Homogenization for active particles in a Stokes fluid

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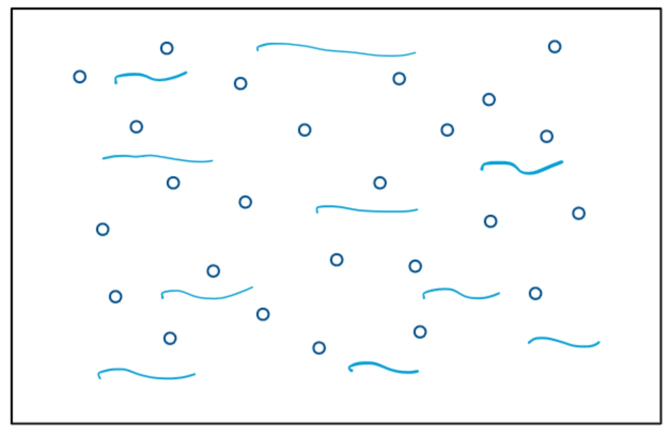
The starting point

A **Stokes fluid** (no inertial effect, no dynamics) enclosed in a domain. Inside lies a **suspension of particles**.



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Neglecting the inter-particle interactions, Einstein obtained his **effective viscosity formula**

$$\eta = \eta_0 \Big(1 + \frac{5}{2}\varphi \Big),$$

where φ is the fraction of volume occupied by the particles (actually Einstein forget the $\frac{5}{2}$ due to a calculational error). Since φ can be directly related to the Avogadro number, and since it was possible to obtain the ratio η/η_0, he could compute an estimation of the Avogadro number (I'm skipping some difficult steps).

Back to the effective viscosity formula

The equation

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tells us how the viscosity is changed by the presence of the suspension. Several challenges are associated to it

1. Rigorous derivation of the formula
2. Validity for larger concentration ?
3. Finer corrections in φ.

Those problems have been the object of intensive research in physics in the second part of the XXth and in the mathematical community during the past decade.

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Remark: Since $\varphi \geq 0$, the presence of passive particles always increases the effective viscosity !

Main approaches

1. The homogenization/constructive approach : goes back to the first description of Einstein $\rightarrow$ Lévy, Sánchez-Palencia (periodic inclusions), Duerinckx, Gloria (random inclusions).
2. The "mean-field approach": Gérard-Varet, Hillairet, Mécherbet...
3. The method of reflections: Höfer, Schubert, Vélazquez, Jabin, Otto
4. Formal asymptotical analysis through the study of the hydrodynamical interactions (Batchelor, Green, Haines, Mazzucato...)

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Hardcore assumption: $\exists \delta > 0$ such that for all $n \neq m$

$$(I_n^\omega + \delta B) \cap (I_m^\omega + \delta B) = \emptyset,$$

where $B = B(0,1)$.

Random suspension II

We define, for all $\omega \in \Omega$, $\epsilon > 0$ $\mathcal{N}_\epsilon^\omega(U) = \{n : \epsilon(I_n^\omega + B) \subset U\}$, and set

$$\mathcal{I}_\epsilon^\omega(U) = \cup_{n \in \mathcal{N}_\epsilon^\omega(U)} \epsilon I_n^\omega .$$

Suspension immersed in a Stokes fluid

Around this random suspension: a Stokes fluid. Write $(u_\epsilon^\omega(x), P_\epsilon^\omega(x)) \in \mathbb{R}^d \times \mathbb{R}$ for the fluid velocity and pressure at $x \in U$. We impose $(u_\epsilon^\omega)_{|\partial U} = 0$.

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Notations: symmetric gradient and Cauchy stress tensor

$$D(u) = \frac{1}{2}\big(\nabla u + \nabla^T u\big), \qquad \sigma(u, P) = 2D(u) - PI_d.$$

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Quasi-static setting (dynamics are hard!) in which inertial forces are neglected, leading us to the Stokes equations, with a source term g.

$$\begin{cases} -\triangle u_\epsilon^\omega + \nabla P_\epsilon^\omega = g & \text{in } U \setminus \mathcal{I}_\epsilon^\omega(U), \\ \operatorname{div}(u_\epsilon^\omega) = 0, & \text{in } U \setminus \mathcal{I}_\epsilon^\omega(U), \\ D(u_\epsilon^\omega) = 0, & \text{in } \mathcal{I}_\epsilon^\omega(U), \end{cases}$$

