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FFT-based homogenization of permeability using a Hashin-Shtrikman type variational framework

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ABSTRACT

A numerical scheme for the computation of the permeability of complex microstructures is presented. As a darcean counterpart of the Fast Fourier Transform (FFT) based scheme in elasticity, the method is designed to be directly coupled with 3D imaging techniques of porous samples, without meshing or definition of an equivalent pore network. The method relies on the variational principle of Hashin-Shtrikman which ensures a rigorous upper bound status to the estimated permeabilities and provides an energetically consistent discretization of Green operators and of the viscosity of heterogeneous voxels comprising both solid and fluid.

1 INTRODUCTION

A pioneering work (Ene, 1975) early clarified the theoretical link between the macroscopic Darcy's law for fluid flow in porous media and the microscopic Stokes flow within the pore space. A quantitatively precise prediction of the intrinsic permeability tensor thus requires an accurate description of the pore geometry. Within this framework, successful predictions of the permeability of porous media have been performed, based on different degrees of idealization of the pore/solid phase descriptions, see e.g. (Boutin, 2000)

Finer description of the fluid flow requires direct full field simulations on real pore geometries. These geometries may be measured thanks to recent advances in imaging techniques, which allow for precise reconstruction of microstructures down to a few nanometers (Desbois, 2011). Most numerical methods are based on approximate solutions of Stokes equations in the pore space, but suffer from high computational cost (memory and time) or complex meshing.

Taking advantage of the fast evaluation of non local terms by FFT, (Wiegmann, 2007) proposed a computationally efficient scheme. Another fruitful approach is the adaptation of the FFT-based scheme initially introduced in linear elasticity (Moulinec, 1994). This scheme was designed to be directly interfaced with imaging techniques and has been adapted to permeability (Monchiet, 2009; Nguyen, 2013). Recently, a variational framework for FFT-based scheme has been introduced in linear elasticity (Brisard, 2010), improving the performances of the so-called basic scheme (Moulinec,

1994). It consists in the minimization of an energy Hashin-Shtrikman functional, allowing for an energetically consistent discretization and providing rigorous bounds of the homogenized properties. Recent advances (Brisard, 2012) made it fairly simple to implement and suitable for computations on large discretization grids.

The present communication proposes a numerical scheme for the computation of permeability combining a new Hashin-Shtrikman like framework for permeability and a FFT-based scheme. In section 2, the framework for the homogenization of the permeability of periodic porous media is recalled, with a specific focus on its variational formulation. In section 3, a Hashin-Shtrikman like variational framework is derived in this context, which is the main result of this paper. As a by-product, an energetically consistent discretization is derived in section 4 to propose an improved FFT-based scheme. A validation of the method is proposed on a simple geometry in section 5 by comparison with Finite Element simulations.

2 FORMULATION OF THE FLUID FLOW PROBLEM

At the macroscopic scale, Darcy's law linearly relates the pressure gradient $\boldsymbol{\alpha}$ to the fluid velocity $\boldsymbol{V}$ through the permeability tensor by $\boldsymbol{V} = -\boldsymbol{K} \cdot \boldsymbol{\alpha}$.

A micromechanical approach to permeability has initially been presented by (Ene, 1975) in the context of periodic boundary conditions. The elementary cell Ω is a rectangular parallelepiped of boundary $\partial\Omega$, comprising a non deformable solid phase in Ω_s and a pore space Ω_f filled with an incompressible Newtonian fluid of viscosity μ. The porosity of the elementary cell is $\varphi = |\Omega_f|/|\Omega|$. The spacial coordinates at the micro scale are denoted by $\boldsymbol{z}$. In this problem (P), the fluid flow is described by the pressure field $p(\boldsymbol{z})$ and the velocity field $\boldsymbol{v}(\boldsymbol{z})$ in Ω_f.

According to the separation of scale principle (Boutin, 2000), the fluid is loaded by the macroscopic pressure gradient $\boldsymbol{\alpha}$, which is equal to the volume average over Ω of the microscopic pressure gradient by considering an extension of the pressure field to the solid phase. The pressure field may thus be rewritten in both fluid and solid phases $p(\boldsymbol{z}) = \boldsymbol{\alpha} \cdot \boldsymbol{z} + \phi(\boldsymbol{z})$ where $\phi(\boldsymbol{z})$ is a periodic pressure fluctuation at the micro-scale.

The velocity field has to comply with several kinematic conditions: 1. no-slip boundary condition at the solid-fluid interface $\mathcal{I}_{sf}$, 2. periodic boundary conditions on $\partial\Omega \cap \Omega_f$, 3. incompressibility or continuity equation $\mathrm{div}(\boldsymbol{v}) = 0$ in Ω_f.

Further on, it will prove convenient to extend the boundary value problem to the whole elementary cell instead of the pore space only. To do so, the rigid solid can be regarded as an incompressible viscous fluid with an infinite viscosity. The essential advantage of this point of view lies in the fact that the no-slip boundary condition at the solid-fluid interface vanishes and will be automatically met by the solution to the problem. The proposed idea however presents a shortcoming: the rigid body motions of the solid domain must be prevented, or it would simply be dragged by the fluid.

