$$

where ϕ is the particle volume fraction.

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More precisely, under straining boundary conditions

$$u_N = Ex \quad \text{on } \partial\Omega, \quad E \in \operatorname{Sym}_0(3)$$

with no external forces, the **energy dissipation** satisfies

$$\int_{\Omega} |Du_N|^2 = |\Omega| |E|^2 \left(1 + \frac{5}{2}\phi + o(\phi) \right)$$

Resistance and mobility of a single particle

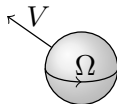
$$-\Delta u + \nabla p = 0, \quad \operatorname{div} u = 0 \quad \text{in } \mathbb{R}^3 \setminus \mathcal{B},$$

$$u(x) = V + \Omega \times (x - X) \quad \text{in } \mathcal{B}.$$

$$\lim_{|x| \rightarrow \infty} u(x) - (u_\infty + \omega_\infty \wedge (x - X) + E_\infty(x - X)) = 0.$$

$$F = - \int_{\partial \mathcal{B}} \sigma[u, p] \nu, \quad T = - \int_{\partial \mathcal{B}} \sigma[u, p] \nu \wedge (x - X),$$

$$S = -\operatorname{sym}_0 \left(\int_{\partial \mathcal{B}} \sigma[u, p] \nu \otimes (x - X) \right),$$

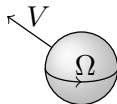


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- **Resistance problem:**

Given $V, \Omega, u_\infty, \omega_\infty \in \mathbb{R}^3$ and $E_\infty \in \operatorname{Sym}_0(3)$,
find F, T, S

$$\begin{pmatrix} F \\ T \\ S \end{pmatrix} = \mathcal{R}_{\mathcal{B}} \begin{pmatrix} V - u_\infty \\ \Omega - \omega_\infty \\ -E_\infty \end{pmatrix}.$$

- **Mobility problem:**

Given $F, T, u_\infty, \omega_\infty \in \mathbb{R}^3$ and $E_\infty \in \operatorname{Sym}_0(3)$,
find V, Ω, S

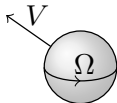
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Sphere of radius R : \mathcal{M}_{B_R} is diagonal.

$$\text{In particular: } F = T = 0 \quad \Rightarrow \quad V = u_\infty, \quad \Omega = \omega_\infty, \quad S = -\frac{5}{2} \frac{4\pi}{3} R^3 E_\infty$$

Formal homogenization through superposition

- N identical spherical particles $B_i = B_R(X_i)$,
- $\frac{1}{N} \sum_i \delta_{X_i} \rightarrow \rho$, $\phi = \frac{4\pi}{3} NR^3 \ll 1$

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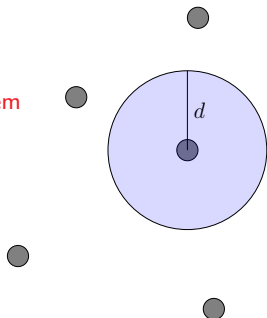
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In $B_d(X_i)$, $R \ll d \ll N^{-1/3}$: approximate **mobility problem** with $F = 0$, $T = 0$, $E_\infty = Du_{\text{eff}}(X_i)$.

Thus, approximate

$$-\Delta u_N + \nabla p_N \approx h - \sum_i \frac{5}{2} \frac{4\pi}{3} R^3 Du_{\text{eff}}(X_i) \nabla \delta_{X_i}$$



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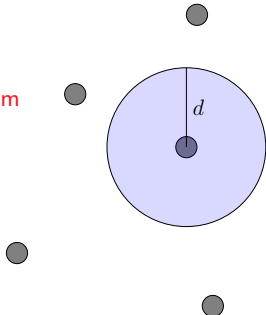
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Taking limits on both sides

$$-\Delta u_{\text{eff}} + \nabla p \approx h - \frac{5}{2} \phi \operatorname{div}(2\rho Du_{\text{eff}})$$



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- H'.–Schubert '21: Time evolution of (buoyant, sedimenting) particles:

$$\begin{aligned} \partial_t \rho + (u + \gamma^{-1}g) \nabla \rho &= 0 \\ -\text{div} \left(2 \left(1 + \frac{5}{2} \phi \rho \right) Du \right) + \nabla p &= \rho g. \end{aligned}$$

