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# A polarization based FFT iterative scheme for computing the effective properties of elastic composites with arbitrary contrast

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## Abstract

It is recognized that the convergence of FFT based iterative schemes used for computing the effective properties of elastic composite materials drastically depends on the contrast between the phases. Particularly, the rate of convergence of the strain based iterative scheme strongly decreases when the composites contain very stiff inclusions and the method diverges in the case of rigid inclusions. Reversely, the stress based iterative scheme converges rapidly in the case of composites with very stiff or rigid inclusions, but leads to low convergence rates when soft inclusions are considered and to divergence for composites containing voids. It follows that the computation of effective properties is costly when the heterogeneous medium contains simultaneously soft and stiff phases. Particularly the problem of composites containing voids and rigid inclusions cannot be solved by the strain or the stress based approaches. In this paper, we propose a new polarization-based iterative scheme for computing the macroscopic properties of elastic composites with an arbitrary contrast which is nearly as simple as the basic schemes (strain and stress based) but which has the ability to compute the overall properties of multiphase composites with arbitrary elastic moduli, as illustrated through several examples.

*Key words:* Elastic composites, Fast Fourier transform, Polarization, Voids, Rigid inclusions

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## 1 Introduction

An alternative approach to FEM and BEM methods [10,8,15] was proposed in the middle of the nineties [20] for the computation of effective properties of linear elastic periodic composite. The local cell problem is solved by means of an iterative scheme which uses the periodic Green's tensor for the strain and exact images of the microstructures. The main advantages of this approach over other existing ones can be summarized as follows: (i) the method is based on a recurrence relation and does not lead to the resolution of a linear system, (ii) the discrete Fourier transform and its inverse are computed with the Fast Fourier Transform (FFT) which significantly increases the performance of the method, (iii) the memory needed for solving the problem is significantly reduced compared to other methods. The approach has been afterwards extended to non linear composites [21,15]. It have been used by the authors themselves but also by other researchers for computing the overall response of visco-elasto-plastic composites (see for instance [2,3,13,11,14]).

The FFT based method [20] allows to expand the elastic solution into Neumann series, along the lines of a method which was first introduced for composite conductors by Brown [6] and later by Kroener [12]. The convergence of this series depends on the elastic properties of the phases but also on the choice of a reference medium. The conditions which ensure the convergence of the Neumann series have been derived in [17] (see also [19] for a study of the convergence in the case of the thermal conduction). It has been found that, from a theoretical point of view, the strain based iterative scheme does not converge in both limited cases of voids and rigid inclusions. New conditions for the convergence of the strain based iterative scheme are derived in the present paper. An interesting modification of the results provided in [17] is given in the paper: it is shown that the convergence can be ensured for composites with voids, as it is confirmed by comparison with numerical calculations. From another point of view, the application of the strain based method for composites containing very stiff inclusions is computational costly and the limited case of rigid inclusions cannot be solved by the method. In the domain of high stiffness of inclusions, the stress based iterative scheme [1,4] is shown to be better suited. However, in the region of low stiffness, the calculation times become very large and the case of void cannot be solved by this dual method. It suggests that the basic schemes are not adapted for solving some specific problems for which the heterogeneous medium contains simultaneously both stiff and soft phases (some examples of such specific problems are given in the last part of the paper).

To circumvent the incapacity of the original approach [20], other iterative schemes have been developed during the ten past years. An "accelerated" scheme has been proposed by Eyre and Milton [7] for conductivity problems and has been generalized to elasticity in [17] (see also [25] for its application to nonlinear periodic composites). The accelerated scheme improves the

rate of convergence of the strain based approach for large values of the contrast. However, similarly to the original scheme [20], the number of iterations at convergence still linearly depends on the contrast (see [17]). As a consequence the method still diverges for rigid inclusions. To address the problems of composites with infinite contrast, alternative methods, based on augmented Lagrangians, have been proposed by Michel et al. [16,17]. In [16], a Lagrangian based on the local strain potential was introduced to treat the case of voids. In [17], a Lagrangian based on the local stress potential is used to solve the problem of an elastic composite reinforced by rigid inclusions. More recently, Brisard and Dormieux [5] have proposed a new method based on the Hashin-Shtrikman variational principle [9,27] and used the conjugate gradient method for solving the problem. We emphasize that the use of conjugate gradient has been also used in the recent paper of Zeman et al. [28] for improving the convergence of the strain based iterative scheme.

In the present paper we propose a simple iterative scheme, based on the polarization, which uses the same ingredients as the basic schemes. The paper contains three parts. In section 2, the equations of the local problem are recalled and new compact notations for representing compatibility and equilibrium equations are introduced: they use a representation by means of the Walpole basis [26]. That representation appears also adequate for putting the Green's tensors into a more compact form. These notations are used to propose new convergence tests for the basic schemes. The second part of the paper is dedicated to recalling the basic schemes. The rate of convergence and the limitations of the methods are discussed and illustrated through a few numerical calculations. In the last part of the paper, we present the new polarization-based method. Its relevance over the basic schemes is shown through several applications for which the studied heterogeneous medium contains simultaneously very soft and very stiff inclusions and also voids and rigid inclusions.

## **2 The cell problem for linear elastic composites with prescribed macroscopic strain or stress**

We consider a periodic composite defined by a parallelepipedic unit cell and three (two for plane strain problems) vectors of translation invariance. The unit cell is made up of  $M$  phases whose elastic tensor (resp. compliance) is denoted by  $\mathbb{C}_\alpha$  (resp.  $\mathbb{S}_\alpha = (\mathbb{C}_\alpha)^{-1}$ ) for  $\alpha = 1..M$ . Classically, the local problem involves compatibility equations, linear elastic constitutive equations, equilibrium and periodic conditions at the boundary of the considered unit cell:

$$\left\{ \begin{array}{l} \underline{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{x}}) = \frac{1}{2}(\nabla \underline{\boldsymbol{u}}(\underline{\boldsymbol{x}}) + \nabla^t \underline{\boldsymbol{u}}(\underline{\boldsymbol{x}})), \quad \forall \underline{\boldsymbol{x}} \in V \\ \underline{\boldsymbol{\sigma}}(\underline{\boldsymbol{x}}) = \mathbb{C}(\underline{\boldsymbol{x}}) : \underline{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{x}}), \quad \forall \underline{\boldsymbol{x}} \in V \\ \operatorname{div}(\underline{\boldsymbol{\sigma}}(\underline{\boldsymbol{x}})) = 0, \quad \forall \underline{\boldsymbol{x}} \in V \\ \underline{\boldsymbol{u}}(\underline{\boldsymbol{x}}) - \mathbf{E} \cdot \underline{\boldsymbol{x}} \text{ periodic} \\ \underline{\boldsymbol{\sigma}}(\underline{\boldsymbol{x}}) \cdot \underline{\boldsymbol{n}} \text{ antiperiodic} \end{array} \right. \quad (1)$$

in which the stiffness tensor  $\mathbb{C}(\underline{\boldsymbol{x}})$  (resp. the compliance) of the heterogeneous medium is given by:

$$\begin{aligned} \mathbb{C}(\underline{\boldsymbol{x}}) &= \sum_{\alpha} I_{\alpha}(\underline{\boldsymbol{x}}) \mathbb{C}_{\alpha}, \quad \mathbb{S}(\underline{\boldsymbol{x}}) = \sum_{\alpha} I_{\alpha}(\underline{\boldsymbol{x}}) \mathbb{S}_{\alpha} \\ \text{with : } I_{\alpha}(\underline{\boldsymbol{x}}) &= \begin{cases} 1 & \text{if } \underline{\boldsymbol{x}} \in V_{\alpha} \\ 0 & \text{if } \underline{\boldsymbol{x}} \in V - V_{\alpha} \end{cases} \end{aligned} \quad (2)$$

$I_{\alpha}(\underline{\boldsymbol{x}})$  for  $\alpha = 1..M$  are the characteristic functions describing volumes  $V_{\alpha}$  which comply with  $\sum_{\alpha} I_{\alpha}(\underline{\boldsymbol{x}}) = 1$ . Prescribed macroscopic strain  $\mathbf{E} = \langle \underline{\boldsymbol{\varepsilon}} \rangle_V$  or macroscopic stress  $\mathbf{\Sigma} = \langle \underline{\boldsymbol{\sigma}} \rangle_V$  are classically considered (the brackets denote the volume average over  $V$ ). Due to periodicity, the strain and stress fields are expanded into Fourier series:

$$\begin{aligned} \underline{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{x}}) &= \sum_n \underline{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{\xi}}_n) \exp(i\underline{\boldsymbol{\xi}}_n \cdot \underline{\boldsymbol{x}}) \\ \underline{\boldsymbol{\sigma}}(\underline{\boldsymbol{x}}) &= \sum_n \underline{\boldsymbol{\sigma}}(\underline{\boldsymbol{\xi}}_n) \exp(i\underline{\boldsymbol{\xi}}_n \cdot \underline{\boldsymbol{x}}) \end{aligned} \quad (3)$$

where the  $\underline{\boldsymbol{\xi}}_n$  are the discrete wave vectors arranged along a discrete network having a period  $2\pi/b_i$  in the direction  $x_i$ . In (3),  $\underline{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{\xi}})$  and  $\underline{\boldsymbol{\sigma}}(\underline{\boldsymbol{\xi}})$  denote the Fourier transforms of the strain and stress fields:

$$\begin{aligned} \underline{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{\xi}}) &= \frac{1}{V} \int_V \underline{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{x}}) \exp(-i\underline{\boldsymbol{\xi}} \cdot \underline{\boldsymbol{x}}) d\underline{\boldsymbol{x}} \quad \text{with : } \underline{\boldsymbol{\varepsilon}}(0) = \mathbf{E} \\ \underline{\boldsymbol{\sigma}}(\underline{\boldsymbol{\xi}}) &= \frac{1}{V} \int_V \underline{\boldsymbol{\sigma}}(\underline{\boldsymbol{x}}) \exp(-i\underline{\boldsymbol{\xi}} \cdot \underline{\boldsymbol{x}}) d\underline{\boldsymbol{x}} \quad \text{with : } \underline{\boldsymbol{\sigma}}(0) = \mathbf{\Sigma} \end{aligned} \quad (4)$$

The difference between quantities in Fourier space and in real space is denoted by adding the variable, for example  $\underline{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{\xi}})$  for the Fourier transform of  $\underline{\boldsymbol{\varepsilon}}(\underline{\boldsymbol{x}})$  with the same symbol "ε" in both cases.

