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A simple extension of FFT-based methods to strain gradient loadings – Application to the homogenization of beams and plates

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Abstract:

Because of their simplicity, efficiency and ability for parallelism, FFT-based methods are very attractive in the context of numerical periodic homogenization, especially when compared to standard FE codes used in the same context. They allow applying to a unit-cell a uniform average strain with a periodic strain fluctuation that is an unknown quantity. Solving the problem allows to evaluate the complete stress-strain fields.

The present work proposes to extend the use of the method from uniform loadings (i.e. uniform applied strain) to strain gradient loadings (i.e. strain fields with a uniform strain gradient) while keeping the algorithm as simple as possible. The identification of a subset of strain gradient loadings allows for a minimally invasive modification of the iterative algorithm so that the implementation is straightforward. In spite of a reduced subset of 9 independent loadings among the 18 available, the second part of the paper demonstrates that it is enough for considering the homogenization of beams and plates. A first application validates the approach and compares it to another FFT-based method dedicated to the homogenization of plates. The second application concerns the homogenization of beams, for the first time considered (to author's knowledge) with an FFT-based solver. The method applies to different beam cross-sections and the proposition of using composite voxels drastically improves the numerical solution when the beam cross-section is not conform with the spatial discretization, especially for torsion loading.

As a result, the massively parallel AMITEX_FFTP code has been slightly modified and now offers a new functionality, allowing the users to prescribe torsions and flexions to beam or plate heterogeneous unit-cells.

Keywords :

FFT; Strain gradients; Beams; Plates; Flexion; Torsion; Composite Voxels; Numerical homogenization;

1 – Introduction

The present paper lies in the overall framework of numerical homogenization of heterogeneous materials for which the mechanical behavior at the upper scale derives from spatial averages of stress-strain fields simulated on heterogeneous unit-cells. The first developments and most common applications focus on first order homogenization, the homogenized behavior relating the displacement gradient tensor to a stress tensor, or more specifically, under the small perturbations assumption, the linearized strain to the Cauchy stress. The type of boundary conditions applied to the unit-cell is quite important in that context. First, they must satisfy the Hill-Mandel condition so that the average microscopic strain energy is equal to the macroscopic one. Then, various choices satisfying this condition are available: Kinematic Uniform Boundary Conditions, Stress Uniform BC, periodic BC or even normal-mixed BC [14]. If the choice of periodic BC is obvious for periodic microstructures, it also provides the best estimate for random microstructures [22] [8] compared to KUBC or SUBC, that provide upper and lower bounds (at least for linear material) [18]. If applying PBC is not straightforward in Finite Element codes and can deteriorate the computation performance, it is natural for the FFT-based methods proposed in the 1990's [26].

These methods have been extensively used and improved during the last decade, reducing the initial drawbacks such as convergence issues for highly contrasted materials, spurious oscillations or sensitivity of the convergence to the reference material behavior (an algorithm parameter). Among significant improvements: modified discrete Green operators reducing spurious oscillations and improving the convergence ([4], [30] [28],...), algorithms replacing the initial fix-point algorithm to improve convergence ([31], [15], [19], [10] ...) or composite voxels accounting for multi-phase materials, for voxels crossed by an interface, to improve the numerical solution and reduce spurious oscillations ([4], [16], [21] ...). The list is not exhaustive and numerous theoretical works reinforce the mathematical basis of the method.

Due to their high numerical efficiency compared to finite element codes used in the same context (periodic boundary conditions), various works intend to extend the method to various applications. Among these applications, we can cite the extension to non-local behaviors such as strain gradient plasticity [25] or damage phase field [10], the coupling with metallurgical phase fields such as martensitic phase transformation [23] or other physics such as magneto-electricity [3], the coupling with DD codes [2]... Once again, this short list is far from exhaustive but gives an idea of the increasing development of the method towards new research fields.

Another kind of extension concerns higher order numerical homogenization [29][11]. In that case, the homogenized behavior is not only dependent of the first gradient of the displacement but also of higher order terms. Following this idea of going beyond the classical application of an average strain loading (i.e. first order displacement gradient) the present paper lies in the same general context. Actually, it focuses on the extension to average strain gradient loadings (i.e. second order displacement gradient), with an additional constraint of simplicity for the implementation. In other words, in the first part of the paper, the question is to propose a method to apply strain gradient loadings within classical FFT-based codes, initially designed for first gradient loadings, with a minimally invasive modification. If the set of strain gradient loadings fulfilling this constraint is

reduced, the second part of the paper demonstrates that it is still large enough to deal with the question of beams and plates numerical homogenization with FFT-based algorithms.

Actually, the questions of beams and plates homogenization can be regarded as second order term homogenizations [12] for which strain gradients are associated to flexion and torsion loadings. For plates, if the classical numerical implementation relies on the finite element method [12] [17], Nguyen also proposes an FFT-based method devoted to this application [27]. It relies on a specific algorithm combined with a dedicated Green operator to account for the traction free boundary conditions applied at the plates' free surfaces. On the contrary, if the finite element method has also been used for beams homogenization [6], to the best of author's knowledge, FFT-based methods have never been proposed in that context. One purpose of the paper is then to demonstrate that the same slightly modified FFT-based code can be used for both classical (i.e. first gradient term), as well as beams and plates, numerical periodic homogenization. This is made possible and quite efficient since recent FFT-based methods (see beginning of the introduction) allow for the simulation of unit-cells enlarged with void voxels (i.e. infinite contrast) to account for traction free boundary conditions.

To sum up, the first part of the paper (section 2) introduces the simple extension of the FFT-based method to a reduced set of strain gradient loadings and the second part (section 3) applies the method to the homogenization of beams and plates. In this part, the first sub-section presents the application to plates homogenization and focuses on the comparison with Nguyen's method using exactly the same cases [27]. Finally, the second sub-section presents the new FFT-based application to beams homogenization with an additional emphasis on the use of composite voxels when the beam cross-section is not conform with the regular grid discretization.

2 – Simple extension of the FFT-based method to strain gradient loadings

Sub-section 2.2 introduces the standard FFT-based algorithm after a small discussion on the different descriptions of the periodicity condition in sub-section 2.1, useful in sub-section 2.3 introducing the simple extension to strain gradient loadings. A final sub-section extends the idea from the small perturbation to the finite strains framework.

2.1 : Periodicity condition

The description of the periodicity condition prescribed on a unit-cell Ω can be done equivalently from two different points of view: whether the unit-cell Ω is considered alone or an infinite periodic medium Ω^{per} is considered. In the first case, fields are defined on Ω and boundary conditions have to be applied on its boundary $\partial\Omega$. In the second case, fields are defined on an infinite space and Ω –periodicities are assumed for the fields. The first description is more appropriate for Finite-Element solvers, the second is well-suited for FFT-based solvers. The two equivalent descriptions of the equilibrium condition, submitted to a periodicity condition, are given in equation (1). Below, " $\sigma \cdot \mathbf{n}$ antiperiodic on $\partial\Omega$ " means that the traction vector ($\sigma \cdot \mathbf{n}$) on opposite points of opposite faces of Ω are opposite.

$$\begin{cases} \mathbf{div}(\sigma(\mathbf{x})) = 0 \\ \sigma \cdot \mathbf{n} \text{ antiperiodic on } \partial\Omega \end{cases} \Leftrightarrow \begin{cases} \mathbf{div}(\sigma(\mathbf{x})) = 0 \\ \sigma \text{ } \Omega \text{ - periodic} \end{cases} \quad (1)$$

The periodicity condition of a displacement field $\tilde{\mathbf{u}}$ in equation (2) is also equivalently formulated on Ω^{per} in terms of strain field $\tilde{\varepsilon}$, adding a compatibility in that case. Below, “ $\tilde{\mathbf{u}}$ periodic on $\partial\Omega$ ” means that the displacement $\tilde{\mathbf{u}}$ evaluated on opposite points of opposite faces are equal.

$$\Omega \left\{ \tilde{\mathbf{u}} \text{ periodic on } \partial\Omega \right. \Leftrightarrow \Omega^{per} \left\{ \tilde{\mathbf{u}} \text{ } \Omega - \text{ periodic} \right. \Leftrightarrow \Omega^{per} \left\{ \begin{array}{l} \tilde{\varepsilon} \text{ compatible} \\ \tilde{\varepsilon} \text{ } \Omega - \text{ periodic} \end{array} \right. \quad (2)$$

2.2 : FFT-based algorithm

When considering classical (i.e. first order term) periodic homogenization under the small perturbations assumption, the problem to solve (3) consists of a heterogeneous unit cell Ω described by its stiffness tensor field c , submitted to an average displacement (first order) gradient ∇U with periodic boundary conditions. The displacement field is written as the sum of the prescribed linear term and the unknown fluctuation field $\tilde{\mathbf{u}}$.

$$\Omega \left\{ \begin{array}{l} \mathbf{div}(\sigma(\mathbf{x})) = 0 \\ \sigma(\mathbf{x}) = c(\mathbf{x}) : \varepsilon(\mathbf{x}) \\ \varepsilon(\mathbf{x}) = (\nabla \mathbf{u})^{sym}(\mathbf{x}) \\ \mathbf{u}(\mathbf{x}) = \nabla U \cdot \mathbf{x} + \tilde{\mathbf{u}}(\mathbf{x}) \\ \tilde{\mathbf{u}} \text{ periodic on } \partial\Omega \\ \sigma \cdot \mathbf{n} \text{ antiperiodic on } \partial\Omega \end{array} \right. \quad (3)$$

Using equations (1) and (2), this problem (3) written on Ω , is equivalent to problem (4) written on Ω^{per} , removing the \mathbf{x} dependence for the sake of concision, the average strain E being equal to the symmetrized average gradient ($E = (\nabla U)^{sym}$).

$$\Omega^{per} \left\{ \begin{array}{l} \mathbf{div}(\sigma) = 0 \\ \sigma = c : \varepsilon \\ \varepsilon = E + \tilde{\varepsilon} \\ \varepsilon \text{ compatible} \\ \tilde{\varepsilon} \text{ } \Omega - \text{ periodic} \\ \sigma \text{ } \Omega - \text{ periodic} \end{array} \right. \quad (4)$$

Now, introducing a homogeneous reference stiffness c_0 allows to define equivalently the problem (5).

$$\Omega^{per} \left\{ \begin{array}{l} \mathbf{div}(c_0 : \varepsilon + \tau) = 0 \\ \tau = (c - c_0) : \varepsilon \\ \varepsilon = E + \tilde{\varepsilon} \\ \tilde{\varepsilon} \text{ compatible} \\ \tilde{\varepsilon} \text{ } \Omega - \text{ periodic} \\ \sigma = c_0 : \varepsilon + \tau \text{ } \Omega - \text{ periodic} \end{array} \right. \quad (5)$$

Temporarily assuming the so-called polarization τ as a known Ω –periodic field, allows defining the auxiliary problem (6) which can be solved by the application of the Green operator Γ_0 , straightforward in Fourier space as the stiffness c_0 is homogeneous (see the annex of [26] for a detailed description).

$$\tilde{\varepsilon} = -\Gamma_0 * \tau \quad (\Leftrightarrow \text{Fourier}) \quad \Leftrightarrow \quad \begin{cases} \mathbf{div}(c_0: \tilde{\varepsilon} + \tau) = 0 \\ \tilde{\varepsilon} \quad \text{compatible} \\ \tilde{\varepsilon} \quad \Omega - \text{periodic} \\ \sigma = c_0: \tilde{\varepsilon} + \tau \quad \Omega - \text{periodic} \end{cases} \quad (6)$$

