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Heat Transfers and Solid Mechanics in Microarchitectured Materials using Periodic Homogenization

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Abstract

Microarchitectured materials are generally made of different compounds bound at the microscopic level using a periodic pattern. This results in a macroscopic material with new properties arising from each of the individual compound properties and the way the microarchitecture binds them. The periodic microstructure can then be optimized to obtain specific macroscopic material properties, but attention must be paid to the microstructure response, such as high thermal gradients in heat transfers or mechanical stresses in structural mechanics. Using a finite element analysis to forecast such behaviors is often computationally challenging due to the abundance of geometrical details, leading to a large number of degrees of freedom to solve for. Modelers must then rely on more sophisticated numerical methods. This paper studies the use of the periodic homogenization method in heat transfers and solid mechanics. This method has the advantage to be built upon a well-established mathematical basis. The initial problem is reformulated into two-scale finite element problem. At the microstructure-scale, unitary stimulations of the material are performed in order to characterize homogenized properties of the material. At the part-scale, homogenized temperature or displacement fields are solved. Each of these steps requires to solve far less degrees of freedom than the initial problem. Ultimately, both results are combined by relocation in order to get an accurate prediction of the local temperature, conductive fluxes, displacement and mechanical stresses.

Keywords: composite materials, equivalent medium, multiscale approach, homogenization, relocation, thermal conduction, elasticity, macroscopic and microscopic medium, heterogeneous medium, unit cell.

1 Introduction

Microarchitectured materials are generally made of different compounds bound at the microscopic level using a periodic pattern, resulting in a macroscopic material with new properties. Modelling such materials using a finite element analysis is computationally unaffordable, because the abundance of geometrical details results in a very large number of degrees of freedom. The modeler must then rely on more sophisticated methods such as the periodic homogenization method.

The periodic homogenization method is a mathematical method to cast PDEs with periodic and rapidly varying coefficients into a set of microscopic and macroscopic equations [1] [2] [3]. The solutions of such equations are far easier to solve than the primal equations, and their combination results in very accurate approximations of the primal solution [4] [5]. For heat transfer in solids and solid mechanics, this method can theoretically predict with high accuracy within the microstructure: hot spots, thermal gradients, strains and stresses. While being mathematically well-established, this method requires a rather careful implementation to take advantage of its power.

This paper studies the COMSOL implementation of the periodic homogenization method for heat transfers and solid mechanics, two physics commonly used by engineers. For solid mechanics, elasticity properties can be homogenized by COMSOL using the Cell Periodicity feature [6]. Beyond homogenizing heat transfer in solids and mechanical properties, the ambition of this work is going further by also relocating variables and their gradients, *i.e.* providing an accurate estimation of temperature, displacement, heat fluxes, and mechanical stresses at the microscale.

2 Theory

a. Basis Problems

The goal is to predict the conductive thermal equilibrium and the mechanical equilibrium of a macrostructure made of a microarchitectured material. Figure 1 illustrates an example of geometry further used for heat transfers. The microstructure is periodic and can be described by a *unit cell* (*e.g.* Figure 1 – right), which is repeated a large number of times within the macrostructure. Each component of the unit cell has its own physical properties.

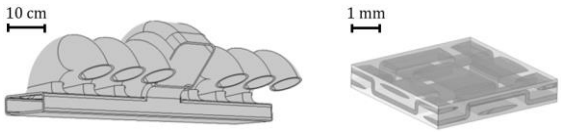

Figure 1. Example of a macrostructure (left) made of a microachitectured material whose the unit cell (right) may be repeated more than tens of thousands times.

The thermal equilibrium within the macrostructure is described by the steady-state heat equation:

$$-\nabla \cdot (\mathbf{K}\,\nabla T) = q, \qquad (1)$$

where T is the temperature, $\mathbf{K}$ the conductivity matrix, and q an external heat source. The mechanical equilibrium solves:

$$\begin{aligned} -\boldsymbol{\nabla}\cdot(\mathbf{C}:\boldsymbol{\epsilon}) &= \boldsymbol{F}, \\ \boldsymbol{\epsilon} &= \tfrac{1}{2}[\boldsymbol{\nabla u} + (\boldsymbol{\nabla u})^{\mathrm{T}}], \end{aligned} \tag{2}$$

where $\boldsymbol{u}$ is the displacement field, $\boldsymbol{\epsilon}$ the linear strain tensor, $\mathbf{C}$ the elasticity tensor, and $\boldsymbol{F}$ external forces. Both of these equations require to be closed using appropriate boundary conditions. The particularity of Eq. 1-2 is that $\mathbf{K}$ and $\mathbf{C}$ vary rapidly in space because of the microscopic structure.