Now, a new tensorial formalism is introduced, which gives a geometrical interpretation of the compatibility and equilibrium equation in the Fourier space. This formalism uses the Walpole basis and will also have the advantage to

give compact forms to Green's operators which are used within FFT iterative solution. In a first step, it is important to notice that all operators such as compatibility operator, Green's tensors,.. are  $\underline{\xi}$  dependent fourth order tensors which are transversely isotropic around wave vector  $\underline{\xi}$ . Therefore, the Walpole basis [26] can be used to represent all these tensors. Let us therefore introduce the fourth order tensors  $\mathbb{P}(\underline{\xi})$  and  $\mathbb{Q}(\underline{\xi})$  defined for every  $\underline{\xi} \neq 0$  by:

$$\mathbb{Q}(\underline{\xi}) = \mathbb{E}_1(\underline{\xi}) + \mathbb{E}_3(\underline{\xi}), \quad \mathbb{P}(\underline{\xi}) = \mathbb{E}_2(\underline{\xi}) + \mathbb{E}_4(\underline{\xi})$$

in which the  $\mathbb{E}_n(\underline{\xi})$  for  $n = 1..4$  are the first four tensors of the Walpole basis [26]. Let us recall the six tensors of this basis:

$$\begin{cases} \mathbb{E}_1(\underline{\xi}) = \frac{1}{2}\mathbf{k}^\perp \otimes \mathbf{k}^\perp, & \mathbb{E}_2(\underline{\xi}) = \mathbf{k} \otimes \mathbf{k} \\ \mathbb{E}_3(\underline{\xi}) = \mathbf{k}^\perp \otimes \mathbf{k}^\perp - \mathbb{E}_1, & \mathbb{E}_4(\underline{\xi}) = \mathbf{k}^\perp \otimes \mathbf{k} + \mathbf{k} \otimes \mathbf{k}^\perp \\ \mathbb{E}_5(\underline{\xi}) = \mathbf{k} \otimes \mathbf{k}^\perp, & \mathbb{E}_6(\underline{\xi}) = \mathbf{k}^\perp \otimes \mathbf{k} \end{cases} \quad (5)$$

where  $\mathbf{k}$  and  $\mathbf{k}^\perp$  are given by:

$$\mathbf{k} = \frac{1}{|\underline{\xi}|^2} \underline{\xi} \otimes \underline{\xi}, \quad \mathbf{k}^\perp = \mathbf{i} - \mathbf{k} \quad (6)$$

where  $\mathbf{i}$  is the two order identity tensor. Since the  $\mathbb{E}_n(\underline{\xi})$  for  $n = 1..4$  are projectors,  $\mathbb{P}(\underline{\xi})$  and  $\mathbb{Q}(\underline{\xi})$  are also two projectors:

$$\forall \underline{\xi} \neq 0 : \begin{cases} \mathbb{P}(\underline{\xi}) : \mathbb{P}(\underline{\xi}) = \mathbb{P}(\underline{\xi}), & \mathbb{Q}(\underline{\xi}) : \mathbb{Q}(\underline{\xi}) = \mathbb{Q}(\underline{\xi}) \\ \mathbb{P}(\underline{\xi}) : \mathbb{Q}(\underline{\xi}) = \mathbb{Q}(\underline{\xi}) : \mathbb{P}(\underline{\xi}) = 0 \\ \mathbb{I} = \mathbb{P}(\underline{\xi}) + \mathbb{Q}(\underline{\xi}) \end{cases} \quad (7)$$

The action of  $\mathbb{Q}(\underline{\xi})$  on a second order tensor  $\mathbf{a}(\underline{\xi})$ , having a zero volume average, gives the projection of  $\mathbf{a}(\underline{\xi})$  along the plane of normal  $\underline{\xi}$  denoted  $\mathcal{Q}_\xi$ . The action of  $\mathbb{P}(\underline{\xi})$  on a second order tensor  $\mathbf{a}(\underline{\xi})$  provides the "out of plane" components, namely along  $\mathcal{P}_\xi$  the supplementary of  $\mathcal{Q}_\xi$ . The two orthogonal subspaces  $\mathcal{P}_\xi$  and  $\mathcal{Q}_\xi$  have both dimension 3 for three dimensional problems. In 2D cases,  $\mathbb{E}_3(\underline{\xi}) = 0$ , the subspaces  $\mathcal{P}_\xi$  and  $\mathcal{Q}_\xi$  are of dimension 2 and 1 respectively.

The compatibility and equilibrium conditions are differential equations which become linear algebraic equations in Fourier space. They can then be represented by algebraic equations which use tensors  $\mathbb{P}(\underline{\xi})$  and  $\mathbb{Q}(\underline{\xi})$ . For instance, the compatibility for every periodic field  $\boldsymbol{\varepsilon}(\underline{x})$  is:

$$\forall \underline{\xi} \neq 0 : \mathbb{P}(\underline{\xi}) : \underline{\boldsymbol{\varepsilon}}(\underline{\xi}) = \underline{\boldsymbol{\varepsilon}}(\underline{\xi}) \quad \text{or} \quad \mathbb{Q}(\underline{\xi}) : \underline{\boldsymbol{\varepsilon}}(\underline{\xi}) = 0 \quad (8)$$

From another hand, the equilibrium condition for the periodic stress field  $\boldsymbol{\sigma}(\underline{x})$ , given by (3), is:

$$\forall \underline{\xi} \neq 0 : \mathbb{P}(\underline{\xi}) : \boldsymbol{\sigma}(\underline{\xi}) = 0 \quad \text{or} \quad \mathbb{Q}(\underline{\xi}) : \boldsymbol{\sigma}(\underline{\xi}) = \boldsymbol{\sigma}(\underline{\xi}) \quad (9)$$

It is worthwhile mentioning that, in this last case, it can be surprising to use a fourth order tensor to express equilibrium equations, while equilibrium equations lead primarily to a third order tensor. However, it is easy to show that a periodic field  $\boldsymbol{\sigma}$  is in equilibrium iff  $\mathbb{P}(\underline{\xi}) : \boldsymbol{\sigma}(\underline{\xi}) = 0$ . The subspace of uniform fields constitute a particular case in the sense that such fields comply with both compatibility and equilibrium equations. Note also that a similar description, using decomposition into orthogonal subspaces, was also proposed by Milton [19] in the context of conduction.

To summarize, the elastic solution of (1) is searched under the form (3), in which  $\underline{\boldsymbol{\varepsilon}}(\underline{\xi}_n)$  and  $\boldsymbol{\sigma}(\underline{\xi}_n)$  comply with conditions (8) and (9).

### 3 The basic iterative schemes

#### 3.1 The strain and stress based iterative schemes

An iterative scheme has been proposed by Moulinec et al. [20] for computing the solution of the linear elastic problem (1), on the basis of previously used similar schemes introduced for conduction problems. The approach introduces a reference medium of rigidity  $\mathbb{C}^0$  to re-write the system of equations (1) as a Lippmann-Schwinger type equation. The solution of that integral equation is expanded along Neumann series [6,12]. Each term of the series is obtained by the following recurrence relations:

$$\left\{ \begin{array}{l} \underline{\boldsymbol{\varepsilon}}^i(\underline{x}) = \mathcal{F}^{-1}(\underline{\boldsymbol{\varepsilon}}^i(\underline{\xi})) \\ \boldsymbol{\sigma}^i(\underline{x}) = \mathbb{C}(\underline{x}) : \underline{\boldsymbol{\varepsilon}}^i(\underline{x}) \\ \boldsymbol{\sigma}^i(\underline{\xi}) = \mathcal{F}(\boldsymbol{\sigma}^i(\underline{x})) \\ \text{convergence test} \\ \underline{\boldsymbol{\varepsilon}}^{i+1}(\underline{\xi}) = \underline{\boldsymbol{\varepsilon}}^i(\underline{\xi}) - \boldsymbol{\Gamma}^0(\underline{\xi}) : \boldsymbol{\sigma}^i(\underline{\xi}) \end{array} \right. \quad (10)$$

which start from the first term given by:

$$\boldsymbol{\varepsilon}^1(\underline{\xi}) = \begin{cases} 0 & \forall \underline{\xi} \neq 0 \\ \mathbf{E} & \text{for } \underline{\xi} = 0 \end{cases} \quad (11)$$

In (10),  $\boldsymbol{\Gamma}^0(\underline{\xi})$  is the periodic "strain Green's tensor", associated to the reference medium of rigidity  $\mathbb{C}^0$ . When an isotropic reference medium is considered, namely  $\mathbb{C}^0 = 3k_0\mathbb{J} + 2\mu_0\mathbb{K}$  with  $\mathbb{J} = \mathbf{i} \otimes \mathbf{i}/3$  and  $\mathbb{K} = \mathbb{I} - \mathbb{J}$  ( $\mathbf{i}$  and  $\mathbb{I}$  being the identity for second and fourth order tensors), the Green's tensor is given, for every  $\underline{\xi} \neq 0$ , by:

$$\boldsymbol{\Gamma}^0(\underline{\xi}) = \frac{1}{\lambda_0 + 2\mu_0} \mathbb{E}_2(\underline{\xi}) + \frac{1}{2\mu_0} \mathbb{E}_4(\underline{\xi}) \quad (12)$$

with  $\boldsymbol{\Gamma}^0(\underline{\xi}) = 0$  when  $\underline{\xi} = 0$ .

In (11),  $\mathcal{F}$  and  $\mathcal{F}^{-1}$  denote the Fourier Transform and its inverse. In (10), the macroscopic strain,  $\mathbf{E}$ , is prescribed whereas the macroscopic stress,  $\boldsymbol{\Sigma}$ , is obtained at convergence of the iterative scheme (10) as follows:  $\boldsymbol{\Sigma} = \boldsymbol{\sigma}(\underline{\xi} = 0)$ . The strain field  $\boldsymbol{\varepsilon}^i(\underline{\xi})$  is compatible at each step,  $\mathbb{Q}(\underline{\xi}) : \boldsymbol{\varepsilon}^i(\underline{\xi}) = 0$ , while the equilibrium for  $\boldsymbol{\varepsilon}^i(\underline{\xi})$  is verified only at convergence of the iterative scheme. The following convergence test can then be used in (10):

$$\frac{\|\mathbb{P}(\underline{\xi}) : \boldsymbol{\sigma}^i(\underline{\xi})\|}{\|\boldsymbol{\sigma}^i(\underline{\xi})\|} < \epsilon \quad (13)$$

where  $\|\bullet\|$  denotes the Frobenius norm. The value  $\epsilon = 10^{-3}$  has been used in this paper.