Finally, the initial problem (4), equivalent to problem (5), reduces to problems (6) and (7). Note that periodicity and compatibility conditions are gathered in problem (6) and automatically fulfilled when applying the Green operator in Fourier space, so that problem (7) gathers a set of equations, which, followed step by step, defines the simple fix-point algorithm proposed initially by Moulinec and Suquet [26]. Initializing the strain field ε (with $\varepsilon = E$) allows to evaluate the polarization field τ (7)_a. Then, the Green operator applies (in Fourier space) on the polarization to evaluate the fluctuation strain field $\tilde{\varepsilon}$ (7)_b, which, added to the average (applied) strain field provides the strain field ε (7)_c (in practice it can be done easily in Fourier space on the null frequency). This strain field allows to begin a second iterate and so on until convergence.

$$\begin{cases} \tau = (c - c_0): \varepsilon & (a) \\ \tilde{\varepsilon} = -\Gamma_0 * \tau \quad (\Leftrightarrow \text{Fourier}) & (b) \\ \varepsilon = E + \tilde{\varepsilon} & (c) \end{cases} \quad (7)$$

2.3 : Extension to strain gradient loadings with a simple implementation

The purpose of this section is to add a non-uniform applied strain ε^* to the homogeneous applied strain E , modifying the initial problem (4) in problem (8).

$$\begin{cases} \mathbf{div}(\sigma) = 0 \\ \sigma = c: \varepsilon \\ \varepsilon = E + \varepsilon^* + \tilde{\varepsilon} \\ \varepsilon \quad \text{compatible} \\ \tilde{\varepsilon} \quad \Omega - \text{periodic} \\ \sigma \quad \Omega - \text{periodic} \end{cases} \quad (8)$$

In addition, for the sake of simplicity, we would like to use exactly the same algorithm as described by problems (6) and (7) with a minor modification that consists in adding the non-uniform applied strain ε^* when evaluating the strain in equation (7)_c, replacing problem (7) by problem (9).

$$\begin{cases} \tau = (c - c_0): \varepsilon & (a) \\ \tilde{\varepsilon} = -\Gamma_0 * \tau \quad (\Leftrightarrow \text{Fourier}) & (b) \\ \varepsilon = E + \varepsilon^* + \tilde{\varepsilon} & (c) \end{cases} \quad (9)$$

The question is now to identify a set of applied strain fields ε^* for which problem (8) reduces to problems (6) and (9).

The first constraint arises from the compatibility equation (8)₄ of the strain field (8)₃ in problem (8). Hence, the applied heterogeneous strain ε^* must be compatible. Among the compatible fields, the simplest ones are linear fields. Actually, the compatibility condition, that involves double derivations of strain components, is satisfied as the double derivations automatically vanish for linear fields. In the following, the heterogeneous applied strain fields are limited to such linear fields characterized by their strain gradients G as follows, assuming ($\mathbf{x} = \mathbf{0}$) the center of the unit-cell:

$$\varepsilon^*(\mathbf{x}) = G \cdot \mathbf{x} \quad \text{or} \quad \varepsilon_{ij}^* = G_{ijk} x_k \quad (10)$$

The second constraint comes from the application of the Green operator in problem (9)_b. Actually, applying the Green operator is equivalent to solve the auxiliary problem (6), derived from problem (4). Instead, the auxiliary problem derived from problem (8) should have read:

$$\left\{ \begin{array}{ll} \mathbf{div}(c_0: \tilde{\varepsilon} + c_0: G \cdot \mathbf{x} + \tau) = 0 & \\ \tilde{\varepsilon} & \text{compatible} \\ \tilde{\varepsilon} & \Omega - \text{periodic} \\ \sigma = c_0: \tilde{\varepsilon} + c_0: G \cdot \mathbf{x} + \tau & \Omega - \text{periodic} \end{array} \right. \quad (11)$$

Hence, the only way to use the auxiliary problem (6) instead of the auxiliary problem (11) is to have the term $c_0: G \cdot \mathbf{x}$ equilibrated ($\mathbf{div}(c_0: G \cdot \mathbf{x}) = 0$) and the term $(c_0: \tilde{\varepsilon} + c_0: G \cdot \mathbf{x} + \tau)$ Ω -periodic. $\tilde{\varepsilon}$ and τ being Ω -periodic, the second condition on G corresponds to the Ω -periodicity of $c_0: G \cdot \mathbf{x}$. Following equation (1), these two conditions on Ω^{per} are now written on Ω as follows:

$$\left\{ \begin{array}{l} \mathbf{div}(c_0: G \cdot \mathbf{x}) = 0 \\ c_0: G \cdot \mathbf{x} \quad \Omega - \text{periodic} \end{array} \right. \Leftrightarrow \left\{ \begin{array}{l} \mathbf{div}(c_0: G \cdot \mathbf{x}) = 0 \\ (c_0: G \cdot \mathbf{x}) \cdot \mathbf{n} \quad \text{antiperiodic on } \partial\Omega \end{array} \right. \quad (12)$$

Assuming an isotropic behavior for c_0 , with Lamé coefficients λ_0 and μ_0 , the first condition on G ($\mathbf{div}(c_0: G \cdot \mathbf{x}) = 0$), expressed in Cartesian coordinates, reads:

$$\left\{ \begin{array}{l} \lambda_0(G_{111} + G_{221} + G_{331}) + 2\mu_0(G_{111} + G_{122} + G_{133}) = 0 \\ \lambda_0(G_{112} + G_{222} + G_{332}) + 2\mu_0(G_{211} + G_{222} + G_{233}) = 0 \\ \lambda_0(G_{113} + G_{223} + G_{333}) + 2\mu_0(G_{311} + G_{322} + G_{333}) = 0 \end{array} \right. \quad (13)$$

The second condition is the anti-periodicity of $(c_0: G \cdot \mathbf{x}) \cdot \mathbf{n}$ on opposite faces of Ω , it reads:

$$\begin{cases}
\lambda_0(G_{111} + G_{221} + G_{331}) + 2\mu_0 G_{111} = 0 \\
G_{211} = 0 \\
G_{311} = 0 \\
G_{122} = 0 \\
\lambda_0(G_{112} + G_{222} + G_{332}) + 2\mu_0 G_{222} = 0 \\
G_{322} = 0 \\
G_{133} = 0 \\
G_{233} = 0 \\
\lambda_0(G_{113} + G_{223} + G_{333}) + 2\mu_0 G_{333} = 0
\end{cases} \quad (14)$$

It is clear that the set equations (13) is automatically satisfied as soon as (14) is fulfilled. Hence, (14) gathers the 9 constraints that must be satisfied by G if we want to solve problem (8), with an applied strain gradient $\varepsilon^*(\mathbf{x}) = G \cdot \mathbf{x}$, using the very simple algorithm described by problem (9). In other words, among the 18 coefficients of G , 6 coefficients G_{ijj} (with $i \neq j$) must be set to zero, nine coefficients G_{ijj} are constrained by 3 equations and the coefficients G_{ijk} (with $i \neq j, a \neq k$ and $k \neq i$) are free. The coefficients G_{ijj} (with $i \neq j$) can be associated to bending loadings and the coefficients G_{ijk} (with $i \neq j, a \neq k$ and $k \neq i$) to torsion loadings.

2.4 : Implementation considerations

Considering an existing FFT-based code able to solve problem (7)+(6), transforming this code to solve problem (9)+(6) is obvious. It consists in adding the applied strain gradient field when adding the homogeneous applied strain field to the periodic strain fluctuation. This is done, first when initializing the strain field (with a null fluctuation) and then, at the end of each iteration. The impact on the memory footprint is null, as no additional field needs to be allocated, and the additional computational cost is low compared to the complete cost of an iteration.

2.5 : Extension to finite strain

Even if not applied in the present paper, an extension to the general framework of finite strains is proposed below.

The extension on the FFT-based method to finite strain proposed initially by Lahellec [24] is quite straightforward, replacing in problems (5) and (6), the Cauchy stress σ by the first Piola-Kirchoff stress π , and strain field ε by the displacement gradient ∇u , the divergence and gradient operators now acting on the initial configuration. The main difference is that these tensors are no more symmetric and involve nine components. Then, the reasoning proposed to account for heterogeneous loadings, under the small perturbation assumption in the previous section, is straightforwardly extendable at finite strain. For the sake of conciseness, we focus on the main ingredients but not recall the complete reasoning below.

The problem to solve at finite strain, accounting for a heterogeneous applied displacement gradient ∇u^* , reads:

$$\Omega^{per} \begin{cases} \mathbf{div}(\pi) = 0 \\ \pi = c(\nabla u) \\ \nabla u = \nabla U + \nabla u^* + \widetilde{\nabla u} \\ \nabla u \quad \text{compatible} \\ \widetilde{\nabla u} \quad \Omega - \text{periodic} \\ \pi \quad \Omega - \text{periodic} \end{cases} \quad (15)$$

A simple way to satisfy the compatibility condition for ∇u^* is to choose a strain gradient field (16) characterized by the tensor G , which is no more symmetric on its two first indices when considering the finite strain context.

$$\nabla u^*(\mathbf{x}) = G \cdot \mathbf{x} \quad \text{or} \quad \nabla u_{ij}^* = G_{ijk} x_k \quad (16)$$

Then, solving problem (15) with the simple fixed-point algorithm described by problem (17) is possible if the applied strain gradient satisfies the same constraints as (12), with a non-symmetric G .

$$\Omega^{per} \begin{cases} \tau = c(\nabla u) - c_0 : \nabla u \\ \widetilde{\nabla u} = -\Gamma_0 * \tau \quad (\Leftrightarrow \text{Fourier}) \\ \nabla u = \nabla U + \nabla u^* + \widetilde{\nabla u} \end{cases} \quad (17)$$

As the set of equations (14) does not account for the symmetry of G , it applies equivalently to the non-symmetric G . Now, the space of available loading has 18 dimensions (27 components minus 9 equations) instead of 9 under the small strain assumption (18 components minus 9 equations).

2.6 : Conclusion

This work proposes to extend in a very simple manner the scope of FFT-based codes, classically implemented to account for uniform applied strain, to account for linearly varying applied strains (i.e. with a constant applied strain gradient). The modification is extremely simple and has a null memory footprint.

The price to pay for this simplicity is a constraint on the components of the applied strain gradient: among the 18 components (or 27 at finite strain) of the strain gradient, 9 equations reduce the space of available loadings to 9 dimensions (or 18 at finite strain). However, the next section will demonstrate that it is enough to consider the problems of the homogenization of beams and plates.

3 : Application to the homogenization of beams and plates

The purpose of this section is to demonstrate that the slight modification proposed in the previous section, applied to an existing FFT-based code that is able to simulate microstructures with null elastic properties, is enough to consider the problem of thin plates or elongated beams homogenization. Nguyen [27] has initially addressed the question of thin plates homogenization with an FFT-based solver, but his approach relied on a dedicated solver whereas our approach relies on any standard FFT-based solver able to account for null elastic properties. For the sake of validation and comparison, section 3.1 reproduces all the simulation cases proposed by Nguyen [27]. Then, section 3.2 extends the approach to the homogenization of beams, treated for the first time, to the author's knowledge, with an FFT-based solver.

