PARALLEL IMPLEMENTATION OF THE AEH TECHNIQUE FOR THE SOLUTION OF PLANE MULTIPHASIC PROBLEMS

BÁRBARA DE M. QUINTELA [1], ANNA PAULA G. FERREIRA [2], MICHÈLE C. RESENDE FARAGE [3] , MARCELO LOBOSCO [4]
Mestrado em Modelagem Computacional, Universidade Federal de Juiz de Fora Campus Universitário, 36036-330, Juiz de Fora, MG, Brasil
[1]barbara@ice.ufjf.br, [2]paula.guida@engenharia.ufjf.br, [3]michele.farage@ufjf.edu.br, [4] marcelo.lobosco@ice.ufjf.br

ABSTRACT

The Asymptotic Expansion Homogenization (AEH) technique is used to estimate the effective properties of heterogeneous media with periodical microstructure. A considerable computational effort can be necessary even though the adopted models are quite simple. For this reason, parallelization is often necessary to achieve good performance. This work presents a first attempt to parallelize the AEH implementation code. Although the parallelization process is in a very early stage, the preliminary results show that the parallel version provides up to a 30% improvement in application speed. This work consists on a step towards a numerical tool for the analysis of more complex and three-dimensional periodic cells. The two-dimensional AEH was implemented in the C programming language for the future generalization to three-dimensional problems employing the available parallelization tools.

KEYWORDS: Asymptotic Homogenization, Heterogeneity, Periodicity, Finite Element Method, Parallel Computing

1. INTRODUCTION

The Asymptotic Expansion Homogenization (AEH) is a multiscale technique applied to the estimation of effective properties of heterogeneous media with periodical microstructure. Synthetic and natural composite materials may be modelled by means of this numerical technique. The macroscopic mechanical behavior of heterogeneous materials - which, in general, may look like homogeneous in a macroscopic level - may be significantly affected by their microscopic structure - where the heterogeneities are observed. For this reason, multiscale techniques, which take into account the microscale characteristics, are important to an adequate simulation of heterogeneous systems, as well as to the industrial development of new materials based on pre-defined properties.

During a preliminary study Ferreira et al. (2007); Farage et al. (2008) developed at the NUMEC (*Núcleo de Pesquisa em Métodos Computacionais em Engenharia* - Research Group on Computational Methods in Engineering, Federal University of Juiz de Fora, Brazil), the AEH was employed to evaluate the effective mechanical properties of plane periodic structures. Even though the adopted models were quite simple, the need for refined meshes resulted in considerable computational efforts, demanding rather long processing time. In order to reduce the processing time, parallelization can be used. In this work we present a first attempt to parallelize the code using OpenMP. Preliminary results show that the parallel version provides up to a 30% improvement in application speed.

The rest of the paper is organized as follows. Section 2 presents the Asymptotic Expansion Homogenization technique, while section 3 presents its implementation. In section 4 we discuss the parallelization approach. Sections 5 and 6 present the experiments, and section 7 concludes the work.

2. ASYMPTOTIC EXPANSION HOMOGENIZATION

The *A*symptotic *E*xpansion *H*omogenization (AEH) is based on the assumption that a heterogeneous medium may be represented by a homogeneous counterpart since its microstructure is periodic or repetitive. The technique is based on the uncoupling of the different scales of a material, extrapolating the results from inferior or heterogeneous scales in order to obtain global or homogenized properties Sanchez-Palencia (1980); Murad et al. (2001); Murad and Moyne (2002); Romkes and Oden (2004); LNCC (2005).

As applying the AEH, a very important aspect is the definition of the geometric characteristics of the periodic cell, which is the smaller microstructural volume able to adequately represent the global constitutive behavior of the medium. By knowing the heterogeneous properties of a cell, it is assumed that those properties are periodically repeated over the structure.

Basically, in periodic structures that present two scales, the AEH consists of uncoupling those scales into a *microscale* and a *macroscale*. The general procedure of the AEH applying the *F*inite *E*lements *M*ethod (FEM) consists of the following steps, as stated in reference Chung et al. (2001):

1. definition of a global body X in a coordinate system x_i, consisting of the structure without the microstructural details, and a local body Y in coordinates y_i, consisting of one microstructure period;

2. meshing of X and Y in finite elements;

3. approximation of a primary variable of the problem into asymptotic series around a scale parameter ϵ, which relates the two coordinate systems (x_i and y_i);

4. derivation of hierarchical equations, specific for the treated problem;

5. definition of a homogenized quantity in the microscale Y;

6. resolution of the homogenized problem in the macroscale X.

