Numerical validation of homogenization models for the case of ellipsoidal particles reinforced composites

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1 Introduction

In the last few decades, several homogenization models have been developed. Homogenization models rely on microstructural information (e.g., constituent properties, volume fractions, shape, orientation, etc.) to predict the effective mechanical properties of heterogeneous materials. The dilute solution of Eshelby [1], the self-consistent scheme (SCS) [2, 3], the Mori-Tanaka model (MT) [4], the model of Ponte Castaneda and Willis (PCW) [5] and the Lielens model [6] are some examples.

To have confidence in these models, an exhaustive validation should be performed by using numerical methods. For a family of microstructures, it would be possible to confirm that a model is more suitable than another. To the knowledge of the authors, there is no rigorous study where the performance of analytical homogenization models are compared for a wide range of mechanical properties, for fibers of various volume fractions and aspect ratios and for particular orientation distributions. If a large validation campaign is planned, numerical methods must be fully automated, i.e., not requiring the user's inputs. The numerical validation tool must address two independent steps. First, the representative microstructures of the composite should be randomly generated. Then, the effective mechanical properties must be accurately computed.

The purpose of this communication is to validate the performance of well-known analytical homogenization models for the case of composites reinforced by ellipsoidal (i.e. 3D) particles. This article is organized as follows: the first part reviews the methods for generating random microstructures and computing the effective properties of composites. Following sections present in summary the algorithm of random generation of artificial microstructures and the necessary steps to compute the effective properties of composites. Then, the methodology adopted to achieve the validation campaign is summarized. Finally, the predictions of some analytical homogenization models are compared with the numerical solution provided by the validation tool.

2 Background

2.1 Generation of random microstructures

Most random microstructures found in the scientific community were generated by the Random Sequential Adsorption (RSA) algorithm [7]. In this algorithm, the position of the first reinforcement is randomly picked. The position of the second fiber is then drawn. If there is interference between the two reinforcements, the position of the second one is again drawn until there is no more contact with the first reinforcement. The process is repeated so on until the desired volume fraction and number of fibers are achieved. The main disadvantage of this algorithm is the difficulty to generate microstructures with high number of fibers and volume fraction in a reasonable computational time [8, 9].

Lubachevsky and Stillinger [10] proposed an algorithm based on molecular dynamics (MD) which can achieve high volume fractions in a short computation time. The authors have developed this algorithm to generate disks and spheres respectively in two and three dimensions. Initially, all spheres are created and have a null volume. A random position and velocity is assigned to each particle. The particles are put in motion and their volumes increase gradually. At each iteration, two types of events have to be checked : binary collisions and collisions between particles and unit cell faces. If two spheres collide, their velocity vector is updated according to the principle of conservation of kinetic energy. On the other side, if a sphere leaves the cell through a face, it must enter through the opposite face to meet the conditions of periodicity. The simulation is stopped when the desired volume fraction is reached.

Donev et al. [11] have used the principle of MD algorithms to generate random packings of elliptical (2D) and ellipsoidal (3D) particles. In addition to a linear velocity, each particle has also an angular velocity. During the simulation, the particles are put in a translational and rotational motion. Due to the complexity of the motion, there is no analytical solution for computing binary collisions. Therefore, a numerical approach should be used. The one proposed by Donev et al. is based on the overlap potentials [11] and takes the form of two optimization subproblems, which leads to a less computationally-efficient algorithm.

Ghossein and Lévesque [12] have proposed a modified version of the algorithm. In their works, the authors present an original and efficient approach to compute the binary collision time between two ellipsoids moving under translational and rotational motions. It has been proved that their algorithm is more efficient than the one developed by Donev et al. Moreover, the new algorithm can generate all types of ellipsoids (prolate, oblate, scalene) with very high aspect ratios (i.e. > 10).

2.2 Computation of composites effective properties

Effective properties of composites are generally computed using finite elements methods (FEM). After meshing the microstructure, periodic boundary conditions are imposed and properties are deduced from the relation between the volume averaged stresses and strains. However, meshing is a craft process and cannot be automated.