As the convergence properties reported below (section 3.1 and 3.2) depends on the FFT-based code used for the simulation, a brief description is necessary. The two main features influencing the convergence properties in our code AMITEX_FFTP [1] are the iterative algorithm and the discrete Green operator. First, the algorithm corresponds to the fixed-point algorithm [26], described by problem (7)+(6), combined with an Anderson convergence acceleration technique reported in ([9], section 3.2.1). This acceleration technique drastically improves the fixed-point algorithm convergence. In addition, compared to the Newton-Raphson implementation also proposed for FFT-based solvers with non-linear behaviors [13], it is interesting because it does not require the tangent matrix behavior, whose analytical evaluation may be tedious. On the other hand, the memory footprint is higher: our implementation requires four couples of (solution field, residual field). Second, the discrete Green operator is associated to a finite element discretization with linear hexaedral elements with reduced integration [30] [28]. It is efficient to reduce spurious oscillations and improve convergence. Thanks to these two elements, the code is able to account, quite efficiently, for unit-cells containing void voxels (null elastic properties).

3.1 : Homogenization of plates

The purpose of this section is to demonstrate that a general FFT-based code, equipped with the minor modification proposed in this study, extends its application domain to the homogenization of plates. Validation comes from comparisons with analytical results and numerical results obtained by Nguyen [27]. Note that an extensive and refined comparison between our simulations and Nguyen's simulations is not easy because of the differences between the iterative algorithms, the discrete Green operators and the convergence criterion. Especially, the convergence criterion used by Nguyen is a 'macroscopic' criterion based on the 'relative' difference of the strain energy between two iterations whereas the criterion used in AMITEX_FFTP relies on the 'absolute' equilibrium condition of the 'local' stress field.

3.1.1 : Method

We consider a thin heterogeneous plate described by a unit cell Ω periodically repeated in the plane $(\mathbf{e}_1, \mathbf{e}_2)$, with direction (\mathbf{e}_3) normal to the plate. Assuming an applied strain field consistent with the Kirchoff-Love modeling for plates, the problem to solve reads:

$$\left\{ \begin{array}{l} \mathbf{div}(\boldsymbol{\sigma}) = 0 \\ \boldsymbol{\sigma} = \mathbf{c} : \boldsymbol{\varepsilon} \\ \boldsymbol{\varepsilon} = \mathbf{E} + \boldsymbol{\chi}\chi_3 + (\nabla \tilde{\mathbf{u}})^{sym} \\ \tilde{\mathbf{u}} \quad \text{periodic on } \partial_{12}\Omega \\ \boldsymbol{\sigma} \cdot \mathbf{n} \quad \text{antiperiodic on } \partial_{12}\Omega \\ \boldsymbol{\sigma} \cdot \mathbf{n} = 0 \quad \text{on } \partial_3\Omega \end{array} \right. \quad (18)$$

Where $\partial_{12}\Omega$ denotes the four faces of normal directions (\mathbf{e}_1) and (\mathbf{e}_2), submitted to periodic boundary conditions and $\partial_3\Omega$ the two faces submitted to a traction-free boundary condition. The macroscopic applied strain and strain gradient are limited to the in-plane components for both the uniform and non-uniform parts, in bold in equation (19). However, due to mechanical couplings between directions, out of plane components do not systematically vanish (i.e. even in the simplest case of an elastic, homogeneous and isotropic material, the components E_{33} and χ_{33} arise from the classical Poisson effect).

$$\mathbf{E} = \begin{pmatrix} \mathbf{E}_{11} & \mathbf{E}_{12} & E_{13} \\ \mathbf{E}_{12} & \mathbf{E}_{22} & E_{23} \\ E_{13} & E_{23} & E_{33} \end{pmatrix} \quad \text{and} \quad \boldsymbol{\chi} = \begin{pmatrix} \chi_{11} & \chi_{12} & \chi_{13} \\ \chi_{12} & \chi_{22} & \chi_{23} \\ \chi_{13} & \chi_{23} & \chi_{33} \end{pmatrix} = \begin{pmatrix} \mathbf{G}_{113} & \mathbf{G}_{123} & G_{133} \\ \mathbf{G}_{123} & \mathbf{G}_{223} & G_{233} \\ G_{133} & G_{133} & G_{333} \end{pmatrix} \quad (19)$$

In their paper, to solve problem (18), Nguyen and al. [27] follow exactly the reasoning described in section 2. However, keeping the traction-free condition on $\partial_3\Omega$, they have to modify the Green operator to account for this condition in the auxiliary problem.

Instead, in the present paper, we make use of the classical periodic Green operator, built with full periodic conditions and available in every FFT-based codes. In order to satisfy the traction-free boundary condition, the full periodic problem is not solved on the unit-cell Ω but on an enlarged unit-cell Ω^* adding to Ω one layer with null elastic properties on each side of $\partial_3\Omega$ (see Figure 1). In practice the added layers are one voxel thickness in the discretized problem and using one layer on each side allows to keep the same middle surface for Ω and Ω^* (helpful for the post-treatment of the stress field). Due to the added void layers, the in-plane components applied to Ω^* must be the same but the out of plane components can be chosen arbitrarily as follows:

$$\mathbf{E}^* = \begin{pmatrix} \mathbf{E}_{11} & \mathbf{E}_{12} & 0 \\ \mathbf{E}_{12} & \mathbf{E}_{22} & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\chi}^* = \begin{pmatrix} \chi_{11} & \chi_{12} & 0 \\ \chi_{12} & \chi_{22} & 0 \\ 0 & 0 & \chi_{33}^* \end{pmatrix} = \begin{pmatrix} \mathbf{G}_{113} & \mathbf{G}_{123} & 0 \\ \mathbf{G}_{123} & \mathbf{G}_{223} & 0 \\ 0 & 0 & G_{333}^* \end{pmatrix} \quad (20)$$

In order to use the method proposed in the previous section to account for linearly varying applied strain, the strain gradient components imposed in equation (20) have to satisfy the constraints established in the general case (set of equations (14)). In the present case, the imposed component G_{123} remains unconstrained; it consists of an elementary torsion plate loading. The unique constraint applies to the G_{ii3} components:

$$\lambda_0(G_{113} + G_{223} + G_{333}^*) + 2\mu_0 G_{333}^* = 0 \quad (21)$$

This constraint allows proposing two elementary flexion plate loadings, governed by the components G_{113} and G_{223} applied to Ω , as follows:

$$\begin{cases} G_{113} \text{ imposed} \\ G_{223} = 0 \\ G_{333}^* = -\frac{\lambda_0}{\lambda_0 + 2\mu_0} G_{113} \end{cases} \quad \begin{cases} G_{113} = 0 \\ G_{223} \text{ imposed} \\ G_{333}^* = -\frac{\lambda_0}{\lambda_0 + 2\mu_0} G_{223} \end{cases} \quad (22)$$

It is worth noting that G_{333}^* , the gradient of ε_{33} according to x_3 is applied to Ω^* in the thickness direction (i.e. direction 3), in which the two additional void layers have been added to Ω . Because of these void layers, Ω is free to deform in direction e_3 (to allow for the mechanical coupling between directions, such as the Poisson effect) and the average value of G_{333}^* on Ω^* can be different from its average on Ω . As a result, if the relations on G_{333}^* in equation (22) must be satisfied on Ω^* , they can be completely disregarded when considering their effect on the unit-cell Ω (without added layers). The same consideration holds for $E_{33}^* = E_{13}^* = E_{23}^* = 0$ and $G_{133}^* = G_{233}^* = 0$ applied to the enlarged unit-cell Ω^* .

Once, the problem solved at the micro-scale (on the heterogeneous unit-cell), the last step consists in defining appropriate averages for the macroscopic quantities used for modeling plates. For an homogenized material, considering $\sigma_{\alpha\beta}$ ($\alpha, \beta = 1$ or 2) as a function of x_3 , the two macroscopic 'stress' tensors are the linear force tensor N (expressed in N/m) and the linear moment tensor M (in N.m/m) defined by:

$$N_{\alpha\beta} = \int_{-h}^h \sigma_{\alpha\beta} dx_3 \quad \text{and} \quad M_{\alpha\beta} = \int_{-h}^h x_3 \sigma_{\alpha\beta} dx_3 \quad (23)$$

Now considering a heterogeneous unit-cell (and $\sigma_{\alpha\beta}$ as a function of x_1, x_2 and x_3), the following averaging procedure is used, with S the area of S_{12} the cross-sections of Ω in plane (1,2) :

$$\begin{aligned} N_{\alpha\beta} &= \int_{-h}^h \left(\frac{1}{S} \int_{S_{12}} \sigma_{\alpha\beta} dS \right) dx_3 = \frac{1}{S} \int_{\Omega} \sigma_{\alpha\beta} dV \\ M_{\alpha\beta} &= \int_{-h}^h \left(\frac{1}{S} \int_{S_{12}} x_3 \sigma_{\alpha\beta} dS \right) dx_3 = \frac{1}{S} \int_{\Omega} x_3 \sigma_{\alpha\beta} dV \end{aligned} \quad (24)$$

Using the in-plane periodicity of $\tilde{\mathbf{u}}$ and the equilibrium condition ($\int_{S_{12}} \sigma_{i3} dS = 0$ for all sections $S_{12}(x_3)$), it can be demonstrated that the average of the microscopic energy is equal to the macroscopic energy. In the case of plates, the energy surface density is considered and the so-called macro-homogeneity condition of Hill-Mandel reads:

$$\frac{1}{S} \int_{\Omega} \sigma : \varepsilon dV = \frac{1}{S} \int_{\Omega} \sigma : (E + \chi x_3 + \tilde{\varepsilon}) dV = N : E^P + M : \chi^P \quad (25)$$

Finally, the homogenized elastic behavior relates the kinematic tensors (E^P, χ^P), restrictions of the tensors (E, χ) to their in-plane components, to the macroscopic 'stress' tensors (N, M) as follows:

$$\begin{bmatrix} N \\ M \end{bmatrix} = \begin{bmatrix} A & B \\ B & D \end{bmatrix} \begin{bmatrix} E^P \\ \chi^P \end{bmatrix} \quad (26)$$

Tensor A describes the membrane behavior, D the flexion and torsion behaviors and B the possible coupling arising, for example, with non-symmetric unit-cells with respect to the middle surface. From this definition, the energy surface density reads:

$$\frac{1}{S} \int_{\Omega} \sigma : \varepsilon dV = E^P \cdot A \cdot E^P + 2E^P \cdot B \cdot \chi^P + \chi^P \cdot D \cdot \chi^P \quad (27)$$

In practice, the identification of the homogenized behavior results from six simulations corresponding to six independent loadings (E^P, χ^P) applied to the unit-cell. The mechanical approach post-treats the stress fields to evaluate the corresponding resultant 'stress' tensors (N, M) with equations (24) in order to identify the coefficients of relation (26). The energetic approach post-treats the stress-strain fields to evaluate the corresponding energies in order to identify the coefficients of relation (27).

As soon as the macro-homogeneity condition (25) holds, the energetic approach followed by Nguyen in [27] is strictly equivalent to the mechanical approach followed in the present paper.

