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A Numerical Tool for Periodic Heterogeneous Media: Application to Interface in Al/SiC Composites

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A wavelet-Galerkin method for periodic heterogeneous media is presented. The advantages are to remove the mesh and to make adaptivity easier. Numerical results are presented. A specific study of interfaces in a Al-SiC composite is given.

1 Introduction

A great number of recent papers are concerned by the solution of partial differential equations by wavelet bases ([1,2]). Mainly, these works deal with one-dimensional or scalar two-dimensional problems. The solution of the elastostatics system by this kind of method is not usual ([3,4]). Boundary problems on open bounded sets are very difficult to treat ([5]). Nevertheless, periodic conditions on elementary bounded sets are natural for the use of wavelet transform. In this paper, we show how to use such a technique and we give applications to interfaces in Al-SiC composite. In the first section we give the notations and the necessary mathematical background. In the second section we present the mechanical problem: the homogenization of periodic heterogeneous media. The third section is concerned with the algorithm: a wavelet-Galerkin method using Daubechies wavelets ([6]). The determination of the macroscopic coefficients is treated in the fourth section. Applications and numerical results are described in the fifth section. Concluding remarks are given.

2 Notations and Mathematical Background

In this section, we present the notations used in the following of the paper. The sets of kinematically and statically admissible fields are denoted H , L , and S . Let

$$L = (L^2(Y))^3 \text{ and } H = (H_p^1(Y))^2$$

$$S = \{v \in L_{loc}^2(Y), v(x_1 + k_1, x_2 + k_2) = v(x_1, x_2) \text{ a.e., } k_1, k_2 \in \mathbb{K}\} \quad (1)$$

$$H_p^1(Y) = \{v \in S, v_{,i} \in L^2(Y), i = 1, 2\}.$$

$u_{,i}$ denotes the i th partial derivative of the function u . We denote C the fourth-order elasticity tensor, e the strain tensor, and σ the stress tensor. In the following $Y =]0, 1[^2$. To construct a wavelet basis of H , we use the compactly supported wavelets introduced by I. Daubechies [6] which is a basis of $L^2(\mathbb{R})$. These wavelets are periodized in order to obtain bases of S . By tensorial and cartesian products wavelet bases of H are obtained ([7]). We denote Ψ^l , $l = 1, 2, 3$, and Ψ^0 the wavelets and the scale functions (six degrees-of-freedom for each point), $N^j = 2^j - 1$ and $\Lambda^j = [0, N^j]^2$.

Let V_j be the subspace of dimension 2^{2j+1} of H generated by this wavelet at approximation level j . An element of $V_{j_{\max}}$ is thus written as

$$u(x_1, x_2) = (u_1(x_1, x_2), u_2(x_1, x_2))$$

$$u_d = \sum_{\kappa \in \Lambda_{j_0}} u_{j_0 \kappa}^{d0} \Psi_{j_0 \kappa}^0 + \sum_{l=1}^3 \sum_{j=j_0}^{j_{\max}} \sum_{\kappa \in \Lambda_j} u_{j \kappa}^{dl} \Psi_{j \kappa}^l. \quad (2)$$

j_0 is a given integer, $d = 1$ or 2 and $\kappa = (k_1, k_2)$.

3 The Mechanical Problem

We consider a multiphase isotropic elastic composite (Fig. 1) and we intend to study the behavior of this heterogeneous media. We introduce the notion of equivalent material, i.e., we mean that under the same loadings, this equivalent material has globally the same response. In former papers ([8,9]) bounds for the bulk and shear moduli of a two-phase composite have been given. Without going into further detail, these bounds depend on the shear and bulk moduli of the two phases and on the volumic fraction of the two phases in the composite. In the same way, the theory of periodic homogenization ([10]) focuses on an idealized composite

Fig. 1 An example of a composite and its representative volume

consisting of the juxtaposition of identical heterogeneities and classically, we need to solve an elastostatics problem on a representative volume Y (Problem P):

Problem. P

$E \in L$ be given, find $u \in H$ such that $a(u, v) = l(v) \quad \forall v \in H$

$$\text{with } a(u, v) = \int_Y \sigma(u) : e(v) dy = \int_Y C(y) e(u) : e(v) dy$$

$$\text{and } l(v) = - \int_Y C E : D(v) dy$$

Because of the nonuniqueness of the solution of problem (P) (defined within a translation), problem (P) is replaced by problem (P_ε) (“viscous” problem):

Problem. P_ε

$E \in L$ be given, find $u \in H$ such that $a_\varepsilon(u, v) = l(v) \quad \forall v \in H$

$$\text{with } a_\varepsilon(u, v) = \int_Y \sigma(u) : e(v) dy + \varepsilon \int_Y u v dy$$

It can be shown that the solution of this problem converges toward the solution of problem (P) with average equal to zero ([4]).

Remarks.

(i) The problem (P) is solved classically by a finite element method or by fast Fourier transform ([11]). We have chosen to introduce wavelet methods in order to eliminate the notion of mesh and to eliminate Gibbs phenomena.

(ii) If the discretization of problem (P) in a orthonormal wave-

Fig. 2 Wavelet element matrix ($j_0 = J, j_{\max} = J+4$)

let basis leads to the system $KU=B$, then the discretization of problem (P_ε) leads to $(K+\varepsilon Id)U=B$, where Id is the identity matrix.

(iii) The tensor C could be given by the image (pixels) of the microstructure.