In the periodic homogenization framework, the microscale is described in a normalized frame: the unit cell is described by a cube of 1 m-length. At the macroscale, the actual size of the unit cell is called ε, allowing to describe the material properties as 1-periodic functions as follows:

$$\begin{aligned} \mathbf{K} &= \mathbf{K}(\boldsymbol{x}/\varepsilon), \\ \mathbf{C} &= \mathbf{C}(\boldsymbol{x}/\varepsilon), \end{aligned} \tag{3}$$

where $\boldsymbol{x}$ is the material coordinate at the macroscale. Note that the theory can be applied to non-cubic unit cells (*e.g.* Figure 1 – right).

The periodic homogenization theory applies under linearity hypotheses: $\mathbf{K}$, q, $\mathbf{C}$ and $\boldsymbol{F}$ are not function of T and $\boldsymbol{u}$.

b. Homogenization

Homogenization is the first step of the method. It consists in numerically submitting the microstructure to unitary solicitations in order to deduce homogenized properties and get the macroscopic behavior of the macrostructure.

Concerning heat transfer in solids, the unit cell is submitted to three unitary thermal gradients. The following heat equations are solved in ω_k within the unit cell:

$$\begin{aligned} -\boldsymbol{\nabla}\cdot[\mathbf{K}\,\boldsymbol{\nabla}\omega_k] &= \boldsymbol{\nabla}\cdot[\mathbf{K}\,\boldsymbol{e}_k], \\ \boldsymbol{e}_1 = (1,0,0), \boldsymbol{e}_2 = (0,1,0), \boldsymbol{e}_3 &= (0,0,1), \\ k &= 1,2,3, \end{aligned} \tag{4}$$

where $\boldsymbol{e}_k$ is the unitary thermal solicitation. These equations are closed with periodic boundary conditions and imposing mean value of ω_k as zero. The homogenized conductivity matrix $\mathbf{K_h}$ is:

$$\mathbf{K_h} = \int_{\mathrm{cell}} \mathbf{K}\,[\mathbf{I} + (\boldsymbol{\nabla}\omega_1\ \boldsymbol{\nabla}\omega_2\ \boldsymbol{\nabla}\omega_3)]\,\mathrm{d}\boldsymbol{x}, \tag{5}$$

where $\mathbf{I}$ designates the identity matrix. The apparent temperature T_0 of the macrostructure can then be solved by replacing $\mathbf{K}$ by $\mathbf{K_h}$ in Eq. 1 and its boundary conditions.

Concerning solid mechanics, the unit cell is submitted to unitary strains. There are nine unitary displacements $\boldsymbol{\gamma}_{jk}$ to solve within the unit cell:

$$\begin{aligned} -\boldsymbol{\nabla}\cdot\left[\mathbf{C}:\boldsymbol{\epsilon}_{jk}\right] &= \boldsymbol{\nabla}\cdot[\mathbf{C}:\boldsymbol{e}_{jk}], \\ \boldsymbol{\epsilon}_{jk} &= \tfrac{1}{2}\left[\boldsymbol{\nabla\gamma}_{jk} + \left(\boldsymbol{\nabla\gamma}_{jk}\right)^{\mathrm{T}}\right], \\ \boldsymbol{e}_{jk} &= \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & 1 & \vdots \\ 0 & \cdots & 0 \end{pmatrix}, 1 \text{ at } jk\text{-th component}, \\ j &= 1,2,3, \\ k &= j,\cdots,3, \end{aligned} \tag{6}$$

where $\boldsymbol{e}_{jk}$ is the unitary strain. These equations are closed with periodic boundary conditions and imposing mean value of $\boldsymbol{\gamma}_{jk}$ as zero. In practice, the number of displacements to solve can be reduced to six by using the symmetry $\boldsymbol{\gamma}_{kj} = \boldsymbol{\gamma}_{jk}$. The homogenized elasticity tensor $\mathbf{C_h}$ is:

$$\mathbf{C_h}_{lmjk} = \int_{\mathrm{cell}} \mathbf{C}_{lmjk} + \left(\mathbf{C}:\boldsymbol{\epsilon}_{jk}\right)_{lm}\,\mathrm{d}\boldsymbol{x}. \tag{7}$$

The apparent displacement field $\boldsymbol{u_0}$ of the macrostructure can then be solved by replacing $\mathbf{C}$ by $\mathbf{C_h}$ in Eq. 2 and its boundary conditions.

c. Relocation

Once unitary microscopic temperature fields ω_k (resp. displacement fields $\boldsymbol{\gamma}_{jk}$) and macroscopic temperature field T_0 (resp. displacement field $\boldsymbol{u_0}$) are solved, they can be combined to obtain accurate microscopic values for the variables and their gradients. This is the *relocation*.