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Last condition is the rigid motion inside the inclusions: for all $n \in \mathcal{N}_\epsilon^\omega(U)$, there exists $\kappa_n \in \mathbb{R}^d$, $\Theta_n \in \mathbb{M}^{\text{Skew}}$ such that

$$u_\epsilon^\omega = \kappa_n + \Theta_n(\cdot - \epsilon x_n^\omega) \qquad \text{in } \epsilon I_n^\omega.$$

Boundary conditions

At the boundary of the inclusions: no buoyancy. For all $n \in \mathcal{N}_\epsilon^\omega(U)$, letting ν be the unit outward normal vector,

$$\int_{\epsilon I_n^\omega} \sigma(u_\epsilon^\omega, P_\epsilon^\omega)\nu = 0,$$

$$\int_{\epsilon I_n^\omega} \Theta(x - \epsilon x_n^\omega) \cdot \sigma(u_\epsilon^\omega, P_\epsilon^\omega)\nu = 0, \qquad \forall \Theta \in \mathbb{M}^{\text{skew}}.$$

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The full colloidal problem

Overall, the system writes

$$\begin{cases} -\triangle u_\epsilon^\omega + \nabla P_\epsilon^\omega = g & \text{in } U \setminus \mathcal{I}_\epsilon^\omega(U), \\ \operatorname{div}(u_\epsilon^\omega) = 0, & \text{in } U \setminus \mathcal{I}_\epsilon^\omega(U), \\ D(u_\epsilon^\omega) = 0, & \text{in } \mathcal{I}_\epsilon^\omega(U), \\ \int_{\epsilon\partial I_n} \sigma(u_\epsilon^\omega, P_\epsilon^\omega)\nu = 0 & \text{for all } n \in \mathcal{N}_\epsilon^\omega(U), \\ \int_{\epsilon\partial I_n} \Theta(x - \epsilon x_n^\omega) \cdot \sigma(u_\epsilon^\omega, P_\epsilon^\omega)\nu = 0 & \text{for all } \Theta \in \mathbb{M}^{\text{skew}}, n \in \mathcal{N}_\epsilon^\omega(U). \end{cases}$$

Goal: analyze this problem in the limit $\epsilon \downarrow 0$.

Theorem (Duerinckx, Gloria, 2021)

We have the following convergence results, as $\epsilon \to 0$,

1. $u_\epsilon^\omega \rightharpoonup \bar{u}$ in $H_0^1(U)^d$,
2. $P_\epsilon^\omega \mathbf{1}_{U \setminus \mathcal{I}_\epsilon^\omega(U)} \rightharpoonup (1-\lambda)(\bar{P} - \bar{b} : D(\bar{u}))$ in $L^2(U)$,

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where $(\bar{u}, \bar{P}) \in H_0^1(U)^d \times L^2(U)$ is the unique solution to the homogenized problem in U:

$$\begin{cases} -\mathrm{div}(2\bar{B}D(\bar{u})) + \nabla \bar{P} = (1-\lambda)g, \\ \mathrm{div}(\bar{u}) = 0, \quad \fint_U \bar{P} = 0, \end{cases}$$

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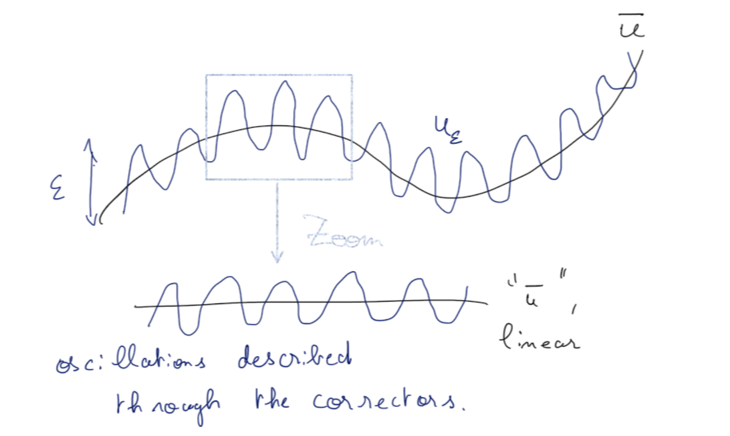
where $\lambda = \mathbb{E}[\mathbf{1}_{\mathcal{I}^\omega}]$ is the particle density, and $\bar{B}, \bar{b}$ are the **effective tensors** of the passive suspension.