Since the proposed method aims at dealing with real microstructures and for the sake of clarity, solid phases with disjoint domains are not considered. Furthermore,

periodicity implies that rotation may not occur if the solid phase spans over the whole cell. Hence only one no-velocity condition will be considered. Note that in the case of a single solid particle isolated in the fluid phase, rotation is not prevented so more complex conditions to prevent rotation or deal with multiple particles could be added (Nguyen, 2013). A more involved treatment would then follow, although the main ideas focused on here would remain valid.

The following developments are based on the condition that for any sub-domain $\Omega_{\mathcal{S}} \subset \Omega_s$ of volume fraction $f_{\mathcal{S}} \neq 0$, the average velocity is null. The set $\mathcal{C}$ of kinematically admissible velocity fields $\boldsymbol{u}$ for the new extended problem (P) defined on the whole elementary cell Ω is then $\mathcal{C} = \{\boldsymbol{u} \mid \boldsymbol{u}$ periodic on $\partial\Omega, \overline{\boldsymbol{u}}^{\mathcal{S}} = \boldsymbol{0}, \operatorname{div}(\boldsymbol{u}) = 0$ on $\Omega\}$, where the notation $\overline{u}^j = |\Omega_j|^{-1} \int_{\Omega_j} u(\boldsymbol{z}) \, \mathrm{d}\, V_z$ is used throughout the paper for the volume average on any domain Ω_j.

The Lagrange multiplier associated to this no-velocity condition is a uniform body force applied on $\Omega_{\mathcal{S}}$. In this specific case where only one no-velocity condition is chosen, the Lagrange multiplier is known. Indeed, according to (Boutin, 2000), momentum balance states that macroscopic stresses in the solid phase, here microscopically described as the Lagrange multiplier, counterbalance the macroscopic fluid pressure gradient. Eventually, momentum balance imposes the body force to be $f_{\mathcal{S}}^{-1}\boldsymbol{\alpha}$.

The unknowns of problem (P) are the velocity field $\boldsymbol{v} \in \mathcal{C}$ and the stress field $\boldsymbol{\sigma}$ or, in an equivalent manner, $\boldsymbol{v}$ and the periodic pressure fluctuation ϕ. The field equations of the new extended problem (P) defined on the whole elementary cell Ω read, for the velocity $\boldsymbol{v} \in \mathcal{C}$ and the strain rate $\boldsymbol{d}(\boldsymbol{z}) = 1/2[\mathbf{grad}(\boldsymbol{v}(\boldsymbol{z})) + {}^t\mathbf{grad}(\boldsymbol{v}(\boldsymbol{z}))]$

$$\mathbf{div}(\boldsymbol{\sigma}(\boldsymbol{z})) = -f_{\mathcal{S}}^{-1}\boldsymbol{\alpha} \text{ if } \boldsymbol{z} \in \Omega_{\mathcal{S}}, \, \boldsymbol{0} \text{ otherwise}, \tag{1a}$$

$$\boldsymbol{\sigma}(\boldsymbol{z}) = 2\mu(\boldsymbol{z})\, \boldsymbol{d}(\boldsymbol{z}) - (\boldsymbol{\alpha} \cdot \boldsymbol{z} + \phi(\boldsymbol{z}))\, \boldsymbol{1} \quad (\boldsymbol{z} \in \Omega), \tag{1b}$$

where the Newtonian behavior (eq. 1b) links the stress $\boldsymbol{\sigma}(\boldsymbol{z})$ to the strain rate with $\mu(\boldsymbol{z}) = \infty$ if $\boldsymbol{z} \in \Omega_s$ and μ otherwise. For Stokes flows, the inertia effects in the momentum balance are neglected (eq. 1a).

These equations are formally identical to a problem of heterogeneous elasticity involving two incompressible phases. We therefore could expect to take advantage of the homogenization methods developed in solid micromechanics. However this analogy breaks down when the boundary conditions and loading parameters are considered. In solid micromechanics, the loading parameter is the macroscopic strain tensor, which defines boundary conditions as an affine displacement with periodic fluctuations. Here, the loading parameter in (P) is the macroscopic pressure gradient vector associated to its equilibrating body forces in $\Omega_{\mathcal{S}}$. However, we shall see later that seminal ideas of solid micromechanics will be of great help in the present context of fluid flow.

Problem (P) is linear with respect to the loading parameter $\boldsymbol{\alpha}$, so the velocity field depends on $\boldsymbol{\alpha}$ through a localization tensor $\boldsymbol{k}(\boldsymbol{z})$ such that $\boldsymbol{v}(\boldsymbol{z}) = -\boldsymbol{k}(\boldsymbol{z}) \cdot \boldsymbol{\alpha}$. Then, the macroscopic velocity relates to the microscopic velocity through $\boldsymbol{V} = \overline{\boldsymbol{v}} = -\overline{\boldsymbol{k}} \cdot \boldsymbol{\alpha}$. Darcy's law is recognized and the permeability tensor appears as $\boldsymbol{K} = \overline{\boldsymbol{k}}$. Hence, the resolution of (P) directly provides the permeability tensor.