Moulinec and Suquet [13] have proposed an algorithm to compute the effective properties of composites based on the Fast Fourier Transform (FFT). The algorithm consists of discretizing the microstructures into voxels and solving, in each voxel, the constitutive law in Fourier space. The mechanical properties were then deduced from the volume averaged stresses and strains in the composite. The technique was accelerated by the work of Eyre and Milton [14]. The advantage of this method stems from its rate of convergence and the fact that it does not require meshing.

3 Generation of periodic ellipsoidal particles

The algorithm of Ghossein and Lévesque [12] was implemented in MATLAB. Initially, all ellipsoids are created in a cube cell but have a null volume. Each particle has a random linear and angular velocity. The ellipsoids are put in translational and rotational motion and their volumes increase gradually. Two types of event are checked at each iteration: binary collisions between ellipsoids and collision between ellipsoids and the cell faces. If the first type of event occurs, velocities of the concerned particles are updated according to the linear and angular momentum conservation principle. On the other side, if a particle collide with a cell face, it should appears on the opposite face to meet the periodicity conditions.

Random microstructures were generated in a low computation time, even those containing a large number of particles at high volume fraction and aspect ratio. Fig. 1 shows a periodic packing

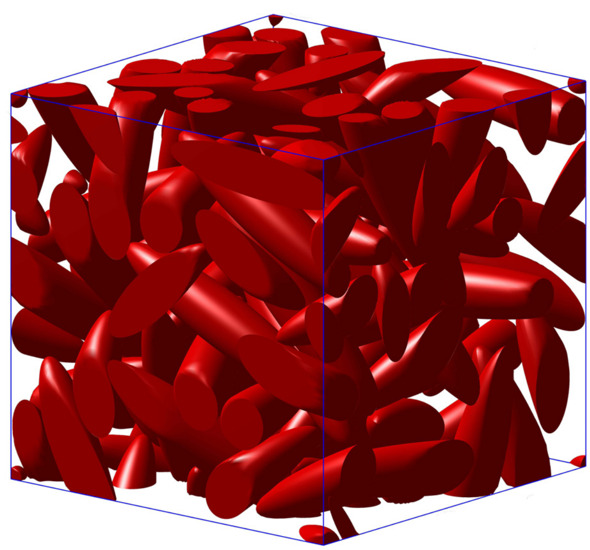

Fig. 1. Random microstructure containing 60 prolate ellipsoids. Volume fraction = 40%. Aspect ratio = 5.

generated by the numerical tool. The microstructure contains 60 prolate ellipsoids with a volume fraction of 40% and an aspect ratio of 5. This microstructure was generated in 11 seconds. Fig. 2 shows a periodic packing containing 50 oblate ellipsoids with an aspect ratio of 20 and a volume fraction of 15%. This packing was generated in less than 7 seconds.

4 Computation of composites effective properties using FFT

The technique based on FFT was chosen to compute the effective properties of the generated microstructures. The main steps required to evaluate the effective properties are presented in the following subsections.

4.1 Discretization of the microstructure

The microstructure is discretized into $N1 \times N2 \times N3$ cubic voxels. For each voxel, a material is assigned by adopting the following rules of arbitration: the position of 9 points uniformly distributed is verified. If most of the points belong to an ellipsoid, then the properties of the ellipsoidal fibers are assigned to the voxel. Otherwise, the voxel is considered to be matrix. In order to determine whether the discretization is representative of the microstructure, a discretized volume fraction is computed, defined as the ratio between the number of voxels considered as fiber and the total number of voxels. This value converges to the true volume fraction when the resolution is fine enough.

Fig. 3 show an example of discretization of a random composite containing 60 prolate ellipsoids with a volume fraction of 40% and an aspect ratio of 5 (shown in Fig. 1). 256 × 256 × 256 voxels are used to represent the microstructure.

4.2 Computation of effective properties

The outline of the algorithm is presented in (Algorithm 1). The coordinates of voxels in real space are represented by x_d, while the frequencies in the Fourier space are represented by ξ_d. It should be noted that FFT and FFT^{-1} mean respectively the Fast Fourier Transform and the inverse Fast Fourier Transform.

