

A POLARIZATION AND FFT BASED NUMERICAL METHOD FOR COMPUTING THE EFFECTIVE PROPERTIES OF ELASTIC COMPOSITES WITH ARBITRARY CONTRAST

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Abstract

In this paper, we present a new Fast Fourier Transform (FFT) based iterative scheme for computing the effective properties of elastic composites materials. The macroscopic properties are computed by solving the standard cell problem with periodic boundary conditions and subjected to a uniform polarization. The solution of this problem is computed by means of an iterative scheme which uses exact expression of the Green operators in the Fourier space. The convergence of the approach is assessed and compared to existing FFT based iterative schemes provided in the literature. Interestingly, it is shown that the polarization based algorithm has the remarkable property to converge independently of the contrast.

1 Introduction

A key problem, of considerable technological importance, is to determine effective properties of composites that are governing the behavior at the macroscopic scale. To reach this objective, standard numerical tools has been used in the literature for solving the problem posed over the unit cell of periodicity, as for example: the finite elements methods [8, 17], the Boundary Element Methods [5], combined integral equations and multipole methods [7, 9, 11].

An alternative method has been proposed in the middle of the nineties by Moulinec et al. [16] for the computation of effective properties of linear elastic periodic composite. The resolution of the local cell problem is effected by an iterative scheme which uses the periodic Green's tensor for the strain and exact images of the microstructures. This method has several advantages over other existing ones. First, it does not require the meshing of the phases but uses a regular grid. The approach is particularly adapted for computing digital images obtained from modern devices that characterizing the microstructure such as tomography. The discrete Fourier transform and its inverse are computed with the Fast Fourier Transform (FFT) which significantly increases the performance of the method. Moreover, the memory needed for solving the problem is significantly reduced compared to other methods.

However, the convergence of the FFT based algorithm introduced in [16] (called strain based iterative scheme) is known to be very sensitive with the contrast between the phases. More precisely, the rate of convergence decreases for stiff inclusions. Moreover the case of perfectly rigid inclusions cannot be handled by the method since the algorithm diverges. A dual (or stress based) formulation [1, 2] is better suited in the domain of contrast corresponding to stiff inclusions. However, it is computationally costly in the domain of soft inclusions. To circumvent

the incapacity of these basic strain or stress based iterative schemes, other methods have been developed during the ten past years (see for instance [6, 12, 13, 3]).

In this paper we present a simple iterative scheme, based on the polarization, which uses the same ingredients as the basic schemes and does not need sophisticated numerical tools. The rate of convergence and the capacity of the method to handle the problem with extreme values of the contrast is highlighted through several examples.

2 The unit cell problem

The composite is defined by a representative volume element (the unit cell) and its local properties, defined by the elastic tensor $\mathbb{C}(\underline{x})$ (and the compliance $\mathbb{S}(\underline{x}) = (\mathbb{C}(\underline{x}))^{-1}$) which depends on the vector position \underline{x} . Classically, the local problem involves compatibility equations, linear elastic constitutive equations, equilibrium and periodic conditions at the boundary of the considered unit cell:

$$\begin{cases} \boldsymbol{\varepsilon}(\underline{x}) = \text{sym}(\nabla \underline{u}(\underline{x})), & \forall \underline{x} \in V \\ \boldsymbol{\sigma}(\underline{x}) = \mathbb{C}(\underline{x}) : \boldsymbol{\varepsilon}(\underline{x}), & \forall \underline{x} \in V \\ \text{div}(\boldsymbol{\sigma}(\underline{x})) = 0, & \forall \underline{x} \in V \\ \underline{u}(\underline{x}) - \mathbf{E} \cdot \underline{x} \text{ periodic} \\ \boldsymbol{\sigma}(\underline{x}) \cdot \underline{n} \text{ antiperiodic} \end{cases} \quad (1)$$