3.1.2 : Laminate plate [27]

Following the validation test used by Nguyen, we consider the case of a two phases laminate plate for which a closed form solution exists (see [27]). The unit-cell Ω represented on Figure 1, is symmetric so that the coupling tensor B vanishes. The volume fractions of phases are equal (50%), and their elastic properties (Young modulus, Poisson coefficient) are respectively (46GPa, 0.3) and (10GPa, 0.3) for phases 1 and 2. According to [27], the spatial resolution used for the simulations are $2^n \times 2^n \times 1$ voxels (the code is 3D) for the unit cell Ω and two additional layers enlarge the unit-cell to simulate traction-free boundary condition in Ω^* (see section 2). The non-null components (E_{22}, χ_{22}) of E^P and χ^P defines the two applied loadings: (1,0) for the tensile loading and (0,1) for the flexion loading. They directly allow to evaluate $A_{22} = N_{22}/E_{22}$ and $D_{22} = M_{22}/\chi_{22}$. The corresponding loadings applied to the enlarged unit-cell Ω^* are:

$$\begin{aligned} E^* &= \begin{pmatrix} \mathbf{0} & \mathbf{0} & 0 \\ \mathbf{0} & E_{22} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \chi^* = 0 & \text{(tension)} \\ E^* &= 0, \chi^* = \begin{pmatrix} \mathbf{0} & \mathbf{0} & 0 \\ \mathbf{0} & \chi_{22} & 0 \\ 0 & 0 & \chi_{33}^* \end{pmatrix} \text{ with } \chi_{33}^* = -\frac{\lambda_0}{\lambda_0 + 2\mu_0} \chi_{22} & \text{(flexion)} \end{aligned} \quad (28)$$

The choice made for the reference material's Lamé coefficients (λ_0, μ_0) is $\lambda_0 = (\lambda_{min} + \lambda_{max})/2$ with $\lambda_{min} = 0$ (for the void layers), and μ_0 adjusted to obtain a Poisson coefficient $\nu_0 = 0.3$, the Poisson coefficient common to both phases.

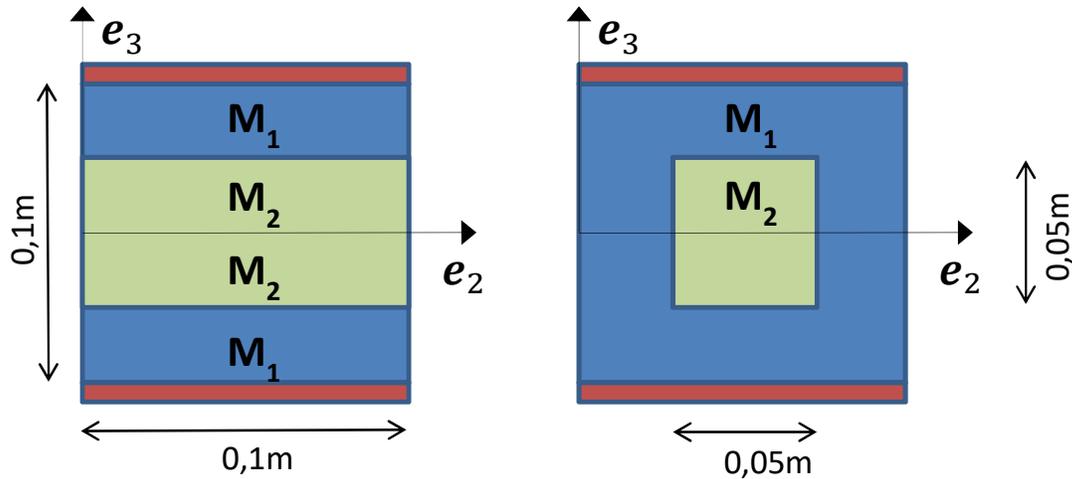


Figure 1 : Description of the two unit-cells used in simulations of heterogeneous plates: laminate plate (left) and composite plate with cylinder (square base) inclusions (right). In orange are represented the additional void layers used in the present simulations.

For the tensile loading, the algorithm reaches convergence after 6 iterations with a convergence criterion on the local equilibrium of 10^{-15} far below the threshold of 10^{-4} used for the simulation. It seems that the solver reaches the exact solution, up to the double precision round-off error. Actually, the exact solution being constant per layer, it can be observed that the FFT-based method is able to find it if the discretization grid is parallel to the layers. From the macroscopic point of view, Table 1 gathers the comparison with analytical results and numerical results from [27]. The comparison with analytical result is exact up to the 8th digit. The comparison with [27] is perfect up to the number of available digits. However, the converged value is obtained after 10 iterations to converge on a macroscopic criterion (10^{-4} on the average energy between two iterations), compared to 6 for this study on a more stringent criterion (local equilibrium). Finally, as the solution is constant per layer, it does not depend on the mesh resolution and exactly the same result is obtained with a resolution 4x4 (i.e. with one voxel per layer in the thickness).

Resolution	Analytical	This work	[27]
8x8	3.07692307	3.07692303	3.077
4x4	3.07692307	3.07692303	

Table 1 : Axial stiffness A_{22} obtained for the laminate case: comparison between analytical results and two FFT-based methods

For the flexion loading, the algorithm reaches convergence after a single iteration with, once again, a convergence criterion on the local equilibrium of 10^{-15} far below the threshold of 10^{-4} . As mentioned earlier, the method is able to find perfectly equilibrated layered stress fields (up to the precision round off and as soon as the layer are parallel to the discretization grid). However, in the case of flexion, the stress field is not constant per phase so that the stress field and consequently the resultant 'stress' tensor M , depends on the mesh size. Table 2 compares the analytical results with the numerical results in [27] and this study, for different spatial resolutions. Both results are in excellent agreement with the analytical case and the error becomes very low as soon as resolution reaches 32x32. For resolution 16x16, results are still in good agreement (relative error $\sim 3.4\%$) and Nguyen's method looks better in that case. On the other hand, it required 10 iterations to reach convergence (on a macroscopic criterion), compared to a single iteration in this study.

Resolution	Analytical (GPa/m)	This study (<i>rel. error</i>)	[27] (<i>rel. error</i>)
16x16	0.003800	0.003670 ($342e-4$)	0.00382 ($52e-4$)
32x32	0.003800	0.003798 ($5e-4$)	0.003805 ($13e-4$)
64x64	0.003800	0.003803 ($7e-4$)	0.003802 ($5e-4$)

Table 2 : Bending stiffness D_{22} obtained for the laminate case: comparison between analytical results and two FFT-based methods

To conclude, the minor modification applied to our general FFT-based solver, allows reproducing the analytical solution obtained for a laminate plate, at least as precisely and as efficiently as an FFT-based solver dedicated to the homogenization of plates.

3.1.3 : Plate with periodic fibers [27]

This second validation test proposed in [27] considers a panel with a periodic distribution of parallelepiped fibers. Figure 1 describes the periodic unit-cell. The matrix and the inclusion have the same Poisson ratio (0.3), and the Young moduli of inclusion / matrix (in GPa) are (0/1), (10/1) and (1/1000). The AMITEX_FFTP code being able to apply whether the average stress or the average strain E^* for each of the six components, applying a null average stress for the components 33, 13 and 23, was found to reduce the number of iterations at convergence of about 30% for the tensile loading. Hence, the loading used in this case is identical to the loading introduced for the laminate case in equation (28), except for these three components, now set to null stress instead of null strain. The flexion loading remains unchanged. The choice made for Lamé coefficients follows the same rule as proposed in the laminate case. The spatial resolution used for the simulations are $2^n \times 2^n \times 1$ voxels (the code is 3D) for the unit cell Ω and two additional layers enlarge the unit-cell to simulate traction-free boundary condition in Ω^* (see section 2).

All the simulations reported in [27] have been reproduced and all the results are gathered in tables of annex A, in which the membrane stiffness A_{22} , bending stiffness D_{22} and number of iterations are given as a function of the spatial resolution for the three elastic contrasts. The convergence criterion being very different between AMITEX_FFTP and [27], the comparison between iteration numbers at convergence is not significant. Hence, the evaluation of strain energy has been implemented in AMITEX_FFTP and the relative difference between two iterations is evaluated as a post-treatment to determine the number of iterations at convergence if using this criterion with a threshold of 10^{-4} (used in [27]).

If not useful to discuss all the tables one by one, their analysis allows drawing a few main conclusions. First, even for the coarsest resolution (16x16), with relative errors below 1%, results obtained with both FFT-based methods are very close to the reference solution obtained from finite element simulations in [27]. Second, if the relative error decreases monotonously with Nguyen's method, the decrease is less monotonous with our approach and, in addition, the relative error do not seem to decrease below 0.1% for the flexion loading cases. If this question could be further investigated, in practice a relative error of 0.1% is yet below the accuracy required by many applications. Third, the number of iterations obtained with our approach (associated to a field equilibrium criterion) remains reasonable with values comprised between 14 and 75. It is lower for

flexion loadings than for tensile loadings, whereas the type of loading has no influence on [27]'s results. Finally, when post-treating our results with the strain energy based criterion, the number of iterations at convergence are rather similar to [27]'s results, a bit higher for tensile loadings and a bit lower for flexion.

To conclude, the minor modification applied to our general FFT-based solver, allows reproducing the numerical results obtained for a matrix/inclusion plate, almost as precisely and as efficiently as a solver dedicated to the homogenization of plates.

3.2 : Homogenization of beams

If the extension of the approach proposed for plates in [27] to the homogenization of beams is not straightforward especially with arbitrary cross-sections, it is direct with our approach. After a description of the method proposed for the homogenization of beams, it is applied to different loadings with various geometries and elastic contrasts. As uniaxial tension is quite straightforward and has already been applied in previous studies [9], the paper focuses on flexion and torsion loadings.

This section considers two different beams with a square and a disk cross-section. In the first case the discretization is conform to the geometry while it is not in the second case. Cubic inclusions, with conform discretization are considered in both cases, so that the effect of a conforming discretization is limited to the shape of the cross-section which is of a prime interest in the present context.

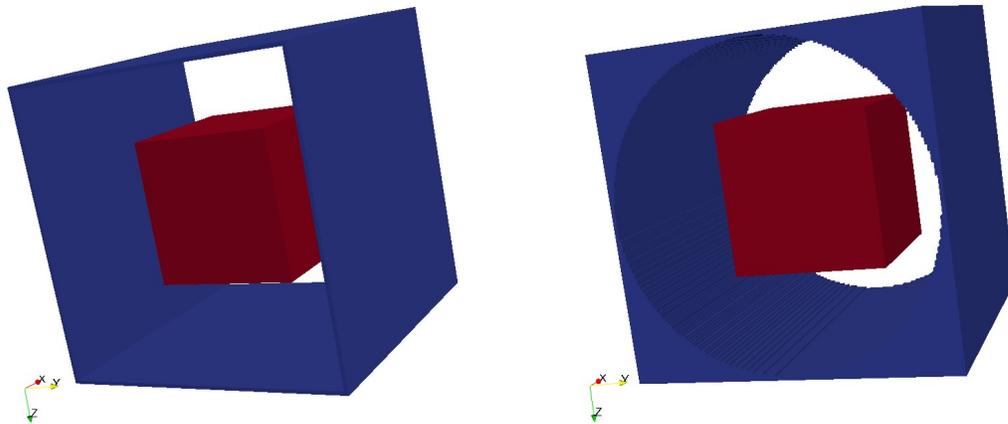


Figure 2 : Rendering of the two unit-cells: on the left with a square cross-section, on the right with a disk cross-section. The cubic inclusion is in red, the added void volume is in blue and the matrix in transparency.