Convergence was checked by calculating two types of errors. The equilibrium error, calculated in Fourier space in step D.3, checks whether the stress field is in equilibrium. The compatibility error, calculated in step D.8, measures the difference between the strain field and another compatible field e_{comp} . This error is computed to check the compatibility of the strain field in the composite at

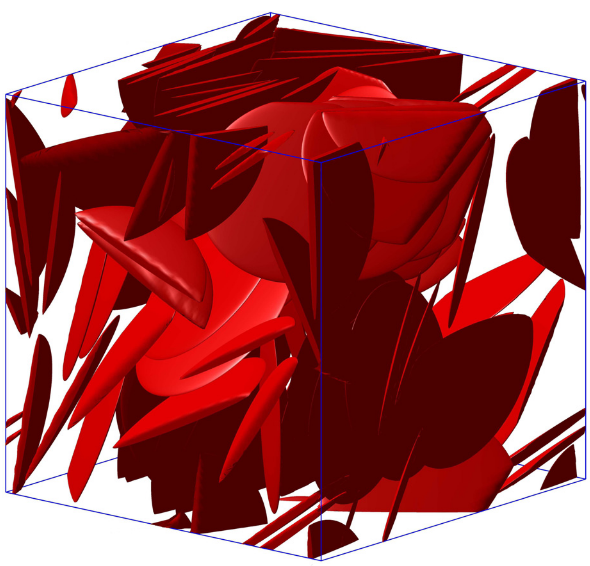

Fig. 2. Random microstructure containing 50 oblate ellipsoids. Volume fraction = 15%. Aspect ratio =20.

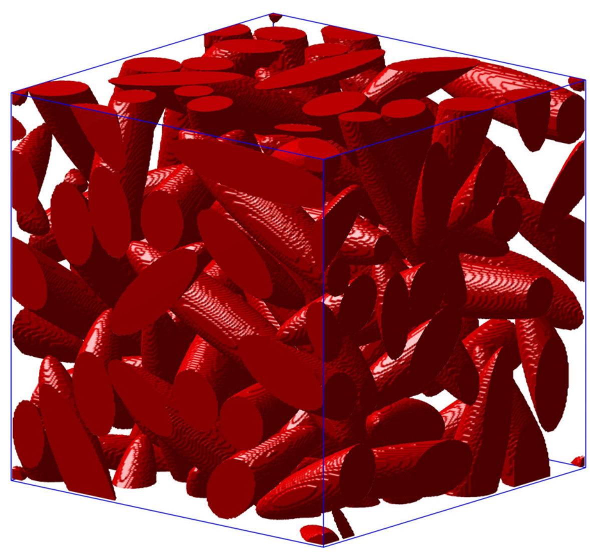

Fig. 3. Discretization of a random microstructure (Fig. 1) on a grid of 256 × 256 × 256 voxels.

each iteration.

The Green operator Γ^0 is introduced in the algorithm. Detailed expressions of this operator for different material symmetries can be found in the book of Mura [15]. When the reference material is isotropic, the expression of this operator is explicit in Fourier space and can be written as follows:

$$\Gamma^0_{ijkl}(\xi) = \frac{1}{4\mu^0|\xi|^2}\left(\delta_{ki}\xi_l\xi_j + \delta_{li}\xi_k\xi_j + \delta_{kj}\xi_l\xi_i + \delta_{lj}\xi_k\xi_i\right) - \frac{\lambda^0+\mu^0}{\mu^0(\lambda^0+2\mu^0)}\frac{\xi_i\xi_j\xi_k\xi_l}{|\xi|^4} \quad (1)$$

where λ^0 and μ^0 represents respectively the Lamé and shear modulus of the reference material. The latter, whose stiffness tensor is denoted by C^0, was chosen so as to have an optimal convergence of the algorithm [14]:

Algorithm 1: Computation of Composites Effective Properties

A. Initialize the deformation field $\varepsilon^0(x_d) = E$, $\forall x_d \in V$, where E denotes the average of the periodic deformation to be imposed.
B. The discretized stiffness tensor is denoted by $C(x_d)$
C. Initialize the equilibrium and compatibility error: $err\_eq = 1$ and $err\_comp = 1$
D. ***WHILE*** $\max(err\_eq, err\_comp) > 10^{-4}$
   1. $\sigma^i(x_d) = C(x_d) : \varepsilon^i(x_d)$
   2. $\hat{\sigma}^i = FFT(\sigma^i)$
   3. Calculate the equilibrium error on the stress field: $err\_eq = f(\hat{\sigma}^i)$
   4. $r^i(x_d) = C(x_d) : \varepsilon^i(x_d) + C^0 : \varepsilon^i(x_d)$
   5. $\hat{r}^i = FFT(r^i)$
   6. $\hat{e}^i_{comp}(\xi_d) = \Gamma^0(\xi_d) : \hat{r}^i(\xi_d) \quad \forall \xi_d \neq 0$ and $\hat{e}^i_{comp}(0) = E$
   7. $e^i_{comp} = FFT^{-1}(\hat{e}^i_{comp})$
   8. Calculate the compatibility error $err\_comp = f(\varepsilon^i, e^i_{comp})$
   9. $\varepsilon^{i+1}(x_d) = \varepsilon^i(x_d) - 2(C(x_d) - C^0)^{-1} : C^0 : (e^i_{comp} - \varepsilon^i)$
E. ***END WHILE***

$$\kappa^0 = -\sqrt{\kappa_1\kappa_2} \quad (2a)$$

$$\mu^0 = -\sqrt{\mu_1\mu_2} \quad (2b)$$

where κ and μ are respectively the bulk and shear modulus. Index 1 refers to the matrix while index 2 refers to the fibers. The number of iterations required for convergence is then proportional to $\sqrt{K}$, where K is the contrast between the properties of the constituent phases [14].

The effective properties of the composite were derived from the volume averaged stress and strain. The effective stiffness tensor $\widetilde{C}$ can be deduced from the following equation :

$$\langle\sigma(x_d)\rangle = \widetilde{C} : \langle\varepsilon(x_d)\rangle \quad (3)$$

where $\langle . \rangle$ denote an average over the volume.

4.3 Parallelization of the algorithm

The six columns of the stiffness tensor (in modified Voigt notation) are calculated independently by imposing a periodic strain field in a particular direction. For example, to calculate the first column, a periodic deformation was imposed in the first principal direction (ε_{11}). The five other columns were determined similarly. Since (Algorithm 1) should be called six times independently, the calculations have been parallelized. In each processor, a column of the effective stiffness tensor was determined. The results were recovered from each processor and the effective tensor was assembled. Using a computer with six processors, the computation time was reduced by almost six.

5 Validation campaign

The numerical tool was used to validate the predictions of some homogenization models. In this paper, the case of composites with isotropic elastic ellipsoidal fibers is considered. The matrix is also isotropic elastic. A wide range of mechanical and geometrical properties has been swept. Two types of ellipsoidal fibers with different aspect ratios have been considered: prolate and oblate. For each case, three types of contrasts were identified, involving the bulk and shear modulus: μ_2 / μ_1, κ_1 /μ_1 and κ_2 / μ_1. For each combination of aspect ratios and contrasts, various volume fractions up to 50% were studied, depending on the maximum volume fraction that has been reached for a given aspect ratio.

The mechanical properties were evaluated using the methodology of Kanit et al. [16] and is summarized as follows. For each combination of contrasts, volume fractions and aspect ratios, the size of the representative volume element (RVE) was determined. Thus, for each number of ellipsoids, several random simulations were launched and mechanical properties were computed. The number of simulations is considered sufficient when the half-length of a confidence interval of 95% is less than 1% of the average. The procedure was repeated for an increasing number of ellipsoids until the mean of the effective properties converge. The representative volume element is then achieved and the resulting mechanical properties are considered to be the exact properties of the composite. In addition, for each simulation, a convergence analysis in number of voxels was performed.