Concerning heat transfer in solids, the relocated temperature T_r is obtained as follows:

$$T_r(\boldsymbol{x}) = T_0(\boldsymbol{x}) + \varepsilon \sum_j \frac{\partial T_0}{\partial x_j}(\boldsymbol{x})\ \omega_j(\boldsymbol{x}/\varepsilon). \tag{8}$$

Then, the gradient of T_r can be used to predict accurate values for the temperature gradient and conductive fluxes within the microstructure.

Concerning solid mechanics, the relocated displacement field $\boldsymbol{u_r}$ is obtained as follows:

$$\boldsymbol{u_r}(\boldsymbol{x}) = \boldsymbol{u_0}(\boldsymbol{x}) + \varepsilon \sum_{j,k} \frac{\partial \boldsymbol{u_0}_j}{\partial x_k}(\boldsymbol{x})\ \boldsymbol{\gamma}_{jk}(\boldsymbol{x}/\varepsilon). \tag{9}$$

Here again, the gradient of $\boldsymbol{u_r}$ can be used to predict accurate values for strains and stresses within the microstructure.

d. Quality of the Approximation

Mathematical analyses of the method have demonstrated its accuracy in multiple configurations (boundary condition combinations), both in heat transfers and solid mechanics [2] [3] [4] [5]. The accuracy results are expressed using *norms* (norms

of Sobolev spaces L^2 and H^1), and are in fact convergence results of the approximate solutions to the solution of the primal equation when the actual size of the unit cell ε tends to zero:

$$\begin{aligned} \|T - T_0\|_{L^2} &\leq C \cdot \varepsilon, \\ \|T - T_r\|_{H^1} &\leq C \cdot \sqrt{\varepsilon}, \\ \|\boldsymbol{u} - \boldsymbol{u_0}\|_{L^2} &\leq C \cdot \varepsilon, \\ \|\boldsymbol{u} - \boldsymbol{u_r}\|_{H^1} &\leq C \cdot \sqrt{\varepsilon}. \end{aligned} \tag{10}$$

where C stands for a constant. In essence, these results mean that accuracy increases as the unit cell is small compared to the macrostructure size. In order to predict hot spots and displacements, T_0 and $\boldsymbol{u_0}$ may suffice, while using T_r and $\boldsymbol{u_r}$ are necessary to predict accurately the thermal fluxes and mechanical stresses within the microstructure.

3 COMSOL Implementation

a. Model Overview

In this section, the COMSOL's features used in the implementation are in *italic*. The implementation is architectured around two *components*: the first one to study the behavior of the unit cell, and the second one to study the macrostructure.

For heat transfers, Eq. 4 is implemented using the *Coefficients Form PDE* physics. This physics allows a great implementation flexibility, and particularly, it eases the implementation of the source term of Eq. 4 by allowing adding natively a source term in the divergent. The zero mean condition is obtained by adding one *Global Equations* introducing a new degree of freedom fixing ω_k at an arbitrary point of the unit cell. For solid mechanics, Eq. 6 is implemented using the *Solid Mechanics* physics. This time, the source terms are implemented in *weak form*. This task must be completed with care, and the ability to automatize the formulae generation using *Methods* within the *Application Builder* is extremely helpful. The unit cell is fixed ($\boldsymbol{\gamma}_{jk} = 0$) at an arbitrary point of the unit cell, and the zero mean condition is obtained at post-treatment by subtracting to the solution its mean.

Once unitary microscopic contributions are solved, the homogeneous properties (Eq. 5 and Eq. 7) are computed and stored as new variables that will be used for the macroscopic computation.

Concerning the relocation formulae (Eq. 8-9), they are implemented as *Variables*, since they only combine already solved variables. Here again, using *Methods* is really helpful. For solid mechanics in 3D, hundreds of variables may be needed to perform relocation of displacements, strains and stresses.