For practical implementations, a classical approach to derive approximate solutions of (P) is the use of a variational framework. For a given strain rate $\boldsymbol{d}$, the density of dissipated energy due to viscosity is $w(\boldsymbol{d}) = \mu\, \boldsymbol{d} : \boldsymbol{d}$. The adaptation of (Dormieux, 2006) provides the variational formulation of the extended fluid flow (P)

$$-\frac{1}{2}\boldsymbol{\alpha} \cdot \boldsymbol{K} \cdot \boldsymbol{\alpha} = \inf_{\boldsymbol{u} \in \mathcal{C}} \overline{w(\boldsymbol{d}(\boldsymbol{u})) + \boldsymbol{\alpha} \cdot \boldsymbol{u}}. \tag{2}$$

For any choice of a kinematically admissible velocity field, (2) provides a lower bound estimate of the permeability. Akin to the minimum of potential energy in linear elasticity, this inequality is the basis for Finite Element Methods (FEM), which explore subsets of $\mathcal{C}$ with finite dimension. Note that the complex description of the solid-fluid interphase for the no-slip boundary condition has been transfered to a problem with infinite contrast in viscosities. Direct use of this variational principle (e.g. FEM) is thus numerically difficult because of the infinite contrast and the incompressibility condition. In the following section, (2) will be used to derive a novel Hashin-Shtrikman variational principle (Hashin, 1962), in which the so-called polarization field to optimize has no condition to fulfill. Another motivation is that the optimization problem associated with the Hashin-Shtrikman variational principle is known in solid micromechanics to lead to a FFT scheme able to deal with infinite contrast (Brisard, 2010).

3 HASHIN-SHTRIKMAN-LIKE VARIATIONAL FRAMEWORK

In the line of reasoning of (Willis, 1977), a transposition of the Hashin-Shtrikman variational principle (Hashin, 1962) to darcean homogenization may be derived. The main idea is to transfer the difficulty arising from a heterogeneity in viscosity to an additional loading parameter $\boldsymbol{\tau}$, called polarization, acting as a prestress.

The Legendre transform of the density of dissipated energy $w(\boldsymbol{d})$ is defined on the space of stress tensors as $w^*(\boldsymbol{\tau}) = \sup_{\boldsymbol{d}} \left(\boldsymbol{\tau} : \boldsymbol{d}(\boldsymbol{u}) - w(\boldsymbol{d}) \right)$. In the case of an incompressible isotropic Newtonian fluid, it equals $w^*(\boldsymbol{\tau}) = (4\mu)^{-1} \boldsymbol{\tau} : \boldsymbol{\tau}$.

Let us consider a reference medium of uniform viscosity μ_0 smaller than any local value of the viscosity in the heterogeneous medium at hand. According to its definition, the Legendre transform $(w - w_0)^*$ associated with a heterogeneous medium of viscosity $\mu(\boldsymbol{z}) - \mu_0$ satisfies $\forall \boldsymbol{\tau}; \forall \boldsymbol{d}; w(\boldsymbol{d}) \geq w_0(\boldsymbol{d}) + \boldsymbol{\tau} : \boldsymbol{d} - (w - w_0)^*(\boldsymbol{\tau})$. After addition of the loading term in $\boldsymbol{\alpha}$ and volume averaging over Ω, the minimum over all kinematically admissible velocity fields in $\mathcal{C}$ yields, using (2)

$$\forall \boldsymbol{\tau}; -\frac{1}{2}\boldsymbol{\alpha} \cdot \boldsymbol{K} \cdot \boldsymbol{\alpha} \geq \inf_{\boldsymbol{u} \in \mathcal{C}} \left(\overline{w_0(\boldsymbol{d}(\boldsymbol{u})) + \boldsymbol{\tau} : \boldsymbol{d}(\boldsymbol{u}) + \boldsymbol{\alpha} \cdot \boldsymbol{u}} \right) - \overline{(w - w_0)^*(\boldsymbol{\tau})}. \tag{3}$$

The result (3) is known as the Hashin-Shtrikman variational principle (Hashin, 1962). The first part of the right term is the variational formulation of an auxiliary problem (P^0), similar to (P), except the viscosity is homogeneous and the polarization field is an additional loading parameter. The second part is known by definition of the Legendre transform. The whole right hand side is a functional of the variable $\boldsymbol{\tau}$

called Hashin-Shtrikman functional $\mathcal{HS}(\boldsymbol{\tau})$. The equality is met for a unique optimum polarization field. The inequality (3) is the basis of the proposed FFT scheme since it may be used to provide upper bound estimates of the permeability for *any choice* of a polarization field $\boldsymbol{\tau}$, with *no condition* on $\boldsymbol{\tau}$.

In order to fully express the quadratic dependence on $\boldsymbol{\tau}$ of the Hashin-Shtrikman functional, the auxiliary problem (P^0) has to be solved for $\boldsymbol{v}^0 \in \mathcal{C}$. The only difference with (P) lies in the prestressed behavior law, which now writes $\boldsymbol{\sigma}^0(\boldsymbol{z}) = 2\mu_0\, \boldsymbol{d}^0(\boldsymbol{z}) - (\boldsymbol{\alpha}\cdot\boldsymbol{z} + \phi^0(\boldsymbol{z}))\,\mathbf{1} + \boldsymbol{\tau} \quad (\boldsymbol{z}\in\Omega)$ instead of (1b).

(P^0) is split using superposition in a reference problem (P^α) loaded by $\boldsymbol{\alpha}$ only and a prestressed problem (P^τ) loaded by the polarization field $\boldsymbol{\tau}$ only. In the following developments, exponent α (resp. τ) refers to the solution of (P^α) (resp. (P^τ)).