4 Wavelet-Galerkin Method

The variational problem (P_ε) is discretized by a Galerkin method. We have introduced a wavelet basis because of their localization and adaptivity properties. The projection of the plane elasticity operator into the wavelet basis ([7]) is given by a stiffness matrix K where the “elementary matrix” of order 2 is

$$K_{jj'\kappa\kappa'}^{ll'} = \begin{bmatrix} F_{1111}+F_{1321}+F_{3112}+F_{3322} & F_{1221}+F_{1311}+F_{3222}+F_{3312} \\ F_{1212}+F_{2322}+F_{3111}+F_{3321} & F_{2222}+F_{2312}+F_{3221}+F_{3311} \end{bmatrix} \quad (3)$$

where

$$F_{pq\alpha\beta} = \int_Y C_{pq} \Psi_{j\kappa,\alpha}^l \Psi_{j'\kappa',\beta}^{l'} dx_1 dx_2.$$

We have chosen to decompose the tensor C on a wavelet basis at level J noted θ . In the numerical applications, Haar wavelet is used with its compact support equal to the square $[l_1/2^j, (l_1+1)/2^j] \times [l_2/2^j, (l_2+1)/2^j]$. This wavelet is constant on this support which is a pixel of the image representation. Thus, the wavelet coefficient θ_{jl} is equal to the value of the tensor C on this pixel. Due to the form of the wavelets (Cartesian and tensorial products of one dimensional wavelets) the computation of the coefficients of the matrix K leads to the determination of elementary terms which are integral of products of three one-dimensional wavelets and their derivatives:

$$\int_0^1 \theta_{jr} \frac{d^m \Psi_{js}}{dx^m} \frac{d^n \Psi_{jt}}{dx^n}, \quad m, n = 0, 1. \quad (4)$$

These terms are obtained by the determination of eigenvectors of a low-order matrix ([7,12]). The right-hand side of the problem corresponding to the term $l(v)$ in problem (P_ε) is computed by a similar technique ([4,5]). Classically, the matrix K is a sparse matrix (Fig. 2). Because of the form of the wavelets bases, it seems natural to solve the linear system which is a discretized version of problem (P_ε) by multigrid techniques ([13,14]). Nevertheless, we have chosen to use a conjugate gradient method.

5 Determination of the Macroscopic Coefficients

The determination of the elastic macroscopic coefficients corresponds to the computation of the macroscopic stress tensor Σ :

$$\Sigma = \int_Y (CE + Ce(u)) dx_1 dx_2. \quad (5)$$

The computation of these terms is in the same way as the matrix and the right-hand side [4].

6 Numerical Results

We present the example of a three-phase fiber-matrix composite (Fig. 3): SiC for the fiber, Al for the matrix and an interface. The Lamé coefficients associated to the interface are $\lambda \eta^\alpha$ and $\mu \eta^\beta$ where $\eta \gamma$ is the thickness of the interface. α and β are real positive parameters and γ is a given function with a sufficient regularity. We have shown in former papers ([15–17]) that when η tends to zero, i.e., the thickness and the rigidity parameters tend to zero, we obtain an elastostatic limit problem with an interface law. This interface law keeps in memory the mechanical and geometrical properties of the layer. The interface law is given in

Fig. 3 Al-SiC composite with an interfacial zone (thickness η)

Table 1 Interface laws

$\mu/\varepsilon \rightarrow 0$	$u_N = 0 \quad \sigma_T = 0$	$\sigma_N = \frac{\bar{\lambda}}{\gamma} u_N \quad \sigma_T = 0$	$\sigma_n = 0$
$\mu/\varepsilon \rightarrow \bar{\mu}$	$u_N = 0 \quad \sigma_T = \frac{\bar{\mu}}{\gamma} u_T$	$\sigma_N = \left(\frac{\bar{\mu}}{\gamma} + 2 \frac{\bar{\lambda}}{\gamma} \right) u_N$	$\sigma_N = 2 \frac{\bar{\lambda}}{\gamma} u_N$
		$\sigma_T = \frac{\bar{\mu}}{\gamma} u_T$	$\sigma_T = \frac{\bar{\mu}}{\gamma} u_T$
$\mu/\varepsilon \rightarrow \infty$	$u = 0$ $\lambda/\varepsilon \rightarrow \infty$	$u = 0$ $\lambda/\varepsilon \rightarrow \bar{\lambda}$	$u = 0$ $\lambda/\varepsilon \rightarrow 0$

Fig. 4 Jump of displacement for different values of α and β ($M=3$)

Table 1 with respect to the value of the parameters α and β . α and β determine how the thickness and the rigidity tend to zero. It is necessary to quantify the limit, in other words we seek an interval in which the initial problem could be approximated by the limit problem for which the solution is more easy to obtain. On the other hand, it is very important to quantify the influence

Fig. 5 Homogenized coefficient for different values of α and β ($M=3$)

of the interface on the macroscopic coefficients, i.e., on the elastic behavior of a structure. Due to the shape and the thickness of the interface this problem is very difficult to treat by classical techniques.

We present, in Fig. 4, a study of the convergence of the jump of displacement in the interface for the case $\gamma=1$, for two values of α and β . λ and μ are chosen as Aluminum coefficients. In this case the jump is equal to zero in the interface law. We have found that for values of η smaller than 0.4 p.c. of the structure the interface law could be considered as valid. Note that the displacement in the interface has the form ([16]) $u(r, \theta) \approx ru(\theta) + u_0$. Figure 5 shows the influence of the thickness parameter on the first component of the homogenized elasticity tensor for different values of α and β . For small values of the thickness (η smaller than 0.2 p.c. of the structure) it is convenient to neglect the interface. Note that for values of the thickness larger than 0.02, the coefficient depends linearly on the thickness.

7 Concluding Remarks

In this paper, we have shown a robust tool to compute the overall response of a composite. In particular, our method is able to compute the influence of an interface even at a very small level. In the future, we want to investigate more complex materials such random materials ([18]) or other kind of interfaces ([19,20]).

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