Thus, COMSOL's flexibility allows to implement such multiscale approach.

b. Numerical Aspects

The numerical implementation of this method requires specific care.

Because of the periodicity boundary conditions of Eq. 4 and Eq. 6, it is strongly recommended to build a mesh of the unit cell such that nodes and edges of opposing faces coincide. Such mesh avoids local artifacts in the unitary microscopic variables.

When solving T_0 or $\boldsymbol{u_0}$, the order of elements must be carefully chosen, depending on the nature of the analysis. When only T_r or $\boldsymbol{u_r}$ are needed, it suffices to use P^1-elements, while when gradients and their products (fluxes, strains, stresses…) are needed, P^2 or *quadratic serendipity* elements must be used, as deriving Eq. 8 (resp. Eq. 9) makes appear second derivatives of T_0 (resp. $\boldsymbol{u_0}$).

Once discretized, microscopic and macroscopic equations are linear and a reasonable number of degrees of freedom are solved, generally allowing to use direct linear solvers.

In order to verify the COMSOL implementation of the method, Eq. 1-2 will be solved directly without the method. Even by using geometries made of a limited number of repetitions of the unit cell, millions of degrees of freedom may be solved, requiring using iterative linear solvers.

4 Results and Discussion

a. Heat Transfers

The method is applied to the case illustrated in Figure 1 for heat transfer in solids, which models the heat dissipation of a hypothetic carbon fiber intake manifold. The unit cell is a carbon fiber textile (Figure 1 – right), where fibers (dark) have a high isotropic conductivity (40 W/m/K) and the matrix (light) has a low isotropic conductivity (4 W/m/K). Homogenization of this microstructure results in an anisotropic conductivity:

$$\mathbf{K_h} = \begin{pmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 6 \end{pmatrix} \text{W/m/K}. \tag{11}$$

This result goes beyond the rule of mixtures and the inverse rule of mixtures, which estimate an isotropic conductivity ranging from 6 W/m/K to 13 W/m/K. Using $\mathbf{K_h}$, the apparent temperature T_0 is solved and illustrated in Figure 2.

The maximal apparent thermal gradient $\boldsymbol{\nabla} T_0$ is compared to a measurement of the relocated thermal gradient $\boldsymbol{\nabla} T_r$ at some point $\boldsymbol{x}_0$ of the geometry:

$$\begin{aligned} \max \|\boldsymbol{\nabla} T_0\| &= 1.02 \times 10^4 \text{ K/m}, \\ \boldsymbol{\nabla} T_r(\boldsymbol{x}_0) &= 2.98 \times 10^4 \text{ K/m}. \end{aligned} \tag{12}$$

High thermal gradients may be correlated with fiber delamination, and Eq. 12 show that the actual gradient may be largely higher than the apparent one.

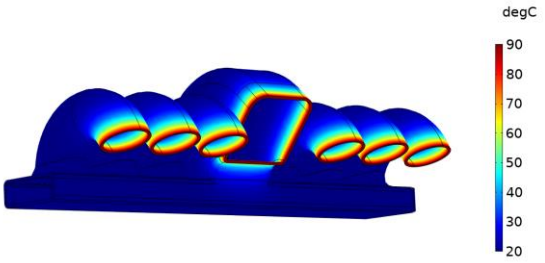

Figure 2. Apparent temperature T_0 at the surface of the macrostructure.

b. Solid Mechanics

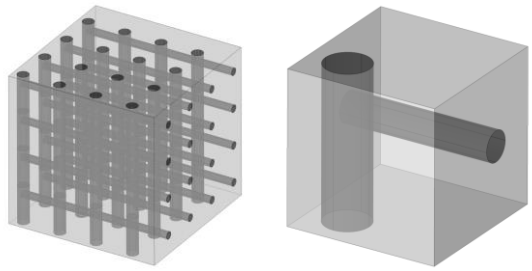

Figure 3. Macrostructure (left) used as test-case for solid mechanics, made of a microachitectured material whose the unit cell (right) is repeted up to tens of times.

In solid mechanics, the method is applied on a non-trivial test case to estimate numerically its accuracy and verify its implementation. The macrostructure (Figure 3 – left) is built upon repetitions of a unit cell (Figure 3 – right) made of fibers (dark) with high Young's modulus and a matrix (light) with low Young's modulus. Different scenarios are evaluated: one of the six faces of the macrostructure is fixed, and either the opposite face is pulled (traction), or adjacent faces are sheared (shearing). Six scenarios are evaluated in total.