In total, about 1500 different ellipsoidal fibers reinforced composites were studied and approximately 66000 simulations were performed. Thus, a large database was established for this family of microstructure and the data generated were used to validate the performance of analytical homogenization models present in literature.

6 Results and discussion

Five analytical homogenization models were studied: dilute solution of Eshelby (Eshelby), Mori-Tanaka (MT), self-consistent scheme (SCS), Lielens and the model of Ponte Canastada and Willis (PCW). The predictions of these models were compared to the exact solution given by the numerical tool (NT). Only the case of prolate ellipsoids are presented in this section.

Two ellipsoids aspect ratios (2 and 10) and two volume fractions (20% and 50%) were considered. For each, several values of contrasts were swept. For the matrix, the bulk and shear modulus were set at 1. For ellipsoidal fibers, these moduli were varied simultaneously from 1 to 100. Furthermore, the numerical results were interpolated using a MATLAB built-in cubic spline interpolation.

Fig. 4 shows the results for a composite containing 20% of fibers with an aspect ratio of 2. For low contrasts (i.e. < 10), all analytical models provide accurate predictions. When the contrasts are high, SCS overestimates the accurate solution while the dilute model underestimates it. In addition, Lielens model seems to be the most accurate model for predicting $\tilde{\kappa}$ and $\tilde{\mu}$ while MT and PCW give accurate results only for the effective bulk modulus.

The same behavior is observed for an aspect ratio of 2 and a volume fraction of 50% (Fig. 5). However, Lielens model is accurate only for contrasts lower than 50. For higher contrasts, Lielens deviate from the interpolation curve when predicting both moduli. Moreover, all analytical models predict a plateau for contrasts higher than 50. This is not the case for the accurate solution.

Fig 6. shows that for a high aspect ratio (i.e. 10) and a volume fraction of 20%, predictions are satisfactory for all models when the contrasts between fibers and matrix are low (i.e. < 10). For higher contrasts, predictions of MT and Lielens are the closest to the accurate effective bulk and shear moduli. However, among these two models, Lielens is still the most accurate.

Finally, Fig. 4, 5 and 6 shows that the contrasts between phases mechanical properties have the greatest impact on the analytical models accuracy Indeed, whatever the fibers volume fraction and aspect ratio, all models predict accurately the effective properties when the contrasts are low (i.e. < 10).

7 Conclusion

In this paper, the performance of analytical homogenization models was numerically validated for the case of composites consisting of an isotropic matrix reinforced with randomly distributed ellipsoidal particles. For the investigated range of aspect ratios, volume fractions and mechanical properties contrasts, it seems that Lielens is the most efficient analytical model to predict the effective bulk and shear moduli for this type of microstructures.

This study will set a range of validity for the analytical homogenization models with a confidence interval. Thus, for a certain family of microstructures, with such contrasts between the mechanical properties and such fibers aspect ratio and volume fraction, it will be possible to identify the most suitable model to predict the properties of composites. A rigorous comparison between different models in the literature can then be made. The authors will also make this tool available to the scientific community. Therefore, other researchers can use it to validate their homogenization models or to obtain the effective properties of some composites.

Future work will aim to validate analytical homogenization models for spherical and ellipsoidal particles reinforced composites with viscoelastic phases.