Figure 2 represents the geometry of the unit-cell with a cube diameter of 50mm, a unit-cell length of 100mm, a square and disk diameter of 100mm for the cross-section. Void volumes in blue complement the unit-cells Ω , with a minimal thickness of two voxels, to form the enlarged unit-cells Ω^* . The center of the inclusion lies on the axis of the unit-cells. The spatial resolutions, defined by the number of voxels on 100mm, are 40, 80 and 160 (so that the unit-cells are 40x44x44, 80x84x84 and 160x164x164). With these resolutions, the discretization of the inclusion is conform to its geometry.

The Young modulus of the matrix is 10MPa with a Poisson coefficient of 0.3 and three elastic behaviors are considered for the inclusion: the matrix behavior, so that the beam is homogeneous, a void behavior leading to an infinite contrast and a behavior stiffer than the matrix with a high contrast 1000.

In addition, the use of composite voxels [16] [21] [20] [7] is tested to improve the description of the geometry when using a non-conforming discretization, as observed with the disk cross-section. The behavior of the composite voxels, crossed by the interface between the matrix and the additional void volume, follows a homogenization rule. Among the three classical rules, the Reuss and laminate homogenization rules are not well-suited with void behavior: the first one simply replaces the voxel by a void voxel and the second leads to an infinitely anisotropic behavior which generates convergence issues in the FFT-based algorithm (observed in torsion loading). In addition, the Voigt homogenization rule, which assumes a homogeneous strain over the phases, is extremely simple to implement, even with non-linear behaviors. Voigt is used in the following. For the sake of simplicity, an approximate definition of volume fractions is used and reported in annex B.

The choice made for the reference material's Lamé coefficients (λ_0, μ_0) is $X_0 = (X_{min} + X_{max})/2$, with X equal to λ or μ . Note that here, min and max are evaluated over the beam material, excluding the additional void volume in Ω^* : for contrasts 0 and 1000, the difference are null or very small, and for contrast 1, the reference material corresponds to the behavior of the homogeneous beam.

3.2.1 : Method

The unit-cell Ω , with an arbitrary cross-section is periodic in direction e_1 and, for numerical resolution purpose, is enlarged by additional voxels of null stiffness to form a parallelepiped unit-cell Ω^* , as shown on the two examples on Figure 2. Assuming an applied strain field consistent with the Bernoulli modeling for beams, the problem to solve reads:

$$\left\{ \begin{array}{l} \mathbf{div}(\sigma) = 0 \\ \sigma = c : \varepsilon \\ \varepsilon = E + \chi_3 \chi_3 + \chi_2 \chi_2 + (\nabla \tilde{\mathbf{u}})^{sym} \\ \tilde{\mathbf{u}} \quad \text{periodic on } \partial_1 \Omega \\ \sigma \cdot \mathbf{n} \quad \text{antiperiodic on } \partial_1 \Omega \\ \sigma \cdot \mathbf{n} = 0 \quad \text{on } \partial_{23} \Omega \end{array} \right. \quad (29)$$

Where $\partial_1 \Omega$ denotes the two faces of normal direction e_1 , submitted to periodic boundary conditions, and $\partial_{23} \Omega$ the external contour of the beam submitted to a traction-free boundary condition. The macroscopic applied strain is limited to components in bold in equation (30). The component E_{11} prescribes a tensile loading, the components G_{112} and G_{113} prescribe two flexion loadings respectively, and $\alpha = G_{132} = -G_{123}$ prescribes the torsion loading. As mentioned for plates in section 3.1.1, due to mechanical coupling between directions, the other components are not prescribed but do not systematically vanish (the simplest example being the Poisson effect).

$$E = \begin{pmatrix} \mathbf{E}_{11} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & E_{22} & E_{23} \\ \mathbf{0} & E_{23} & E_{33} \end{pmatrix}; \quad \chi_3 = \begin{pmatrix} \mathbf{G}_{113} & -\alpha & \mathbf{0} \\ -\alpha & G_{223} & G_{233} \\ \mathbf{0} & G_{233} & G_{333} \end{pmatrix} \quad \text{and} \quad \chi_2 = \begin{pmatrix} \mathbf{G}_{112} & \mathbf{0} & \alpha \\ \mathbf{0} & G_{222} & G_{232} \\ \alpha & G_{232} & G_{332} \end{pmatrix} \quad (30)$$

In order to satisfy the traction-free boundary condition, the full periodic problem is solved on the enlarged unit-cell Ω^* with a void volume surrounding Ω in order to fulfil the traction free boundary condition on $\partial_{23}\Omega$. Due to the added void layers, the out of plane components prescribed to Ω^* are the same (in bold) but the in plane components can be chosen arbitrarily as follows:

$$E^* = \begin{pmatrix} \mathbf{E}_{11} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 0 & 0 \\ \mathbf{0} & 0 & 0 \end{pmatrix}; \quad \chi_3^* = \begin{pmatrix} \mathbf{G}_{113} & -\boldsymbol{\alpha} & \mathbf{0} \\ -\boldsymbol{\alpha} & G_{223}^* & 0 \\ \mathbf{0} & 0 & G_{333}^* \end{pmatrix} \text{ and } \chi_3^* = \begin{pmatrix} \mathbf{G}_{112} & \mathbf{0} & \boldsymbol{\alpha} \\ \mathbf{0} & G_{222}^* & 0 \\ \boldsymbol{\alpha} & 0 & G_{332}^* \end{pmatrix} \quad (31)$$

In order to use the method proposed in section 2 to account for linearly varying applied strain, the strain gradient components imposed in equation (31) have to satisfy the constraints established in the general case (set of equations (14)). In the present case, the torsion component $\alpha = G_{132} = -G_{123}$ remains unconstrained and two constraints apply to G_{ii3} and G_{ii2} components:

$$\begin{cases} \lambda_0(G_{112} + G_{222}^* + G_{332}^*) + 2\mu_0 G_{222}^* = 0 \\ \lambda_0(G_{113} + G_{223}^* + G_{333}^*) + 2\mu_0 G_{333}^* = 0 \end{cases} \quad (32)$$

These constraints allow proposing two elementary flexion beam loadings, governed by the components G_{113} and G_{112} applied to Ω , as follows:

$$\begin{cases} G_{113} \text{ imposed} \\ G_{223}^* = \beta G_{333}^* \\ G_{333}^* = -\frac{\lambda_0}{\lambda_0(1+\beta) + 2\mu_0} G_{113} \end{cases} \quad \begin{cases} G_{332}^* = \beta G_{222}^* \\ G_{112} \text{ imposed} \\ G_{222}^* = -\frac{\lambda_0}{\lambda_0(1+\beta) + 2\mu_0} G_{112} \end{cases} \quad (33)$$

These two loadings are very similar to the flexion plate loadings (one is identical with $\beta = 0$) given in equation (22). As mentioned in the case of plates, because of the void volume surrounding Ω in Ω^* , the volume Ω is free to deform in the directions \mathbf{e}_2 and \mathbf{e}_3 , so that the values of G_{ij} and G_{ij2} (with $(i,j) \in \{1,2\}^2$) evaluated over Ω can be different from their corresponding values G_{ijk}^* over the enlarged cell Ω^* . The same consideration holds for the null components 22, 33 and 23 of E^* . The parameter β is set to 1 in the present paper.

Once, the problem solved at the micro-scale (on the heterogeneous unit-cell), the last step consists in defining appropriate spatial averages for the macroscopic quantities used for modeling beams. Classically, integrations of the traction vector ($\sigma \cdot \mathbf{e}_1$) over the cross-section provide the macroscopic force \mathbf{N} (expressed in N) and moments \mathbf{M} (in N.m) as follows:

$$\begin{aligned} \mathbf{N} &= \int_{S_{23}} \sigma \cdot \mathbf{e}_1 dS = \int_{S_{23}} \begin{pmatrix} \sigma_{11} \\ \sigma_{12} \\ \sigma_{13} \end{pmatrix} dS \\ \mathbf{M} &= \int_{S_{23}} \begin{pmatrix} 0 \\ x_2 \\ x_3 \end{pmatrix} \wedge (\sigma \cdot \mathbf{e}_1) dS = \int_{S_{23}} \begin{pmatrix} \sigma_{13}x_2 - \sigma_{12}x_3 \\ \sigma_{11}x_3 \\ -\sigma_{11}x_2 \end{pmatrix} dS \end{aligned} \quad (34)$$

The N_1 component of the force vector is the axial force and the other components are shear forces. The M_1 component of the moment vector is the torsion moment and the other components are

bending moments. For homogenization purpose, these quantities evaluated on a cross section are averaged over the \mathbf{e}_1 direction of the unit-cell Ω so that they can be evaluated from volume integrations over the complete unit-cell Ω :

$$\begin{aligned}\mathbf{N} &= \frac{1}{l_1} \int_{L_1} \left(\int_{S_{23}} \sigma \cdot \mathbf{e}_1 dS \right) dx_1 = \frac{1}{l_1} \int_{\Omega} \sigma \cdot \mathbf{e}_1 dV \\ \mathbf{M} &= \frac{1}{l_1} \int_{L_1} \left(\int_{S_{23}} \begin{pmatrix} 0 \\ x_2 \\ x_3 \end{pmatrix} \wedge (\sigma \cdot \mathbf{e}_1) dS \right) dx_1 = \frac{1}{l_1} \int_{\Omega} \begin{pmatrix} 0 \\ x_2 \\ x_3 \end{pmatrix} \wedge (\sigma \cdot \mathbf{e}_1) dV\end{aligned}\quad (35)$$

Using the axial periodicity of $\tilde{\mathbf{u}}$ and the equilibrium condition ($\int_{S_{12}(x_3)} \sigma_{i3} dS = \int_{S_{13}(x_2)} \sigma_{i2} dS = 0$, for all longitudinal sections $S_{12}(x_3)$ and $S_{13}(x_2)$), it can be demonstrated that the average of the microscopic energy is equal to the macroscopic energy. In the case of beams, the energy linear density is considered and the so-called macro-homogeneity condition of Hill-Mandel reads:

$$\frac{1}{l_1} \int_{\Omega} \sigma : \varepsilon dV = \frac{1}{l_1} \int_{\Omega} \sigma : (E + \chi_2 x_2 + \chi_3 x_3 + \tilde{\varepsilon}) dV = N_1 : E_{11} + M_2 : G_{113} - M_3 : G_{112} + 2M_1 : \alpha \quad (36)$$

The different terms are respectively associated to the uniaxial, the two bendings and the torsion loadings. The minus sign of the third term comes from the minus sign of M_3 in equation (34).

Finally, the homogenized elastic behavior relates the kinematic quantities $\mathbf{U} = (E_{11}, \alpha, G_{112}, G_{113})$ to the forces and moments $\mathbf{F} = (N_1, M_1, M_2, M_3)$ with a linear relationship:

$$\mathbf{F} = \mathbf{K} : \mathbf{U} \quad (37)$$

As mentioned for plates, the Hill-Mandel condition allows using indifferently the energetic or the mechanical approach. The last one is used in the following: a single kinematic loading is applied and the stress field is post-treated to evaluate forces and moments and identify the stiffness components of \mathbf{K} .