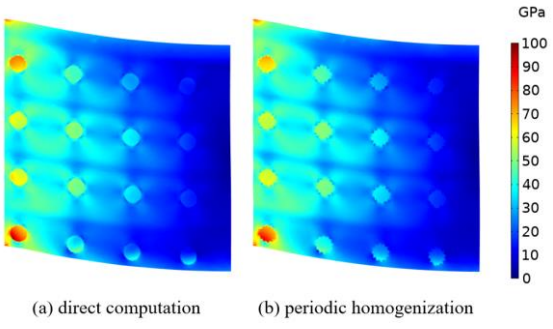

Figure 4. Reference (a) and periodic homogenization method (b) von Mises constraint results obtained in a shearing scenario, on a cut plane.

Figure 4 shows results of von Mises constraints obtained by solving directly Eq. 2 with $4 \times 4 \times 4$ repetitions of the unit cell (a), and by using the periodic homogenization method Eq. 6-7, 9 (b). Even with a low number of repetitions of the unit cell, the method predicts accurately the locations and the magnitudes of high constraint spots.

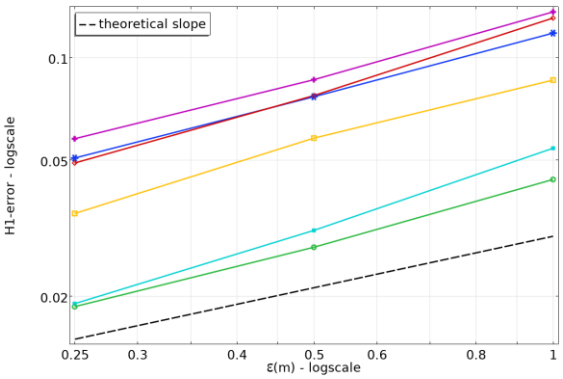

Figure 5. Evolution of the H^1-error of the implementation for each scenario when $\varepsilon \to 0$.

The implementation of the method is quantitatively tested by evaluating the left-hand sides of Eq. 10. Figure 5 shows the evolution of the H^1-error of the numerical implementation for each scenario, when $\varepsilon \to 0$. The graphs are in log-log scale, allowing to compare the numerical slope to the theoretical slope (Eq. 10: $\text{slope} = 1/2$), which is actually attained. This result shows that the implementation of the method is correct, as it is capable to predict with accuracy displacement fields, strains and constraints.

Table 1. Number of degrees of freedom and computation time of the direct method and the periodic homogenization method, with $4 \times 4 \times 4$ repetitions of the unit cell.

Method	#DOF	Comp. time (min)
Direct (Eq. 2)	1.8 M	33
Micro Eq. 6-7	6×37 K	2
Macro Eq. 7 → 2	80 K	0.5
Homogenization	0.3 M	2.5

The computational cost of solving directly Eq. 2 is compared to the periodic homogenization method in Table 1. The periodic homogenization method requires far less degrees of freedom to solve for simultaneously and a far below computation time compared to the direct method, even with a low number of repetitions of the unit cell. The computation cost of the periodic homogenization method does not depend on ε. This means that the speedup should be far greater with smaller values of ε. The method thus allows for studying cases where a direct computation is impossible.

5 Conclusions

The goal of this work is to predict heat transfer in solids and solid mechanics of parts made of microarchitectured materials using the periodic homogenization. The method reformulates the solution of PDEs having rapidly varying periodic coefficients as a combination of macroscale and microscale solutions *via* the steps of *homogenization* and *relocation*. This multiscale approach is

implemented within COMSOL Multiphysics® thanks to its great flexibility.

Numerical results in heat transfer show the ability of the method to predict anisotropies from a combination of isotropic materials, and the importance of relocation: apparent (macroscopic) variables may hide huge variations within the microarchitecture. The method is also applied to solid mechanics, showing its accuracy to relocate stresses within the microstructure. Numerical convergence results are obtained by comparing results of the method with a solution obtained by directly solving the primal equation, showing both the correctness of the implementation and the gain in terms of computational costs.

The method is very general and can be directly applied to industrial cases to predict and optimize microarchitectures. Nonlinearities still require specific care, and the method may need to be customized to specific purposes. Future works include handling more physics, in particular fluid dynamics in porous media.

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