The homogenization deals with partial differential equations related to heterogeneous materials with periodical structure considering the assumption that the amount of periodic cells tends to infinity. The scale parameter ϵ is the characteristic dimension of the period (or periodic cell). Figure 1, adapted from reference Cioranescu and Donato (1999), illustrates the physical meaning of periodicity and the scales uncoupling in a two-dimensional problem.

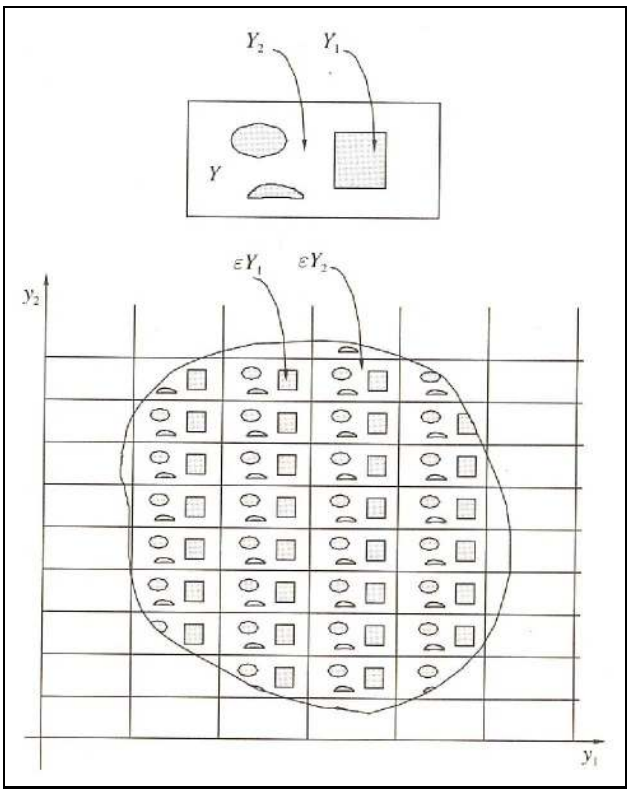


FIGURE 1: Periodic structure adapted from Cioranescu and Donato (1999).

In practical purposes, the main interest is getting to know the global behavior of a composite by considering that the heterogeneities dimensions - or that the scale parameter ϵ - tends to zero Cioranescu and Donato (1999).

The coefficients of the describing differential equations are the characteristics of the studied material, depending on ϵ. Concerning a composite with a ϵ-periodic distribution, those coefficients are not easy to evaluate. Consideration of the limit case of $\epsilon \rightarrow 0$ leads to a *homogenized* problem, with constant coefficients that may be calculated with the help of numeric techniques, such as the Finite Element Method Sanchez-Palencia (1980); Cioranescu and Donato (1999); LNCC (2005).

In the present work, the AEH is employed to evaluate the homogenized elastic properties of composites. The primary variable is a smooth displacement function $u^i(x, y)$, which presents periodicity in the microscale Y, related to the macroscale by means of the equation: $y = x/\epsilon$.

2.1 AEH applied to Linear Elasticity

By considering a material whose microstructure is composed of multiple phases, periodically distributed over the body Sanchez-Palencia (1980); Chung et al. (2001), the periodic elastic material properties are defined by the following relation:

$$D^{\epsilon}_{ijkl} = D_{ijkl}\left(\frac{x}{\epsilon}\right) \tag{1}$$

where $(\ )^{\epsilon}$ denotes quantities related to the *actual* non-homogeneous medium; the function D^{ϵ}_{ijkl} stands for the material's properties variations in the heterogeneous microstructure Y.