Dually, the solution of the inhomogeneity problem (1), can be computed by using the following iterative scheme:

$$\begin{cases} \boldsymbol{\sigma}^i(\underline{x}) = \mathcal{F}^{-1}(\boldsymbol{\sigma}^i(\underline{\xi})) \\ \boldsymbol{\varepsilon}^i(\underline{x}) = \mathbb{S}(\underline{x}) : \boldsymbol{\sigma}^i(\underline{x}) \\ \boldsymbol{\varepsilon}^i(\underline{\xi}) = \mathcal{F}(\boldsymbol{\varepsilon}^i(\underline{x})) \\ \text{convergence test} \\ \boldsymbol{\sigma}^{i+1}(\underline{\xi}) = \boldsymbol{\sigma}^i(\underline{\xi}) - \boldsymbol{\Delta}^0(\underline{\xi}) : \boldsymbol{\varepsilon}^i(\underline{\xi}) \end{cases} \quad (14)$$

which starts from the first term given by:

$$\boldsymbol{\sigma}^1(\underline{\xi}) = \begin{cases} 0 & \forall \underline{\xi} \neq 0 \\ \boldsymbol{\Sigma} & \text{for } \underline{\xi} = 0 \end{cases} \quad (15)$$



The macroscopic stress  $\Sigma$  is prescribed over the unit cell. It means that the macroscopic strain  $\mathbf{E}$  is now considered as an unknown and is obtained at convergence. In (14),  $\Delta^0(\underline{\xi})$  is the "stress Green's tensor", given, for  $\underline{\xi} \neq 0$ , by:

$$\Delta^0(\underline{\xi}) = \mathbb{C}^0 - \mathbb{C}^0 : \Gamma^0(\underline{\xi}) : \mathbb{C}^0 = \frac{2\mu_0(3\lambda_0 + 2\mu_0)}{\lambda_0 + 2\mu_0} \mathbb{E}_1(\underline{\xi}) + 2\mu_0 \mathbb{E}_3(\underline{\xi}) \quad (16)$$

with  $\Delta^0(\underline{\xi}) = 0$  when  $\underline{\xi} = 0$ . In (14), the stress field  $\sigma^i(\underline{\xi})$  in (14) is equilibrated at each step while the strain field  $\varepsilon^i(\underline{\xi})$  is compatible only at convergence of the iterative scheme. The following convergence test is then used:

$$\frac{\|\mathbb{Q}(\underline{\xi}) : \varepsilon(\underline{\xi})\|}{\|\varepsilon(\underline{\xi})\|} < \epsilon \quad (17)$$

In which the value  $\epsilon = 10^{-3}$  will be used in the following.

### 3.2 Estimation of the convergence of the basic schemes

The condition giving the convergence of the strain based iterative scheme has been derived in [17]. Here we present a modification of that result which is specially interesting for voided composites. Next, this result will be extended to the stress based iterative scheme.

#### 3.2.1 The convergence of the strain based iterative scheme

In [17], the authors investigate the conditions giving the convergence of the Neumann series. It is well known that the Neumann series converges only if the eigenvalues of the operator are strictly comprised between  $-1$  and  $1$ . From another point of view, the original iterative scheme used by these authors can be written as a Neumann series in the operator  $-\Gamma^0(\underline{x}) * (\mathbb{C}(\underline{x}) - \mathbb{C}^0)$ . Studying the eigenvalues of this operator, they found that the convergence cannot be ensured when the composite material comprises voids, because this case produces eigenvalues of the operator equal to  $1$ .

In the present paragraph we propose to establish a modification of that result. For this, we focus our attention on the convergence of the iterative scheme (10) instead of the Neumann series. Let us therefore define by  $\phi$  and by  $\underline{e}_\phi$  respectively an eigenvalue and the associated eigenvector of the linear operator  $\mathbb{I} - \Gamma^0(\underline{x}) * \mathbb{C}(\underline{x})$ . They comply with:

$$\phi \underline{e}_\phi(\underline{x}) = \underline{e}_\phi(\underline{x}) - \mathbf{\Gamma}^0(\underline{x}) * \mathbb{C}(\underline{x}) : \underline{e}_\phi(\underline{x}) \quad (18)$$

As shown in appendix A the convergence of such an iterative scheme is ensured if the eigenvalues comply with:  $-1 < \phi \leq 1$ . In (18), it can be observed that  $\underline{e}_\phi(\underline{x})$  is compatible and has a null volume average if  $\phi \neq 1$ . However, for every compatible field  $\underline{\varepsilon}(\underline{x})$ , such that  $\langle \underline{\varepsilon}(\underline{x}) \rangle_V = 0$ , one has:

$$\underline{\varepsilon}(\underline{x}) = \mathbf{\Gamma}^0(\underline{x}) * \mathbb{C}^0 : \underline{\varepsilon}(\underline{x}) \quad (19)$$

Then, equation (18) can be also put into the form:

$$\mathbf{\Gamma}^0(\underline{x}) * \left[ \mathbb{C}(\underline{x}) - (1 - \phi)\mathbb{C}^0 \right] : \underline{e}_\phi(\underline{x}) = 0 \quad (20)$$

This relation (which is also obviously true for  $\phi = 1$ ) indicates that  $(\mathbb{C}(\underline{x}) - (1 - \phi)\mathbb{C}^0) : \underline{e}_\phi(\underline{x})$  is an equilibrated field. As explained in [17],  $\underline{e}_\phi(\underline{x})$  is then the solution of an elasticity problem corresponding to an elastic heterogeneous material with stiffness  $\mathbb{C}'(\underline{x}) = \mathbb{C}(\underline{x}) - (1 - \phi)\mathbb{C}^0$ , and subjected to a zero macroscopic strain. Such a problem has the trivial solution  $\underline{e}_\phi(\underline{x}) = 0$  if  $\mathbb{C}'(\underline{x})$  is positive or negative definite.

At this stage, the procedure is identical to that conducted in [17] with the substantial modification that the value  $\phi = 1$  is now allowed. It leads to the following result (the reader will refer to the paper of Michel et al. [17] for more details about the procedure):

$$k_{max} < 2k_0, \quad k_{min} \geq 0 \quad \text{and} \quad \mu_{max} < 2\mu_0, \quad \mu_{min} \geq 0 \quad (21)$$

with:  $k_{min} = \min[k_1, k_2, \dots, k_N]$ ,  $k_{max} = \max[k_1, k_2, \dots, k_N]$  and  $\mu_{min} = \min[\mu_1, \mu_2, \dots, \mu_N]$ ,  $\mu_{max} = \max[\mu_1, \mu_2, \dots, \mu_N]$ . It is worthwhile mentioning that the value  $k_{min} = 0$  and  $\mu_{min} = 0$  are acceptable contrarily to the result of [17].

In fact, the very reason of such a difference with the result of [17] is that two iterative schemes can be used : the one corresponding to (10) and an alternative scheme leading to a Neumann series in  $-\mathbf{\Gamma}^0(\underline{x}) * (\mathbb{C}(\underline{x}) - \mathbb{C}^0)$ . Studying the spectra of the operator used in the alternative scheme seems to lead to no convergence in the case of void-containing materials. However, it has been proved by [20] that both schemes are strictly equivalent. As a consequence, the previous proof that scheme (10) converges even for void containing materials proves that the the alternative scheme converges also in this case, as show also numerous numerical tests.

### 3.2.2 The convergence of the stress based iterative scheme

Our purpose is now to establish a similar result in the case of the stress based iterative scheme (14). To this aim, the eigenvalues of the linear operator  $\mathbb{I} - \Delta^0(\underline{x}) * \mathbb{S}(\underline{x})$  are now studied. As effected in the previous section, we introduce an eigenvalue  $\phi$  and the associated eigenvector  $\mathbf{e}_\phi$  such that:

$$\phi \mathbf{e}_\phi(\underline{x}) = \mathbf{e}_\phi(\underline{x}) - \Delta^0(\underline{x}) * (\mathbb{S}(\underline{x}) : \mathbf{e}_\phi(\underline{x})) \quad (22)$$

If  $\phi \neq 1$ , the eigenvector complies with equilibrium and has a null volume average. It follows that  $\mathbf{e}_\phi$  complies with:

$$\mathbf{e}_\phi(\underline{x}) = \Delta^0(\underline{x}) * \mathbb{S}^0 : \mathbf{e}_\phi(\underline{x}) \quad (23)$$

Consequently, (22) can be written as:

$$\Delta^0(\underline{x}) * \left[ (\mathbb{S}(\underline{x}) - (1 - \phi)\mathbb{S}^0) : \mathbf{e}_\phi(\underline{x}) \right] = 0 \quad (24)$$

Similarly to the case of the strain based iterative scheme, one observes that  $(\mathbb{S}(\underline{x}) - (1 - \phi)\mathbb{S}^0) : \mathbf{e}_\phi(\underline{x})$  is a compatible field. So,  $\mathbf{e}_\phi$  is the solution of an elasticity problem corresponding to an elastic heterogeneous material with the compliance  $\mathbb{S}'(\underline{x}) = (\mathbb{S}(\underline{x}) - (1 - \phi)\mathbb{S}^0) : \mathbf{e}_\phi(\underline{x})$  and subjected to a zero macroscopic stress. There exists a non trivial solution for  $\mathbf{e}_\phi(\underline{x})$  if  $\mathbb{S}'(\underline{x})$  is not strictly positive or negative definite. Again, applying the procedure described in [17], we obtain:

$$\frac{1}{k_0} > \frac{1}{2k_{min}}, \quad \frac{1}{2k_{max}} \geq 0 \quad \text{and} \quad \frac{1}{\mu_0} > \frac{1}{2\mu_{min}}, \quad \frac{1}{2\mu_{max}} \geq 0 \quad (25)$$

Which shows that the case of rigid inclusion corresponding to the case of  $k_{max}$  or  $\mu_{max}$  being infinite corresponds to admissible bounds for the inverses of these moduli. In the next subsection, we propose to present a few numerical examples to show the features of the convergence, more specially for infinite contrasts, and showing that improvements are necessary if one wants to deal with microstructures containing simultaneously voids and rigid inclusions.