The minimum of the potential energy in the Hashin-Shtrikman functional meets its minimum in $\mathcal{C}$ for $\boldsymbol{v}^0$ solution of (P^0). The functional is simplified by repeatedly using the divergence theorem and boundary conditions to

$$\mathcal{HS}(\boldsymbol{\tau}) = \frac{1}{2}\boldsymbol{\alpha}\cdot\overline{\boldsymbol{v}^\alpha} + \overline{\boldsymbol{d}^\alpha : \boldsymbol{\tau}} + \frac{1}{2}\overline{\boldsymbol{\tau} : \boldsymbol{d}^\tau} - \frac{1}{2}\overline{(2\mu - 2\mu_0)^{-1}\boldsymbol{\tau} : \boldsymbol{\tau}}. \tag{4}$$

Since the viscosity is uniform in both sub problems, they may be solved using Green operators. The solutions of problems (P^α) and (P^τ) are expressed thanks to the different order Green operators as defined in Appendix A

$$\begin{aligned} \boldsymbol{v}^\alpha(\boldsymbol{z}) &= \overline{\boldsymbol{v}^\alpha} + \left(\boldsymbol{G}_0 * f_{\mathcal{S}}^{-1}\chi^{\mathcal{S}}\boldsymbol{\alpha}\right)(\boldsymbol{z}) \quad ; \quad \boldsymbol{d}^\alpha(\boldsymbol{z}) = \left({}^t\boldsymbol{\mathcal{G}}_0 * f_{\mathcal{S}}^{-1}\chi^{\mathcal{S}}\boldsymbol{\alpha}\right)(\boldsymbol{z}), \\ \boldsymbol{v}^\tau(\boldsymbol{z}) &= \overline{\boldsymbol{v}^\tau} + \left(\boldsymbol{\mathcal{G}}_0 * \boldsymbol{\tau}\right)(\boldsymbol{z}) \quad ; \quad \boldsymbol{d}^\tau(\boldsymbol{z}) = -\left(\boldsymbol{\Gamma}_0 * \boldsymbol{\tau}\right)(\boldsymbol{z}). \end{aligned}$$

The average velocities in both problems may be computed thanks to the no velocity boundary condition. For problem (P^α) namely, $0 = \overline{\boldsymbol{v}^\alpha\chi^{\mathcal{S}}} = \overline{\overline{\boldsymbol{v}^\alpha}\chi^{\mathcal{S}}} + \overline{\chi^{\mathcal{S}}\left(\boldsymbol{G}_0 * f_{\mathcal{S}}^{-1}\chi^{\mathcal{S}}\boldsymbol{\alpha}\right)}$, where the auto-influence term of the Green function over $\Omega_{\mathcal{S}}$ is recognized (appendix B). Finally, $\overline{\boldsymbol{v}^\alpha} = -\boldsymbol{G}_0^{\mathcal{SS}}\cdot\boldsymbol{\alpha}$. The auto-influence term $\boldsymbol{G}_0^{\mathcal{SS}}$ may thus be considered as the permeability of the fictitious reference problem (P^α). The Hashin-Shtrikman functional is now explicited as a quadratic form in $\boldsymbol{\tau}$, and the upper bound on the permeability writes

$$\begin{aligned} \forall\boldsymbol{\tau},\, \frac{1}{2}\boldsymbol{\alpha}\cdot\boldsymbol{K}\cdot\boldsymbol{\alpha} \leqslant & \frac{1}{2}\boldsymbol{\alpha}\cdot\boldsymbol{G}_0^{\mathcal{SS}}\cdot\boldsymbol{\alpha} - \overline{\left({}^t\boldsymbol{\mathcal{G}}_0 * f_{\mathcal{S}}^{-1}\chi^{\mathcal{S}}\boldsymbol{\alpha}\right) : \boldsymbol{\tau}} \\ & + \frac{1}{2}\overline{\boldsymbol{\tau} : \boldsymbol{\Gamma}_0 * \boldsymbol{\tau}} + \frac{1}{2}\overline{(2\mu - 2\mu_0)^{-1}\boldsymbol{\tau} : \boldsymbol{\tau}}. \end{aligned} \tag{5}$$

4 FROM DISCRETIZATION TO A FFT SCHEME

The d-dimensional domain Ω is divided in a regular $N_1 \times ... \times N_d$ grid of $N = N_1...N_d$ sub-domains $\Omega_{\boldsymbol{\beta}}$ (pixels for d = 2, voxels for d = 3) of length (or resolution) r along the d axis of an orthonormal basis $(\boldsymbol{e}_1, ..., \boldsymbol{e}_d)$. The multi-index $\boldsymbol{\beta} = (\beta_1, ..., \beta_d) \in \mathcal{I} = [0..N_1 - 1] \times ... \times [0..N_d - 1]$ is used to position the pixel in the d directions.

In order to optimize the Hashin-Shtrikman functional, we restrict to the exploration of the space of pixel-wise constant polarization fields. For any choice of a sequence $(\boldsymbol{\tau_\beta})_{\boldsymbol{\beta}\in\mathcal{I}}$, a polarization field is associated by $\boldsymbol{\tau}(\boldsymbol{z}) = \sum_{\boldsymbol{\beta}\in\mathcal{I}} \boldsymbol{\tau_\beta}\, \chi^{\boldsymbol{\beta}}(\boldsymbol{z})$, where $\chi^{\boldsymbol{\beta}}$ is the characteristic function of pixel $\Omega_{\boldsymbol{\beta}}$ defined as $\chi^{\boldsymbol{\beta}}(z_1\boldsymbol{e}_1 + ... + z_d\boldsymbol{e}_d) = 1$ if $\forall i, 2|z_i - r\beta_i| \leqslant r$, 0 otherwise.

