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The boundary-due terms in the Green operator of inclusion patterns from distant to contact and to connected situations using radon transforms: Illustration for spheroid alignments in isotropic media

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ABSTRACT

We examine the boundary-due components in the mean modified Green operator integral (Green operator for short) of an inclusion pattern in distant-contact and contact-connection transitions. The Direct (RT) and inverse (IRT) Radon Transforms, which allow specification of the different contributions to the mean Green operator of the pattern in simple geometrical terms, are used. The already well-documented case of axially symmetric alignments of equidistant identical oblate spheroids, in an infinite matrix of isotropic (elastic-like or dielectric-like) properties is treated up to infinite alignments and for any aspect ratio from unity (spheres) to infinitesimal (platelets). Simple closed forms for this mean Green operator and for its different parts are newly obtained. These closed forms allow an easy parametric study of the operator variations in terms of the alignment characteristics from distant to contact situations. From contact to connection of the inclusions, the changes in the Green operator's contributions are pointed, what provides relevant operator forms for the connected patterns. These results are of interest in problems where phase percolation, connectivity inversions or co-continuity are implied.

1. Introduction

In heterogeneous structures, where one or several phases are embedded in a matrix under the form of bounded and separated domains (inclusions), an effective property (elasticity, conductivity, . . .) cannot be correctly approached if the inclusion interactions are ignored, except where concentrations are "dilute enough" (Willis and Acton, 1976; Christensen, 1979). For "high" concentrations, the isolated (one site) inclusion approximation has been significantly improved by using either the solution for the pair interaction problem between two ellipsoids (Berveiller et al., 1987; Kouris and Tsuchida, 1991; Anttreter and Fisher, 1996) or statistical estimates that are based on correlation functions of rank two and more (Davis, 1991; Helsing, 1993; Ponte Castaneda and Willis, 1995; Kanaun, 2003). However, when inclusions are not homogeneously or randomly distributed within a matrix, the estimate of the cluster or pattern effects needs to approach some mean, or effective, interaction contribution in the arrangement (De Bartolo and Hillberry, 1998; Estevez et al., 1995, 1999). In practice, it is currently accepted that only the interaction pairs of one inclusion with its nearest neighbors will significantly affect inclusion clustering. However, as has already been examined by Willis and Acton (1976) in the case of random arrangements of spheres, such a simplification remains an approximation even when no long range order exists. Consequently, this becomes more unlikely for highly anisotropic spatial distributions of elements in patterns with a long range order as is the case to be considered in this study for alignments in a matrix that has isotropic and linear properties.

Applications of this linear "pair interaction problem" in isotropic media extend to anisotropic materials, with the help of appropriate transformation or homogenization methods (Pouya and Zaoui, 2006; Franciosi et al., 1998; Franciosi and Berbenni, 2008), as well as to non linear behavior, as in plasticity theory for modeling the pile up of martensitic variants (Cherkaoui et al., 2000; Aubry et al., 2003) or slip bands (Franciosi and Berbenni, 2007, 2008), which are responsible for forest hardening (Kocks et al., 1991; Mecif et al., 1997). Note that most of these abovementioned plasticity problems somehow pile flat, platelet-like, inclusions.

These varieties of morphological situations that involve complex patterns can, today, be approached on an individual basis with numerical calculations. However, the goal of obtaining simpler expressions for the "representative operators" that are related to various inclusion or pattern shapes and matrix property symmetry is to simplify the numerical implementation or to obtain new analytical solutions; and this is still a topic of active research (Meisner and Kouris, 1995; Ju and Sun, 1999; Nakasone et al., 2000; Kushch et al., 2005; Zheng et al., 2006; Agnolin and Roux, 2008). If the transition from dilute to concentrated volume fractions of inclusions has been widely explored, an important and yet unanswered

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question is the specific changes of these operators when inclusions at contact become a connected cluster. Addressing this is of particular interest when aiming, for example, to model the evolution of the effective properties in a material that is submitted to some thermal-physical-mechanical process that causes one (or several) phase(s) to change from discontinuous to continuous (or the reverse).

Thus, in support of investigating the operator changes, from dilute to compact filling and from contact to connection between inclusions, the present paper analytically examines, in detail, the mean modified Green operator integral (the "Green operator" or "operator" for short) of an axially symmetric alignment. The alignment is of n equidistant identical oblate spheroids in an isotropic medium, with essentially elastic-like properties and, secondarily, with dielectric-like properties. At first, this Green operator, which provides the mean Eshelby tensor for the considered domains or patterns, is given a simple and new closed-form solution. This closed-form solution allows an easy parametric study which helps highlight the properties of composite materials involving such inclusion patterns.