### 3.3 Numerical study of the rate of convergence of the basic schemes

The rate of convergence of the basic schemes is examined through numerical calculations in the case of composites reinforced by long fibers arranged along

a hexagonal array (the unit cell being defined in figure 1). The unit cell is a rectangle and contains an inclusion centered at  $\underline{x} = 0$  and four quarters of inclusions located at the corner of the cell. In our computations, the radii of the fibers are chosen as  $R = 0.4$  (the area of the unit cell being taken as  $S = 1$ ) and  $N = 64$  wave vectors are taken along each space direction. Both phases, matrix and inclusions, are assumed to be incompressible and we denote the "contrast"  $c$  as  $c = \mu_I/\mu_M$ . Plane strain conditions are assumed and the unit cell is subjected to the macroscopic strain  $E_{11} = -E_{22} = 1$  when the strain based method is used. For the illustrations of the stress based iterative scheme, the macroscopic stress  $\Sigma_{11} = -\Sigma_{22} = 1$  is applied over the unit cell. The exact Fourier transform is thereafter replaced by the discrete

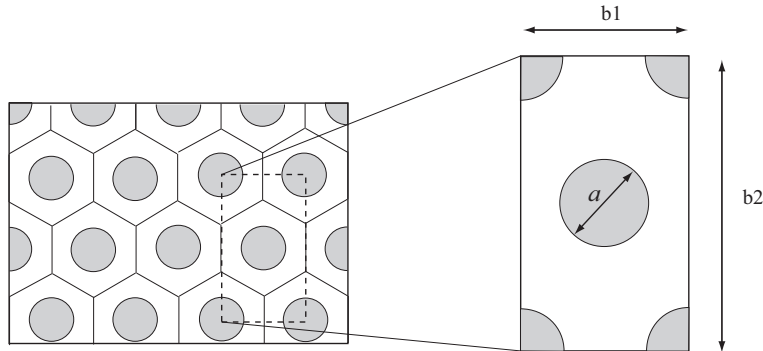


Fig. 1. Unit cell of the composite reinforced by long fibers arranged along a hexagonal array.

Fourier transform which is computed by means of the FFT algorithm. In [20], the stress-strain relation is applied in the real space at each point along a regular grid. For many inclusion-matrix problems, such a description is only approximated. As an example, if cylindrical fibers are concerned, the cross section of the fiber must be described within the real space by using a regular mesh, which approximates the form of the inclusion. In [4], exact expressions for the Fourier transforms of the characteristic functions  $I_\alpha(\underline{x})$  have been used. These Fourier transforms are named "shape coefficients" and are the basis of the approximation for the elastic properties of elastic media obtained by Nemat-Nasser and Hori [23]. These "shape coefficients" are defined by:

$$I_\alpha(\underline{\xi}) = \int_{V_\alpha} \exp(-i\underline{\xi} \cdot \underline{x}) dx \quad (26)$$

The use of shape functions improves the convergence of the iterative scheme. On figure 2, we represent the logarithm of the number of iterations ( $\log(N)$ ), needed for obtaining the convergence of the strain based iterative scheme (10), as a function of the logarithm of the "contrast" ( $\log(c)$ ). On this figure, we compare the original approach [20] (full line with points), and the method which uses the shape functions (full line with circles). The results show that the con-

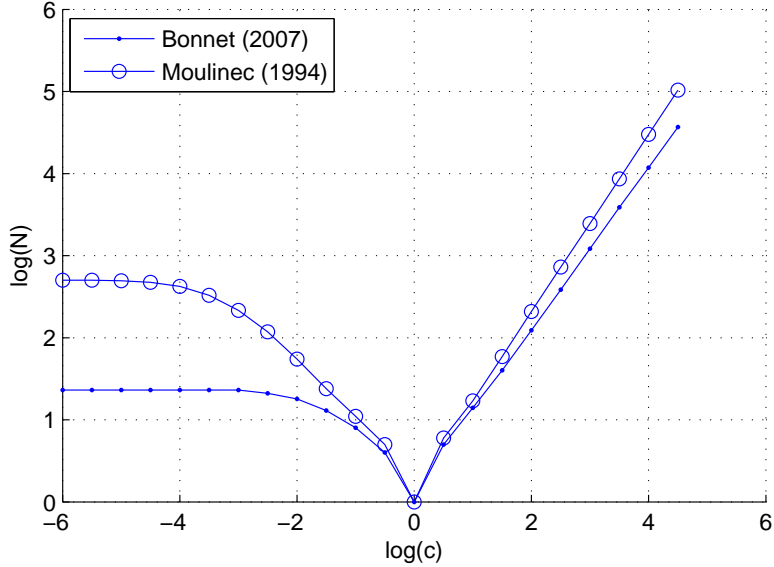


Fig. 2. Number of iterations at convergence as a function of the "contrast". Comparison between the initial strain based iterative scheme [20] and the method using shape functions [4].

vergence is obtained when  $c = 0$  for both approaches, with or without using the shape coefficients. However, one observes that the use of the shape functions improves the convergence of the basic scheme, and this, whatever the value of the contrast. When the value of  $c = \mu_I/\mu_M$  is higher than 1, it can be observed that the number of iterations linearly increases with the contrast (in the log-log frame). The strain based iterative scheme diverges therefore for an infinite "contrast". The case of a composite with rigid inclusions cannot be handled by the method. Note that the shear modulus of the reference medium used in [20] and also used here is defined by:  $\mu_0 = (\mu_M + \mu_I)/2$ . With that choice, the convergence of the iterative scheme is found to be obtained with the lowest number of iterations. When the shape coefficients are used, it has been found that the better choice for  $\mu_0$  does not coincide exactly with  $\mu_0 = (\mu_M + \mu_I)/2$ . The reference shear modulus is chosen on the form:  $\mu_0 = (1 - \omega)\mu_M + \omega\mu_I$  where the value  $\omega = 0.5$  is taken for  $c > 1$  but the value  $\omega = 0.45$  is taken for  $c < 1$ . Note that the convergence is still achieved when the value  $\omega = 0.5$  is used and for a contrast  $c < 1$ , however the choice  $\omega = 0.45$  instead of  $\omega = 0.5$  leads to a gain of convergence rate.

On Figure 3 we represent the logarithm of the number of iterations at convergence as a function of  $\log(c) = \log(\mu_I/\mu_M)$  for the strain based scheme (full line with points), and for the stress based scheme (full line with circles). Both iterative schemes are computed with a representation of the elastic tensors using the shape functions. It can be observed that the stress based approach converges rapidly in the domain of high values of the contrast  $c$ . However, for soft inclusions, namely in the region defined by  $c < 1$ , it can be seen that the number of iterations increases linearly when the logarithm of  $c$  decreases. It means

that the case of materials containing voids cannot be treated by the stress based method. The optimal reference medium, leading to the lowest number of iterations, has been found to be defined by  $\mu_0 = ((1 - \omega)/\mu_M + \omega/\mu_I)^{-1}$ . The value  $\omega = 0.5$  is considered when  $c < 1$  while  $\omega = 0.45$  when  $c > 1$ . To

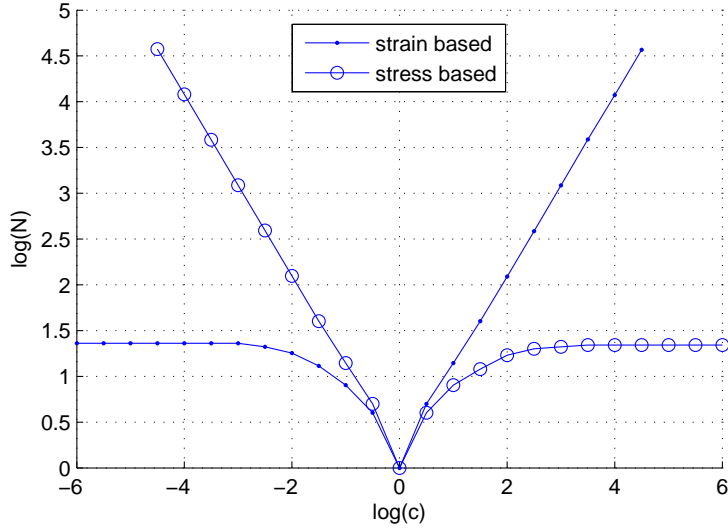


Fig. 3. Number of iterations at convergence as a function of the "contrast": comparison between the strain based and the stress based formulations.

summarize, the strain based approach is better suited for composites containing soft inclusions, namely for which  $\mu_I < \mu_m$ . However, when the composite is made up of stiff inclusions ( $\mu_I > \mu_M$ ), the stress based iterative scheme is better suited. Nevertheless, it suggests that the basic schemes are not adapted for computing the effective properties of composites which contain both stiff and soft inclusions. Moreover the case of composites with rigid inclusions and voids cannot be handled by any of these methods. In the next section, we propose therefore a new iterative scheme which improves the convergence, by comparison with the basic schemes.

## 4 A new iterative scheme based on the polarization

### 4.1 Description of the algorithm

Let us introduce in the system of equations (1) the "polarization tensor"  $\boldsymbol{\tau}(\underline{x}) = (\mathbb{C}(\underline{x}) - \mathbb{C}^0) : \boldsymbol{\varepsilon}(\underline{x})$ :

$$\left\{ \begin{array}{l} \boldsymbol{\varepsilon}(\underline{x}) = \frac{1}{2}(\nabla \underline{u}(\underline{x}) + \nabla^t \underline{u}(\underline{x})), \quad \forall \underline{x} \in V \\ \operatorname{div}(\boldsymbol{\sigma}(\underline{x})) = 0, \quad \forall \underline{x} \in V \\ \boldsymbol{\varepsilon}(\underline{x}) = (\mathbb{C}(\underline{x}) - \mathbb{C}^0)^{-1} : \boldsymbol{\tau}(\underline{x}), \quad \forall \underline{x} \in V \\ \boldsymbol{\sigma}(\underline{x}) = \boldsymbol{\tau}(\underline{x}) + \mathbb{C}^0 : \boldsymbol{\varepsilon}(\underline{x}), \quad \forall \underline{x} \in V \\ \underline{u}(\underline{x}) - \mathbf{E} \cdot \underline{x} \text{ periodic} \\ \boldsymbol{\sigma}(\underline{x}) \cdot \underline{n} \text{ antiperiodic} \\ \langle \boldsymbol{\tau}(\underline{x}) \rangle_V = \mathbf{T} \end{array} \right. \quad (27)$$

In this problem, the uniform polarization  $\mathbf{T}$  is now prescribed over the unit cell. It follows that the macroscopic strain  $\mathbf{E}$  and stress  $\boldsymbol{\Sigma}$  are now both considered as unknowns. However, due to the linearity of the equations, the relations giving the macroscopic stress and strain fields as functions of the uniform polarization  $\mathbf{T}$  can be expressed as:

$$\mathbf{E} = \boldsymbol{\varepsilon}(\underline{\xi} = 0) = \mathbb{A} : \mathbf{T}, \quad \boldsymbol{\Sigma} = \boldsymbol{\sigma}(\underline{\xi} = 0) = \mathbb{B} : \mathbf{T} \quad (28)$$

Note that  $\boldsymbol{\Sigma} = \mathbf{T} + \mathbb{C}^0 : \mathbf{E}$ . As a consequence, it follows that the fourth order tensors  $\mathbb{A}$  and  $\mathbb{B}$  are linked by  $\mathbb{B} = \mathbb{I} + \mathbb{C}^0 : \mathbb{A}$ . The effective elastic tensor  $\mathbb{C}^{hom}$  and the effective compliance  $\mathbb{S}^{hom}$ , are then defined by:

$$\mathbb{C}^{hom} = \mathbb{A}^{-1} + \mathbb{C}^0 \quad \text{or} \quad \mathbb{S}^{hom} = \mathbb{S}^0 : (\mathbb{I} - \mathbb{B}^{-1}) \quad (29)$$

