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Vorwort

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Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.



Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

FAST NUMERICAL COMPUTATION OF PRECISE BOUNDS OF EFFECTIVE ELASTIC MODULI

M. KABEL AND H. ANDRÄ

ABSTRACT. A fast numerical solver to compute precise bounds of effective properties of multi-phase elastic composites is presented in contrast to analytical estimates like Hashin-Shtrikman bounds. Integral equations of Lippmann-Schwinger type are solved by using FFT. This approach is particularly suited for digital images (CT images) of complex microstructures and needs much less computational effort than finite element schemes to predict the effective properties. The different variants of this method are first reviewed and combined. Secondly, they are extended to the computation of lower and upper bounds. A numerical test for a simple microstructure demonstrates the convergence of the bounds with respect to the resolution of the microstructure. The number of iterations necessary for convergence are compared for the different variants. Finally, the quality of the new bounds is compared with analytical bounds.

1. INTRODUCTION

Analytical homogenization methods fulfil the requirements (with respect to accuracy, computational effort and generality of the microstructures) for predicting effective properties of multi-phase elastic composites only for simple shaped inclusions. Curved fibers and even more complex non-convex inclusions cannot be considered or lead to bad approximations at least for higher stiffness ratios, as shown by Klusemann and Böhm and Svendsen [1] for a realistic microstructure. Furthermore, the usage of analytical homogenization on base of micro-tomographies often requires additional image processing and image analysis steps. Since micro-tomographies become more and more mainstream in material science, numerical homogenization as additional tool for image processing software is qualified for highly precise predictions directly from three-dimensional segmented images.

For numerical homogenization we use a method originally introduced by Moulinec and Suquet [2] that allows the computation of local and overall response of (non-) linear composites. This method applies the Fast Fourier Transformation (FFT) to efficiently solve the integral equation of Lippmann-Schwinger type [3, 4] which is equivalent to the periodic boundary value problem in elasticity. The standard iterative numerical solution, which is based on the Neumann series expansion (basic scheme) [2], can be accelerated by Krylov subspace methods [5].

The main disadvantage of this method is the fact, that the number of iterations needed for convergence grows linearly with the phase contrast ρ for the Neumann series approximation resp. $\sqrt{\rho}$ for the Krylov subspace methods. This problem was overcome by Monchiet and Bonnet [6], who derived a generalization of the

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accelerated scheme of Michel, Moulinec and Suquet [7] for composites with high contrast. This numerical scheme, which iterates on the polarization resp. eigen-strain, can also handle pores and rigid inclusions (even in the same microstructure). The trade-off is the dependence of the applied macroscopic load on parameters of the algorithm (the stiffness of the reference material). Therefore, this scheme is less applicative for nonlinear problems. Additionally, it needs twice as much memory as the basic scheme.

Another numerical method that also converges for arbitrary contrast of the phases and does not have the trade-offs of the scheme of Monchiet and Bonnet was derived by Brisard and Dormieux [8] from the upper Hashin-Shtrikman bound [9] for the effective stiffness. We will show that it is indeed possible to compute rigorous upper and lower bounds on the overall response by carrying over the results of Brisard and Dormieux to the Hashin-Shtrikman bound for the effective compliance. The resulting numerical method for the lower bound iterates on the local stresses instead of the local strains. Therefore the lower bound on the overall response can be also calculated for composites with rigid inclusions.

The outline of the paper is as follows: In Section 2 we introduce the periodic boundary value problem which has to be solved in the numerical homogenization procedure and the equivalent Lippmann-Schwinger type equation. Then the Hashin-Shtrikman bounds are formulated for anisotropic elastic materials. In Section 3 the new bounds of Hashin-Shtrikman type for the effective elastic coefficients are derived. In Section 4 the derived results are numerically validated for a simple fiber reinforced composite by comparing the effective elastic moduli with analytical estimations and bounds [10, 11, 12] for varying spatial resolution of the microstructure.

2. MATHEMATICAL BACKGROUND

2.1. Periodic boundary value problem for homogenization. For the homogenization of an heterogeneous, periodic medium with local stiffness $C(x)$ we have to solve periodic boundary value problems (BVP) for the displacement fluctuations u^* on a rectangular cuboid Ω which is often called unit-cell, statistic or representative volume element:

$$(1) \quad \begin{cases} \operatorname{div} \sigma(x) = 0, & x \in \Omega, \\ \sigma(x) = C(x) : \epsilon(x), & x \in \Omega, \\ 2\epsilon(x) = 2E + \operatorname{grad} u^*(x) + (\operatorname{grad} u^*(x))^T, & x \in \Omega, \\ u^*(x) \text{ periodic}, & x \in \partial\Omega, \\ \sigma \cdot n(x) \text{ anti-periodic}, & x \in \partial\Omega. \end{cases}$$

For all constant strains E the problem (1) is uniquely solvable in the space

$$\left\{ u^* \in (H^{1,\#}(\Omega))^3 : \langle u_i^* \rangle_\Omega := \int_\Omega u_i^*(x) dx = 0, \quad i = 1, 2, 3 \right\},$$

with $H^{1,\#}(\Omega)$ being the closure of $C^{\infty,\#}(\Omega) = \{v \in C^\infty(\Omega) : v \text{ periodic}\}$ in $H^1(\Omega)$ (see [13, 14]).