Now, special attention will be paid to the transition from the contact to the connection of the inclusions; this investigation requires separately calculating the Green operator at the interior and exterior points of the bounded single (simply connected) domains and, more specifically, the boundary-due contributions. Even when taking into account the various calculation methods used (Fourier transform, multi-potential modelling, F.E. calculations, etc.), literature that specifically addresses determining the inclusion "exterior operators" remains relatively scarce (Mura and Cheng, 1977; Johnson et al., 1980; Mura, 1987; Hasegawa et al., 1992; Wu and Du, 1995). In addition, literature that explains the boundary-due parts, even for simple patterns, appears to be entirely absent.

This study's calculations and comparisons, involving interior and exterior operators of inclusions, are performed using the Radon Transform (RT) method and its inversion formula (Gel'fand et al., 1966), a widely used method in 2D tomographic analyses (Natterer, 1986; Ramm and Katsevitch, 1996), but used less often in the field of 3D solid structure analyses (Wang, 1997; Pan and Tonon, 2000; Franciosi and Lormand, 2004; Franciosi, 2005). One advantage of the Inverse Radon Transform (IRT) method is that it provides simple access to the boundary-due part of the Green operator of a domain; thus, the method is useful when boundary effects are important, with regards to connectivity, compaction or debonding considerations (Drissi-Habtia et al., 1999; Martina et al., 2003; Ricotti et al., 2006), or in the analysis of percolation events. Using the IRT, closed forms for each (and especially for the boundary-due) operator part are obtained.

Finally, it is worth specifying that we did not intend to enter the application domain to estimate the effective properties of the heterogeneous materials of which the patterns discussed here would be representative. Too many frameworks are likely to be used for this estimation, as discussed in several books, with different viewpoints, by Mura (1987), Cherkaev (2000) and Buryachenko (2007). The effective properties of spheroid alignments have been recently examined by Buryachenko et al., 2007). We are not saying that the overall pattern operators can be used within any existing framework; they are, for example, suitable with models such as the one by Ponte Castaneda and Willis (1995), which accounts for pair correlation functions in spatial inclusion distributions that have ellipsoidal symmetry. Such "mean field approximations" have also been proposed for patterns, as in Bornert et al., 1996) and in Buryachenko (2001). In many cases, it would be necessary to not only consider a mean pattern operator, but also the mean operators of each pattern element. The present discussion focuses on the decomposition of the overall pattern operator being similar to that of the mean operators of the pattern elements as it will be exemplified for spheroid alignments.

Section 2 briefly presents the calculation of the Green operator at the interior and exterior points of an inclusion, using the IRT method. From its application to calculating the mean operator of an inclusion pair, as recalled in Section 3, the case of two axially symmetric oblate spheroids is fully examined, from the sphere shape to the platelet (laminate) extreme. Section 4 addresses the mean operator of an aligned assemblage of oblate spheroids, from spheres to platelets. The noticeable characteristics are also stressed and discussed. *Finally*, Section 5 examines the transition from an alignment at contact to a connected alignment and proposes relevant forms for operators of connected patterns.

2. Interior and exterior inclusion characteristic functions and Green operators, from the IRT

2.1. Summary of the general IRT framework

Let $\mathbf{C}$, which can either be a four-rank (elasticity-like) or a second-rank (dielectric-like) tensor, denote the considered linear property of an infinite matrix that contains the V inclusion. Take $\Gamma(\mathbf{r}-\mathbf{r}')$ to be the related modified Green tensor, which is defined from the $\mathbf{G}(\mathbf{r}-\mathbf{r}')$ Green function as:

$$\mathbf{C} : \Gamma(\mathbf{r}-\mathbf{r}') = \mathbf{C} : (-\partial\partial\mathbf{G}(\mathbf{r}-\mathbf{r}')) = -\delta(\mathbf{r}-\mathbf{r}') \tag{1}$$