The linear elasticity problem is described by the equilibrium equation 2, boundary conditions 3 and 4, strain-displacement relation 5 and constitutive relation 6:

$$\frac{\partial \sigma^{\epsilon}_{ij}}{\partial x^{\epsilon}_j} + f_i = 0 \text{ in } \Omega \tag{2}$$

$$u^{\epsilon}_i = 0 \text{ in } \partial_1\Omega \tag{3}$$

$$\sigma^{\epsilon}_i n_j = F_i \text{ in } \partial_2\Omega \tag{4}$$

$$\varepsilon_{ij}(u^{\epsilon}) = \frac{1}{2}\left(\frac{\partial u^{\epsilon}_i}{\partial x^{\epsilon}_j} + \frac{\partial u^{\epsilon}_j}{\partial x^{\epsilon}_i}\right) \tag{5}$$

$$\sigma^{\epsilon}_{ij} = D^{\epsilon}_{ijkl}\varepsilon_{kl}(u^{\epsilon}) \tag{6}$$

where the scale parameter ϵ identifies quantities related to the *actual* heterogeneous material behavior; σ^{ϵ}_{ij} is the $_{ij}$ term of the internal stresses tensor and f_1 is the body force in the dominium Ω; u^{ϵ}_i is the displacement in direction i; n_j is the vector normal to the boundary $\partial\Omega$ and F_1 is the external force applied on the boundary and ε_{ij} is the $_{ij}$ term of the strains tensor.

The displacements are approximated by an asymptotic series in ϵ, given by equation 7:

$$u^{\epsilon}_i(x^{\epsilon}) = u^{(0)}_i(x, y) + \epsilon u^{(1)}_i(x, y) + \epsilon^2 u^{(2)}_i(x, y) + \dots \tag{7}$$

where $u^{(0)}_i$ is the macroscopic displacement and $u^{(1)}_i, u^{(2)}_i, \dots$ stand for the periodic displacements in more refined scales. As the heterogeneous *actual* medium is represented by two coordinate systems (x and $y = x/\epsilon$), the derivatives originally in x^{ϵ} must

be expanded in a chain rule given by:

$$\frac{\partial}{\partial x_i^\epsilon} = \frac{\partial}{\partial x_i} + \frac{1}{\epsilon}\frac{\partial}{\partial y_j} \tag{8}$$

In order to obtain the uncoupled equations that describe the microscale and the macroscale problems, the displacement u_i is replaced by equation 7 in the set of equations 2 to 6. The basis of the approximation is the assumption of $\epsilon \to 0$, indicating that the number of periodic cells tends to infinity and the actual non-homogeneous structure is then approximated by a homogeneous one. In order to validate such an approximation, the resulting coefficients of ϵ with negative exponent must be identically nulls. That leads to the conclusion that the homogenized solution $u^{(0)}$ is constant over the microscopic scale ($u^{(0)}$ does not depend on y), as indicated by the following equation:

$$\frac{\partial}{\partial y_j} D_{ijkl}\left(\frac{\partial u_k^0}{\partial y_l}\right) = 0 \tag{9}$$

Microscale and macroscale equation Equation 10 relates the perturbation term $u_i^{(1)}$ to the homogenized term $u_i^{(0)}$ and represents the microscale problem:

$$-\frac{\partial}{\partial y_j} D_{ijkl}\frac{\partial u_k^{(1)}}{\partial y_l} = \frac{\partial}{\partial y_j} D_{ijkl}\frac{\partial u_k^{(0)}}{\partial x_l} \tag{10}$$

where $u^{(0)}$ is a known quantity and $u^{(1)}$ is the unknown.

The variational formulation of the problem described by equation 10 is:

$$\int_Y D_{ijkl}\frac{\partial u_k^{(1)}}{\partial y_l}\frac{\partial \nu}{\partial y_k}dy = \frac{\partial u_k^{(0)}}{\partial x_l}\int_Y \frac{\partial D_{ijkl}}{\partial y_l}\nu dy \tag{11}$$

where ν is a weight function. In order to avoid the necessity of solving $u_i^{(1)}$ in the periodic cell for every variation of $u_i^{(0)}$, the solution of the variational problem described by expression 11 is given by an auxiliary equation in Y, solved through the Finite Element Method, relating $u_i^{(1)}$ to $\frac{\partial u_i^{(0)}}{\partial x_j}$ as follows:

$$u_i^{(1)} = \xi_i^{kl}\frac{\partial u_k^{(0)}}{\partial x_l} + \tilde{u}_i^{(1)}(x) \tag{12}$$

where $\tilde{u}_i^{(1)}(x)$ is an integration constant and ξ_i^{kl} is the solution to the auxiliary variational problem consisting of determining $\xi_i^{kl} \in V_Y$ so that:

$$\int_Y D_{ijkl}\frac{\partial \xi_k^{mn}}{\partial y_l}\frac{\partial \nu_i}{\partial y_j}dy = \int_Y \nu_j \frac{\partial D_{ijmn}}{\partial y_i}dy; \forall \nu_i \in V_Y \tag{13}$$

The function ξ_i^{kl} is known as elastic corrector or characteristic function Chung et al. (2001), independent of $u^{(0)}$. Once ξ_i^{kl} is determined, the stresses and strains in the microscale are calculated with the help of the following relations:

$$\varepsilon_{ij}^{(0)} = \left(\delta_{im}\delta_{jn} + \frac{\partial \xi_i^{mn}}{\partial y_i}\right)\frac{\partial u_m^{(0)}}{\partial x_n} \tag{14}$$

$$\sigma_{ij}^{(0)} = D_{ijmn}\left(\delta_{im}\delta_{jn} + \frac{\partial \xi_i^{mn}}{\partial y_i}\right)\frac{\partial u_m^{(0)}}{\partial x_n} \tag{15}$$

which describe the microscopic problem (in y).

In order to solve the macroscale problem it is necessary to determine the elastic properties tensor relating the homogenized stresses and strains in x. To this end, the average operator defined as $\langle . \rangle = \frac{1}{Y}\int_Y (.)dy$ is applied to $\sigma^{(0)}$ and $\varepsilon^{(0)}$ in expression 15, leading to:

$$\langle \sigma^{(0)} \rangle = D_{ijmn}^h \langle \varepsilon^{(0)} \rangle \tag{16}$$

where $\langle \sigma^{(0)} \rangle$ and $\langle \varepsilon^{(0)} \rangle$ are the macroscale stresses and strains, respectively, and the homogenized elastic properties tensor is given by:

$$D_{ijmn}^h = \frac{1}{|Y|}\int_Y D_{ijmn}\left[\delta_{im}\delta_{jn} + \frac{\partial \xi_i^{mn}}{\partial y_j}\right]dy \tag{17}$$

Equations 16 and 17 define the macroscale problem.

3. AEH IMPLEMENTATION

3.1 Problem Description

This work derives from two previously published studies Ferreira et al. (2007); Farage et al. (2008, 2009) in which the HEA2D program was introduced. These works validated the use of the HEA2D program to the evaluation of homogenized elastic properties of plane periodic cells. For this purpose, numerical results obtained via the HEA2D program were compared to experimental measurements of lightweight aggregate concretes Ke et al. (2006b,a), showing good agreement.

The current versions of the program evaluate the effective or homogenized elastic tensor of two-dimensional cells through the finite element methods, employing six-noded finite triangular elements. The HEA2D application was initially implemented in the integrated technical computing environment MATLAB© Mathworks (2007). However, by observing that complex meshes severely hurts performance, it was decided to port the application to the C programming language Quintela et al. (2009). The C version of HEA2D was then used to implement the parallel version. Its purpose is the same: the evaluation of the effective elastic tensor for periodic cells, to obtain the

macroscopic properties of periodic n-component composites.

3.2 The program

The HEA2D inputs are the geometrical and mechanical characteristics of the cell and the output is the effective elastic tensor for the material. The following steps are performed to calculate the homogenized properties:

1. Data input. Information about the finite element mesh, boundary conditions of the periodic cell and mechanical properties of their α phasis (elastic modulus E_α and Poisson's ratio ν_α);

2. Assemblage of the stiffness matrix $[K]$ and the independent tensor $[F]$ (right-hand side of the equilibrium equation).

$$[K] = \left[\sum_{i=1}^{nelm} B^T DBJ\right] \tag{18}$$

and

$$[F] = \left[\sum_{i=1}^{nelm} B^T DJ\right] \tag{19}$$

where *nelm* is the number of elements in the mesh, *B* is the derivation tensor, *D* is the local elastic property tensor (for each α phase that composes the microstruture) and *J* is the Jacobian tensor, which relates the coordinate system to the parametric representation of the geometry;