The solution of (27) can be computed by using the following iterative scheme:

$$\left\{ \begin{array}{l} \boldsymbol{\tau}^i(\underline{x}) = \mathcal{F}^{-1}(\boldsymbol{\tau}^i(\underline{\xi})) \\ \boldsymbol{\varepsilon}^i(\underline{x}) = (\mathbb{C}(\underline{x}) - \mathbb{C}^0)^{-1} : \boldsymbol{\tau}^i(\underline{x}) \\ \boldsymbol{\varepsilon}^i(\underline{\xi}) = \mathcal{F}(\boldsymbol{\varepsilon}^i(\underline{x})) \\ \boldsymbol{\sigma}^i(\underline{\xi}) = \mathbb{C}^0 : \boldsymbol{\varepsilon}^i(\underline{\xi}) + \boldsymbol{\tau}^i(\underline{\xi}) \\ \text{convergence test} \\ \boldsymbol{\tau}^{i+1}(\underline{\xi}) = \boldsymbol{\tau}^i(\underline{\xi}) - \alpha \mathbb{C}^0 : \boldsymbol{\Gamma}^0(\underline{\xi}) : \boldsymbol{\sigma}^i(\underline{\xi}) - \beta \boldsymbol{\Delta}^0(\underline{\xi}) : \boldsymbol{\varepsilon}^i(\underline{\xi}) \end{array} \right. \quad (30)$$

where  $\alpha$  and  $\beta$  are coefficients which will be chosen thereafter in order to obtain the best rate of convergence. In (30), tensors  $\boldsymbol{\Gamma}^0(\underline{\xi})$  and  $\boldsymbol{\Delta}^0(\underline{\xi})$  are respectively the periodic Green's tensors for strain and stress defined by equations (12) and (16). In this iterative scheme, the stress field  $\boldsymbol{\sigma}^i(\underline{\xi})$  and the strain field  $\boldsymbol{\varepsilon}^i(\underline{x})$  are respectively equilibrated and compatible fields only at convergence of the

iterative scheme. Indeed, the convergence is achieved when  $\boldsymbol{\tau}^{i+1}(\underline{\xi}) = \boldsymbol{\tau}^i(\underline{\xi})$  in (30) and then, when:

$$\alpha \boldsymbol{\Gamma}^0(\underline{\xi}) : \boldsymbol{\sigma}^i(\underline{\xi}) + \beta \mathbb{S}^0 : \boldsymbol{\Delta}^0(\underline{\xi}) : \boldsymbol{\varepsilon}^i(\underline{\xi}) = 0 \quad (31)$$

However, the projection of equation (31) along  $\mathbb{Q}(\underline{\xi})$  and  $\mathbb{P}(\underline{\xi}) : \mathbb{C}^0$  provides  $\mathbb{Q}(\underline{\xi}) : \boldsymbol{\varepsilon}^i(\underline{\xi})$  and  $\mathbb{P}(\underline{\xi}) : \boldsymbol{\sigma}^i(\underline{\xi})$  respectively. Then, it means that  $\boldsymbol{\varepsilon}^i(\underline{\xi})$  and  $\boldsymbol{\sigma}^i(\underline{\xi})$  are compatible and equilibrated respectively.

The iterative scheme is stopped when:

$$\max \left( \frac{\|\mathbb{Q}(\underline{\xi}) : \boldsymbol{\varepsilon}^i(\underline{\xi})\|}{\|\boldsymbol{\varepsilon}^i(\underline{\xi})\|}, \frac{\|\mathbb{P}(\underline{\xi}) : \boldsymbol{\sigma}^i(\underline{\xi})\|}{\|\boldsymbol{\sigma}^i(\underline{\xi})\|} \right) < \epsilon \quad (32)$$

and the first term of the series is defined by:

$$\boldsymbol{\tau}^1(\underline{\xi}) = \begin{cases} 0 & \forall \underline{\xi} \neq 0 \\ \mathbf{T} & \text{for } \underline{\xi} = 0 \end{cases} \quad (33)$$

It is worthwhile mentioning that this polarization based iterative scheme has some similarities with the accelerated scheme used in [17]. More precisely, it is shown in appendix A that the accelerated scheme coincides with (30) for  $\alpha = 2$  and  $\mathbf{T} = (< \mathbb{C}(\underline{x}) >_V - \mathbb{C}_0) : \mathbf{E}$ . Note that, with that choice, the prescribed polarization  $\mathbf{T}$  diverges for rigid inclusions while, in our approach, the uniform polarization  $\mathbf{T}$  is finite, being prescribed over the unit cell, its value being chosen independently of the elastic properties of the heterogeneous medium. In addition, a specific feature of the polarization based scheme is that it involves always finite linear relations between local stress, strain and polarization fields (second and fourth lines of (30)) even if the elasticity and compliance tensors are not finite.

Note also that a dual form, of the iterative scheme (30), can also be used. This iterative scheme is based on the eigenstrain  $\boldsymbol{\eta}$  and reads:

$$\begin{cases} \boldsymbol{\eta}^i(\underline{x}) = \mathcal{F}^{-1}(\boldsymbol{\eta}^i(\underline{\xi})) \\ \boldsymbol{\sigma}^i(\underline{x}) = (\mathbb{S}(\underline{x}) - \mathbb{S}^0)^{-1} : \boldsymbol{\eta}^i(\underline{x}) \\ \boldsymbol{\sigma}^i(\underline{\xi}) = \mathcal{F}(\boldsymbol{\sigma}^i(\underline{x})) \\ \boldsymbol{\varepsilon}^i(\underline{\xi}) = \boldsymbol{\eta}^i(\underline{\xi}) + \mathbb{S}^0 : \boldsymbol{\sigma}^i(\underline{\xi}) \\ \text{convergence test} \\ \boldsymbol{\eta}^{i+1}(\underline{\xi}) = \boldsymbol{\eta}^i(\underline{\xi}) - \alpha \mathbb{S}^0 : \boldsymbol{\Delta}^0(\underline{\xi}) : \boldsymbol{\varepsilon}^i(\underline{\xi}) - \beta \boldsymbol{\Gamma}^0(\underline{\xi}) : \boldsymbol{\sigma}^i(\underline{\xi}) \end{cases} \quad (34)$$



In (34), the stress is computed in the real space and uses the compliance tensor  $\mathbb{S}(\underline{x})$  whereas in (30) the rigidity  $\mathbb{C}(\underline{x})$  is used. The convergence test is still given by (31). The first term of the series is associated to a uniform eigenstrain, denoted  $\mathbf{N}$ , prescribed over the unit cell. Using this "eigen-strain-based" scheme, it has been found that its rate of convergence is comparable to the one of the polarization scheme. For this reason, only results for the polarization scheme are presented in the following.

#### 4.2 The convergence of the polarization-based iterative scheme

In the iterative scheme (30), the values of coefficients  $\alpha, \beta$  and of the elastic moduli of the reference medium,  $\lambda_0, \mu_0$ , will be chosen in order to obtain the convergence. In other words, they must be chosen in order to ensure that eigenvalues of the operator

$$\mathbb{I} - \alpha \mathbb{C}^0 : \mathbf{\Gamma}^0(\underline{x}) * (\mathbb{C}(\underline{x}) : \delta \mathbb{C}^{-1}(\underline{x})) - \beta \mathbf{\Delta}^0(\underline{x}) * \delta \mathbb{C}^{-1}(\underline{x}) \quad (35)$$

are comprised in the interval  $] - 1, 1]$ . In (35), we have introduced  $\delta \mathbb{C}^{-1}(\underline{x}) = (\mathbb{C}(\underline{x}) - \mathbb{C}^0)^{-1}$ .

Let us introduce an eigenvalue  $\phi$  of that operator and its associated eigenvector  $\mathbf{e}_\phi(\underline{x})$ . They comply with:

$$\begin{aligned} \phi \mathbf{e}_\phi(\underline{x}) = & \mathbf{e}_\phi(\underline{x}) - \alpha \mathbb{C}^0 : \mathbf{\Gamma}^0(\underline{x}) * (\mathbb{C}(\underline{x}) : \delta \mathbb{C}^{-1}(\underline{x}) : \mathbf{e}_\phi(\underline{x})) \\ & + \alpha \mathbf{\Delta}^0(\underline{x}) * (\delta \mathbb{C}^{-1}(\underline{x}) : \mathbf{e}_\phi(\underline{x})) \end{aligned} \quad (36)$$

If  $\phi \neq 0$ , one has  $\langle \mathbf{e}_\phi(\underline{x}) \rangle = 0$  and for any such second order tensor:

$$\mathbf{e}_\phi(\underline{x}) = (\mathbf{\Delta}^0(\underline{x}) : \mathbb{S}^0 + \mathbb{C}^0 : \mathbf{\Gamma}^0(\underline{x})) * \mathbf{e}_\phi(\underline{x}) \quad (37)$$

It follows that (36) can be put into the form:

$$\mathbb{C}^0 : \mathbf{\Gamma}^0(\underline{x}) * \boldsymbol{\sigma}_\phi(\underline{x}) + \mathbf{\Delta}^0(\underline{x}) * \boldsymbol{\varepsilon}_\phi(\underline{x}) = 0 \quad (38)$$

with:

$$\begin{aligned} \boldsymbol{\sigma}_\phi(\underline{x}) = & \alpha \mathbb{C}(\underline{x}) : \delta \mathbb{C}^{-1}(\underline{x}) : \mathbf{e}_\phi(\underline{x}) - (1 - \phi) \mathbf{e}_\phi(\underline{x}) \\ \boldsymbol{\varepsilon}_\phi(\underline{x}) = & \beta \delta \mathbb{C}^{-1}(\underline{x}) : \mathbf{e}_\phi(\underline{x}) - (1 - \phi) \mathbb{S}^0 : \mathbf{e}_\phi(\underline{x}) \end{aligned} \quad (39)$$

Owing to property (38) and following an argument similar to the one used previously for (31),  $\boldsymbol{\varepsilon}_\phi(\underline{x})$  and  $\boldsymbol{\sigma}_\phi(\underline{x})$  are compatible and equilibrated fields. They are solutions of an elasticity problem related to a heterogeneous material having a stiffness  $\mathbb{C}'(\underline{x})$  given by:

$$\mathbb{C}'(\underline{x}) = \left[ \alpha \mathbb{C}(\underline{x}) : \delta \mathbb{C}^{-1}(\underline{x}) - (1 - \phi) \mathbb{I} \right] : \left[ \beta \delta \mathbb{C}^{-1}(\underline{x}) - (1 - \phi) \mathbb{S}^0 \right]^{-1} \quad (40)$$

and subjected to a zero polarization. That problem does not lead to the trivial solution  $\boldsymbol{e}_\phi(\underline{x}) = 0$ , if  $\mathbb{C}'(\underline{x})$  is not strictly positive or negative definite. Let us recall that the convergence of the iterative scheme is ensured if  $-1 < \phi \leq 1$ . So, a sufficient condition for having the convergence is that  $\mathbb{C}'(\underline{x})$  must be strictly positive or negative definite only within the interval  $] -\infty, -1]$  and  $]1, +\infty[$ .