3.2.2 : Beam flexion

The flexion loading applies to the unit-cell Ω^* with G_{112} and the other strain gradient components set to 0. For the homogeneous strain loading, three different propositions have been tested: all the average strain components equal to 0, all the average stress components equal to 0, average strain components $(1j)_{j=1,2,3}$ and average stress components $(ij)_{i=1,2 \ j=1,2}$ equal to zero. All the propositions provide the same bending moment M_3 (up to a relative difference of $\sim 10^{-4}$) and none of them outperforms the others regarding the number of iterations at convergence. Results below are presented with all the average strain components equal to 0.

In practice, G_{112} is set to 1 in the simulations so that the bending moment is directly the bending stiffness.

3.2.2.1 : Homogeneous beam flexion

The case of a homogeneous beam is interesting, at first as a validation case for which the analytical solution is known, but also to focus on the question of the non-conforming discretization of the beam (for the disk cross-section) and the potential interest of using composite voxels (with Voigt homogenization rule in that case). This specific case is also interesting because the initialization of the strain field in the FFT-based algorithm directly provides the solution of the problem and convergence should achieve at the first iterate. Actually, the initial strain field is a null homogeneous strain field added to a linearly varying strain field associated to G_{112} and $G_{222}^* = G_{332}^* = -\frac{\lambda_0}{2(\lambda_0 + \mu_0)} G_{112}$ (see equation (33)). Hence, the initialization of the strain field imposes $\varepsilon_{12} = \varepsilon_{13} = \varepsilon_{23} = 0$ for shear strains, $\varepsilon_{11} = G_{112} x_2$ for the axial strain and $\varepsilon_{22} = \varepsilon_{33} = -\frac{\lambda_0}{2(\lambda_0 + \mu_0)} \varepsilon_{11} = -\nu_0 \varepsilon_{11}$ for the transverse strains. This strain field initialized on the whole unit-cell Ω^* also applies on the sub-volume Ω so that, if the Poisson coefficient of the reference medium ν_0 is equal to the Poisson coefficient of the beam material ν , the initial strain field is directly the solution of the flexion problem. As a validation part, the implementation in the AMITEX_FFTP code confirms this property (convergence reached at the first iterate).

The bending moments derived from the Euler-Bernoulli beam theory are:

$$M_3 = E \frac{\pi D^4}{64} G_{112} \quad (\text{disk cross section}) \quad \text{and} \quad M_3 = E \frac{D^4}{12} G_{112} \quad (\text{square cross section}) \quad (38)$$

Figure 3 represents the evolution of the relative error of the bending moments as a function of the spatial resolution. For the square cross-section, with a conform discretization the error is very low even for the lowest resolution ($6 \cdot 10^{-4}$) and decreases to around 10^{-5} . On the contrary, for the disk cross section, the error is much higher and decreases with the spatial resolution from 0.01 to reach a value around $1 \cdot 10^{-4}$ for the highest resolution. This difference clearly exhibits, on the macroscopic property, the difference between conforming and non-conforming discretization. For the square cross-section, the error is purely associated to the numerical integration of a quadratic field ($\sigma_{11} x_2$) on a rectilinear grid, whereas for the disk cross-section, an additional and predominant error due to the non-conforming discretization of the cross-section is added. In that case, the composite voxels demonstrate their efficiency to improve the results: the error is $3 \cdot 10^{-4}$ for the lowest resolution and stabilizes around 10^{-5} . From the stress field point of view, as observed on Figure 4, the composite voxels only modify the stress within the voxels crossed by the interface. In that case, their effect is purely local (it will be different for torsion loading).

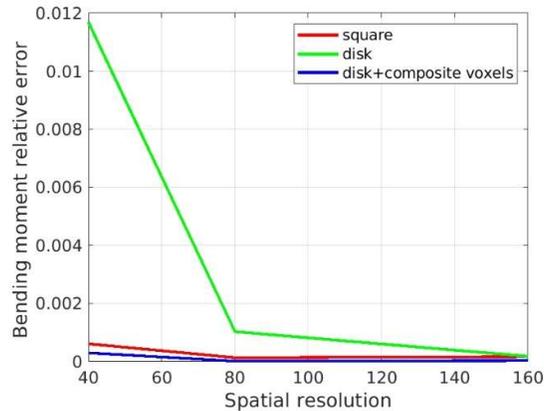


Figure 3 : Evolution of the relative error on the evaluation of the bending moment as a function of the spatial resolution, for homogeneous beams with square and disk cross-sections, and with the use of composite voxels for disk cross-sections.

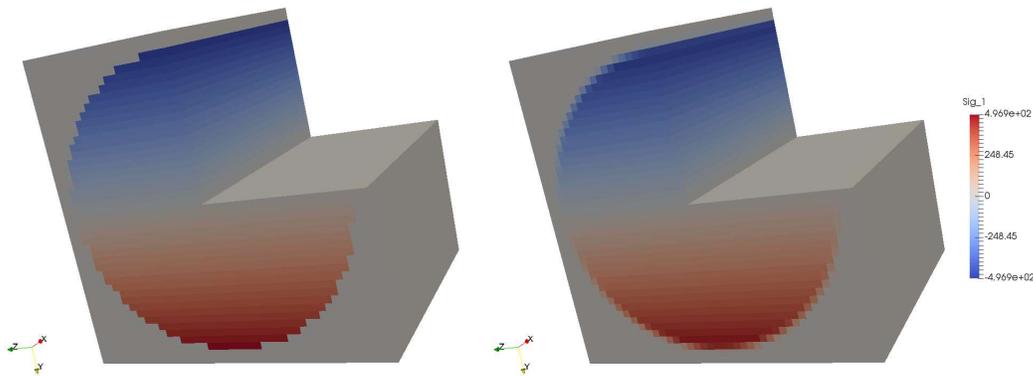


Figure 4 : Axial stress field obtained for the disk cross-section with (right) and without (left) composite voxels, for the lowest spatial resolution (40) (for visualization purpose a quarter of the unit-cell is removed) and an homogeneous beam.

3.2.2.2 : Heterogeneous beam flexion

Figure 5 (right) represents the evolution of the bending moments (or bending stiffness as $G_{112} = 1$) for the three different elastic contrasts. It is worth noting that in spite of high contrasts, the evolution of the bending stiffness is moderate. Different observations can explain this result. At first, the volume fraction of inclusions is not so high (12.5% and 15.9%, respectively for the square and disk cross-sections). Then, and probably more importantly, the inclusions are located at the center of the beam, which is the less stressed region of the beam. It is also noticeable that the difference on the moments between square and disk cross-sections is almost independent of the contrast (respectively $(3.42, 3.42, 3.45) \times 10^7$ for the contrasts $(0,1,1000)$). In other words, the stiffening (or softening) induced by these stiff (or soft) inclusions, with respect to the homogeneous beam, corresponds to an additional positive (or negative) bending stiffness that is rather independent of the beam cross-section.

Figure 5 (left) proposes a convergence analysis, as a function of the spatial resolution, of the bending moments, normalized by their converged value (obtained for resolution 160). The same conclusions

as obtained for the homogeneous beam still hold for heterogeneous beams: convergence is very fast for the square cross-section, unlike the case of the disk cross-section without composite voxels, and using composite voxels significantly improves the convergence. The effect of the contrast, moderate on the converged values of the moments (see Figure 5 (right)), is also quite moderate on the convergence curves (see Figure 5 (left)).

Regarding the convergence analysis of the FFT-based algorithm (in our case, a fixed-point algorithm combined with a convergence acceleration procedure), presented on Table 3, four main conclusions can be drawn. First, the convergence is very efficient for void inclusions. Second, stiff inclusions drastically deteriorate the convergence. Note that, in that case, the unit-cell Ω^* exhibits two types of large elastic contrast: between the matrix and the infinitely soft voids and between the matrix and the 1000 times stiffer inclusions. Such high and opposite contrasts are not really well suited for FFT-based methods. However, convergence is achieved and the number of iteration remains reasonable. Third, the use of composite voxels deteriorates the convergence by a factor of around 2. Fourth, for the square cross-section, increasing the spatial resolution deteriorates the convergence, but it tends to stabilize in the worst case with the contrast of 1000. The understanding of these last two unexpected results is still under investigation.

The analysis of the local stress fields focuses on the simulations with an elastic contrast of 1000 that induces the highest contribution to the bending stiffness (compared to the homogeneous beam, see Figure 5 (right)) and exhibits the worst algorithm convergence (see Table 3). The worse convergence of the algorithm is probably to be correlated with the spurious oscillations arising in and around the stiff inclusion. Comparing the disk and square cross-sections, the stress fields in and around the inclusion are almost identical, independent of the cross-section. This is consistent with the previous observation, at the macroscopic scale, of an additional contribution to the bending stiffness independent of the cross-section. Finally, comparing the disk cross-section with and without composite voxels, the conclusion reported for homogeneous beam still holds in the heterogeneous cases: they essentially affect the voxels crossed by the interface, keeping unchanged the rest of the volume (it will be different for torsion loading).

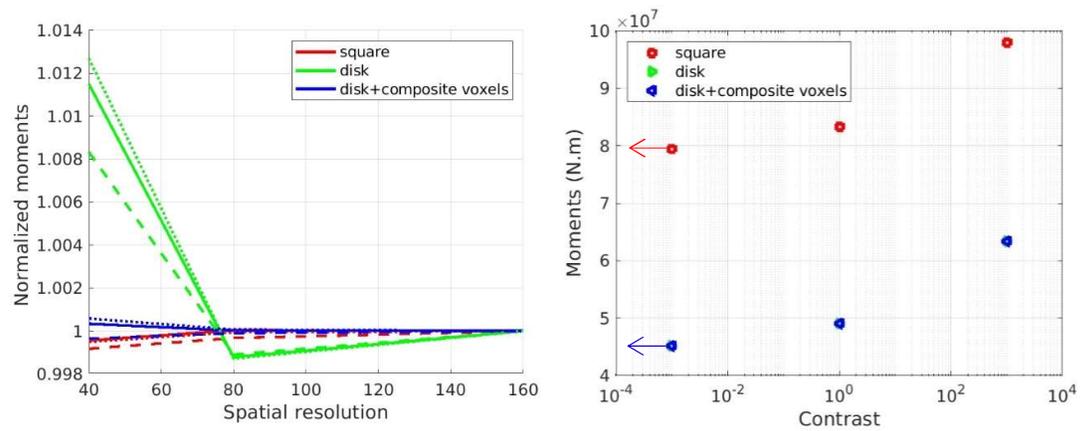


Figure 5 : Evolution of the bending moments (normalized by their converged values obtained for the highest resolution) as a function of the spatial resolution; with solid, dotted and dashed lines respectively for contrasts 1, 0 and 1000 (left). Evolution of the converged values of the moments (obtained for the highest resolution) as a function of the contrast (the arrows symbolize null contrasts in log axis) (right). Note that 'disk' and 'disk+composite voxels' symbols are superimposed, confirming that the moments obtained with the 'disk' (without composite voxel) at resolution 160 are converged values.