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

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

$I_{\alpha}(\underline{x})$ for $\alpha = 1..M$ are the characteristic functions describing volumes V_{α} which comply with $\sum_{\alpha} I_{\alpha}(\underline{x}) = 1$. Prescribed macroscopic strain $\mathbf{E} = \langle \boldsymbol{\varepsilon} \rangle_V$ or macroscopic stress $\boldsymbol{\Sigma} = \langle \boldsymbol{\sigma} \rangle_V$ are classically considered (the brackets denote the volume average over V). The effective or homogenized elastic properties are denoted \mathbb{C}^{hom} and \mathbb{S}^{hom} and are defined such that $\boldsymbol{\Sigma} = \mathbb{C}^{hom} : \mathbf{E}$, $\mathbf{E} = \mathbb{S}^{hom} : \boldsymbol{\Sigma}$ and $\mathbb{S}^{hom} = (\mathbb{C}^{hom})^{-1}$

3 Resolution with the strain or stress based iterative scheme

On the basis of the earlier works of [4, 10], Moulinec and Suquet [16] have proposed an original method for computing the solution of the linear elastic problem (1). This approach uses an iterative scheme for computing the solution of the Lippmann- Schwinger equation associated to the elasticity problem (1). Indeed, by introducing a reference medium of rigidity \mathbb{C}^0 , the system of equations (1) can be rewritten into the form:

$$\boldsymbol{\varepsilon}(\underline{x}) = \mathbf{E} - \Gamma^0(\underline{x}) * [(\mathbb{C}(\underline{x}) - \mathbb{C}^0) : \boldsymbol{\varepsilon}(\underline{x})] \quad (3)$$

in which the symbol "*" denotes the convolution product and $\Gamma^0(\underline{x})$ is the periodic Green function for the strain. Its, expression, in the Fourier space and for an isotropic elastic reference material, is:

$$\Gamma_{ijkl}^0(\underline{\xi}) = \frac{1}{4\mu_0|\underline{\xi}|^2} [\delta_{ik}\xi_j\xi_l + \delta_{jk}\xi_i\xi_l + \delta_{il}\xi_j\xi_k + \delta_{jl}\xi_i\xi_k] - \frac{\lambda_0 + \mu_0}{\mu_0(\lambda_0 + 2\mu_0)} \frac{\xi_i\xi_k\xi_j\xi_l}{|\underline{\xi}|^4} \quad (4)$$

where λ_0 and μ_0 are Lamé coefficients of the reference medium. The solution of that integral equation is expanded along Neumann series, each term being computed by means of the

following recurrence relations:

$$\left\{ \begin{array}{l} \underline{\varepsilon}^i(\underline{x}) = \mathcal{F}^{-1}(\underline{\varepsilon}^i(\underline{\xi})) \\ \underline{\sigma}^i(\underline{x}) = \mathbb{C}(\underline{x}) : \underline{\varepsilon}^i(\underline{x}) \\ \underline{\sigma}^i(\underline{\xi}) = \mathcal{F}(\underline{\sigma}^i(\underline{x})) \\ \text{convergence test} \\ \underline{\varepsilon}^{i+1}(\underline{\xi}) = \underline{\varepsilon}^i(\underline{\xi}) - \Gamma^0(\underline{\xi}) : \underline{\sigma}^i(\underline{\xi}) \end{array} \right. \quad (5)$$

which start from the first term given by: $\underline{\varepsilon}^1(\underline{\xi}) = \underline{E}$. In (5), \mathcal{F} and \mathcal{F}^{-1} denote the Fourier Transform and its inverse. The macroscopic strain, \underline{E} , is prescribed whereas the macroscopic stress, $\underline{\Sigma}$, is obtained at convergence of the iterative scheme (5). The algorithm is stopped when:

$$\frac{|\underline{\varepsilon}^{i+1}(\underline{x}) - \underline{\varepsilon}^i(\underline{x})|}{|\underline{\varepsilon}^{i+1}(\underline{x})|} < e \quad \text{and} \quad \frac{|\underline{\sigma}^{i+1}(\underline{x}) - \underline{\sigma}^i(\underline{x})|}{|\underline{\sigma}^{i+1}(\underline{x})|} < e \quad (6)$$

in which the value $e = 10^{-3}$ has been used in our calculations.