The elastic properties of each phase and the reference modulus being isotropic,  $\mathbb{C}'(\underline{x})$  is also isotropic and can be put into the form  $\mathbb{C}'(\underline{x}) = 3k'(\underline{x})\mathbb{J} + 2\mu'(\underline{x})\mathbb{K}$ , where  $k'(\underline{x})$  and  $\mu'(\underline{x})$  are given by:

$$\begin{aligned} k'(\underline{x}) &= k_0 \frac{\alpha k(\underline{x}) - (1 - \phi)(k(\underline{x}) - k_0)}{\beta k_0 - (1 - \phi)(k(\underline{x}) - k_0)} \\ \mu'(\underline{x}) &= \mu_0 \frac{\alpha \mu(\underline{x}) - (1 - \phi)(\mu(\underline{x}) - \mu_0)}{\beta \mu_0 - (1 - \phi)(\mu(\underline{x}) - \mu_0)} \end{aligned} \quad (41)$$

So, a sufficient condition for having the convergence is that  $k'(\underline{x})$  and  $\mu'(\underline{x})$  must be strictly positive or negative definite only within the interval  $] -\infty, -1]$  and  $]1, +\infty[$ . Functions  $k'(\underline{x})$  and  $\mu'(\underline{x})$  are zero if:

$$\phi = 1 - \frac{\alpha k(\underline{x})}{k(\underline{x}) - k_0}, \quad \phi = 1 - \frac{\alpha \mu(\underline{x})}{\mu(\underline{x}) - \mu_0} \quad (42)$$

and are singular if:

$$\phi = 1 - \frac{\beta k_0}{k(\underline{x}) - k_0}, \quad \phi = 1 - \frac{\beta \mu_0}{\mu(\underline{x}) - \mu_0} \quad (43)$$

It can be easily verified that, if  $\alpha, \beta, k_0, \mu_0$  comply with:

$$0 \leq \alpha < 2, \quad -2 < \beta \leq 0, \quad -\infty < \mu_0 < 0, \quad -\infty < k_0 < 0 \quad (44)$$

the values of  $\phi$  given by (42) and (43) are comprised in the interval  $] -1, 1]$  and then  $k'(\underline{x})$  and  $\mu'(\underline{x})$  are strictly positive or negative definite within the

interval  $] -\infty, -1]$  and  $]1, +\infty[$ . The inequalities in (44) give then a sufficient condition for having the convergence of the polarization based iterative scheme. It is worth noting that the conditions of convergence of the basic schemes (see (21) and (25)) depend on the properties of the elastic moduli of the heterogeneous medium while the conditions (44) do not depend anymore on these properties. Thus, it is expected that the convergence of the polarization based iterative scheme will be reached independently of the values of the contrast. This is investigated in the next section through several numerical applications. In addition, it is also interesting to notice that the elastic properties of the reference medium are negative, a feature which is common with the "accelerated" scheme [7]

### 4.3 Numerical investigation of the rate of convergence

#### 4.3.1 Application to a two phase composite

We now investigate the rate of convergence of the polarization based iterative scheme through some numerical examples. As a first illustration of the method, we still consider the example of the section 3.3. The composite is made up of long fibers which are periodically arranged along a hexagonal array (see figure 1). The radius of the fibers is  $R = 0.4$  (where it is recalled that the area of the unit cell is  $S = 1$ ) and  $N = 64$  wave vectors are used in each direction. The matrix and the inclusions are assumed to be incompressible and we denote by  $c = \mu_I/\mu_M$  the contrast. Plane strain conditions are considered and a prescribed uniform polarization is defined by its components:  $T_{11} = -T_{22} = 1$ , other ones being null. Du to the similarity between the conditions on  $\alpha$  and  $-\beta$  for the conditions ensuring convergence of the polarization scheme, it is set  $\beta = -\alpha$ . For an incompressible composite, the conditions in (44) reduce to  $\mu_0 < 0$  and  $0 \leq \alpha < 2$ . We propose to validate that condition with numerical calculations. For this, we consider fixed values of  $\alpha$  within the interval  $]0, 2[$  and we measure the rate of convergence of the iterative scheme as a function of the choice of  $\mu_0$ . For instance, on figure 4 we represent the number of iterations at convergence of the iterative scheme as a function of the shear modulus of the reference medium,  $\mu_0$ , for a fixed  $\alpha = 3/2$  and for the two limit cases of rigid inclusions and voids. It can be observed that the convergence is attained whatever the value of  $\mu_0 < 0$  (excepted for  $\mu_0 = -\infty$ ). It is also observed that each curve has a minimum which defines the optimal reference medium. At a distance of this minimum, the logarithm of the number of iterations increases linearly with the logarithm of  $\mu_0$  and it suggests that the iterative scheme diverges for  $\mu_0 = 0$  and  $\mu_0 = -\infty$ .

The determination of the optimal reference medium is of a great importance but is a very difficult task since it depends on several parameters such as the contrast, the resolution, the geometry and the size of the inclusions. The opti-

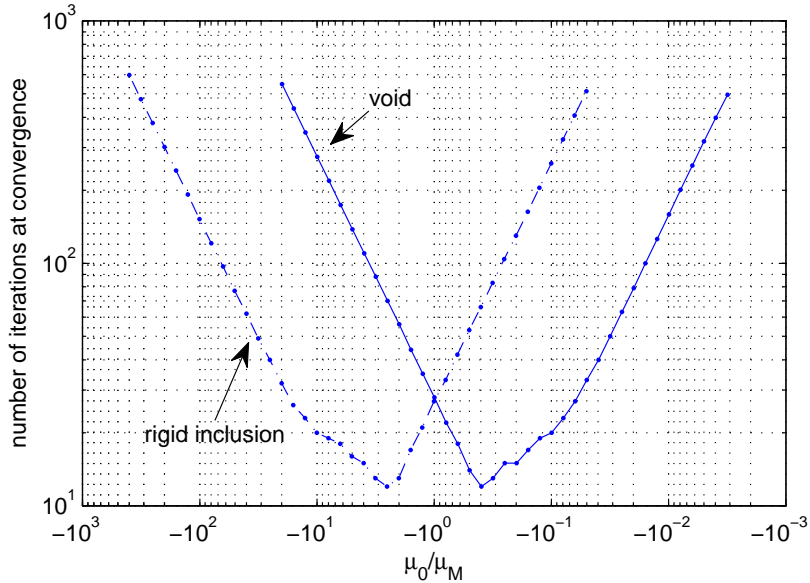


Fig. 4. Number of iterations at convergence as a function of the ratio  $\mu_0/\mu_M$  for  $\alpha = -\beta = 3/2$ .

mal reference medium is very sensitive to the contrast when the basic schemes (strain based or stress based) are considered. For example, the optimal reference medium defined for the strain based iterative scheme depends linearly on the contrast and tends to infinity in the case of rigid inclusion. In the present work, the polarization scheme uses additional parameters, namely  $\alpha$  and  $\beta$ , which have to be optimized in order to obtain the lowest number of iterations at convergence. In the absence of theoretical arguments yielding to the optimal choice of  $(\alpha, \beta, \mu_0, k_0)$ , they must be determined numerically. For example, in figure 5 are reported the interval for  $\mu_0/\mu_M$  ( $\mu_M$  being the shear modulus of the matrix) corresponding to the optimal value of  $\mu_0$  for several values of the contrast varying from  $10^{-6}$  to  $10^6$  and for  $\alpha = -\beta = 3/2$ . It can be observed that, contrarily to the basic approaches, the optimal reference medium of the polarization based method does not diverge in the limited cases of voided and rigid inclusions.

When other values of the coefficients  $\alpha$  are considered within the interval  $]0, 2[$ , the results are similar to the ones given on figures 4 and 5. However, the choice  $\alpha = 3/2$  has been found to lead to the better rate of convergence of the iterative scheme. So, in the absence of any other arguments, the choice  $\alpha = 3/2$  is kept for the other examples treated in the following.

We now compare the new iterative scheme with the basic ones. In Figure 6 we represent the number of iterations at convergence as a function of the contrast (in a log-log frame), the optimal value of  $\mu_0$  being determined numerically (see figure 5). On the same figure the results obtained with the strain and the stress based approaches were also reported. The polarization based approach clearly appears to be more efficient since the convergence is reached

after a lower number of iterations and this, whatever the value of the contrast. It has been found that the convergence is obtained after 12 iterations when  $\log(\mu_I/\mu_M) = \pm 6$ .

In figure 7, is plotted the prediction for the effective shear modulus as a function of the number of wave vectors (used for computing the Fourier transform and its inverse). The contrast has been chosen as  $\mu_I/\mu_M = 10$ . It can be seen that, as observed currently by users of basic schemes, the strain based iterative scheme leads to an upper type estimate of the homogenized elastic tensor whereas the stress based approach leads to a lower type estimate of that modulus. By comparison, the prediction obtained with the polarization based method is always comprised between the estimates of the basic methods. As a consequence, the number of wave vectors needed for ensuring the convergence is lower.