Each term of the Hashin-Shtrikman functional may be numerically computed *exactly* thanks to the consistently discretized operators introduced by (Brisard, 2010) and briefly recalled in appendix B. These operators allow for the use of Discrete Fourier Transforms while no truncation of the Fourier series are made. The discrete convolution products $\circledast$ are computed as a direct product in the Fourier space, using the Fast Fourier Transform (FFT) to compute the discrete Fourier transforms.

The constant term may be computed *exactly* if $\Omega_{\mathcal{S}}$ is chosen as a union of pixels, resorting to the discrete convolution product to compute the auto-interaction term

$$\boldsymbol{G}_0^{\mathcal{SS}} = \frac{1}{N f_{\mathcal{S}}^2} \sum_{\boldsymbol{\beta}\in\mathcal{I}} \chi_{\boldsymbol{\beta}}^{\mathcal{S}} \left(\boldsymbol{G}_0^c \circledast \chi^{\mathcal{S}}\right)_{\boldsymbol{\beta}} = \sum_{\boldsymbol{\beta}\in\mathcal{I}} \chi_{\boldsymbol{\beta}}^{\mathcal{S}} \boldsymbol{G}_0^{\mathcal{S}\boldsymbol{\beta}}.$$

The linear term relates to the mean value of $\boldsymbol{d}^\alpha$ over pixel $\Omega_{\boldsymbol{\beta}}$, denoted $\boldsymbol{d}_{\boldsymbol{\beta}}^\alpha$, since $\boldsymbol{d}_{\boldsymbol{\beta}}^\alpha = \left({}^t\boldsymbol{\mathcal{G}}_0^c \circledast f_{\mathcal{S}}^{-1}\chi^{\mathcal{S}}\boldsymbol{\alpha}\right)_{\boldsymbol{\beta}} = {}^t\, \boldsymbol{\mathcal{G}}_0^{\boldsymbol{\beta}\mathcal{S}} \cdot \boldsymbol{\alpha}$. and is calculated using the relation

$$\overline{\boldsymbol{\tau} : \left({}^t\boldsymbol{\mathcal{G}}_0 * f_{\mathcal{S}}^{-1}\chi^{\mathcal{S}}\boldsymbol{\alpha}\right)} = \frac{1}{N}\sum_{\boldsymbol{\beta}\in\mathcal{I}} \boldsymbol{\tau_\beta} : \left({}^t\boldsymbol{\mathcal{G}}_0^c \circledast f_{\mathcal{S}}^{-1}\chi^{\mathcal{S}}\boldsymbol{\alpha}\right)_{\boldsymbol{\beta}} = \frac{1}{N}\sum_{\boldsymbol{\beta}\in\mathcal{I}} \boldsymbol{\tau_\beta} : \boldsymbol{d}_{\boldsymbol{\beta}}^\alpha,$$

Similarly, the first quadratic term is computed thanks to the property

$$\overline{\boldsymbol{\tau} : \boldsymbol{\Gamma}_0 * \boldsymbol{\tau}} = \frac{1}{N^2}\sum_{\boldsymbol{\beta}\in\mathcal{I}}\sum_{\boldsymbol{\delta}\in\mathcal{I}} \boldsymbol{\tau_\beta} : \boldsymbol{\Gamma}_0^{\boldsymbol{\beta\delta}} : \boldsymbol{\tau_\delta} = \frac{1}{N}\sum_{\boldsymbol{\beta}\in\mathcal{I}} \boldsymbol{\tau_\beta} : \left(\boldsymbol{\Gamma}_0^c \circledast \boldsymbol{\tau}\right)_{\boldsymbol{\beta}},$$

where the computation is quicker in the second option than in the first option by resorting to FFTs by the order of magnitude $N\log(N)$ versus N^2 operations.

The second quadratic term leads to the introduction of an energetically consistent averaging rule for the equivalent viscosity of a composite pixel comprising fluid and solid. Introducing the equivalent viscosities $\mu_{\boldsymbol{\beta}}$ defined on each pixel by the averaging rule $(\mu_{\boldsymbol{\beta}} - \mu_0)^{-1} = N\,\overline{\chi^{\boldsymbol{\beta}}(\mu - \mu_0)^{-1}}$, this term containing the local information may be expressed as

$$\overline{(2\mu - 2\mu_0)^{-1}\boldsymbol{\tau} : \boldsymbol{\tau}} = \frac{1}{N}\sum_{\boldsymbol{\beta}\in\mathcal{I}} (2\mu_{\boldsymbol{\beta}} - 2\mu_0)^{-1}\boldsymbol{\tau_\beta} : \boldsymbol{\tau_\beta}.$$