3. Solution of the linear equations system. The system of equations is solved to obtain the elastic corrector tensor *U*, represented by ξ_i in Eq. (13):

$$\left[\sum_{i=1}^{nelm} B^T DBJ\right][U] = \left[\sum_{i=1}^{nelm} B^T DJ\right] \tag{20}$$

4. Determination of the homogenized property tensor, by means of the averaging procedure described by Eq. (17), rewritten herein as:

$$[D_{ef}] = \frac{1}{Y}\left[\sum_{i=1}^{nelm} D(I - BU)|J|\right] \tag{21}$$

where Y is the total body area and I the identity matrix.

Three factorization methods (LU, Cholesky, QR) can be choosen to deal specifically with sparse matrices such as those arising from the finite element method. Also, the approximate minimum degree (AMD) permutation vector is used, since its choice can have a dramatic effect on the amount of fill that occurs during the factorization George and Liu (1989). Thus, the rows and columns of the matrix are reordered before performing the factorization. The user can choose the type of permutation to be performed: natural (no permutation), amd($A + A^T$), amd($S^T * S$) and amd($A^T * A$). The CSparse (Concise Sparse Matrix Package) library Davis (2006) was used to implement the factorization methods and the AMD permutation.

4. PARALLEL VERSION

The parallel version of HEA2D was implemented using OpenMP (*Open Specifications for Multi Processing*) Chapman et al. (2007). OpenMP offers a programming interface for shared memory parallel machines. The programmer uses compilation directives to identify the portions of the source code that should be executed in parallel. The programmer can also specify how the code should be executed. So the first step is to identify the time consuming parts of the HEA2D code.

Two portions of the sequential code were identified as hotspots. The first one is related to the resolution of the system of algebraic equations (the third step described in subsection 3.2) and the other one is the initialization of the sparse matrix using the CSparse library.

```
for i = 0 to 2 do
{
   case i = 0 : b = column 1
   case i = 1 : b = column 2
   case i = 2 : b = column 3

   solve system choosing one
   of the methods having
   b as the unknown

   case i = 0 : x1 = b
   case i = 0 : x2 = b
   case i = 0 : x3 = b
}
```

FIGURE 2: Algorithm for the sequential resolution of the system of equations.

The system of equations can be solved with QR, LU or Cholesky. The system is represented by a matrix with dimensions gll x gll and a matrix of independent terms with dimensions gll x 3, where the unknowns are a matrix with gll x 3. The dimension gll means the total number of degrees of freedom on the global structure. The result is a variational problem of finite elements. The function that solves the system of equations

is called *solve*. It was the first part of the code to be parallelized.

To solve the unknown matrix, the *solve* function calls three times the resolution of the chosen method (QR, LU or Cholesky), one for each column of the unknown matrix. This part can be easily parallelized just solving these three columns at the same time. Figure 2 shows the sequential schema for this portion of code.

```
for i = 0 to (gll - 1) do
{
   for j = 0 to (gll -1) do
   {
      if the ij^th element of
      coefficients matrix
      is not null then
      {
         call function cs_entry
      }
   }
}
```

FIGURE 3: Algorithm for the assemblage of the sparse matrix.

The assemblage of the sparse matrix requires dynamic memory allocation and reallocation. The CSparse function *cs_entry* is responsible for this work. Figure 3 shows the sequential version of the code that uses the *cs_entry* function.

```
#pragma omp parallel for private (b)
#pragma omp shared (c)
for (i =0; i <= 2 ; i++) {
  switch(i){
    case 0: b = Prob->b1; break;
    case 1: b = Prob->b2; break;
    case 2: b = Prob->b3; break;
  }
  ok = cs_cholsol (C, b, order);
  switch(i){
    case 0: Prob->x1 = b; break;
    case 1: Prob->x2 = b; break;
    case 2: Prob->x3 = b; break;
  }
}
```

FIGURE 4: Parallelized code using OpenMP for the resolution of the system.