Back to viscoelasticity

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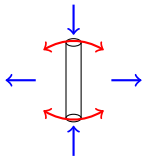
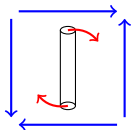
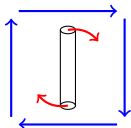
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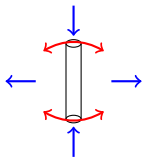
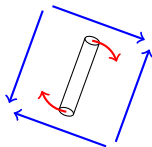
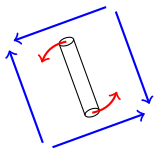
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A single Brownian particle

Mobility problem

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$$u = V + \Omega \times (x - X) \quad \text{in } \mathcal{B}.$$

$$\lim_{|x| \rightarrow \infty} u(x) = 0.$$

with random forces F^B, T^B given through a 6-dim Brownian motion according to the fluctuation-dissipation-theorem (Stokes-Einstein relation)

$$(F^B, T^B) = \sqrt{2k_B \Theta \mathcal{R}_{red}} \circ dB,$$

$$\mathcal{R}_B = \begin{pmatrix} \mathcal{R}_1 & \mathcal{R}_{12} & \mathcal{R}_{13} \\ \mathcal{R}_{12}^T & \mathcal{R}_2 & \mathcal{R}_{23} \\ \mathcal{R}_{13}^T & \mathcal{R}_{23}^T & \mathcal{R}_3 \end{pmatrix}.$$

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For Axisymmetric particles $\mathcal{B}_R = RO(\xi)\mathcal{B}$ with orientation ξ , $O(\xi) \in SO(3)$:

$$\mathcal{R}_{\mathcal{B}_R} = \begin{pmatrix} \boxed{\mathcal{R}\mathcal{R}_1(\xi)} & 0 & 0 \\ 0 & \mathcal{R}^3\mathcal{R}_2(\xi) & \mathcal{R}^3\mathcal{R}_{23}(\xi) \\ 0 & \mathcal{R}^3\mathcal{R}_{23}^T(\xi) & \mathcal{R}^3\mathcal{R}_3(\xi) \end{pmatrix}.$$

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Thus, in a fluid at rest,

$$V = R^{-1}\mathcal{R}_1^{-1}(\xi)F^B = R^{-1/2}\sqrt{\mathcal{R}_1^{-1}(\xi)} \circ dB^t, \quad \Omega = R^{-3/2}\sqrt{\mathcal{R}_2^{-1}(\xi)} \circ dB^r$$

$$S = R^3\mathcal{R}_{23}^T(\xi)\Omega = R_{23}^T(\xi)\sqrt{\mathcal{R}_2^{-1}(\xi)} \circ dB^r$$

Microscopic model of N Brownian particles

- N identical axissymmetric particles $\mathcal{B}_i = O(\xi_i)R\mathcal{B}$ with centers X_i and orientations ξ_i , orientation matrix $O(\xi_i) \in SO(3)$ and $R = R_N \rightarrow 0$, $\phi = NR^3 \ll 1$.

$$\begin{aligned} -\Delta u_N + \nabla p_N &= h, & \operatorname{div} u_N &= 0 & \text{in } \mathbb{R}^3 \setminus \cup_i \mathcal{B}_i, \\ u_N(x) &= V_i + (x - X_i) \wedge \Omega_i & & & \text{in } \cup_i \mathcal{B}_i, \\ \int_{\partial \mathcal{B}_i} \sigma[u_N, p_N] \nu &= F_i^B, & \int_{\partial \mathcal{B}_i} \sigma[u_N, p_N] \nu \wedge (x - X_i) &= T_i^B, \\ (F_i^B, T_i^B)_i &= \sqrt{\mathcal{R}_N} \circ dB, \\ \dot{X}_i &= V_i, & \dot{\xi}_i &= \Omega_i \wedge \xi_i. \end{aligned}$$

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 \partial_t f + u \cdot \nabla_x f + \operatorname{div}_\xi (P_{\xi^\perp}(\xi \cdot \nabla u) f) &= D_t \Delta_x f + D_r \Delta_\xi f, \\
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 \partial_t f + \operatorname{div}_\xi ((P_{\xi^\perp} h f - \nabla_\xi f)) = 0, & \quad \text{Deborah number } De = 1 \\
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Statement of the result

- well separated particles: $\min_{i \neq j} |X_i - X_j| \geq cN^{-\frac{1}{3}}$
- small volume fraction: $\phi_N \log N = NR_N^3 \log N \rightarrow 0$
- Convergence of initial data: $\mathbb{E}[\mathcal{W}_1(\frac{1}{N} \sum \delta_{X_i, \xi_i^0}, f_0)] \rightarrow 0$, $f_0 \in L^2(\mathbb{R}^3 \times \mathbb{S}^2)$