2.2. Equivalent strain and stress based Lippmann-Schwinger equation.

By introducing a *reference material* of homogeneous stiffness C^0 and the *polarization*

$$(2) \quad \tau(x) = (C(x) - C^0) : \epsilon(x),$$

the constitutive equation for the *stress* $\sigma(x) = C(x) : \epsilon(x)$ can be transformed as follows

$$(3) \quad \sigma(x) = C^0 : \epsilon(x) + \tau(x).$$

For known residual stresses $\tau(x)$ with support in Ω , i.e. $\text{supp}(\tau) \subseteq \Omega$, the solution of $\text{div } \sigma(x) = 0$ can be expressed by using the nonlocal elastic *Green operator* Γ^0 for strains associated with the reference Material C^0 [4], see Appendix B,

$$(4) \quad \epsilon(x) = E - (\Gamma^0 * \tau)(x),$$

where the convolution is defined by

$$(\Gamma^0 * \tau)(x) = \int_{\Omega} \Gamma^0(x-y) : \tau(y) dy.$$

Plugging (2) into (4) we arrive at the strain based formulation of the *Lippmann-Schwinger equation*:

$$(5) \quad (I + B_{\epsilon}) \epsilon := \epsilon + \Gamma^0 * ((C - C^0) : \epsilon) = E.$$

This integral equation is equivalent to an integral equation for the stress [15]

$$(6) \quad (I + B_{\sigma}) \sigma := \sigma + \Delta^0 * ((D - D^0) : \sigma) = S,$$

with $D(x) = C^{-1}(x)$ the local compliance, $D^0 = (C^0)^{-1}$ the compliance of the reference material and the *macroscopic stress* $S = \langle C(x) : \epsilon(x) \rangle_{\Omega}$. The *Green operator* Δ^0 for stresses associated with the reference Material C^0 can be determined from the Green operator Γ^0 for strains by

$$(7) \quad \Delta^0 = C^0 - C^0 : \Gamma^0 : C^0.$$

2.3. Lippmann-Schwinger equations for the Hashin-Shtrikman bounds.

The energy principle of Hashin and Shtrikman [9] states that for any choice of the polarization field $\tau(x)$ the following bounds on the elastic energy in the unit-cell hold true

$$(8) \quad \langle \epsilon : C : \epsilon \rangle \underset{(\geq)}{\leq} E : C^0 : E + 2 \langle \tau : E \rangle - \langle \tau : (C - C^0)^{-1} : \tau \rangle - \langle \tau : (\Gamma^0 * \tau) \rangle,$$

if $C \leq C^0$ ($C \geq C^0$). Equality is reached when $\tau = (C - C^0) : \epsilon$. These bounds are applied to the subspace of voxel-wise constant polarization fields [8]. It is shown that by introducing the *periodized Green operator* $\Gamma^{\#}$, the bounds (8) or to be more precise $\Gamma^0 * \tau$, can be calculated in this subspace without approximation error by a discrete Fourier transformation (DFT). Since Willis [16] has shown that the Hashin-Shtrikman bounds are quadratic positive (negative) definite forms on the space of all polarization fields, an optimal polarization field τ_{HS} in this subspace must exist.

Applying this result for the polarization fields to the associated strain field $\epsilon_{HS} := (C - C^0)^{-1} : \tau_{HS}$ leads us to the following equation

$$(9) \quad \epsilon_{HS}(x) + (\Gamma^{\#} * ((C - C^0) : \epsilon_{HS}))(x) = E,$$

which has the same form as (5). This means that the bounds of Hashin-Shtrikman can be calculated by the methods discussed for the strain based formulation of the Lippmann-Schwinger equation. The difficulties which arise in the calculation of the periodized Green operator are discussed in [8].

Now we want to carry over these results to the stress based formulation of the Lippmann-Schwinger equation, which will have the advantage, that rigid inclusions can be treated without problems. Following Hill [17] we introduce the eigenstrain η by

$$(10) \quad \eta = D^0 : \tau = (D^0 - D) : \sigma.$$

This leads us to the following formulation of the bounds of Hashin-Shtrikman [16]

$$(11) \quad \langle \sigma : D : \sigma \rangle \underset{(\geq)}{\leq} S : D^0 : S + 2 \langle \eta \rangle : S + \langle \eta : (D - D^0)^{-1} : \eta \rangle + \langle \eta : (\Delta^0 * \eta) \rangle,$$

if $C \leq C^0$ ($C \geq C^0$) or equivalently $D \geq D^0$ ($D \leq D^0$). Again, equality is reached for $\eta = (D^0 - D) : \sigma$. Applying the above arguments to the associated stress field $\sigma_{HS} := (D^0 - D)^{-1} : \eta_{HS}$ of the optimal eigenstrain field η_{HS} in the subspace of voxel-wise constant eigenstrain fields, we obtain the following equation

$$(12) \quad \sigma_{HS}(x) + (\Delta^\# * ((D - D^0) : \sigma_{HS}))(x) = S,$$

with $\Delta^\#$ being the *periodized Green operator for stresses* which is defined in the same way as the periodized Green operator for strains

3. HASHIN-SHTRIKMAN BOUNDS ON THE EFFECTIVE MODULI

Now we will show that it is possible to use the solutions of the Lippmann-Schwinger equations (9) and (12) to obtain upper and lower bounds on the effective moduli (see Appendix A). Additionally, the assumptions of the Hashin-Shtrikman bounds on C^0 will have the consequence that it is not possible to numerically calculate an upper (lower) bound of the effective stiffness, if the composite contains any rigid (porous) region. This is no real limitation because in the first case the upper Hashin-Shtrikman bound is a rigid material and in the second case the lower Hashin-Shtrikman bound is a material without any elastic stiffness. In the case of a composite having both, rigid and porous regions, the assumptions of the Hashin-Shtrikman bounds can not be fulfilled. In this case only the polarization scheme (see section 4.3) can give an estimation of the effective moduli.