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

$$\left\{ \begin{array}{l} \underline{\sigma}^i(\underline{x}) = \mathcal{F}^{-1}(\underline{\sigma}^i(\underline{\xi})) \\ \underline{\varepsilon}^i(\underline{x}) = \mathbb{S}(\underline{x}) : \underline{\sigma}^i(\underline{x}) \\ \underline{\varepsilon}^i(\underline{\xi}) = \mathcal{F}(\underline{\varepsilon}^i(\underline{x})) \\ \text{convergence test} \\ \underline{\sigma}^{i+1}(\underline{\xi}) = \underline{\sigma}^i(\underline{\xi}) - \Delta^0(\underline{\xi}) : \underline{\varepsilon}^i(\underline{\xi}) \end{array} \right. \quad (7)$$

which starts from the first term given by: $\underline{\sigma}^1(\underline{x}) = \underline{\Sigma}$. The macroscopic stress $\underline{\Sigma}$ is prescribed to the unit cell, the macroscopic strain \underline{E} is now considered as an unknown and is obtained at convergence of the iterative scheme. In (7), $\Delta^0(\underline{\xi})$ is the "stress Green's tensor", given by $\Delta^0(\underline{\xi}) = \mathbb{C}^0 - \mathbb{C}^0 : \Gamma^0(\underline{\xi}) : \mathbb{C}^0$. The convergence test (6) is used for evaluating the accuracy of the local solution.

Remarks:

1. The exact Fourier transform is thereafter replaced by the discrete Fourier transform. The discrete wave vectors, denoted $\underline{\xi}_n$, are taken from $n = -N$ to $n = N - 1$. The discrete Fourier transform and its inverse are computed by means of the Fast Fourier Transform (FFT) algorithm which makes the algorithm faster.
2. In the real space, the unit cell is discretized along a regular grid. Each node of that grid are denoted \underline{x}_n for $n = -N..N - 1$. The resolution of the image is $2N \times 2N$ for 2D-problems.
3. The elasticity tensors $\mathbb{C}(\underline{x})$ and $\mathbb{S}(\underline{x})$ are computed at each nodes of a regular grid and from the exact images of the microstructures. Note that, for simple geometry of inclusions, elasticity tensors are obtained from characteristic functions of the phase $I_\alpha(\underline{x})$ for which the use of level-set functions makes their computation easier.
4. The elastic coefficients, λ_0 and μ_0 , of the reference medium must be chosen adequately in order to obtain the convergence of the iterative schemes. It has been proved (see [13] and later in [14]) that the convergence of the basic iterative schemes is ensured if:

$$\begin{array}{ll} +\infty > 2k_0 > k(\underline{x}), \quad +\infty > 2\mu_0 > \mu(\underline{x}) & \text{strain based scheme} \\ 0 < k_0 < 2k(\underline{x}), \quad 0 < \mu_0 < 2\mu(\underline{x}) & \text{stress based scheme} \end{array} \quad (8)$$

with $k_0 = \lambda_0 + 2\mu_0/3$ and $k(\underline{x}) = \lambda(\underline{x}) + 2\mu(\underline{x})/3$.

5. For the numerical implementation of the strain and stress based iterative schemes, the optimal values (giving the better rate of convergence) for λ_0 and μ_0 are:

$$\begin{aligned} k_0 &= \frac{1}{2}(k_{max} + k_{min}), \quad \mu_0 = \frac{1}{2}(\mu_{max} + \mu_{min}) && \text{strain based scheme} \\ k_0 &= \frac{2}{k_{max}^{-1} + k_{min}^{-1}}, \quad \mu_0 = \frac{2}{\mu_{max}^{-1} + \mu_{min}^{-1}} && \text{stress based scheme} \end{aligned} \quad (9)$$

4 An iterative scheme based on the polarization

To circumvent some incapacities of the basic iterative schemes for high values of the contrast (this will be shown in the next section), a new approach, formulated with the polarization, has been proposed in [14] for elasticity problems and in [15] for the problem of thermal conduction. In this section we propose to recall this new algorithm.