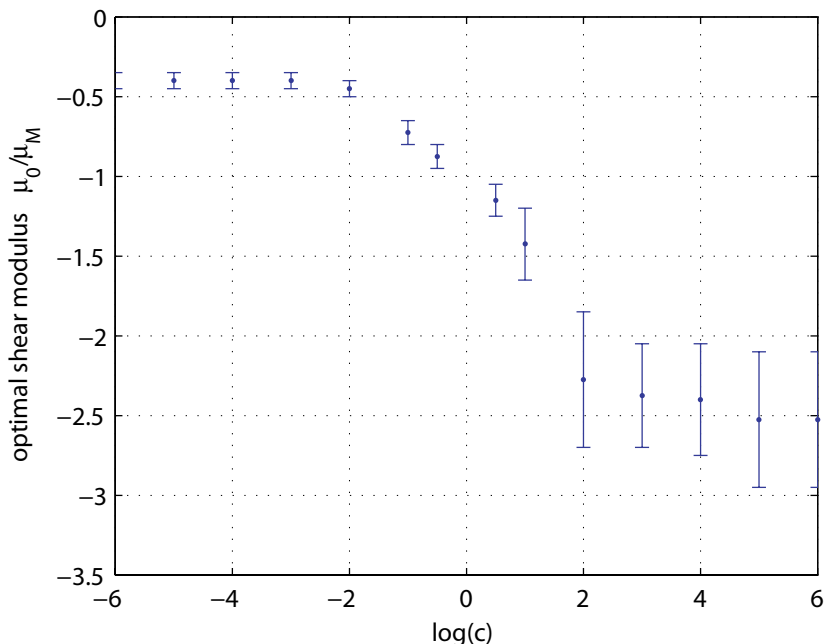


Fig. 5. Value of the optimal reference medium as a function of the logarithm of the contrast

#### 4.3.2 Application to three phases composites

To check the ability of the polarization based method to deal with highly contrasted microstructures, we investigate the rate of convergence for three-phases composites which contain both soft and stiff constituents. Two examples are considered and are represented by their unit cell on figure 8. Those microstructures are depicted below:

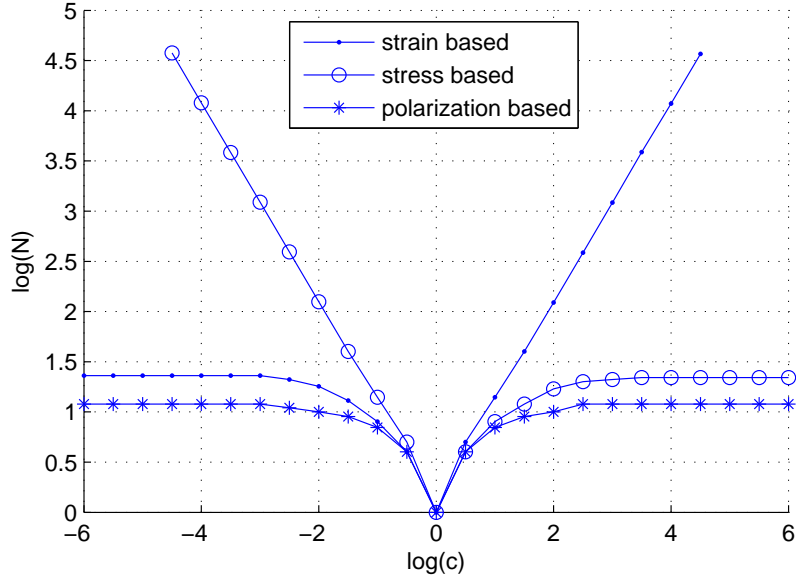


Fig. 6. Number of iterations at convergence as a function of the contrast: comparison between the strain, the stress and the polarization based approaches.

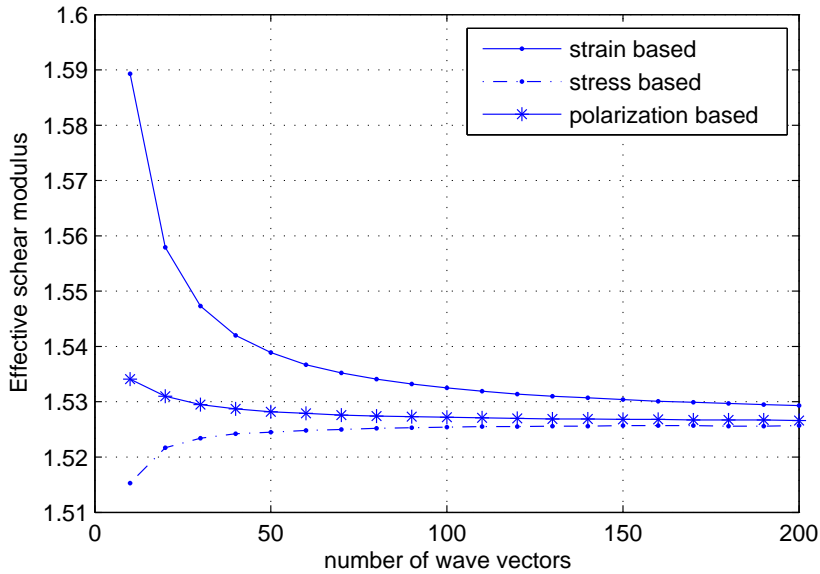


Fig. 7. The effective shear modulus for a contrast  $c = 10$ . Comparison of the estimations obtained from the strain, the stress and the polarization approaches.

- *Microstructure a*: the composite is made up of an incompressible elastic matrix whose shear modulus is  $\mu_M$  which contains circular inclusions being arbitrary distributed within the unit cell. Two kinds of inclusions, with the same proportion, are considered: (i) circular inclusions with the shear modulus  $\mu_{I1} = p\mu_M$ , (ii) circular inclusions with modulus  $\mu_{I2} = \mu_M/p$  (the inclusions are also considered incompressible). The unit cell is squared

(with the area  $S = 1$ ) and the inclusions have the same radius  $R = 0.05$ . The volume fraction of stiff and soft inclusions is  $f_{I1} = f_{I2} = 0.0785$ . The contrast between the phases is controlled by the parameter  $p$  which varies from 1 to  $10^6$  in our applications. Note that the particular case  $p = 1$  corresponds to a homogeneous material whereas the limited case  $p = +\infty$  corresponds to a composite which contains both cavities and rigid inclusions.

- *Microstructure b*: the composite is made of an incompressible elastic matrix whose shear modulus is  $\mu_M$  and containing circular inclusions having a circular interphase. A squared unit cell is still considered (with the area  $S = 1$ ), the radius of the inclusions (the cores) is  $R = 0.05$  and the external radius of the interphase (the circular shells) is  $R = 0.075$ . The volume fraction of the inclusions is  $f_{I1} = 0.118$  and the volume fraction of the interphase is  $f_{I2} = 0.147$ . The inclusions and the interphase are both chosen incompressible. The shear modulus of the inclusions is  $\mu_{I1} = p\mu_M$  whereas the shear modulus of the interphase is  $\mu_{I2} = \mu_M/p$ . The contrast is again controlled by the parameter  $p$  whose value is taken from  $10^{-6}$  to  $10^6$ .

In our calculations a grid  $256 \times 256$  is considered, the macroscopic loading is the same as in the last example. The number of iterations at convergence is plotted in figure 9 as a function of the parameter  $p$ , in the case of the microstructure "a", constituted of soft and stiff inclusions. The logarithm of the number of iterations increases linearly with  $\log(p)$  for the two basic schemes. As expected, the case of a composite made up of both voids and rigid inclusion (corresponding to  $p = +\infty$ ) cannot be handled by these methods. When the polarization based iterative scheme is used, the number of iteration increases with  $p$  but reaches moderate values. Indeed, for higher values of  $p$ , the number of iterations converges at  $N = 19$  iterations.

In figure 10 is plotted the number of iterations at convergence as a function of  $p$  for the second microstructure involving interphases surrounding circular inclusions (microstructure "b" on figure 8). When the basic schemes are used, it is observed again that the computation times become very long when  $p$  is large (corresponding to a very soft interphase surrounding a stiff inclusion) and when  $p$  is low (the case of a soft inclusion with a very stiff interphase). Again, it is observed that the convergence is attained with the polarization based method and this for any value of the parameter  $p$ . It can be also noticed that the number of iterations for having the convergence, for this kind of microstructure, is higher than for the first microstructure (microstructure *a* on figure 8). When  $\log(p) = -6$  the number of iterations at convergence is  $N = 52$  whereas  $N = 57$  iterations are needed when  $\log(p) = 6$ . This diminution of the rate of convergence can be attributed to the fact that the soft and the stiff phases are connected for the microstructure "b", leading to high local fluctuations of the mechanical fields near the interface between core and shell. Some indications on the numerical parameters which were used in the iterative schemes are of interest. When the strain based iterative scheme is used, the reference modulus given in [17] has been considered:  $\mu_0 = (\mu_{min} + \mu_{max})/2 =$

$\mu_M(p + 1/p)/2$ . When the stress based iterative scheme is used, the reference modulus is chosen as  $1/\mu_0 = (1/\mu_{min} + 1/\mu_{max})/2 = (p + 1/p)/(2\mu_M)$ . When the polarization based iterative scheme is used, the optimal reference medium has been determined numerically. In the case of the composite made up of stiff and soft inclusions (microstructure "a") it has been found that the optimal shear modulus is  $\mu_0 = -\mu_m$  and then is independent of the parameter  $p$ . In the case of the composite with circular interphases (microstructure "b") it has been found that  $\mu_0 = -\mu_M$  does not correspond to the optimal reference medium (squares on figure (10)). In this case, the use of an optimized reference medium (stars on figure (10)) leads to a gain on the rate of convergence. It suggests that the optimal reference not only depends on the elastic properties of constituents but also on their spatial distribution within the unit cell. The question relative to the determination of the optimal reference medium needs to be further investigated in order to be able to predict the relation between the microstructure and this optimum.

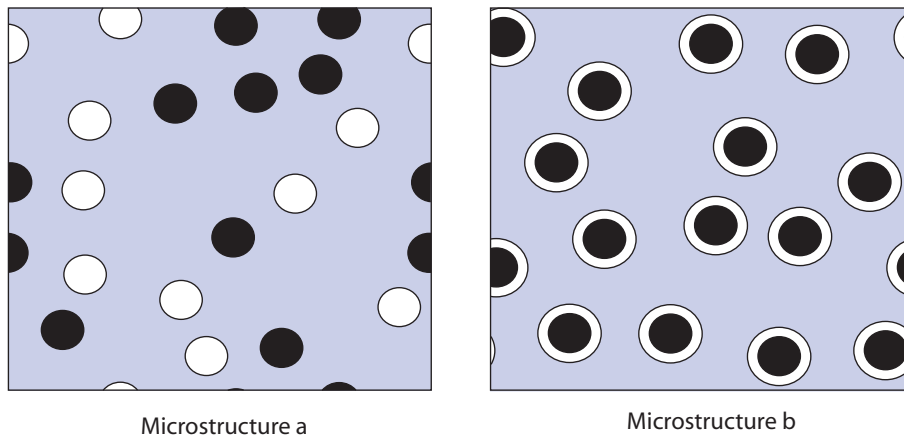


Fig. 8. The unit cell of the three phase composite. Case a: composite with soft and stiff circular inclusions. Case b: composite reinforced with circular inclusions surrounded by circular interphases.