Combining (19) and (21) with (8) yields

$$\begin{aligned} & E : C_{\text{eff}} : E \\ &= \langle \epsilon : C : \epsilon \rangle \\ &\underset{(\geq)}{\leq} E : C^0 : E + \langle \tau_{HS} \rangle : E - \langle \tau_{HS} : (C - C^0)^{-1} : \tau_{HS} \rangle - \langle \tau_{HS} : (\Gamma^0 * \tau_{HS}) \rangle \\ &= E : C^0 : E + \langle \tau_{HS} \rangle : E - \langle \tau_{HS} : \epsilon_{HS} \rangle - \langle \tau_{HS} : (E - \epsilon_{HS}) \rangle \\ &= E : C^0 : E + \langle \tau_{HS} \rangle : E \\ &= E : \langle C : \epsilon_{HS} \rangle \\ &= E : C_\epsilon^{HS} : E. \end{aligned}$$

Therefore

$$C \underset{(\geq)}{\leq} C^0 \Rightarrow C_{\text{eff}} \underset{(\geq)}{\leq} C_\epsilon^{HS}.$$

Combining (20) and (22) with (11) yields an analogous result for the compliance

$$\begin{aligned}
 & S : D_{eff} : S - S : D^0 : S \\
 &= \langle \sigma : D : \sigma \rangle - S : D^0 : S \\
 &\stackrel{(\leq)}{=} \langle \eta_{HS} : S \rangle + \left\langle \eta_{HS} : (D - D^0)^{-1} : \eta_{HS} \right\rangle + \langle \eta_{HS} : (\Delta^0 * \eta_{HS}) \rangle \\
 &= \langle \eta_{HS} : S \rangle - \langle \eta_{HS} : \sigma_{HS} \rangle + \langle \eta_{HS} : (C^0 - C^0 : \Gamma^0 : C^0) * (D^0 : \tau_{HS}) \rangle \\
 &= \langle \eta_{HS} : S \rangle - \langle \eta_{HS} : \sigma_{HS} \rangle + \langle \eta_{HS} : (\tau_{HS} - C^0 : \Gamma^0 * \tau_{HS}) \rangle \\
 &= \langle \eta_{HS} : S \rangle - \langle \eta_{HS} : \sigma_{HS} \rangle + \langle \eta_{HS} : (\tau_{HS} - C^0 : (E - \epsilon_{HS})) \rangle \\
 &= \langle \eta_{HS} : S \rangle - \langle \eta_{HS} : \sigma_{HS} \rangle + \langle \eta_{HS} : (C : \epsilon_{HS} - S) \rangle \\
 &= \langle \eta_{HS} : S \rangle \\
 &= S : (D^0 - D_\sigma^{HS}) : S.
 \end{aligned}$$

Therefore if $D \stackrel{(\leq)}{\geq} D^0$

$$D_{eff} \stackrel{(\leq)}{(\geq)} 2D^0 - D_\sigma^{HS} \stackrel{(\leq)}{(\geq)} 2D_{eff} - D_\sigma^{HS},$$

which means that

$$D \stackrel{(\leq)}{\geq} D^0 \Rightarrow D_\sigma^{HS} \stackrel{(\leq)}{(\geq)} D_{eff}.$$

For non-rigid materials this means

$$C \stackrel{(\leq)}{(\geq)} C^0 \Rightarrow C_{eff} \stackrel{(\leq)}{(\geq)} C_\sigma^{HS}.$$

Thanks to the convergence analysis of [7] and [18] it is clear that the convergence of the Neumann series expansion (14) for the strain based formulation of the Lippmann-Schwinger equation (9) is only guaranteed for $C \leq C^0$. The opposite is true for the stress based formulation for which only the case $D \leq D^0$ guarantees the convergence of the Neumann expansion (14). To sum up, the strain (stress) based formulation allows the determination of an upper (lower) bound of the effective stiffness if the composite does not contain any rigid inclusion (pore space)

$$(13) \quad C_\sigma^{HS} \leq C_{eff} \leq C_\epsilon^{HS}.$$

4. NUMERICAL ALGORITHMS AND RESULTS

For completeness we shortly present the different iterative schemes which are used in the numerical tests for the computation of the estimations resp. the Hashin-Shtrikman bounds of the effective stiffness [2, 8, 6]. In section 4.3 we will combine Krylov subspace methods with the polarization scheme.

4.1. Basic scheme. Both, the strain based formulation (5) as well as the stress based formulation (6) of the Lippmann-Schwinger equation, can be iteratively solved using the Neumann series expansion for inverting the operator $(I + B_\epsilon)$ resp. $(I + B_\sigma)$. To be more precise, the iterates of the local strain resp. stress read

$$(14) \quad \epsilon^n = \sum_{i=0}^n (-B_\epsilon)^i E \quad \sigma^n = \sum_{i=0}^n (-B_\sigma)^i S$$

which can be also written as

$$(15) \quad \epsilon^0 = E \quad \sigma^0 = S$$

$$(16) \quad \epsilon^{n+1} = -B_\epsilon \epsilon^n + E \quad \sigma^{n+1} = -B_\sigma \sigma^n + S$$

The iterates (16) can be efficiently calculated in four simple steps using FFT by the so called *basic scheme* for polarization and eigenstrain, resp. [7]:

$$\begin{aligned} \tau &= (C - C^0) : \epsilon^n & \eta &= (D - D^0) : \sigma^n \\ \hat{\tau} &= \text{DFT}(\tau) & \hat{\eta} &= \text{DFT}(\eta) \\ \hat{\eta} &= -\hat{\Gamma}^0 : \hat{\tau}, \quad \hat{\eta}(0) = E & \hat{\tau} &= -\hat{\Delta}^0 : \hat{\eta}, \quad \hat{\tau}(0) = S \\ \epsilon^{n+1} &= \text{DFT}^{-1}(\hat{\eta}) & \sigma^{n+1} &= \text{DFT}^{-1}(\hat{\tau}) \end{aligned}$$

In these equations we have changed the sign of the eigenstrain η , previously defined in (10), to get an identical algorithm for the strain and stress formulation. A formula for the Fourier coefficients $\hat{\Gamma}^0$ of the Green operator Γ^0 the can be found for isotropic reference materials in the Appendix B. Combining this formula with (7) results in a formula for the Fourier coefficients $\hat{\Delta}^0$ of the Green operator for stresses Δ^0 .