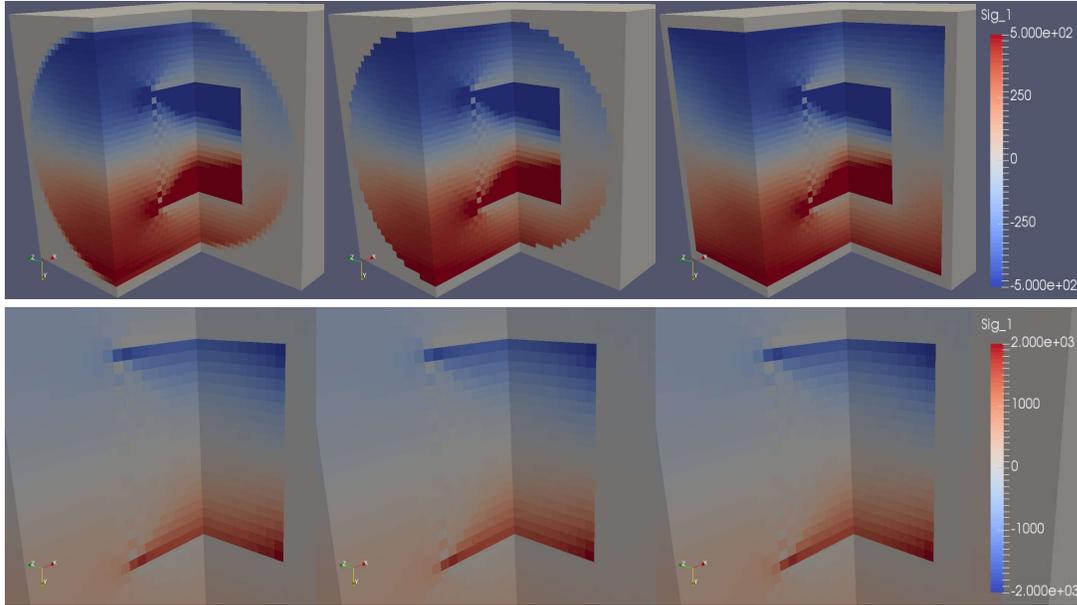


Figure 6 : Axial stress field obtained for the square cross-section (right), and the disk cross-section with (left) and without (middle) composite voxels, for the lowest spatial resolution (40) and a contrast of 1000 for the inclusion (for visualization purpose a quarter of the unit-cell is removed). Bottom figures are zooms on the inclusion with an appropriate color bar.

Resolution	Square			Disk			Disk with Composite Voxel		
	C=0	C=1	C=1000	C=0	C=1	C=1000	C=0	C=1	C=1000
40	16	1	387	16	1	351	25	1	642
80	21	1	585	15	1	372	24	1	864
160	28	1	849	15	1	399	24	1	645
320	39	1	840						

Table 3 : Number of iteration at convergence for the different beams, contrasts, resolutions and use of composite voxels (flexion loading case)

3.2.3 : Beam torsion

The torsion loading applies to the unit-cell Ω^* with $\alpha = G_{132} = -G_{123}$ and the other strain gradient components set to 0. For the homogeneous strain loading, three different propositions have been tested: all the average strain components equal to 0, all the average stress components equal to 0, average strain components $(1j)_{j=1,2,3}$ and average stress components $(ij)_{i=1,2 j=1,2}$ equal to zero. All the propositions provide the same torsion moment M_1 (up to a relative difference of $\sim 10^{-4}$) and none of the proposition outperforms the others regarding the number of iterations at convergence. Results below are presented with all the average strain components equal to 0.

In practice, G_{132} is set to 1 in the simulations so that the torsion moment is directly the torsion stiffness.

3.2.3.1 : Homogeneous beam torsion

The torsion of homogeneous beams, submitted to flexion in the previous section, is also interesting for validation purpose. However, when the initialization of the strain field solution directly provides the solution in the flexion case, the torsion case requires iterating the algorithm for equilibrating the stress field. The torsion moments derived from the Euler-Bernoulli beam theory are:

$$M_1 = \mu \frac{\pi D^4}{32} \alpha \quad (\text{disk cross section}) \quad \text{and} \quad M_1 = \mu D^4 \alpha \times 0.1406 \quad (\text{square cross section}) \quad (39)$$

For the square cross-section, the expression is not analytical but deduced from numerical simulation and reported in various handbooks (see for example [5]).

Figure 7 reports the evolution of the relative error of the torsion moment (or torsion stiffness) as a function of the spatial resolution. For the square cross-section, the error is very small ($5 \cdot 10^{-4}$) for the lowest resolution (40) and decreases up to $2 \cdot 10^{-4}$ for the highest resolution (160). The shear stress field σ_{13} , observed on Figure 8 (right), is not a simple linear function of x_2 but also depends on x_3 , emphasizing that the solution, obtained after 9 iterations, is quite different from the initial stress field (linear function of x_2). In spite of an infinite contrast (with the surrounding void volume), the solution is perfectly smooth without any spurious oscillations. On the other hand, for the disk cross-section, the relative error is much larger: decreasing from 1.4% to 0.6% between resolution 40 and 160. Here, the stress field, on Figure 8 (left), is almost a linear function of x_2 but exhibits important spurious oscillations in the neighborhood of the beam interface. These important fluctuations are suspected to maintain a quite high error (0.6%) for the highest resolution, whereas in the flexion case, without any spurious oscillations, the error reduces to $1 \cdot 10^{-4}$. Finally, the use of composite voxels is, once again, of a great help for improving the solution. Macroscopically, the relative error is very low, compared to the solution without composite voxels: decreasing from $12 \cdot 10^{-4}$ up to $4 \cdot 10^{-4}$ between resolution 40 and 160. The effect is also very important on the stress field, observed on Figure 8 (left and middle): it drastically reduces the amount of spurious oscillations. Compared to the flexion loading case for which the effect is purely local, here, composite voxels also affect the solution in their neighborhood. Surprisingly, in spite of a smoother solution, the number of iterations at convergence is higher with composite voxels (see Table 4). This unexpected result is still not well understood.

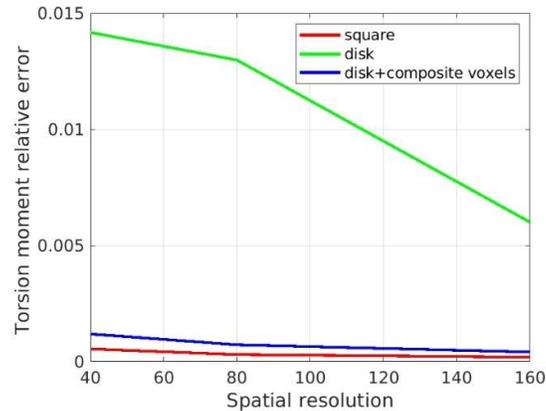


Figure 7 : Evolution of the relative error on the evaluation of the torsion moment as a function of the spatial resolution, for homogeneous beams with square and disk cross-sections, and with the use of composite voxels for disk cross-sections.

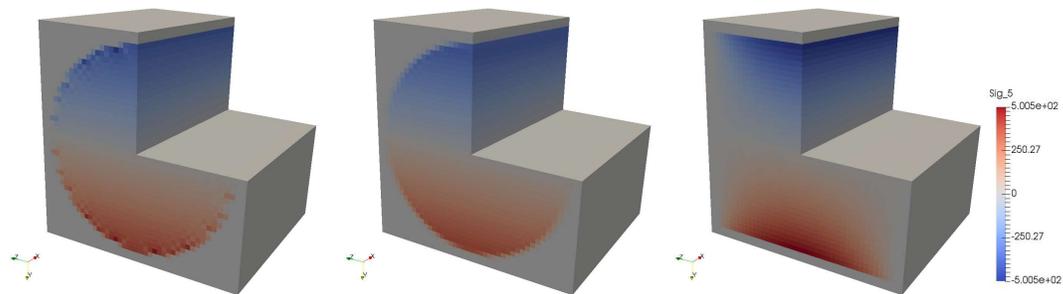


Figure 8 : Shear stress (σ_{13}) field obtained for the square cross-section (right), disk cross-section without (left) and with (middle) composite voxels, for the lowest spatial resolution (40) (for visualization purpose a quarter of the unit-cell is removed) with an homogeneous beam (torsion loading).

3.2.3.2 : Heterogeneous beam torsion

Figure 9 (right) represents the evolution of the torsion moments (or torsion stiffness as $\alpha = 1$) for the three different contrasts. Similarly to the flexion loading cases, the effect of inclusions on the stiffness is quite moderate, even if a bit more pronounced for the highest contrast (1000) with an increase from $1.08 \cdot 10^8$ N.m to $1.41 \cdot 10^8$ N.m. In addition, and in agreement with the flexion loading case: the stiffening (or softening) induced by the stiff (or soft) inclusions, with respect to the homogeneous beam, corresponds to an additional positive (or negative) torsion stiffness that is rather independent of the beam cross-section.

The convergence analysis of the FFT-based algorithm (fixed-point algorithm combined with a convergence acceleration procedure), presented on Table 4, draws conclusions very similar to the flexion loading case. For the sake of conciseness, the reader is invited to refer to the analysis of Table 3 for flexion in section 3.2.2.2. The main difference arises from the fourth conclusion: in the torsion

case, for the square cross-section, increasing the spatial resolution do not deteriorates the convergence.

Finally, the analysis of the local stress fields focuses on the simulations with an elastic contrast of 1000 that induces the highest contribution to the torsion stiffness (compared to the homogeneous beam, see Figure 9 (right)) and exhibits the worst algorithm convergence (see Table 4). As for the flexion loading case, the stress field in and around the inclusion (zooms in Figure 9) does not seem affected by the beam cross-section (square or disk), which is also consistent with the macroscopic observation of an additional contribution on the torsion stiffness independent of the cross-section. If spurious oscillations almost disappear in torsion, these smoother solutions are not associated to a better convergence of the algorithm when comparing Table 3 with Table 4.

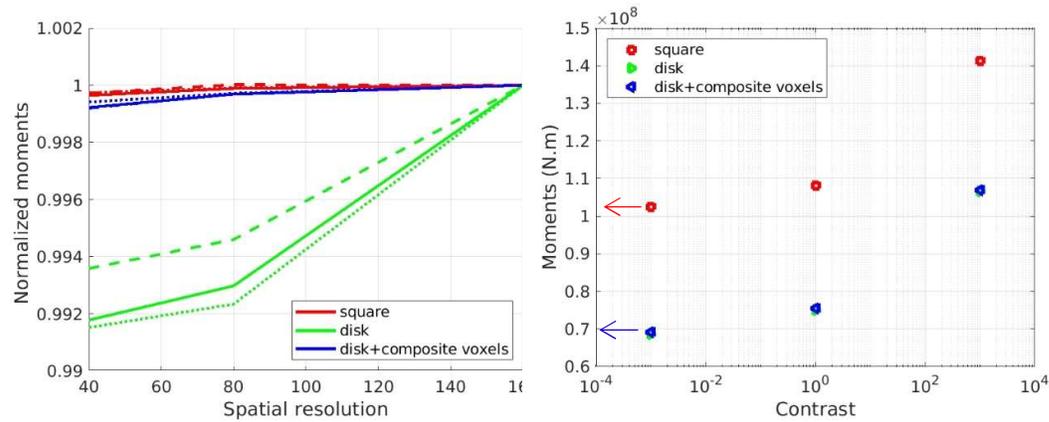


Figure 9 : Evolution of the torsion moments (normalized by their converged values obtained for the highest resolution) as a function of the spatial resolution; with solid, dotted and dashed lines respectively for contrasts 1, 0 and 1000 (left). Evolution of the converged values of the moments (obtained for the highest resolution) as a function of the contrast (the arrows symbolize infinite contrasts) (right). Note that 'disk' and 'disk+composite voxels' symbols are superimposed, confirming that the moments obtained with the 'disk' (without composite voxel) at resolution 160 are converged values.