In the elasticity problem (1), we propose to replace the classic conditions $\mathbf{E} = \langle \boldsymbol{\varepsilon}(\underline{x}) \rangle_V$ or $\boldsymbol{\Sigma} = \langle \boldsymbol{\sigma}(\underline{x}) \rangle_V$ by the following new condition $\mathbf{T} = \langle \boldsymbol{\tau}(\underline{x}) \rangle_V = \langle (\mathbb{C}(\underline{x}) - \mathbb{C}^0) : \boldsymbol{\varepsilon}(\underline{x}) \rangle_V$ for the local polarization $\boldsymbol{\tau}(\underline{x})$. In that last condition, \mathbf{T} represents a uniform polarization prescribed to the unit cell. The solution of (1) with that new, non conventional, loading condition for the unit cell, can be computed by using the following iterative scheme:

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

where the coefficient α is chosen in order to obtain the better rate of convergence. At convergence, $\boldsymbol{\varepsilon}^i(\underline{\xi})$ and $\boldsymbol{\sigma}^i(\underline{\xi})$ are the local strain and stress field generated by the application of the uniform polarization \mathbf{T} . It is then possible to compute the associated macroscopic strain and stress: $\mathbf{E} = \langle \boldsymbol{\varepsilon}^i(\underline{x}) \rangle_V$ or $\boldsymbol{\Sigma} = \langle \boldsymbol{\sigma}^i(\underline{x}) \rangle_V$. Subsequently, due to the linearity of the equations, the relations giving the macroscopic strain and stress as functions of the uniform polarization \mathbf{T} can be read: $\mathbf{E} = \mathbb{A} : \mathbf{T}$ and $\boldsymbol{\Sigma} = \mathbb{B} : \mathbf{T}$. The effective elasticity tensors are then defined by $\mathbb{C}^{hom} = \mathbb{B} : \mathbb{A}^{-1}$ and $\mathbb{S}^{hom} = \mathbb{A} : \mathbb{B}^{-1}$.

Remarks:

1. The polarization based iterative scheme uses the same ingredients that the basic (strain or stress based) iterative schemes: the Green operators, the FFT algorithm, a representation of the elasticity tensor $\mathbb{C}(\underline{x})$ with a regular grid in the real space... The implementation of this new iterative scheme is then nearly as simple as the strain or stress based algorithms.
2. It has been demonstrated in [14] that the convergence of the polarization based iterative scheme is ensured if:

$$0 \leq \alpha < 2, \quad -\infty < \mu_0 < 0, \quad -\infty < k_0 < 0 \quad (11)$$

The above conditions have the remarkable property to be independent of the local elastic properties. In this way, it is expected that the convergence is reached independently of the contrast between the phases. This will be shown through numerical examples proposed in the next section.

5 Applications

We now investigate the rate of convergence of the basic schemes and the polarization based algorithm through two numerical examples. The first one corresponds to a composite reinforced by very soft or stiff long fibers. In the second example we consider two populations of very soft an very stiff fibers.

5.1 Example 1:

We consider a 2D squared unit cell, represented on figure 1 (at the left), and containing circular inclusions randomly distributed with a condition of non interpenetration. The radius of the inclusions is $R = 0.05$ (the width of the cell has been normalized to 1). The cell contains 30 inclusions defining then a volume fraction of $f = 0.24$. Both phases, the matrix and the inclusions are assumed to be incompressible and we denote by μ_M and μ_I their shear modulus.