4.2. Accelerated basic scheme. A faster but less memory efficient method for the iterative solution of (5) and (6) has been proposed by Zeman et al [5]. Instead of using the the Neumann expansion, Krylov subspace methods are applied. In each iteration of these methods the application of the linear operator $(I + B_\epsilon)$ resp. $(I + B_\sigma)$, i.e.

$$(17) \quad (I + B_\epsilon) \epsilon^n = \epsilon^n + \Gamma^0 * ((C - C^0) : \epsilon^n)$$

$$(18) \quad (I + B_\sigma) \sigma^n = \sigma^n + \Delta^0 * ((D - D^0) : \sigma^n)$$

need to be computed. This can be done by a slight modifications of the basic scheme presented in section 4.1 which we call *accelerated basic scheme*

$$\begin{aligned} \tau &= (C - C^0) : \epsilon^n & \eta &= (D - D^0) : \sigma^n \\ \hat{\tau} &= \text{DFT}(\tau) & \hat{\eta} &= \text{DFT}(\eta) \\ \hat{\eta} &= -\hat{\Gamma}^0 : \hat{\tau}, \quad \hat{\eta}(0) = 0 & \hat{\tau} &= -\hat{\Delta}^0 : \hat{\eta}, \quad \hat{\tau}(0) = 0 \\ \eta &= \text{DFT}^{-1}(\hat{\eta}) & \tau &= \text{DFT}^{-1}(\hat{\tau}) \\ (I + B_\epsilon) \epsilon^n &= \epsilon^n - \eta & (I + B_\sigma) \sigma^n &= \sigma^n - \tau \end{aligned}$$

4.3. Polarization scheme. By prescribing a uniform polarization T instead of a constant macroscopic strain E , Monchiet and Bonnet introduce the so called *polarization scheme* [6]

$$\begin{aligned} \epsilon &= (C - C^0)^{-1} : \tau^n \\ \hat{\epsilon} &= \text{DFT}(\epsilon) \\ \hat{\tau}^{n+1} &= \hat{\tau}^n - \alpha C^0 : \hat{\Gamma}^0 : (C^0 : \hat{\epsilon} + \hat{\tau}^n) - \beta \hat{\Delta}^0 : \hat{\epsilon}, \quad \hat{\tau}^{n+1}(0) = T \\ \tau^{n+1} &= \text{DFT}^{-1}(\hat{\tau}^{n+1}) \end{aligned}$$

which converges for arbitrary contrast, as long as the elastic properties of the reference material are negative and the parameters α , β of the scheme are chosen according to

$$0 \leq \alpha < 2, \quad -2 < \beta \leq 0$$

This scheme can also be formulated for the eigenstrain $\eta = (D - D^0) : \sigma$ as follows

$$\begin{aligned} \sigma &= (D - D^0)^{-1} : \eta^n \\ \hat{\sigma} &= \text{DFT}(\sigma) \\ \hat{\eta}^{n+1} &= \hat{\eta}^n - \alpha D^0 : \hat{\Delta}^0 : (D^0 : \hat{\sigma} + \hat{\eta}^n) - \beta \hat{\Gamma}^0 : \hat{\sigma}, \quad \hat{\eta}^{n+1}(0) = H \\ \eta^{n+1} &= \text{DFT}^{-1}(\hat{\eta}^{n+1}) \end{aligned}$$

Again, the matrix vector products (17), (18) for Krylov subspace methods can be computed by a slight modification of the polarization scheme which we call *accelerated polarization scheme*

$$\begin{aligned} \epsilon &= (C - C^0)^{-1} : \tau^n \\ \hat{\epsilon} &= \text{DFT}(\epsilon) \\ \hat{\tau} &= \hat{\tau}^n - \alpha C^0 : \hat{\Gamma}^0 : (C^0 : \hat{\epsilon} + \hat{\tau}^n) - \beta \hat{\Delta}^0 : \hat{\epsilon}, \quad \hat{\tau}(0) = 0 \\ \tau &= \text{DFT}^{-1}(\hat{\tau}) \\ (I + B_\tau) \tau^n &= \tau^n - \tau \end{aligned}$$

and *accelerated eigenstrain scheme*

$$\begin{aligned} \sigma &= (D - D^0)^{-1} : \eta^n \\ \hat{\sigma} &= \text{DFT}(\sigma) \\ \hat{\eta} &= \hat{\eta}^n - \alpha D^0 : \hat{\Delta}^0 : (D^0 : \hat{\sigma} + \hat{\eta}^n) - \beta \hat{\Gamma}^0 : \hat{\sigma}, \quad \hat{\eta}(0) = 0 \\ \eta &= \text{DFT}^{-1}(\hat{\eta}) \\ (I + B_\eta) \eta^n &= \eta^n - \eta \end{aligned}$$

4.4. Variational scheme. The computation of the Hashin-Shtrikman bounds (9) and (12) can be done by replacing the Green operators Γ^0 and Δ^0 in the basic scheme and the accelerated basic scheme by their periodized counterparts $\Gamma^\#$ resp. $\Delta^\#$ [8].