Gathering all these results, a bound on the permeability is obtained for any choice of the sequence $(\boldsymbol{\tau_\beta})_{\boldsymbol{\beta}\in\mathcal{I}}$

$$\begin{aligned}\frac{1}{2}\boldsymbol{\alpha}\cdot\boldsymbol{K}\cdot\boldsymbol{\alpha} \leqslant & \frac{1}{2}\boldsymbol{\alpha}\cdot\boldsymbol{G}_0^{\mathcal{SS}}\cdot\boldsymbol{\alpha} + \frac{1}{N}\sum_{\boldsymbol{\beta}\in\mathcal{I}}\Big(-\boldsymbol{d}_{\boldsymbol{\beta}}^\alpha : \boldsymbol{\tau_\beta} \\ & + \frac{1}{2}\left[\boldsymbol{\tau}_\beta : \left(\boldsymbol{\Gamma}_0^c \circledast \boldsymbol{\tau}\right)_{\boldsymbol{\beta}} + (2\mu_{\boldsymbol{\beta}} - 2\mu_0)^{-1}\boldsymbol{\tau_\beta} : \boldsymbol{\tau_\beta}\right]\Big).\end{aligned} \tag{6}$$

The comparison of (6) with linear elasticity (Eq. (17) in (Brisard, 2010)) shows great similarities, although the difference in loading parameter and boundary conditions lead to a more complicated reference solution: constant strain in linear elasticity versus Green operator dependent strain rate here.

Among the subset of pixel wise constant polarization fields, the optimal choice $(\boldsymbol{\tau}_{\boldsymbol{\beta}}^{opt})_{\boldsymbol{\beta}\in\mathcal{I}}$ in the sense of the Hashin-Shtrikman energy complies with the system

$$\forall \boldsymbol{\beta} \in \mathcal{I}, \left(\boldsymbol{\Gamma}_0^c \circledast \boldsymbol{\tau}\right)_{\boldsymbol{\beta}} + (2\mu_{\boldsymbol{\beta}} - 2\mu_0)^{-1}\boldsymbol{\tau}_{\boldsymbol{\beta}} = \boldsymbol{d}_{\boldsymbol{\beta}}^{\alpha}. \tag{7}$$

In the case were the pixel averaged viscosity matches the reference viscosity, the polarization is forced to zero on the corresponding pixels.

The quadratic form associated with the Hashin and Shtrikman functional has been shown to be definite positive (Willis, 1977), so the system (7) has a unique solution. To take advantage of the fast evaluation of the discrete convolution product by FFT, the matrix underlying this system is not explicited, although its expression is known through the pixel to pixel interaction terms of the fourth order Green operator. Instead, (Brisard, 2010) suggests using iterative linear solvers such as the conjugate gradient. The optimum bound on the permeability for a given discretization is then

$$\boldsymbol{\alpha}\cdot\boldsymbol{K}\cdot\boldsymbol{\alpha} \leqslant \boldsymbol{\alpha}\cdot\boldsymbol{G}_0^{\mathcal{SS}}\cdot\boldsymbol{\alpha} - \frac{1}{N}\sum_{\boldsymbol{\beta}\in\mathcal{I}} \boldsymbol{\tau}_{\boldsymbol{\beta}}^{opt} :^t \boldsymbol{\mathcal{G}}_0^{\boldsymbol{\beta}\mathcal{S}}\cdot\boldsymbol{\alpha}.$$

The average on pixel $\Omega_{\boldsymbol{\beta}}$ of the associated velocity field is

$$\boldsymbol{v}_{\boldsymbol{\beta}}^{opt} = \left(\boldsymbol{G}_0^{\mathcal{S}\boldsymbol{\beta}} - \boldsymbol{G}_0^{\mathcal{SS}}\right)\cdot\boldsymbol{\alpha} + \left(\boldsymbol{\mathcal{G}}_0^c \circledast \boldsymbol{\tau}^{opt}\right)_{\boldsymbol{\beta}} - \frac{1}{N}\sum_{\boldsymbol{\delta}\in\mathcal{I}} \boldsymbol{\mathcal{G}}_0^{\mathcal{S}\boldsymbol{\delta}} : \boldsymbol{\tau}_{\boldsymbol{\delta}}^{opt}. \tag{8}$$

Eq. (8) will be shown to be a good approximation of the solution of the initial problem (P) in section 5. Furthermore, it also proves to be energetically consistent since at the optimum the identity $\boldsymbol{\alpha}\cdot\boldsymbol{K}\cdot\boldsymbol{\alpha} \leqslant -\boldsymbol{\alpha}\cdot N^{-1}\sum_{\boldsymbol{\beta}\in\mathcal{I}}\boldsymbol{v}_{\boldsymbol{\beta}}^{opt}$ holds.

5 VALIDATION

In this section, the 2D problem a flow past a regular array of square cylinders is numerically studied. The square has half the size of the unit cell which is of size 1 and the same orientation of the faces ($\boldsymbol{e}_1$ and $\boldsymbol{e}_2$). Thanks to the symmetry of the problem, no rotation of the solid phase occurs. A bound is obtained on the component K_{11} of the intrinsic permeability tensor by setting $\mu_f = 1$ and $\boldsymbol{\alpha} = \boldsymbol{e}_1$. The discretization grid is of $N_1 = N_2$ pixels in each direction. FEM computations have been carried out using quadratic elements on a 256^2 square elements grid using the Finite Element Method (FEM) code Cast3M.