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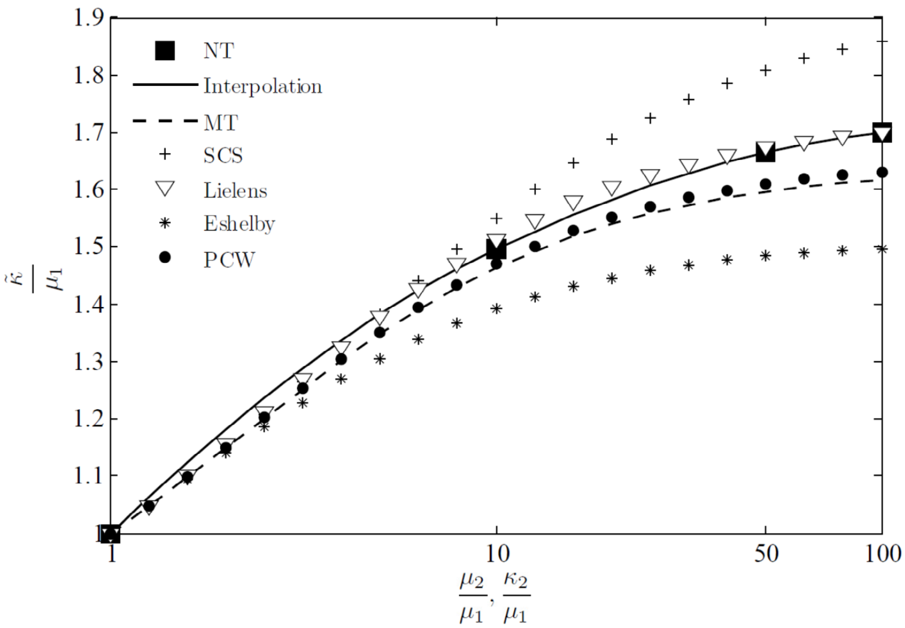
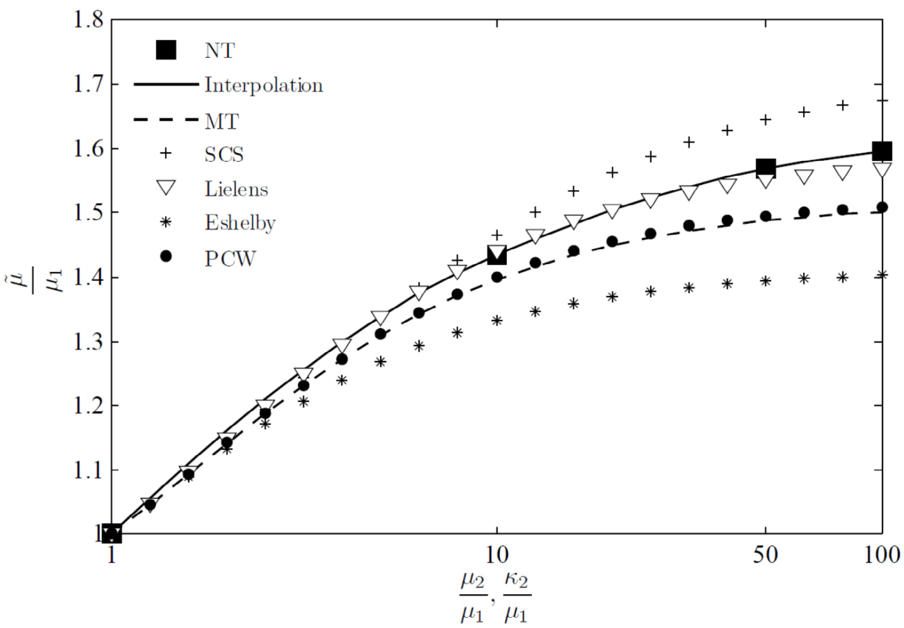
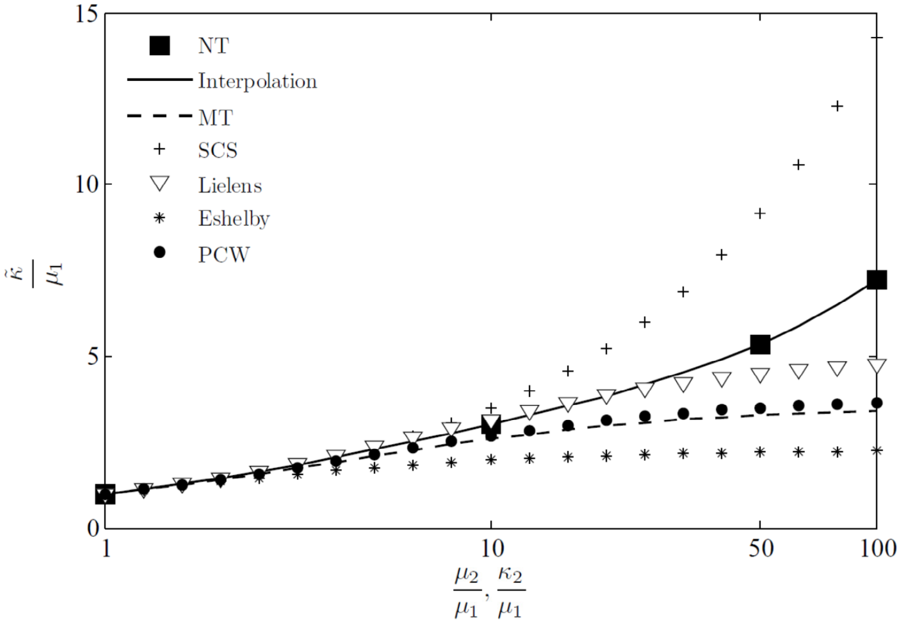