We get the *variational scheme*

$$\begin{aligned} \tau &= (C - C^0) : \epsilon_{HS}^n & \eta &= (D - D^0) : \sigma_{HS}^n \\ \hat{\tau} &= \text{DFT}(\tau) & \hat{\eta} &= \text{DFT}(\eta) \\ \hat{\eta} &= -\hat{\Gamma}^\# : \hat{\tau}, \quad \hat{\eta}(0) = E & \hat{\tau} &= -\hat{\Delta}^\# : \hat{\eta}, \quad \hat{\tau}(0) = S \\ \epsilon_{HS}^{n+1} &= \text{DFT}^{-1}(\hat{\eta}) & \sigma_{HS}^{n+1} &= \text{DFT}^{-1}(\hat{\tau}) \end{aligned}$$

As *accelerated variational schema* we get

$$\begin{aligned} \tau &= (C - C^0) : \epsilon_{HS}^n & \eta &= (D - D^0) : \sigma_{HS}^n \\ \hat{\tau} &= \text{DFT}(\tau) & \hat{\eta} &= \text{DFT}(\eta) \\ \hat{\eta} &= -\hat{\Gamma}^\# : \hat{\tau}, \quad \hat{\eta}(0) = 0 & \hat{\tau} &= -\hat{\Delta}^\# : \hat{\eta}, \quad \hat{\tau}(0) = 0 \\ \eta &= \text{DFT}^{-1}(\hat{\eta}) & \tau &= \text{DFT}^{-1}(\hat{\tau}) \\ (I + B_\epsilon) \epsilon_{HS}^n &= \epsilon_{HS}^n - \eta & (I + B_\sigma) \sigma_{HS}^n &= \sigma_{HS}^n - \tau \end{aligned}$$

Material	Young's modulus [GPa]	Poisson's ratio [-]
Glas fibers	73.0	0.2
Polypropylene (PP)	1.665	0.36

TABLE 1. The material parameters for the glas fiber reenforced polypropylene (GFPP) shown in Figure 1.

Just like the polarization scheme the variational scheme converges for arbitrary contrast of the material phases.

4.5. Numerical results. Since the analytical estimations of Hashin-Shtrikman¹ can only be calculated if the Eshelby tensor of the inclusion is known, we choose a rather simple geometry for the comparison of analytical estimations with our numerically calculated bounds. Therefore we decided to analyse the effective stiffness for unidirectional fiber composites. This means that the unit-cell Ω only contains a single fiber that is aligned with one of the coordinate axes (see Figure 1).

We calculate the effective transversal isotropic material properties for varying discretization with the material parameters chosen as shown in Table 1. Since the Poisson's ratio is the same for both, the fiber and the matrix material, there are only four (instead of five) unknown material parameters of the composite.

The volumetric amount of the different discretizations is shown in Table 2 and has of course an influence on the effective macroscopic property. Depending on the parameter of interest the different upper resp. the lower Hashin-Shtrikman bound give better results for low resolution, but in all cases both bounds can be used if only the resolution is high enough.

In contrast to other authors [2, 8, 6] we use a more memory efficient and less time consuming convergence test that only needs the L^2 norm of the iterates. Depending on the numerical scheme we use one of the following four convergence tests

$$\begin{aligned} \frac{\left| \|\epsilon^{n+1}\|^2 - \|\epsilon^n\|^2 \right|}{\|E\|^2} < \varepsilon & \qquad \frac{\left| \|\sigma^{n+1}\|^2 - \|\sigma^n\|^2 \right|}{\|S\|^2} < \varepsilon \\ \frac{\left| \|\tau^{n+1}\|^2 - \|\tau^n\|^2 \right|}{\|T\|^2} < \varepsilon & \qquad \frac{\left| \|\eta^{n+1}\|^2 - \|\eta^n\|^2 \right|}{\|H\|^2} < \varepsilon \end{aligned}$$

The number of iterations necessary for convergence ($\varepsilon = 10^{-5}$) are shown in Table 3. Since the matrices B_ϵ and B_σ as well as the matrices B_τ and B_η are asymmetric, the convergence of the conjugate gradient method (CG) is not guaranteed. In contrast to Zeman et al [5] who studied the convergence behavior in the scalar case, we observe convergence problems of the CG method for the stress based basic scheme, while the BiCGStab method converges and decreases the number of iterations necessary for convergence. The same holds true for the polarization scheme. Since the BiCGStab method needs two instead of one matrix vector products for each iteration, it does not seem to be useful to combine Krylov subspace methods with the polarization scheme of Monchiet and Bonnet.

¹The lower Hashin-Shtrikman bound coincides with the Mori-Tanaka estimate for two-phase composites.

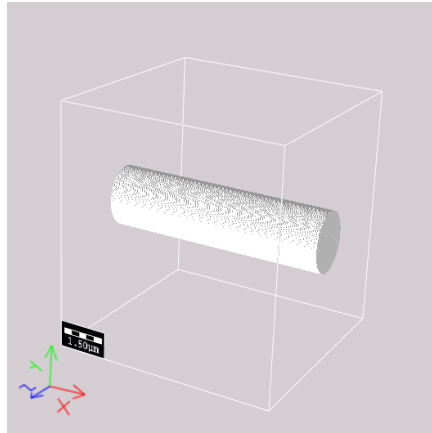


FIGURE 1. Single fiber with radius $1\mu\text{m}$.

Resolution [-]	Fiber radius/Voxel length [-]	Volumetric fiber fraction [%]
8	1	6.25
16	2	4.69
32	4	5.08
64	8	5.08
128	16	4.96
256	32	4.93
512	64	4.92
1024	128	4.91

TABLE 2. The volumetric amount of the single fiber shown in Figure 1 with increasing resolution.

Scheme	Neumann Series	CG	BiCGStab
Strain based basic	34.00	9.83	6.67
Stress based basic	79.83	-	13.17
Polarization	19.67	-	6.83
Eigenstrain	45.33	-	6.67
Strain based variational	90.00	13.67	11.50
Stress based variational	140.33	17.50	16.17

TABLE 3. Average number of iterations per loadcase for the different schemes to converge at the resolution 128.