Structure and oscillations

Key point of the theory: ∇u_ϵ^ω has some small scale oscillations $O(\epsilon)$, but $u_\epsilon^\omega \rightharpoonup \bar{u}$ in $H_0^1(U)^d$ with $\bar{u}$ solution of a new equation. Our goal: describing the oscillations at the scale ϵ through **correctors**.



Passive corrector problem

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Encapsulates the contribution of the presence of particles given a uniform velocity gradient $E \in \mathbb{M}_0^{\mathrm{Sym}}$. Idea: fix the velocity gradient of the fluid (as if it was the one of $\bar{u}$), what is the correction required ?

Passive corrector problem II

For a fixed deformation $E \in \mathbb{M}_0^{\mathrm{Sym}}$,

$$\begin{cases} -\triangle \psi_E^\omega + \nabla \Sigma_E^\omega = 0, & \text{in } \mathbb{R}^d \setminus \mathcal{I}^\omega, \\ \mathrm{div}(\psi_E^\omega) = 0, & \text{in } \mathbb{R}^d \setminus \mathcal{I}^\omega, \\ D(\psi_E^\omega + Ex) = 0, & \text{in } \mathcal{I}^\omega, \\ \int_{\partial I_n^\omega} \sigma(\psi_E^\omega + Ex, \Sigma_E^\omega)\nu = 0, & \forall n, \\ \int_{\partial I_n^\omega} \Theta(x - x_n^\omega) \cdot \sigma(\psi_E^\omega + Ex, \Sigma_E^\omega)\nu = 0, & \forall \Theta \in \mathbb{M}^{\mathrm{skew}}, \forall n. \end{cases}$$

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One can show that $\nabla \psi_E$ and $\Sigma_E \mathbf{1}_{\mathbb{R}^d \setminus \mathcal{I}^\omega}$ are stationary, have bounded second moments and vanishing expectations. The **diffusion tensor associated to the presence of particles**, $\bar{B}$, is expressed through (ψ, Σ).

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Indeed,

$$E : \bar{B}E = \mathbb{E}[|D(\psi_E) + E|^2] > |E|^2$$

so the contribution of this correction **increases the viscosity**, in accordance with the physical results.

Towards Einstein formula... and beyond

Duerinckx-Gloria 2020: expect

$$\bar{B} \sim I_d + \sum_{j \geq 1} \frac{1}{j!} \bar{B}^j,$$

where $\bar{B}^j$ accounts for interactions between j particles (actually this is very subtle).

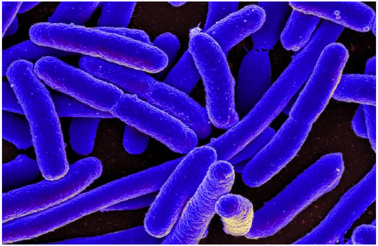
For the case here, explicit formulae:

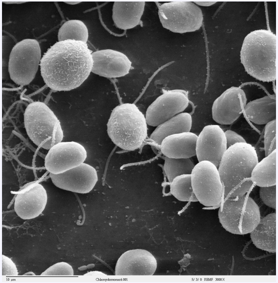
$$\bar{B}^1 = \lambda \frac{d+2}{2} I_d.$$

and for $\bar{B}^2$, more complicated and depending on the structure of the point process, recovering the estimates of Batchelor-Green (and justifying it).

Motivation

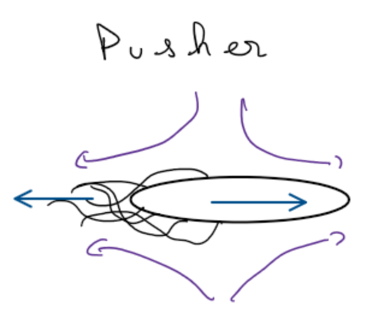
We are typically interested in considering motile bacteria (Escherichia coli, left) or microalgae (Chlamydomonas reinhardtii, right), which are flagellated organisms, rather than passive particles.