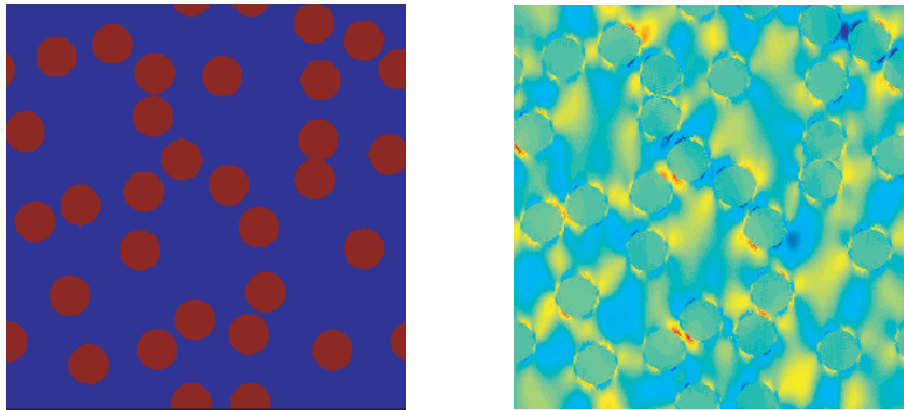


Figure 1: At the left: the unit cell of the two-phases composite. At the right: strain distribution when applying the uniform polarization $T_{12} = 1$ and other $T_{ij} = 0$.

The contrast between the phases is denoted $c = \mu_I/\mu_M$, the case $c = +\infty$ corresponds to perfectly rigid inclusions while the case $c = 0$ corresponds to voids. For the numerical implementation of the iterative schemes a grid 256×256 has been used. Plane strain conditions are considered and the unit cell is subjected to the macroscopic strain component $E_{12} = 1$ when the strain based iterative scheme is used. For the stress and polarization based approaches, the components $\Sigma_{12} = 1$ and $T_{12} = 1$ are respectively applied to the unit cell.

On figure 2, we represent the number of iterations, needed for obtaining the convergence of the strain, the stress and the polarization based iterative schemes, as function of the contrast c (in a log-log frame). The results show that the convergence of the strain based approach is obtained when $c < 1$, i.e. in the domain of soft inclusions. In the domain of stiff inclusions, one observes a linear dependence of the number of iterations with the contrast (in the log-log frame). It suggests that for large values of c , the strain based iterative scheme becomes computationally expensive and it diverges in the case of perfectly rigid inclusions ($c = +\infty$). Reversely, the stress based algorithm converges quickly in the domain of stiff inclusions but diverges in the case of the cavity. When the polarization based iterative scheme is used, the convergence is reached whatever the value of the contrast c . Note that, for the numerical implementation of the polarization iterative scheme, we have put $\alpha = 3/2$ and $\mu_0 = -\mu_M/2$ for $c < 1$ but $\mu_0 = -2\mu_M$ for $c > 1$.

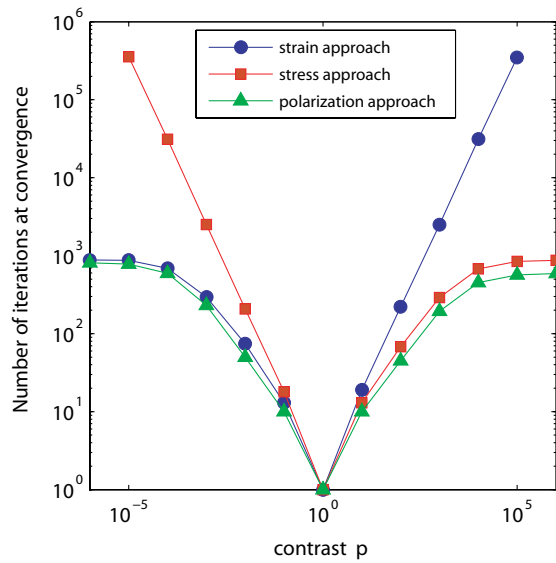


Figure 2: Number of iterations at convergence as function of the contrast $c = \mu_I/\mu_M$ in the case of the two phases composite.