The reference viscosity is chosen equal to the fluid velocity, so that only the solid phase is polarized. This choice experimentally provides the best bound for a given

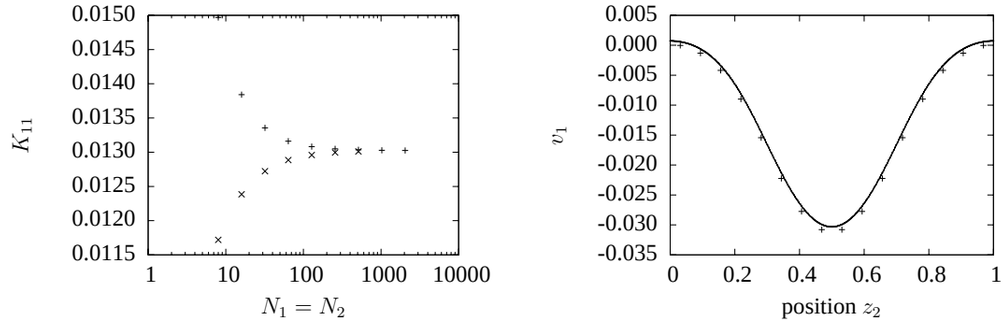

Figure 1. Square inclusion problem. Left: bounds on permeability: FFT (+), FEM (×). Right: velocity field for FEM (fine ×), FFT: $N_1 = 16$ (+), $N_1 = 1024$ (fine −).

discretization. Note that this is valid only for geometries in which the viscosity averaging rule is not needed. This choice also results in less iterations of the linear iterative solver, since the space of explored polarization fields is shrunk. In this example, the choice $\Omega_{\mathcal{S}} = \Omega_s$ is made and consistent discrete Green operators have been used.

Results for the bound on K_{11} are shown in Fig. 1. Since the FFT (resp. FEM) method is based on the principle of Hashin-Shtrikman (resp. minimum potential energy (2)), refinement of the discretization provides increasingly better upper (resp. lower) bounds on the permeability, and both methods steadily converge to the same value.

The local velocities computed using (8) prove to be good approximations of the solution velocity field on Fig. 1, even at low discretization grid (16×16).

6 CONCLUSION

The present work introduced a Hashin-Shtrikman variational framework for the darcean flow problem with periodic boundary conditions. This formulation proved to be a solid basis for the development of numerical approximate solutions. The variational framework ensures the status of upper bound on the permeability of any derived estimate as well as an improvement of the estimates with grid refinement, and provides a consistent discretization of heterogeneous pixels and of the Green operators. The proposed method is computationally faster than FEM and easier to implement: no meshing operation has to be realized, since images may be directly used as an input.

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A ON THE DIFFERENT ORDER GREEN OPERATORS

The Green function $\boldsymbol{G}_0$ solves for the velocity $\boldsymbol{u}$ in a RVE Ω comprising a uniform material with linear properties loaded by a body force field $\boldsymbol{f}$ through $\boldsymbol{u}(\boldsymbol{z}) = \int_\Omega \boldsymbol{G}_0(\boldsymbol{z}-\boldsymbol{y})\cdot\boldsymbol{f}(\boldsymbol{y})\,\mathrm{d}\,V_y = (\boldsymbol{G}_0 * \boldsymbol{f})(\boldsymbol{z})$. In the Fourier space, the convolution product is simply expressed as the dot product $\hat{\boldsymbol{u}}(\boldsymbol{k}) = \hat{\boldsymbol{G}}_0(\boldsymbol{k})\cdot\hat{\boldsymbol{f}}(\boldsymbol{k})$, where, in the Fourier space: $\boldsymbol{k}$ is the wave vector, $\boldsymbol{n}$ its normalization, $\hat{f}$ the Fourier transform of a function f. The Fourier transform of the Green function is known as $\hat{\boldsymbol{G}}_0(\boldsymbol{k}) = (\mu_0|k|^2)^{-1}\left(\boldsymbol{1} - (2(1-\nu_0))^{-1}\boldsymbol{n}\otimes\boldsymbol{n}\right)$, with $\nu_0 = 1/2$. For $\boldsymbol{k}=\boldsymbol{0}$ the convention is that all operators are null. The operator $\boldsymbol{G}_0$ is symmetric.

A third order Green operator may be defined. This operator links polarization to velocity through $\boldsymbol{v} = \boldsymbol{\mathcal{G}}_0 * \boldsymbol{\tau}$ and its Fourier transform is $\hat{\boldsymbol{\mathcal{G}}}_0(\boldsymbol{k}) = -\imath\hat{\boldsymbol{G}}_0(\boldsymbol{k}) \overset{s}{\otimes} \boldsymbol{k}$, where the superscript s indicates symmetrization. Then body force is linked to strain rate through $\boldsymbol{d} = ({}^t\boldsymbol{\mathcal{G}}_0 * \boldsymbol{f})$. Use of the Maxwell-Betti theorem indicates that the operator $\boldsymbol{\mathcal{G}}_0$ is anti-symmetric in the sense $\overline{\boldsymbol{f}\cdot(\boldsymbol{\mathcal{G}}_0*\boldsymbol{\tau})} = -\overline{\boldsymbol{\tau}:({}^t\boldsymbol{\mathcal{G}}_0*\boldsymbol{f})}$.