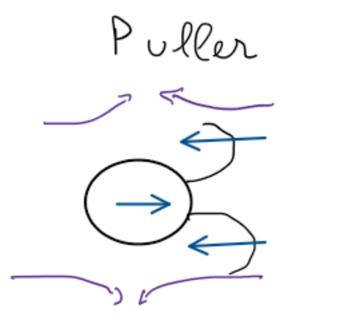




Two swimming mechanisms

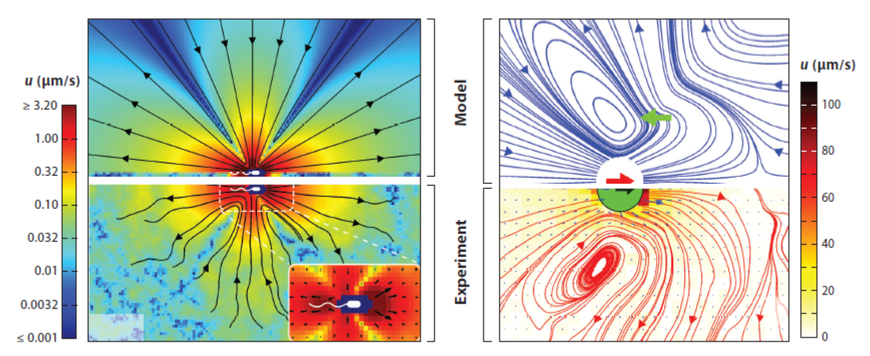
There are two main types of active particles: extensile swimmers (pushers, E. coli) and contractile ones (pullers, C. reinhardtii). The rheological properties strongly depends on this swimming mechanism.





Confirmation from experimental data

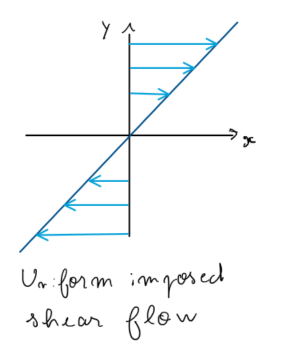
Those broad pictures are actually confirmed by experiments.

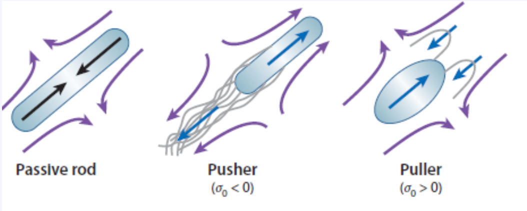


Model vs experimental results for the disturbance flow near a bacterium. Pusher on the left, puller on the right. From Saintillan (Ann. Rev. in Fl. Mech. 2017).

Physical (rough) explanation of the rheological behavior

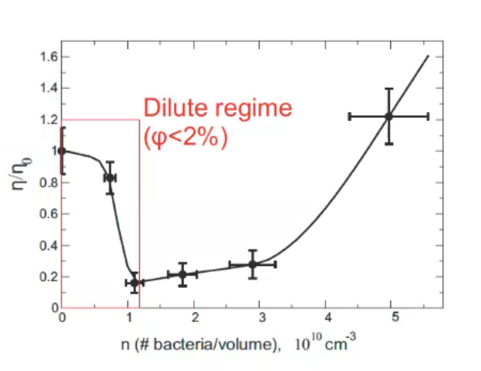
Extensile mechanisms enhance the disturbance flow, while contractile mechanisms (also the one in place when considering passive particles) resist it.





Experimental confirmation

From Sokolov-Aranson (PRL, 2009), the solution is Bacillus subtilis, a pusher. The viscosity decreases, as expected.



Some references from the mathematical physics communit

1. Haines-Aranson-Berlyand-Karpeev (2008): 2D model, computation of the perturbation due to 1 particle to understand the rheology (in the spirit of Einstein).
2. Potomkyn, Ryan, Berlyand (2016): kinetic model with the orientations, very strong hypothesis.
3. Same approach in Ryan, Haines, Karpeev, Berlyand (2013)
4. Gluzman-Karpeev-Berlyand (2013): renormalization approach. Main novelty in our approach: the retroaction of the fluid on particles is a part of the problem (not prescribed). Also, possibility for a development of the further terms with the road-map from the colloidal case.

Our modeling assumptions

We make the following hypotheses:

1. particles have an orientation, along which a swimming device acts (typically, the flagella);
2. this swimming device acts both on the particle, and on the fluid;
3. if the fluid is at rest, the distribution of orientation is isotropic.

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Fluid not at rest: the distribution depends on the velocity gradient (at large scales) E felt by the particles: the larger $|E|$, the more peaked the distribution of orientations in some direction.

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Of course, orientations will play a key role !