5.2 Example 2

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. The unit cell considered in this second example is given on figure 3 (at the left). It is made up of an incompressible elastic matrix whose shear modulus is μ_M which contains circular inclusions being arbitrary distributed within the unit cell. Two kinds of inclusions are considered: (i) circular inclusions with the shear modulus $\mu_{I1} = p\mu_M$ and the radius $R = 0.1$, (ii) circular inclusions with modulus $\mu_{I2} = \mu_M/p$ and the radius $R = 0.03$. The inclusions are also considered incompressible. The contrast between the phases is controlled by the parameter p which varies from 1 to 10^6 in our applications. Moreover, a resolution of 512×512 has been considered for our calculations. 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 perfectly rigid inclusions.

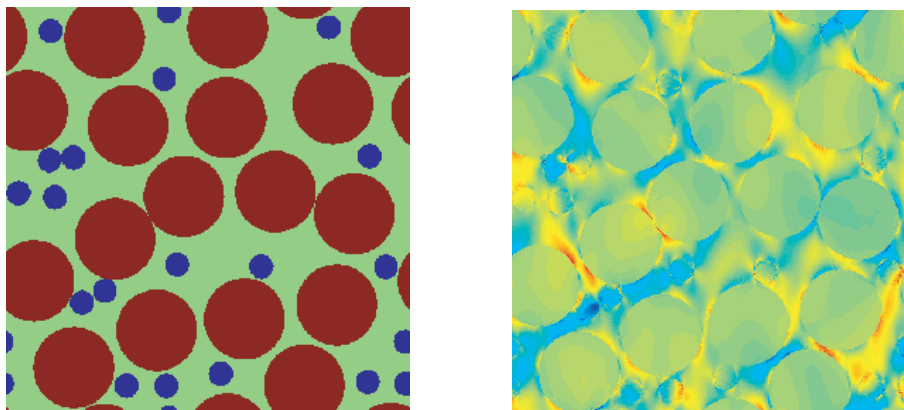


Figure 3: At the left: the unit cell of the three phases composite. At the right: strain distribution when applying the uniform polarization $T_{12} = 1$ and other $T_{ij} = 0$.

In our calculations a grid 256×256 is considered, the macroscopic loading is the same as in the last example. The number of iterations at convergence is plotted in figure 4 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. Note that, for the numerical implementation of the polarization iterative scheme, the shear modulus of the reference medium is $\mu_0 = -\mu_M$.

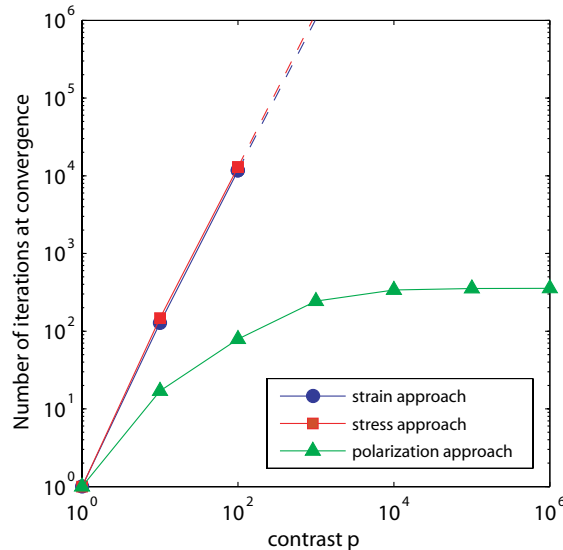


Figure 4: Number of iterations at convergence as a function of the contrast $p = \mu_{I1}/\mu_M = \mu_M/\mu_{I2}$ in the case of the three phases composite.

6 Conclusion

A new iterative scheme has been proposed for the computation of the macroscopic properties of elastic composites. 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. The approach uses an iterative scheme for solving an elasticity problem expressed in terms of the polarization. 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 good rate of convergence.

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