(a)



(b)

Fig. 4. Comparison between the mechanical properties obtained with the numerical tool (NT) and those predicted by analytical models: Mori-Tanaka (MT), self-consistent scheme (SCS), Lielens, dilute solution of Eshelby (Eshelby) and Ponte Castaneda and Willis model (PCW). Volume fraction = 20%. Aspect ratio = 2. $\kappa_1 = \mu_1 = 1$. (a) Normalized effective bulk modulus. (b) Normalized effective shear modulus.



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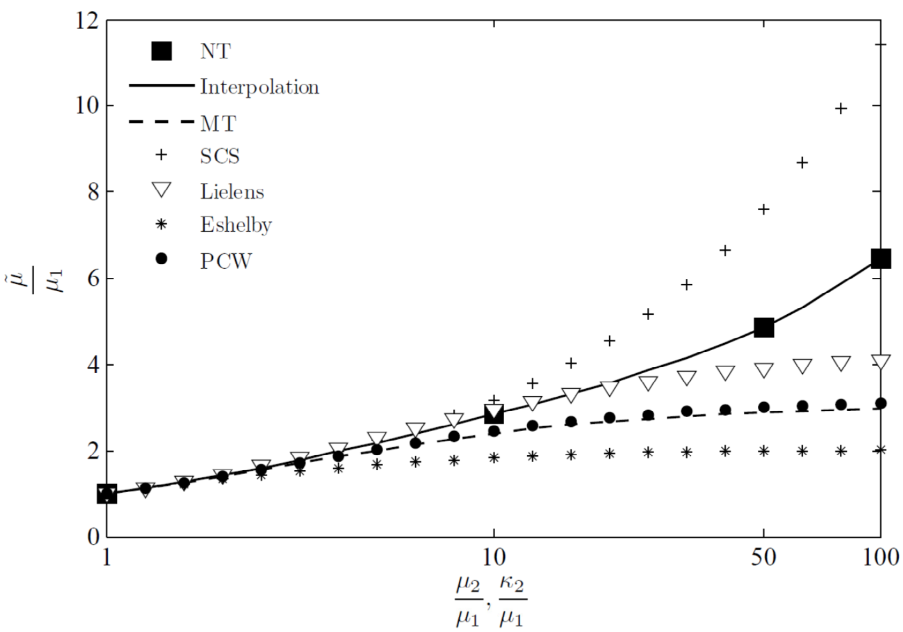
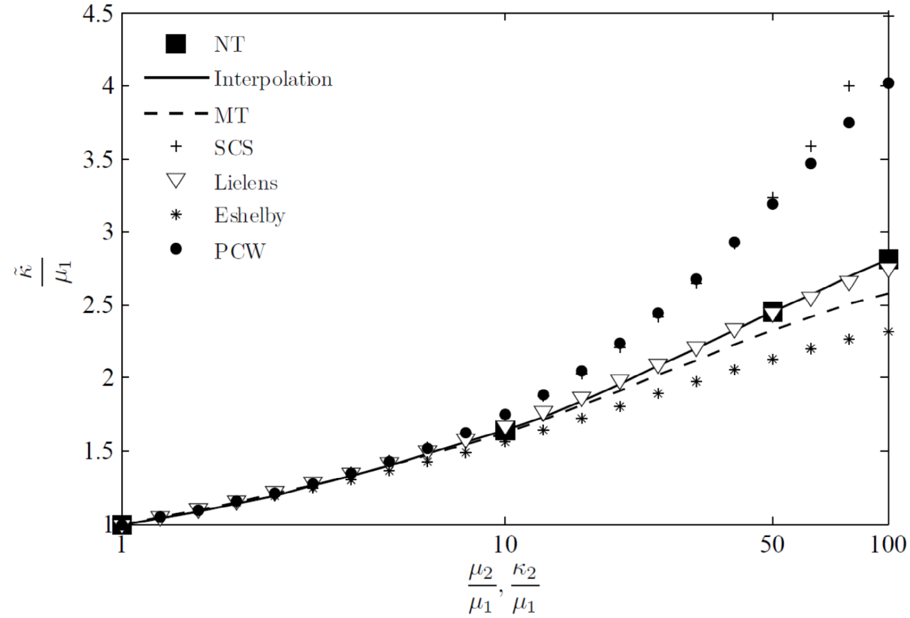