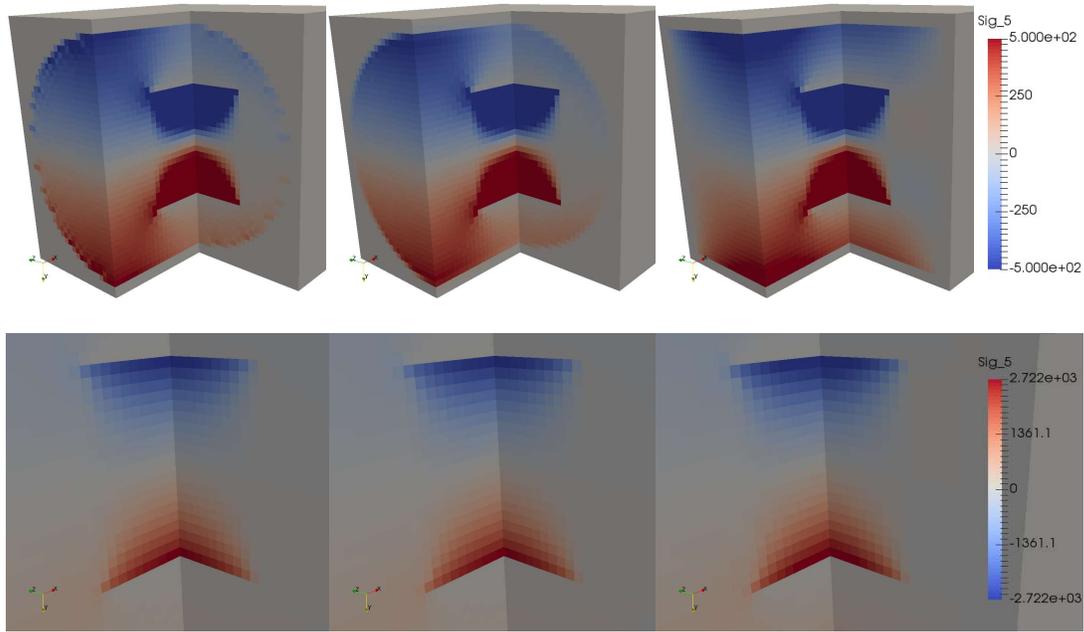


Figure 10 : Shear stress (σ_{13}) field obtained for the square cross-section (right), and the disk cross-section without (left) and without (middle) composite voxels, for the lowest spatial resolution (40) and a contrast of 1000 for the inclusion (for visualization purpose, a quarter of the unit-cell is removed). Bottom figures are zooms on the inclusion with an appropriate color bar.

Resolution	Square			Disk			Disk with Composite Voxel		
	C=0	C=1	C=1000	C=0	C=1	C=1000	C=0	C=1	C=1000
40	18	9	462	19	12	475	57	48	1236
80	19	12	453	21	12	648	57	51	1437
160	25	16	378	21	10	744	51	36	1350

Table 4 : Number of iteration at convergence for the different beams, contrasts, resolutions and use of composite voxels (torsion loading case).

4 : Conclusion

The method described in the present paper allows extending the application domain of any existing FFT-based code, from homogeneous applied strain loading to strain gradient loadings, with a minor and low invasive modification. Actually, the modification consists in adding the applied strain gradient field when adding the homogeneous applied strain field to the periodic strain fluctuation. This is done, first when initializing the strain field and then, at the end of each iteration. The impact on the memory footprint is null, as no additional field needs to be allocated. The price to pay for this simplicity is that only a subset of strain gradients can be applied in that context. However, this subset has proven to be large enough to consider the problems of heterogeneous beams and plates homogenization. As a practical result, the massively parallel code AMITEX_FFTP [1] now offers a new functionality, allowing the users to prescribe torsion and flexion loadings to beam or plate heterogeneous unit-cells.

The approach proposed for the homogenization of beams and plates relies on this method to apply flexion and torsion loadings to heterogeneous unit-cells enlarged with void voxels to account for traction free boundary conditions. As an FFT-based method dedicated to the homogenization of plates had previously been proposed in [27], all the simulations reported in [27] have been reproduced. These comparisons, together with analytical and Finite Element comparisons, validate the approach and demonstrates that a non-specific FFT-based solver, with a minor modification, can be almost as precise and efficient as a dedicated one.

The extension of the method proposed for plates in [27], to the homogenization of beams with any arbitrary cross-section do not seem straightforward. To the best of the author's knowledge, it has been considered here, for the first time with an FFT-based solver. The approach is partially validated from simulations of homogeneous beams, with disk and square cross-sections, submitted to flexion and torsion. Simulations of heterogeneous beams with void or stiff inclusions (with a high elastic contrast of 1000) demonstrates the robustness of the solver. In addition, the use of composite voxels, proves once again its ability to improve the numerical solution when voxels are crossed by an interface. Here, the interface is the beam boundary, and composite voxels consist of two phases: the void and the beam material. Applied to a beam with a disk cross-section, composite voxels with the Voigt homogenization rule improve the estimation of macroscopic moments (torsion, flexion) and reduces spurious oscillations observed in torsion in the neighborhood of the beam boundary. Surprisingly, in spite of smoother fields, the use of composite voxels deteriorates the convergence of the algorithm. This point should be clarified. From the application point of view, it is noticeable that for the considered heterogeneities, located at the beam center, the additional stiffness induced by the presence of inclusions is quite moderate and independent of the beam cross-section.

As future prospects, the approach proposed for the homogenization of beams and plates could now be applied to more complex, but of practical interest, microstructures such as stranded cables and corrugated beams or plates, as studied in [6]. Its straightforward extension to non-linear behaviors should also be tested, as well as the extension to finite strains proposed but not applied in the paper. Finally, another interesting application comes with the use of FFT-based solvers to simulate volume elements for which DIC or DVC (Digital Image or Volume Correlation) measurements have been performed [9]. Up to now, FFT-based solvers can apply the average strain measured experimentally. The present method will allow extending the loading to strain gradients components measured experimentally. It could be useful for example if the in-situ tensile test device induces spurious flexion or torsion loadings.

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Annex A

All the simulation cases reported in [27] have been reproduced with our approach and results are gathered in the following tables for the different contrasts and loading cases. The absolute values are respectively the tension and bending stiffness $A_{22} = N_{22}/E_{22}$ and $D_{22} = M_{22}/\chi_{22}$ (in GPa/m).

Regarding the column “iteration” : the first value is the number of iteration at convergence of our code AMITEX_FFTP, based on a field equilibrium criterion, and the second value correspond to the number of iterations to reach the convergence criterion used in [27] (relative difference of strain energy between two iterations less than 10^{-4}).

Contrast 0 : $(E_{inclusion}/E_{matrix}) = (0/1)$ GPa

Tension

Resolution	FEM [27]	This study (<i>rel.error</i>)	FFT [27] (<i>rel. error</i>)	Iterations	Iterations [27]
16x16	0.5840	0.5822(-0.3%)	0.5826(-0.24%)	27/8	8
32x32	0.5840	0.5834(-0.1%)	0.5837(-0.05%)	44/11	9
64x64	0.5840	0.5838(-0.07%)	0.5839(-0.01%)	44/14	9
128x128	0.5840	0.5838(-0.07%)	0.5840(~0%)	47/15	9

Flexion

Resolution	FEM [27]	This study (<i>rel.error</i>)	[27] (<i>rel. error</i>)	Iterations	Iterations [27]
16x16	8.224e-4	8.204e-4(-0.24%)	8.242e-4(0.22%)	14/5	8
32x32	8.224e-4	8.219e-4(-0.06%)	8.228e-4(0.05%)	14/5	8
64x64	8.224e-4	8.230e-4(0.07%)	8.225e-4(0.01%)	14/5	8
128x128	8.224e-4	8.216e-4(-0.1%)	8.224e-4(~0%)	17/5	8

Contrast 0.001 : $(E_{inclusion}/E_{matrix}) = (1/1000)$ GPa

Tension

Resolution	FEM [27]	This study (<i>rel.error</i>)	FFT [27] (<i>rel. error</i>)	Iterations	Iterations [27]
16x16	58.495	58.329(-0.28%)	58.363(-0.23%)	27/8	8
32x32	58.495	58.455(-0.07%)	58.472(-0.04%)	38/11	9
64x64	58.495	58.484(-0.02%)	58.502(0.01%)	44/14	9
128x128	58.495	58.487(-0.01%)	58.506(0.02%)	47/15	9

Flexion

Resolution	FEM [27]	This study (<i>rel.error</i>)	FFT [27] (<i>rel. error</i>)	Iterations	Iterations [27]
16x16	0.08225	0.08206(-0.23%)	0.08244(0.23%)	14/5	8
32x32	0.08225	0.08221(-0.05%)	0.08230(0.06%)	14/5	8
64x64	0.08225	0.08232(0.08%)	0.08227(0.02%)	14/5	8
128x128	0.08225	0.08217(-0.1%)	0.08226(0.01%)	17/5	8

Contrast 10: ($E_{inclusion}/E_{matrix}$) = (10/1) GPa

Tension

Resolution	FEM [27]	This study (<i>rel.error</i>)	FFT [27] (<i>rel. error</i>)	Iterations	Iterations [27]
16x16	0.16288	0.16267(-0.13%)	0.16209(-0.49%)	48/14	15
32x32	0.16288	0.16284(-0.02%)	0.16257(-0.19%)	38/17	16
64x64	0.16288	0.16287(-0.01%)	0.16279(-0.06%)	59/17	16
128x128	0.16288	0.16290(0.01%)	0.16287(-0.01%)	75/17	16

Flexion

Resolution	FEM [27]	This study (<i>rel.error</i>)	FFT [27] (<i>rel. error</i>)	Iterations	Iterations [27]
16x16	1.0652e-4	1.0597e-4(-0.5%)	1.0701e-4(0.46%)	32/6	18
32x32	1.0652e-4	1.0638e-4(-0.13%)	1.0659e-4(0.07%)	30/6	18
64x64	1.0652e-4	1.0659e-4(0.07%)	1.0654e-4(0.02%)	35/6	18
128x128	1.0652e-4	1.0642e-4(-0.1%)	1.0654e-4(0.02%)	32/6	18

Annex B

The volume fraction of beam (cylinder with disk cross-section) within composite voxels is approximated from the intersection area between two disks: the disk base of the cylinder and a disk of radius R_{cv} centered on the voxel, with R_{cv} the radius of the encompassing circle.

$$\begin{aligned} S &= S_1 + S_2 \\ S_1 &= R_0^2 \arccos\left(\frac{d_i}{R_0}\right) - d_i \sqrt{R_0^2 - d_i^2} \\ S_2 &= R_{cv}^2 \arccos\left(\frac{d_1 - d_i}{R_{cv}}\right) - (d_1 - d_i) \sqrt{R_{cv}^2 - (d_1 - d_i)^2} \\ d_i &= \frac{R_0^2 - R_{cv}^2 + d_1^2}{2d_1} \\ f &= \frac{S}{\pi R_{cv}^2} \end{aligned} \tag{40}$$

In practice, in order to avoid too low (or high) volume fractions, the detection of composite voxels uses a distance of $0.9345R_{cv}$ which corresponds to a threshold of 1% of volume fraction (i.e. below this value a voxel is not considered as composite).