E_1 **Young’s modulus in fiber direction:** The basic scheme, the polarization scheme, the upper bound of the variational scheme, the lower and upper Hashin-Shtrikman bounds as well as the Voigt bound almost give identical results. For a good estimation of the lower bound by the variational scheme

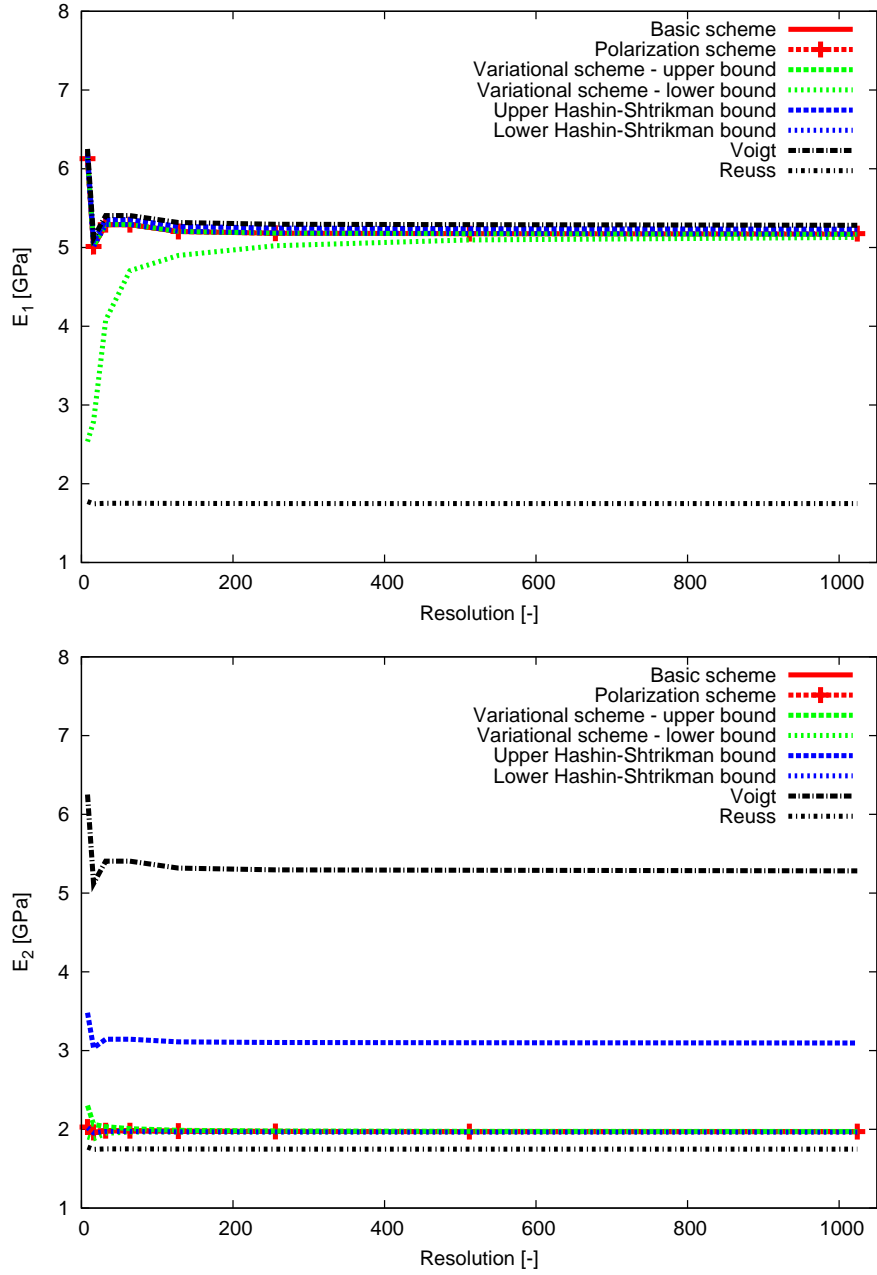


FIGURE 2. Young's moduli of the transversal isotropic microstructure.

a very high resolution of 32 voxel per fiber radius is needed. The Reuss bound does not give satisfactory results (see Figure 2).

E_2 **Young's modulus orthogonal to the fiber direction:** Both numerical bounds gives already good results for 2 voxel per fiber radius. The basic