The fourth order Green operator $\boldsymbol{\Gamma}_0$ links the polarization to strain rate through $\boldsymbol{d} = -\boldsymbol{\Gamma}_0 * \boldsymbol{\tau}$. In Fourier space, $\hat{\boldsymbol{\Gamma}}_0(\boldsymbol{k}) = -\boldsymbol{k}\overset{s}{\otimes}\hat{\boldsymbol{G}}_0(\boldsymbol{k})\overset{s}{\otimes}\boldsymbol{k}$. $\boldsymbol{\Gamma}_0$ is symmetric.

B ON DISCRETIZED PERIODIC GREEN OPERATORS

The periodized Green operator introduced in (Brisard, 2010; 2012) may be generalized to different order operators. Consider an operator $\mathcal{H}$ operating as $\boldsymbol{x}(\boldsymbol{z}) = (\mathcal{H} * \boldsymbol{y})(\boldsymbol{z})$ and two sub-domains Ω_I and Ω_J of Ω whose characteristic functions are denoted χ^I and χ^J, of volume fractions f_I and f_J. To capture the interaction of the two sub-domains, the interaction term $\mathcal{H}^{IJ} = \overline{f_I^{-1}\chi^I\mathcal{H} * f_J^{-1}\chi^J}$ is introduced.

Physically speaking, the interaction term $\mathcal{H}^{IJ}$ yields the average velocity (or strain) on domain Ω^I resulting from a uniform body force (or polarization) applied on domain Ω^J (depending on the choice of Green operator). Using the properties of the Fourier transform, $\mathcal{H}^{IJ} = f_I^{-1}f_J^{-1}\sum_{\boldsymbol{b}\in\mathbb{Z}^d}\hat{\chi}^{I^*}(\boldsymbol{k_b})\hat{\mathcal{H}}(\boldsymbol{k_b})\hat{\chi}^J(\boldsymbol{k_b})$, where the superscript $*$ denotes the complex conjugate. Note that the influence term is null if Ω_I or Ω_J is equal to Ω in the case of Green operators, since they are null for $\boldsymbol{k}=\boldsymbol{0}$.

Now assume Ω_I and Ω_J are both a union of pixels, as defined in section 4. The finite data series $(\chi^I_{\boldsymbol{\beta}})_{\boldsymbol{\beta}\in\mathcal{I}}$ is introduced, such as $\chi^I_{\boldsymbol{\beta}} = 1$ if the pixel Ω_β is in Ω_I, and is null otherwise. For this particular choice, the Fourier transform of $\hat{\chi}^I(\boldsymbol{k_b})$ is linked to the discrete Fourier transform (DFT) $\hat{\chi}^I_{\boldsymbol{b}}$ by $\hat{\chi}^I(\boldsymbol{k_b}) = [\prod_{c\in(1,..,d)}N_c^{-1}\operatorname{sinc}(\pi b_c/N_c)]\hat{\chi}^I_{\boldsymbol{b}}$. The sum over $\mathbb{Z}^d$ is reorganized to take advantage of the DFT periodicity. Reorganization leads to the introduction of the consistently discretized operator $\hat{\mathcal{H}}^c$ whose DFT is $\hat{\mathcal{H}}^{\boldsymbol{c}}_{\boldsymbol{b}} = \sum_{\boldsymbol{n}\in\mathbb{Z}^d}\hat{\mathcal{H}}(\boldsymbol{k}_{b_1+n_1N_1,\ldots,b_d+n_dN_d})\prod_{c\in(1,..,d)}\operatorname{sinc}^2(\pi[b_c/N_c+n_c])$. The influence term is then expressed as $\mathcal{H}^{IJ} = (N^2f_If_J)^{-1}\sum_{\boldsymbol{b}\in\mathcal{I}}\hat{\chi}^{I^*}_{\boldsymbol{b}}\hat{\mathcal{H}}^c_{\boldsymbol{b}}\hat{\chi}^J_{\boldsymbol{b}}$.

A discrete convolution product $\circledast$ may be defined by introducing the sequence $\left(\mathcal{H}^c\circledast\chi^J\right)_{\boldsymbol{\beta}}$ whose DFT is $\widehat{(\mathcal{H}^c\circledast\chi^J)}_{\boldsymbol{b}} = \hat{\mathcal{H}}^c_{\boldsymbol{b}}\hat{\chi}^J_{\boldsymbol{b}}$. Use of the Plancherel theorem provides the useful relation $\mathcal{H}^{IJ} = (Nf_If_J)^{-1}\sum_{\boldsymbol{\beta}\in\mathcal{I}}\chi^I_{\boldsymbol{\beta}}(\mathcal{H}^c\circledast\chi^J)_{\boldsymbol{\beta}}$. Thus, the convolution

products may be exactly computed if Ω_I and Ω_J are both a union of pixels thanks to the relation $\overline{\chi_I \mathcal{H} * \chi_J} = N^{-1} \sum_{\boldsymbol{\beta} \in \mathcal{I}} \chi^I_{\boldsymbol{\beta}} \left(\mathcal{H}^c \circledast \chi^J \right)_{\boldsymbol{\beta}}$, where the discrete convolution product may numerically be efficiently computed by FFT of $(\chi^J_{\boldsymbol{\beta}})_{\boldsymbol{\beta} \in \mathcal{J}}$, product with the consistent operator in the Fourier space and inverse FFT.

The consistent operators require computation of infinite sums, but for sufficiently refined grids, (Brisard, 2012) proved they could be advantageously replaced by so-called filtered non consistent operators in a very satisfactory approximation, which neither require involved computations nor storage.

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