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Also, $\exists \bar{O} : \mathbb{M}_0^{\mathrm{Sym}} \to \mathbb{S}^1$ such that for all $E \in \mathbb{S}^1$,

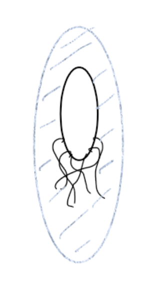
$$\lim_{t \downarrow 0} \bar{\mu}(tE) = d\sigma_{\mathbb{S}^1}, \qquad \lim_{t \uparrow \infty} \bar{\mu}(tE) = \delta_{\bar{O}E},$$

where $d\sigma_{\mathbb{S}_1}$ denotes the uniform measure on the sphere $\mathbb{S}^1$.

On the particle, strength $\bar{f}(E) = \ell F(E)$. Here, $\ell = 1$ to simplify.

Modeling the swimming mechanism: on the fluid

Backflow force $f(E) := \ell F(E)\zeta(F(E))$ for some function $\zeta \geq 0$, with $\text{supp}(\zeta) \subset (I+B) \setminus I$ with mass 1.



Note that $\bar{f}(E) = \int_{I+B} f(E)$.

Some simplifying assumptions here

- Constant strength $\ell = 1$ of the swimming device (otherwise, add a function $h(|E|)$ in the previous framework).
- No torque mechanism (see next slide).

Associated boundary conditions

Condition at the boundary of ϵI_n^ω for all $n \in \mathcal{N}_\epsilon^\omega(U)$: letting ν be the unit outward normal vector,

$$\int_{\epsilon \partial I_n} \sigma(u_\epsilon^\omega, P_\epsilon^\omega)\nu + \frac{\kappa}{\epsilon} \bar{f}_n \Big(\fint_{\epsilon I_n^\omega} \chi * D(u_\epsilon^\omega) \Big) = 0,$$

where κ small is a coupling parameter,
$\bar{f}_n(E) = \int_{I+B} f_n^\omega(E, \frac{x}{\epsilon} - x_n^\omega) = \ell F_n(E)$ and the $(F_n)_{n \geq 0}$ are i.i.d. with the hypotheses above.

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No torque: for all $\Theta \in \mathbb{M}^{\text{skew}}$

$$\int_{\epsilon \partial I_n} \Theta(x - x_n^\omega) \cdot \sigma(u_\epsilon^\omega, P_\epsilon^\omega)\nu = 0,$$

Our full problem

The final problem takes the following form

$$\begin{cases} -\triangle u_\epsilon^\omega + \nabla P_\epsilon^\omega & \\ \quad = g - \frac{\kappa}{\epsilon} \sum_{n \in \mathcal{N}_\epsilon^\omega(U)} f_{n,\epsilon}^\omega \Big(\fint_{\epsilon I_n} \chi * D(u_\epsilon^\omega) \Big) & \text{in } U \setminus \mathcal{I}_\epsilon^\omega(U), \\ \operatorname{div}(u_\epsilon^\omega) = 0, & \text{in } U \setminus \mathcal{I}_\epsilon^\omega(U), \\ D(u_\epsilon^\omega) = 0, & \text{in } \mathcal{I}_\epsilon^\omega(U), \\ \int_{\epsilon \partial I_n} \sigma(u_\epsilon^\omega, P_\epsilon^\omega)\nu & \\ \quad + \frac{\kappa}{\epsilon} \bar{f}_{n,\epsilon}^\omega \Big(\fint_{\epsilon I_n^\omega} \chi * D(u_\epsilon^\omega) \Big) = 0 & \text{for all } n \in \mathcal{N}_\epsilon^\omega(U), \\ \int_{\epsilon \partial I_n} \Theta(x - \epsilon x_n^\omega) \cdot \sigma(u_\epsilon^\omega, P_\epsilon^\omega)\nu = 0 & \text{for all } \Theta \in \mathbb{M}^{\text{skew}}, n \in \mathcal{N}_\epsilon^\omega(U). \end{cases}$$

Goal: analyze this problem in the limit $\epsilon \downarrow 0$.