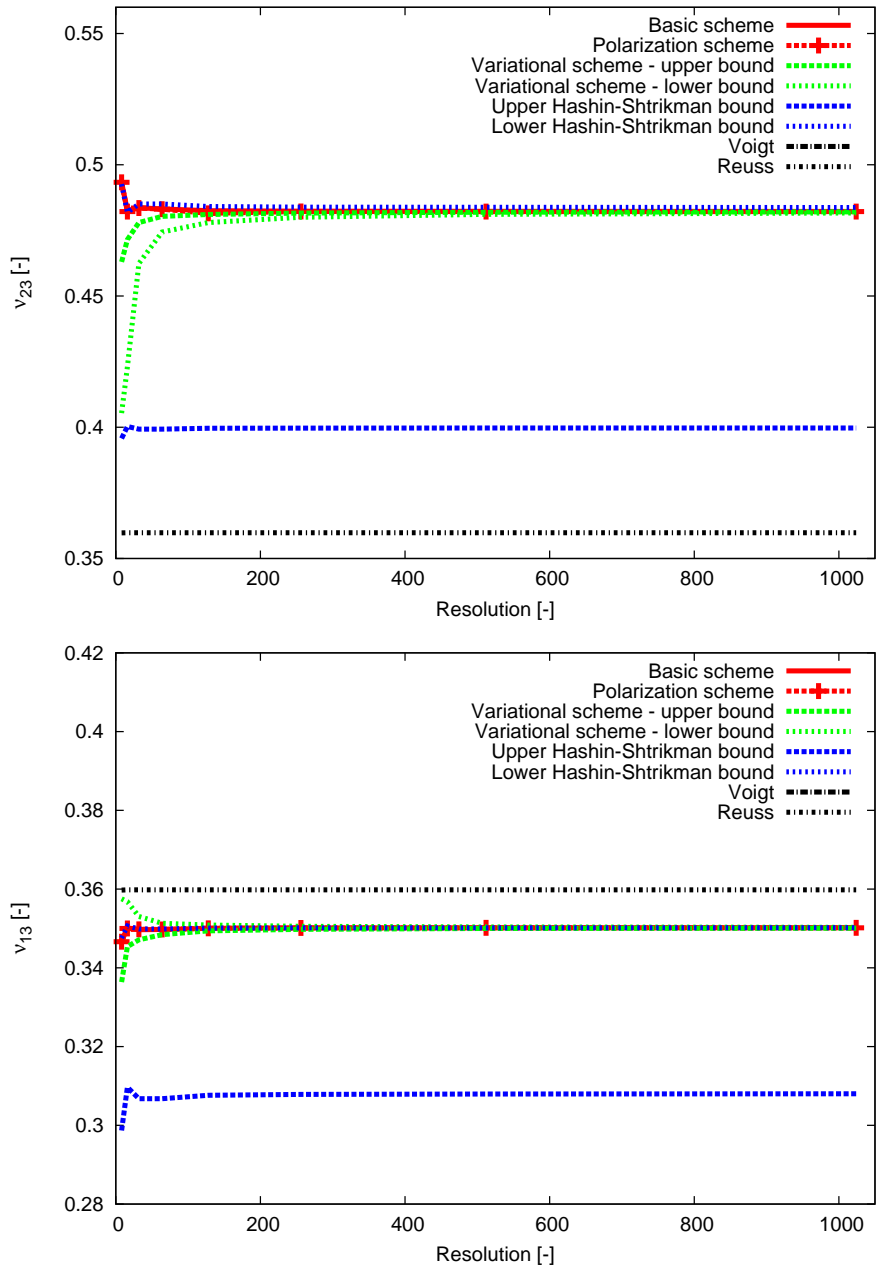


FIGURE 3. Poisson's ratios of the transversal isotropic microstructure.

scheme, the polarization scheme and the lower Hashin-Shtrikman bound coincide whereas the Reuss and upper Hashin-Shtrikman bound do not give satisfactory results (see Figure 2).

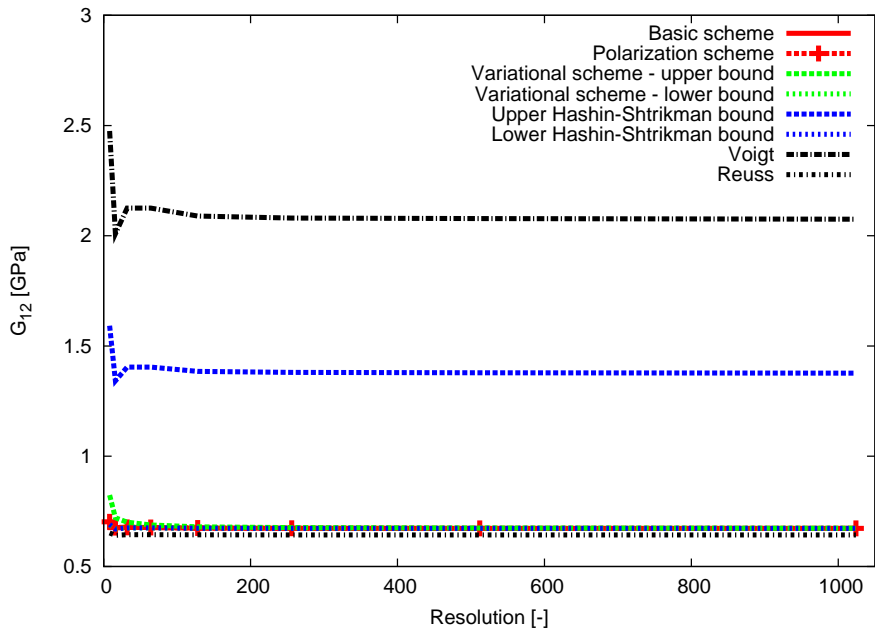


FIGURE 4. Shear modulus of the transversal isotropic microstructure.

ν_{23} **Poisson's ratio in the plane orthogonal to the fiber:** The upper and lower bound of the variational scheme give good results for 16 voxel per fiber radius. The basic scheme, the polarization scheme, the lower Hashin-Shtrikman bound as well as the Voigt bound coincide, but the Reuss and the upper Hashin-Shtrikman bound do not give satisfactory results (see Figure 3).

ν_{13} **Poisson's ratio in the plane parallel to the fiber:** The upper and lower bound of the variational scheme give good results for 4 voxel per fiber radius. The basic scheme, the polarization scheme, the lower Hashin-Shtrikman bound as well as the Voigt bound coincide, but the Reuss and the upper Hashin-Shtrikman bound do not give satisfactory results (see Figure 3).

G_{12} **Shear modulus in the the plane parallel to the fiber:** The basic scheme, the polarization scheme, the lower Hashin-Shtrikman bound as well as the lower bound of the variational scheme coincide. For the upper bound of the variational scheme to give a good approximation a resolution of 2 voxel per fiber radius is needed. The Voigt, the Reuss and the upper Hashin-Shtrikman bound do not give satisfactory results. (see Figure 4).

5. CONCLUSION

Rigorous numerical upper and lower bounds (13) on the macroscopic properties of elastic composites have been derived from the Hashin-Shtrikman bounds (8), (11).

For the calculation of the lower bound, the variational scheme of Brisard and Dormieux has been transferred to the stress formulation of the Hashin-Shtrikman bounds (11). The resulting scheme is comparable to the basic scheme for the stress formulation of the Lippmann-Schwinger equation (6). Additionally, for fast calculation of the effective properties, we have investigated the combination of the polarization schemes with Krylov subspace methods (Section 4.3).

The numerical convergence of the bounds with increasing resolution against analytical and numerical estimations of the macroscopic properties has been validated by three-dimensional simulations for a simple fiber reinforced composite (Section 4.5). Results for complicated microstructures are shown in a preceding publication [19, 20].

In contrast to most analytical estimations and bounds, the numerical bounds can be calculated for any geometry and any contrast of the material phases. By increasing the resolution (i.e. upsampling) the bounds can be improved. On the other hand, it is also possible to fastly calculate rough bounds by first downsampling the geometry.