(b)

Fig. 5. Comparison between the mechanical properties obtained with the numerical tool (NT) and those predicted by analytical models: Mori-Tanaka (MT), self-consistent scheme (SCS), Lielens, dilute solution of Eshelby (Eshelby) and Ponte Castaneda and Willis model (PCW). Volume fraction = 50%. Aspect ratio = 2. $\kappa_1 = \mu_1 = 1$. (a) Normalized effective bulk modulus. (b) Normalized effective shear modulus.



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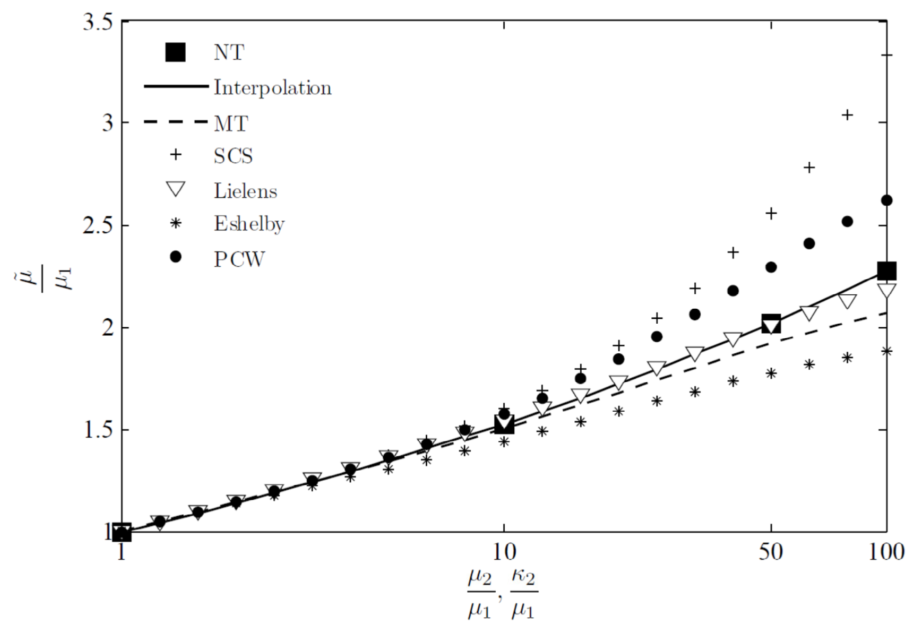

(b)

Fig. 6. Comparison between the mechanical properties obtained with the numerical tool (NT) and those predicted by analytical models: Mori-Tanaka (MT), self-consistent scheme (SCS), Lielens, dilute solution of Eshelby (Eshelby) and Ponte Castaneda and Willis model (PCW). Volume fraction = 20%. Aspect ratio = 10. $\kappa_1 = \mu_1 = 1$. (a) Normalized effective bulk modulus. (b) Normalized effective shear modulus.