Well-posedness

$\exists\bar{\kappa}$ s.t. for all $0 \le \hat{\kappa} \le \bar{\kappa}$, all $\delta > 1$, all $\epsilon \in (0, 1]$ and all forcing terms $g \in L^2(U)^d$, the full problem above with $\kappa = \hat{\kappa}\delta^d$ is well-posed almost surely: there exists a unique weak solution $(u_\epsilon^\omega, P_\epsilon^\omega) \in H_0^1(U)^d \times L^2(U \setminus \mathcal{I}_\epsilon^\omega(U))$ and we have the estimate

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$$\int_U |\nabla u_\epsilon^\omega|^2 + \int_{U \setminus I_\epsilon^\omega(U)} |P_\epsilon^\omega|^2 \lesssim \int_U |g|^2 + 1.$$

Theorem (B., Duerinckx, Gloria, 2022^+)

We have the following convergence results, as $\epsilon \to 0$,

1. $u_\epsilon^\omega \rightharpoonup \bar{u}$ in $H_0^1(U)^d$,
2. $P_\epsilon^\omega \mathbf{1}_{U\setminus\mathcal{I}_\epsilon^\omega(U)} \rightharpoonup (1-\lambda)(\bar{P}-\bar{b}:D(\bar{u})-\bar{c}:D(\chi*\bar{u}))$ in $L^2(U)$,

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where $(\bar{u}, \bar{P}) \in H_0^1(U)^d \times L^2(U)$ is the unique solution to the homogenized problem in U:

$$\begin{cases} -\mathrm{div}(2\bar{B}D(\bar{u})) - \mathrm{div}(2\bar{C}D(\chi * \bar{u})) + \nabla \bar{P} = (1-\lambda)g, \\ \mathrm{div}(\bar{u}) = 0, \quad \fint_U \bar{P} = 0, \end{cases}$$

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where $\lambda = \mathbb{E}[\mathbf{1}_{\mathcal{I}^\omega}]$ is the particle density, $\bar{B}, \bar{b}$ are the effective tensors of the passive suspension, $\bar{C}, \bar{c}$ are maps connected to the active behavior of the particles.

Post-processing: getting rid of χ

Recall that the velocity gradient is evaluated through some the convolution with some kernel $\chi \to$ quite artificial.

We can get rid of this assumption by considering the case where $\chi \to$ Dirac weakly-* in measure. Then, we obtain the local equation

$$-\operatorname{div}(2\bar{B}D(\bar{u})) - \operatorname{div}(2\bar{C}D(\bar{u})) + \nabla\bar{P} = (1-\lambda)g. \qquad (1)$$

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In progress: diagonal argument. Target: having the convergence of χ depend on ϵ in order to do all at once. Requirements: some quantitative mixing assumptions on the inclusion process, e.g. hardcore Poisson process.

Post-processing II: from non-linear to linear

One further difficulty: at first, $\bar{C}$ obtained through the corrector problem is not linear. Write, for $t \in (0,1)$, $(\bar{u}^t, \bar{P}^t) \in H_0^1(U)^d \times L^2(U)$ the solution of the homogenized equation (1) with source term $t(1-\lambda)g$.

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Then, there exists a linear map $\hat{C} : \mathbb{M}_0^{\mathrm{Sym}} \to \mathbb{M}_0^{\mathrm{Sym}}$ such that

$$\lim_{t \downarrow 0} \frac{\|(\nabla \bar{u}^t, \bar{P}^t) - t(\nabla \tilde{u}, \tilde{P})\|_{L^2(U)}}{t} = 0,$$

where $(\tilde{u}, \tilde{P}) \in H_0^1(U)^d \times L^2(U)$ solves the linear local equation

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$$-\mathrm{div}(2(\bar{B} + \hat{C})D(\tilde{u})) + \nabla \tilde{P} = (1-\lambda)g.$$

This equation (and the induced viscosity) can be directly compared with the initial problem.
Moreover, $\hat{C}$ satisfies, for all $E \in \mathbb{M}_0^{\mathrm{Sym}}$,

$$\hat{C}E = \lim_{t \downarrow 0} \frac{1}{t} \hat{C}(tE).$$

Active corrector problem

As before, the tensors $\bar{C}$ and $\bar{c}$ are obtained through the **active corrector problem** $\rightarrow$ new !

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Encapsulates the contribution of the swimming device given a uniform velocity gradient $E \in \mathbb{M}_0^{\mathrm{Sym}}$. Idea: fix the velocity gradient of the fluid (as if it was the one of $\bar{u}$), what is the correction induced by the swimming mechanism ?