Theorem 1: For $De = 1$, for all $t > 0$, $s > 1/2$

$$\forall \varepsilon > 0 \lim_{N \rightarrow \infty} \mathbb{P}[\|\phi_N^{-1} u_N - u\|_{H^{-s}((0,t), H^{-s}(\mathbb{R}^3))} + \sup_{\tau \in [0,t]} \mathcal{W}_1(f_N(\tau), f(\tau)) > \varepsilon] = 0,$$

where (f, u) solve

$$\begin{aligned} \partial_t f + \operatorname{div}_\xi((P_{\xi^\perp} h f - \nabla_\xi f) &= 0 & f(0, \cdot) &= f_0 \\ -\Delta u + \nabla p = \gamma_B \int_{\mathbb{S}^2} (3\xi \otimes \xi - \operatorname{Id}) f \, d\xi, & & \operatorname{div} u &= 0. \end{aligned} \quad (1)$$

Theorem 2: For $De = \phi_N \rightarrow 0$, for all $t > 0$, $s_1 > 1/2$, $s_2 > 0$, $s_3 > 3/2$

$$\forall \varepsilon > 0 \lim_{N \rightarrow \infty} \mathbb{P}[\|u_N - u\|_{H^{-s_1}((0,t); H^{-s_1}(\mathbb{R}^3))} + \|f_N - f\|_{H^{-s_2}(0,t; H^{-s_3}(\mathbb{R}^3 \times \mathbb{S}^2))} > \varepsilon] = 0,$$

where u solves (1) and f solves

$$\operatorname{div}_\xi((P_{\xi^\perp} h f - \nabla_\xi f) = 0, \quad \int f \, d\xi = \int f_0 \, d\xi.$$

Strategy of the proof

Consider $u_N \approx u_{N,app}$, the solution to

$$-\Delta u_{N,app} + \nabla p_{N,app} = -\frac{\phi_N}{N} \sum_i (S_i + T_i) \nabla \delta_{X_i}, \quad \operatorname{div} u_{N,app} = 0 \quad \text{in } \mathbb{R}^3,$$

$$T_i := \sqrt{\mathcal{R}_2(\xi_i)} \circ dB_i \quad S_i := \mathcal{R}_{23}^T(\xi_i) \mathcal{R}_2^{-1}(\xi_i) T_i := \mathcal{S}(\xi_i) \circ dB_i$$

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Recall

$$d\xi_i = \xi_i \times \sqrt{\mathcal{R}_2(\xi_i)} \circ dB_i + P_{\xi_i^\perp} h dt, \quad d\mathcal{S}(\xi_i) = \nabla_{\xi_i} \mathcal{S}(\xi_i) \xi_i \times \sqrt{\mathcal{R}_2(\xi_i)} \circ dB_i + \dots dt$$

Compute by **Itô-Stratonovitch conversion**

$$\begin{aligned} \mathbb{E} \left[\int_0^t S_i dt \right] &= \mathbb{E} \left[\int_0^t \mathcal{S}(\xi_i) \circ dB_i \right] = \mathbb{E} \left[\int_0^t \mathcal{S}(\xi_i) dB_i \right] + \frac{1}{2} \mathbb{E} \left[[S(\xi_i), B_i]_t \right] \\ &= \dots = \gamma_B \mathbb{E} \left[\int_0^t (3\xi_i \otimes \xi_i - \operatorname{Id}) ds \right] \end{aligned}$$

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Similarly, $\mathbb{E}[\int_0^t T_i dt] = 0$. Thus, formally, by the **Law of Large Numbers**,

$$\phi_N^{-1} u_{N,app} \rightarrow u, \quad -\Delta u + \nabla p = \operatorname{div} \sigma := \gamma_B \operatorname{div} \int_{S^2} (3\xi \otimes \xi - \operatorname{Id}) f d\xi$$

Main obstacles

Need to make sense of

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Solution: Denote $L_N : (S^2)^N \rightarrow \mathcal{L}(\mathbb{R}^{3N}; \dot{H}^1(\mathbb{R}^3))$ the solution operator to (2) with given torques (T_1, \dots, T_N) instead of $R^3 \sqrt{\mathcal{R}_2(\xi_i)} \circ dB_i$.

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Show

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Key ingredient: **Method of reflections** that allows to write L_N in terms of single particle solution operators with more explicit shape derivatives.

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Thank you!