where "$\partial\partial$" stands for "$\partial^2/\partial x_p \partial x_q$", which acts on $\mathbf{r} = (x_1, x_2, x_3)$; Δ is the Kronecker tensor or unity when $\mathbf{C}$ is either a four-rank or a second-rank tensor, respectively; and $\delta(\mathbf{r})$ is the delta function in R^3. We a priori denote $\mathbf{t}^V(\mathbf{r}) = \int_V \Gamma(\mathbf{r}-\mathbf{r}')\,d\mathbf{r}'$ as the modified Green operator integral over V for $\mathbf{r}$, which is either inside or outside V, while $\overline{\mathbf{t}^V} = \frac{1}{V}\int_V \mathbf{t}^V(r)\,d\mathbf{r}$ is the interior mean (volume average) operator value; these are thus referred to as the (Green) operator and the mean (Green) operator, respectively. The related Eshelby and mean Eshelby tensors for V are defined by $\mathbf{E}^V(\mathbf{r}) = \mathbf{C} : \mathbf{t}^V(\mathbf{r})$ and $\overline{\mathbf{E}^V} = \mathbf{C} : \overline{\mathbf{t}^V}$, respectively. Thus, V is a general, regular, possibly multiply connected, bounded domain, whether it is convex or not. The IRT in R^3 of the Green operator $\mathbf{t}^V(\mathbf{r})$ (resp. of the mean Green operator $\overline{\mathbf{t}^V}$ over V) is a weighted angular average of the elementary operators $\mathbf{t}^P(\boldsymbol{\omega})$ over the vectors $\boldsymbol{\omega} = (\theta, \phi)$ of the unit sphere Ω. This is a result of writing the following (see Franciosi and Lormand, 2004):

$$\begin{aligned} t^V_{pqjn}(\mathbf{r}) &= \int_V \Gamma_{pqjn}(\mathbf{r}-\mathbf{r}')\,d\mathbf{r}' \\ &= \frac{1}{8\pi^3}\int_V \left(\int_{\mathbf{K}} ((M^{-1})_{pj}(\boldsymbol{\omega})\omega_q\omega_n)\Big|_{(pq),(jn)} \exp^{-i\mathbf{K}(\mathbf{r}-\mathbf{r}')}\,d\mathbf{K}\right) d\mathbf{r}' \\ &= \frac{1}{8\pi^3}\int_V \left(\int_\Omega t^P_{pqjn}(\boldsymbol{\omega}) \int_{k=0}^{\infty} k^2 \exp^{-i\mathbf{K}(\mathbf{r}-\mathbf{r}')}\,dk\,d\omega\right) d\mathbf{r}' \\ &= \int_\Omega t^P_{pqjn}(\boldsymbol{\omega})\psi_V(\boldsymbol{\omega},\mathbf{r})\,d\boldsymbol{\omega} \end{aligned}$$

with $\boldsymbol{\omega} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, $d\boldsymbol{\omega} = \sin\theta\,d\theta d\phi$. Thus, the following equation is arrived at:

$$\begin{aligned} \mathbf{t}^V(\mathbf{r}) &= \int_\Omega \mathbf{t}^P(\boldsymbol{\omega})\psi_V(\boldsymbol{\omega},\mathbf{r})\,d\boldsymbol{\omega}; \\ \overline{\mathbf{t}^V} &= \frac{1}{V}\int_{\mathbf{V}} \mathbf{t}^V(\mathbf{r})\,d\mathbf{r} = \int_\Omega \mathbf{t}^P(\boldsymbol{\omega})\overline{\psi_V}(\boldsymbol{\omega})\,d\boldsymbol{\omega}, \end{aligned} \tag{2}$$

where

$$\begin{cases} t^P_{pqjn}(\boldsymbol{\omega}) = \left((M^{-1})_{pj}(\boldsymbol{\omega})\boldsymbol{\omega}_q\boldsymbol{\omega}_n\right)_{(pq),(jn)}; & M_{mp}(\boldsymbol{\omega}) = C_{mipj}\omega_j\,\omega_i \quad (i) \\ \text{or} & \\ t^P_{qn}(\boldsymbol{\omega}) = \left((M^{-1})(\boldsymbol{\omega})\omega_q\omega_n\right); & M(\boldsymbol{\omega}) = C_{ij}\omega_j\omega_i \quad (ii) \end{cases}, \tag{3a}$$

$$\begin{aligned} \psi_V(\boldsymbol{\omega},\mathbf{r}) &= \frac{1}{8\pi^3}\int_{\mathbf{V}}\left(\int_{k=0}^{\infty} k^2 \exp^{-ik\boldsymbol{\omega}(\mathbf{r}-\mathbf{r}')}\,dk\right) d\mathbf{r}' \\ &= \frac{1}{8\pi^3}\int_{\mathbf{V}} (-\pi)\delta''(\boldsymbol{\omega}.(\mathbf{r}-\mathbf{r}'))\,d\mathbf{r}' = -\frac{s''_V(z,\boldsymbol{\omega})}{8\pi^2}. \end{aligned} \tag{3b}$$