Active corrector problem II

For a fixed deformation $E \in \mathbb{M}_0^{\mathrm{Sym}}$,

$$\begin{cases} -\triangle \phi_E^\omega + \nabla \Pi_E^\omega = -\sum_n f_n(E), & \text{in } \mathbb{R}^d \setminus \mathcal{I}^\omega, \\ \operatorname{div}(\phi_E^\omega) = 0, & \text{in } \mathbb{R}^d \setminus \mathcal{I}^\omega, \\ D(\phi_E^\omega) = 0, & \text{in } \mathcal{I}^\omega, \\ \int_{\partial I_n^\omega} \sigma(\phi_E^\omega, \Pi_E^\omega)\nu + \bar{f}_n(E) = 0, & \forall n, \\ \int_{\partial I_n^\omega} \Theta(x - x_n^\omega) \cdot \sigma(\phi_E^\omega, \Pi_E^\omega)\nu = 0, & \forall \Theta \in \mathbb{M}^{\mathrm{skew}}, \forall n. \end{cases}$$

Again, one can show that $\nabla \phi_E^\omega$ and $\Pi_E \mathbf{1}_{\mathbb{R}^d \setminus \mathcal{I}^\omega}$ are stationary, have bounded second moments and vanishing expectations. However, here

$$E : \bar{C} E = -\mathbb{E}[D(\phi_E) : D(\psi_E)] + \mathbb{E}\Big[\sum_n \frac{\mathbf{1}_{I_n}}{|I_n|}\Big(\int_{I_n + B} (\bar{f}_n \frac{\mathbf{1}_{I_n}}{|I_n|} - f_n\Big)\psi_E\Big)\Big].$$

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In particular, it is possible to have $E : (\bar{B} + \bar{C})E < |E|^2$ (and the same with $\hat{C}$ → this corresponds to the **superfluid behavior**, since the viscosity is then smaller than when the diffusion tensor is I_d (our starting point).

Method of proof

We use a two-scale expansion. The first idea is that

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$$u_\epsilon \sim \bar{u}_\epsilon + \epsilon \sum_{E \in \mathcal{E}} \psi_E(\tfrac{\cdot}{\epsilon}) \nabla_E \bar{u}_\epsilon + \epsilon \phi_{\chi * D(u_\epsilon)}(\tfrac{\cdot}{\epsilon}),$$

$$P_\epsilon \mathbf{1}_{\mathbb{R}^d \setminus \epsilon\mathcal{I}} \sim \bar{P}_\epsilon + \bar{b} : D(\bar{u}_\epsilon) + \bar{c} : D(\chi * u_\epsilon) + \sum_{E \in \mathcal{E}} (\Sigma_E \mathbf{1}_{\mathbb{R}^d \setminus \mathcal{I}})(\tfrac{\cdot}{\epsilon}) \nabla_E \bar{u}_\epsilon$$
$$+ (\Pi_{\chi * D(u_\epsilon)} \mathbf{1}_{\mathbb{R}^d \setminus \mathcal{I}})(\tfrac{\cdot}{\epsilon}),$$

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where $\mathcal{E}$ orthonormal basis of $\mathbb{M}_0^{\mathrm{Sym}}$ and $(\bar{u}_\epsilon, \bar{P}_\epsilon) \in H_0^1(U)^d \times L^2(U)$ is the unique solution to the intermediate equation

$$-\mathrm{div}(2\bar{B}D(\bar{u}_\epsilon)) + \nabla \bar{P}_\epsilon = (1-\lambda)f + \mathrm{div}(2\bar{C}D(\chi * u_\epsilon))$$

(note that there is no $\bar{u}_\epsilon$ on the right-hand side !)

Step 2: convergence to the fully homogenized equation

It follows from the properties of χ and energy estimates that if $u_\epsilon \rightharpoonup u_0$ in $H_0^1(U)$ along a subsequence, then $\bar{u}_\epsilon \rightharpoonup \bar{u}_0$ in $H_0^1(U)$ as well, with $\bar{u}_0$ solution to

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$$-\operatorname{div}(2\bar{B}D(\bar{u}_0)) + \nabla \bar{P}_\epsilon = (1-\lambda)f + \operatorname{div}(2\bar{C}D(\chi * u_0)).$$

Moreover, our convergence result to $\bar{u}_\epsilon$ shows that $u_\epsilon - \bar{u}_\epsilon \to 0$ in $L^2(U)$. From this, we conclude that $u_0 = \bar{u}_0$, leading to a unique solution of the homogenized equation.

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Thank you for your attention !