## 5 Conclusion

A new iterative scheme has been proposed for the computation of the macroscopic properties of elastic composites. The main features and advantages of the present method can be summarized as follows:

- The method uses the same ingredients as the basic schemes: the periodic Green tensors for the strain and the stress, the FFT algorithm for computing the Fourier Transform and its inverse... No additional treatment or numerical tools (Lagrangian, conjugate gradient,...) are required for its implementation.



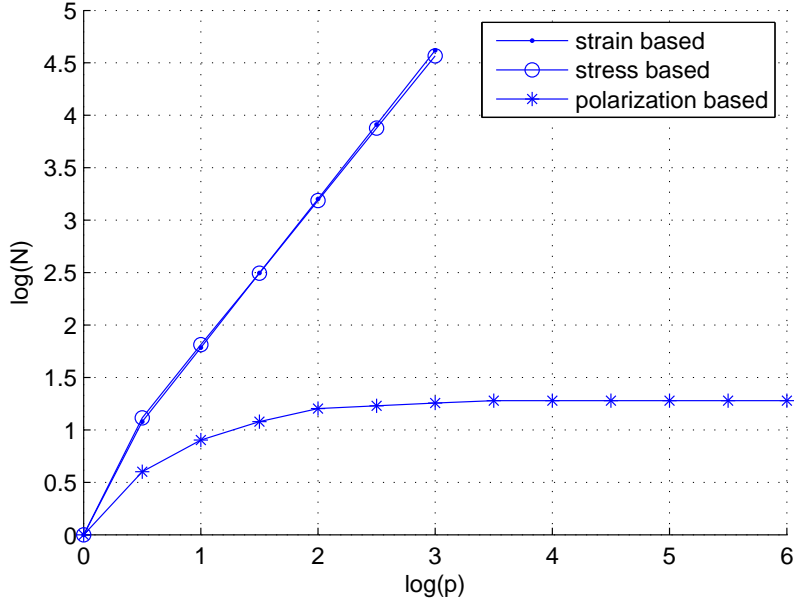


Fig. 9. Number of iterations as a function of the ratio  $p = \mu_{I1}/\mu_M = \mu_M/\mu_{I2}$  in the case of three phases composite constituted of both stiff and soft circular inclusions.

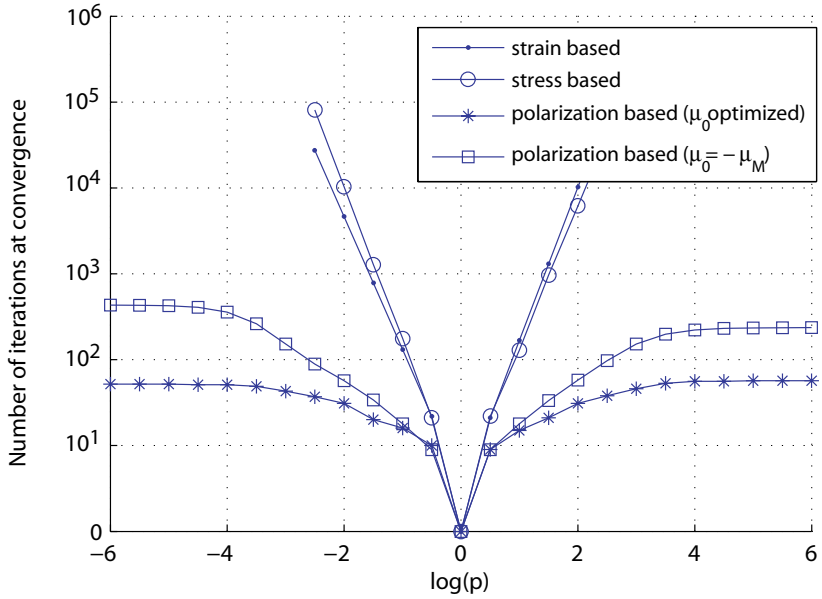


Fig. 10. Number of iterations as a function of the ratio  $p = \mu_{I1}/\mu_M = \mu_M/\mu_{I2}$  in the case of coated circular inclusions.

- The approach uses an iterative scheme for solving an elasticity problem expressed in terms of the polarization. In that problem a uniform polarization is prescribed over the unit cell instead of a uniform macroscopic strain or stress in the classical approaches.
- It has been shown that the condition ensuring the convergence of this new

iterative scheme is independent of the elastic moduli of the heterogeneous material. This result has been proven theoretically and tested numerically through several examples. More specifically, it has been shown that the problem of composites containing both voids and rigid inclusions can be solved by the method with a very good rate of convergence.

The application of the method for determining the overall properties of composites with soft or stiff interphases has been addressed in the next part of the paper. The method can be extended to the context of non linear composites; this point will be the subject of a forthcoming work.

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## A Condition of convergence of a recurrence relation

Let us consider a recurrence relation on the form:

$$\mathbf{a}^{i+1} = \mathbb{L} : \mathbf{a}^i \quad (\text{A.1})$$

and starting from  $\mathbf{a}^1 = \mathbf{A}$ . denoting by  $\phi_k$  and  $\mathbf{e}_{\phi_k}$  for  $k = 1..K$  the eigenvalues and the associated eigenvectors of the linear operator  $\mathbb{L}$ . It follows that at the iterate  $i + 1$ , one has:

$$\mathbf{a}^{i+1} = \sum_{k=1}^{k=K} (\phi_k)^i \mathbf{A}_k \mathbf{e}_{\phi_k} \quad (\text{A.2})$$

where the  $\mathbf{A}_k$  are such that:

$$\mathbf{A} = \sum_{k=1}^{k=K} \mathbf{A}_k \mathbf{e}_{\phi_k} \quad (\text{A.3})$$

Three case are distinguished:

- if  $\phi_k \leq -1$  or  $\phi_k > 1$ , the factor  $(\phi_k)^i$  increases at each iteration and the iterative scheme diverges if  $\mathbf{A}_k \neq 0$ .
- if  $\phi_k = 1$ , then  $(\phi_k)^i = 1$  and the component of  $\mathbf{a}^i$  along  $\mathbf{e}_{\phi_k}$  remains unchanged and equal to  $\mathbf{A}_k$ .
- if  $-1 < \phi_k < 1$ , the factor  $(\phi_k)^i$  decreases at each iteration and tends to zero when  $i \rightarrow \infty$ .

Consequently, the convergence is ensured if  $-1 < \phi_k \leq 1$ . Moreover, assuming that the  $K'$  first eigenvalues are equal to 1 while  $-1 < \phi_k < 1$  for  $k = K' + 1..K$ , when the limit  $i \rightarrow +\infty$  is taken, one has:

$$\mathbf{a}^\infty = \sum_{k=1}^{k=K'} \mathbf{A}_k \mathbf{e}_{\phi_k} \quad (\text{A.4})$$

Which shows that  $\mathbf{a}^\infty = 0$  if all the eigenvalues are strictly comprised between 1 and  $-1$ . There must exist some eigenvalues equal to 1 if one hopes that the iterative scheme does not converge to  $\mathbf{a}^\infty = 0$ .

## B Connection with the accelerated scheme

The recurrence relation of the accelerated scheme is[17]:

$$\begin{aligned} \boldsymbol{\varepsilon}^{i+1}(\underline{x}) = \boldsymbol{\varepsilon}^i(\underline{x}) - 2(\mathbb{C}(\underline{x}) - \mathbb{C}^0)^{-1} : \mathbb{C}^0 : \\ \left[ \boldsymbol{\Gamma}^0(\underline{x}) * (\mathbb{C}^0 : \boldsymbol{\varepsilon}^i(\underline{x})) - \boldsymbol{\varepsilon}^i(\underline{x}) + \mathbf{E} + \boldsymbol{\Gamma}^0(\underline{x}) * (\mathbb{C}(\underline{x}) : \boldsymbol{\varepsilon}^i(\underline{x})) \right] \end{aligned} \quad (\text{B.1})$$

which is initialized by  $\boldsymbol{\varepsilon}^1(\underline{x}) = \mathbf{E}$ .

We multiply the terms at the right and at the left of the equality by  $(\mathbb{C}(\underline{x}) - \mathbb{C}^0)$ . It leads to:

$$\begin{aligned} \boldsymbol{\tau}^{i+1}(\underline{x}) = \boldsymbol{\tau}^i(\underline{x}) - 2\mathbb{C}^0 : \left[ \boldsymbol{\Gamma}^0(\underline{x}) * (\mathbb{C}^0 : \boldsymbol{\varepsilon}^i(\underline{x})) - \boldsymbol{\varepsilon}^i(\underline{x}) + \mathbf{E} \right. \\ \left. + \boldsymbol{\Gamma}^0(\underline{x}) * (\mathbb{C}(\underline{x}) : \boldsymbol{\varepsilon}^i(\underline{x})) \right] \end{aligned} \quad (\text{B.2})$$

Using now the following equality:

$$\mathbb{C}^0 : \left[ \boldsymbol{\Gamma}^0(\underline{x}) * (\mathbb{C}^0 : \boldsymbol{\varepsilon}^i(\underline{x})) - \boldsymbol{\varepsilon}^i(\underline{x}) + \mathbf{E} \right] = -\boldsymbol{\Delta}^0(\underline{x}) * \boldsymbol{\varepsilon}^i(\underline{x}) \quad (\text{B.3})$$

and introducing  $\boldsymbol{\sigma}^i(\underline{x}) = \mathbb{C}(\underline{x}) : \boldsymbol{\varepsilon}^i(\underline{x})$ , it gives:

$$\boldsymbol{\tau}^{i+1}(\underline{x}) = \boldsymbol{\tau}^i(\underline{x}) - 2\mathbb{C}^0 : \boldsymbol{\Gamma}^0(\underline{x}) * \boldsymbol{\sigma}^i(\underline{x}) + 2\boldsymbol{\Delta}^0(\underline{x}) * \boldsymbol{\varepsilon}^i(\underline{x}) \quad (\text{B.4})$$

Which reads, in the Fourier space:

$$\begin{cases} \boldsymbol{\tau}^{i+1}(\underline{\xi}) = \boldsymbol{\tau}^i(\underline{\xi}) - 2\mathbb{C}^0 : \boldsymbol{\Gamma}^0(\underline{x}) : \boldsymbol{\sigma}^i(\underline{\xi}) + 2\boldsymbol{\Delta}^0(\underline{\xi}) : \boldsymbol{\varepsilon}^i(\underline{\xi}) \\ \boldsymbol{\tau}^{i+1}(\underline{\xi}) = \mathbf{T} \end{cases} \quad (\text{B.5})$$

In the recurrence relation (B.1), the macroscopic strain is prescribed over the unit cell. It follows that  $\mathbf{T} = \langle \boldsymbol{\tau}(\underline{x}) \rangle_V = (\langle \mathbb{C}(\underline{x}) \rangle_V - \mathbb{C}_0) : \mathbf{E}$ .