APPENDIX A. ENERGY AND STRAIN EQUIVALENCE PRINCIPLE

With the use of the energy equivalence principle

$$(19) \quad \frac{1}{2} \langle \epsilon_i(x) : C(x) : \epsilon_j(x) \rangle_\Omega = \frac{1}{2} \langle \epsilon_i(x) \rangle_\Omega : C_{eff} : \langle \epsilon_j(x) \rangle_\Omega$$

it is possible to determine the effective (homogeneous) stiffness C_{eff} by solving (1) for a basis of the six dimensional space of macroscopic strains E . The same can be done for the effective compliance D_{eff}

$$(20) \quad \frac{1}{2} \langle \sigma_i(x) : D(x) : \sigma_j(x) \rangle_\Omega = \frac{1}{2} \langle \sigma_i(x) \rangle_\Omega : D_{eff} : \langle \sigma_j(x) \rangle_\Omega$$

By applying the results of Bishop and Hill [21, 22], the effective stiffness and compliance can be obtained by the strain equivalence principle

$$(21) \quad \langle C(x) : \epsilon_j(x) \rangle_\Omega = C_{eff} : \langle \epsilon_j(x) \rangle_\Omega,$$

$$(22) \quad \langle D(x) : \sigma_j(x) \rangle_\Omega = D_{eff} : \langle \sigma_j(x) \rangle_\Omega.$$

APPENDIX B. LIPPMANN-SCHWINGER EQUATION IN ELASTICITY

We shortly introduce the Lippmann-Schwinger equation by using the Fourier transformation and the notation similar as in [23, 2]. Alternative derivations are given in [3, 24, 25, 26]. In Fourier space the constitutive equation (3) and the equilibrium condition (first equation in (1)) have the form

$$\hat{\sigma}_{kl}(\xi) = iC_{klmn}^0 \xi_n \hat{u}_m(\xi)^* + \hat{\tau}_{kl}(\xi), \quad i\hat{\sigma}_{kl}(\xi) \xi_l = 0.$$

Eliminating $\hat{\sigma}_{kl}$ yields

$$C_{klmn}^0 \xi_l \xi_n \hat{u}_m^*(\xi) = i\hat{\tau}_{kl}(\xi) \xi_l.$$

Using the notations $K_{km}(\xi) = C_{klmn}^0 \xi_l \xi_n$ and $X_k(\xi) = i\hat{\tau}_{kl}(\xi) \xi_l$ we obtain

$$\hat{u}_m^*(\xi) = N_{mk}(\xi) X_k(\xi) / D(\xi),$$

where $N_{mk}(\xi)$ are the cofactors of the matrix $K(\xi)$ and $D(\xi)$ is the determinant of $K(\xi)$. The corresponding strains are obtained from the last equation by using $\hat{\epsilon}_{kl} = \frac{i}{2}(\xi_k \hat{u}_l^* + \xi_l \hat{u}_k^*)$ as

$$\hat{\epsilon}_{kl}(u^*) = -\frac{1}{2} \hat{\tau}_{mn}(\xi) \xi_n \{ \xi_l N_{km}(\xi) + \xi_k N_{lm}(\xi) \} D^{-1}(\xi) =: -\hat{\Gamma}_{klmn}^0(\xi) \hat{\tau}_{mn}(\xi)$$

Expressions for $\hat{\Gamma}^0$ can be found in [23] for different types of anisotropy. In the case of an isotropic material with Lamé coefficients λ_0 and μ_0 the Green operator in the Fourier space reads

$$\hat{\Gamma}_{klmn}^0(\xi) = \frac{\delta_{km} \xi_l \xi_n + \delta_{lm} \xi_k \xi_n + \delta_{kn} \xi_l \xi_m + \delta_{ln} \xi_k \xi_m}{4\mu_0 |\xi|^2} - \frac{\lambda_0 + \mu_0}{\mu_0 (\lambda_0 + 2\mu_0)} \frac{\xi_m \xi_n \xi_k \xi_l}{|\xi|^4}.$$

If τ_{mn} is given in the Fourier integral form

$$\tau_{mn}(x) = \int_{\mathbb{R}^3} \hat{\tau}_{mn}(\xi) \exp(i\xi \cdot x) d\xi,$$

where

$$\hat{\tau}_{mn}(\xi) = (2\pi)^{-3} \int_{\mathbb{R}^3} \tau_{mn}(y) \exp(-i\xi \cdot y) dy$$

then we obtain

$$\epsilon_{kl}(u^*)(x) = -(2\pi)^{-3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \hat{\Gamma}_{klmn}^0(\xi) \tau_{mn}(y) \exp\{i\xi \cdot (x - y)\} d\xi dy$$

After introducing the Green's tensor for the strains

$$\Gamma^0(x - y) := (2\pi)^{-3} \int_{\mathbb{R}^3} \hat{\Gamma}^0(\xi) \exp\{i\xi \cdot (x - y)\} d\xi,$$

the corresponding expression for the strain becomes

$$\epsilon_{kl}(u^*)(x) = - \int_{\mathbb{R}^3} \Gamma_{klmn}^0(x - y) \tau_{mn}(y) dy$$

or shortly written as convolution

$$\epsilon(u^*) = -\Gamma^0 * \tau.$$

By adding the constant strain E , the usual Lippmann-Schwinger equation in elasticity follows

$$\epsilon(u) = E - \Gamma^0 * \tau.$$

The Green's tensor Γ^0 for the strains is sometimes called fundamental solution and can be derived from the usual displacement fundamental solution U^0 by [24, 27, 28]

$$\Gamma_{klmn}^0 = -\frac{1}{2} \left(\frac{\partial}{\partial x_l} \frac{\partial}{\partial y_n} U_{km}^0 + \frac{\partial}{\partial x_k} \frac{\partial}{\partial y_n} U_{lm}^0 \right).$$

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