Three different approaches were adopted to parallelize the code:

1. Parallelization of the resolution of the system of equations (Figure 4);
2. Parallelization of the sparse matrix assemblage (Figure 5);
3. Parallelization of both (Figure 4+Figure 5).

```
#pragma omp parallel for ordered private (j)
#pragma omp shared (gll,kg,list_gll,T)
for (i = 0; i < gll; i++) {
  #pragma omp ordered
  for (j = 0; j < gll; j++) {
    if (kg[list_gll[i] - 1][list_gll[j] - 1] != 0)
      cs_entry (T, i, j, kg[list_gll[i] - 1]
        [list_gll[j] - 1]);
  }
}
```

FIGURE 5: Parallelized code using OpenMP for the assemblage of the sparse matrix.

It should be emphasized that the directive *ordered* must be used to avoid conflicts between the threads. Since the *cs_entry* method reallocs the memory used to store the sparse matrix, the reallocation must be performed in order. The *ordered* directive specifies that code under a parallelized for loop should be executed exactly like a sequential loop Wilkinson and Allen (2005).

5. NUMERICAL EXPERIMENTS

This section presents the results for numerical experiments performed with a 2 GHz Intel Core 2 Quad processor (Q8200), with 4 GB RAM and 2 MB L2 cache. The system runs Rocks 5.2 (kernel 2.6.18). The gcc version 4.1.2 was used to compile the program.

5.1 Experimental Methodology

Aiming to compare the performance of the sequential and parallel versions of the program, distinct types of periodical cells were considered to represent composite materials.

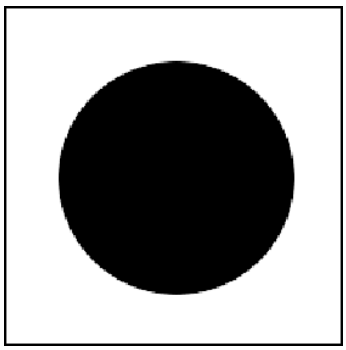


FIGURE 6: Circular.

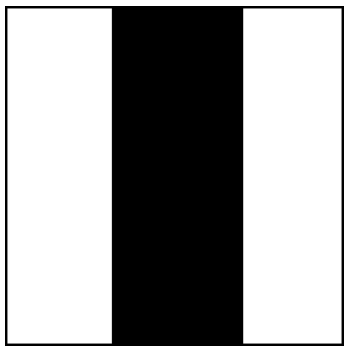


FIGURE 7: Long fiber.

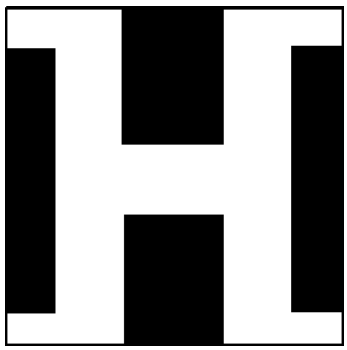


FIGURE 8: Short fiber.

Figure 6 represents a square cell with a circular inclusion that may represent the cross section of a composite reinforced with long aligned fibers. This composite material exhibits isotropic behavior in the represented plane.

The cell shown in Figure 7 is the elementary volume of a laminated composite, for which the elastic tensor may be exactly evaluated. The laminate structured composites are hierarchically a class of great importance among the macroscopically anisotropic composites Torquato (2001). This structural conformation is largely employed to the construction of structures from prescribed properties Torquato (2001).

Figure 8 represents another important class of composite materials, standing for materials reinforced with short fibers. This example, taken from reference Ghosh et al. (1995), presents anisotropic behavior and the effective properties are not exactly evaluated - the quality of the approximated results depend strongly on the refinement of the finite elements mesh.

6. RESULTS

In all the numerical tests, the sequential and parallel versions of the program generated the same homogenized tensor.

The circular inclusion (Figure 6) was analysed with a 1512 elements mesh. The mechanical properties of the components were adopted, for validation purposes, as: matrix elastic modulus $E_m = 1$, inclusion elastic modulus $E_i = 10$, matrix Poisson's ratio $\nu_m = 0.3$ and inclusion Poisson's ratio $\nu_i = 0.03$.

The obtained effective isotropic tensor was:

$$Def = \begin{bmatrix} 1.205 & 0.0713 & 0 \\ 0.0713 & 1.205 & 0 \\ 0 & 0 & 0.5582 \end{bmatrix} \tag{22}$$

The long fiber cell (Figure 7) and the short fibers cell (Figure 8) were taken from reference Ghosh et al. (1995), where the same multiscale technique was employed to analyze a composite with the following properties: $E_m = 72.5GPa$, $E_i = 400GPa$, $\nu_m = 0.33$ and $\nu_i = 0.2$.

The long fiber cell (Figure 7) was modeled by a 1332 elements mesh. The evaluated tensor agrees with the one obtained by Ghosh et al. (1995), given in Eq. 23:

$$Def = \begin{bmatrix} 136.1 & 36.25 & 0 \\ 36.08 & 245.8 & 0 \\ 0 & 0 & 47.31 \end{bmatrix} \tag{23}$$

The short fiber model (Figure 8) presented some differences in comparison to the homogenized tensor obtained by Ghosh et al. (1995), whose non-null values are shown in Table 1. Three different meshes, with varying refinement degrees, were adopted in this case and the obtained results are compared to the reference ones in Table 1. The

first mesh, with 2516 elements, generated the following non-null values for the coefficients Def_{13}, Def_{23}, Def_{31} and Def_{32}: 0.0001, 0.0004, 0.0005 and 0.0009, respectively. This problem was not observed for the two more refined meshes, with 7440 and 22000 elements. As observed in Table 1, some improvements were accomplished with the higher refinement, specially concerning the D_{22} and D_{33} coefficients.

TABLE 1: Comparison of homogenized properties of the three short fiber meshes and reference values.

	Ghosh et al. (1995)	**2516 el**	**7440 el**	**22000 el**
D_{11}	122.4	122.3	122.3	122.3
D_{12}	36.23	36.30	36.32	36.32
D_{21}	36.23	36.29	36.31	36.31
D_{22}	151.2	151.5	151.3	151.2
D_{33}	42.10	42.22	42.16	42.11

A performance comparison between the sequential and the parallel code is presented in Table 2. S_{amd} represents the theoretical speedup calculated using the *Amdahl's law* Wilkinson and Allen (2005) and S is the speedup obtained for each approach. The indexes 1, 2 and 3 represents, respectively, the parallelization of the matrix assemblage (Figure 5), the parallelization of the system solving (Figure 4) and the usage of both approaches (Figure 4 $+$ Figure 5).

TABLE 2: Ideal and obtained speedup factor for each analised case.

	$S_{amd(1)}$	$S_{(1)}$	$S_{amd(2)}$	$S_{(2)}$	$S_{amd(3)}$	$S_{(3)}$
Circular 1512 el	1.2	0.9	1.5	1.3	2.0	1.2
Long 1332 el	1.2	0.9	1.3	1.3	1.7	1.2
Short 2516 el	1.2	0.9	1.3	1.2	1.6	1.1
Short 7440 el	1.3	0.9	1.3	1.2	1.8	1.1
Short 22000 el	1.5	0.9	1.3	1.0	2.0	0.9

As one can see, the parallelization of the system solving ($S_{(2)}$) obtained good results. In particular, we can observe that the ideal speedup is achieved for the long fiber case. The circular and the short fiber cases, with 2516 and 7440 elements, achieved a speedup near to the maximum theoretical values. The only exception is the short fiber with 22000 elements, where the obtained speedup was not so good. The $S_{(1)}$ values indicate a slowdown for all cases. This has impacted also in the third case, when both approaches are used: the speedup factor decreased, when compared to the $S_{(2)}$ case.

7. CONCLUSIONS

In this work, we presented the parallel implementation of the asymptotic expansion homogenization technique using OpenMP. The experiment has shown that the parallelization was effective in improving the performance, providing gains up to 30%.

We intend to continue our work developing a 3D version of the asymptotic expansion homogenization method. We also plan to implement another parallel version of our code, using new high-performance platforms, such as GPGPUs (General-Purpose computation on Graphics Processing Units) Luebke et al. (2004). We hope that, by using this new parallel 3D version, our code will be able to analyze more complex and realistic models of composite materials.

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ACKNOWLEDGEMENTS

The authors would like to thank CAPES, FAPEMIG, CNPq and UFJF for supporting this study.