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# Numerization of a memory effect for an homogenized composite material with a large contrast in the phase thermal conductivities $\stackrel{\text{tr}}{\Rightarrow}$

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#### ABSTRACT

In this article, we propose a systematic numerical solution method for deriving the homogenized material parameters in the case where a large contrast in the phase thermal properties leads to a macroscopic memory effect. Focus is therefore set on the determination of this memory effect for a periodic microstructure. As for other and more classical homogenized parameters, the possibility of analyzing with the finite element method a single periodic cell is used, and a transient simulation allows to provide the incremental evolution of the memory effect function. Additionally, some approximations are proposed for a low cost estimate of this function, and validated on two examples.

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#### 1. Introduction

Models with memory effects (or heredity models) have been used quite extensively in structural mechanics for viscoelasticity behaviors. Especially when the structures are subjected to forced vibration loading, their response may be easily found, analytically in simple cases, or numerically. For transient responses, concurrent models, mainly with internal variables have proved their ability to be used numerically [1].

Several justifications can be stated for the physical meaning of memory effects, one being the presence of a microstructure in the material, leading to a delayed response at the macroscopic scale, therefore related to upscaling [2] and a kind of time non-locality. This is for instance the case for scattering of elastic waves for hyperbolic problems [3], for composite materials where the constituents themselves exhibit a memory effect [4], or for particular non-linear behaviors or time-dependent material properties [5].

In this article we focus on the case of evolution (elliptic) problems, even with linear constituents, but where the contrast of constitutive properties is large. The delayed effect is therefore

directly provided by the homogenization procedure [6–9]. We proposed to study a thermal problem for illustration purpose, though the same framework also applies to different physics [10].

The aim is to be able to compute numerically the memory effect function as a macroscopic material characteristic from simulations on the microstructure (i.e. a periodic cell), as it is classically done for the homogenized other parameters, such as the thermal capacity and the thermal conductivity.

In this article, Section 2 states the reference problem, Section 3 recalls the results of the periodic homogenization method for the kind of problem that is under concern. Section 4 proposes a numerical procedure for the memory effect function determination. Finally, Section 5 provides two numerical examples: (i) a 1D problem with an analytical solution, allowing to test the numerical procedure, and whose study provides approximations for determining the memory function at small and large times; (ii) a 3D problem for testing the discretization choices and for validation of the previous approximations.

#### 2. Reference problem and notations

We are concerned herein in an heterogeneous solid media subjected to a transient thermal loading. For sake of simplicity, linear conduction is assumed, and the media is composed of two phases, denoted with *S* and *F* with different thermal properties, and occupying two complementary domains  $\omega_S$  and  $\omega_F$ . The interface  $\gamma$ 

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between these two phases is assumed to be perfect, ensuring continuity of temperature and thermal flux. The reference problem consists in finding the temperature field  $\theta(X, t)$ , where *X* denotes the position within the studied domain  $\omega = \omega_S \cup \omega_F$ , and *t* the time. This temperature field, once restricted to each phase is denoted with  $\theta_S$  and  $\theta_F$ . Apart from the external boundary conditions, the problem at the microscopic scale over the whole structure reads:

$$-\nabla \cdot \boldsymbol{q}_{S} = c_{S} \frac{\partial \theta_{S}}{\partial t} \quad \text{on } \omega_{S} \text{ with } \boldsymbol{q}_{S} = -k_{S} \boldsymbol{Z}_{S} \text{ and } \boldsymbol{Z}_{S} = \nabla \theta_{S}$$
$$-\nabla \cdot \boldsymbol{q}_{F} = c_{F} \frac{\partial \theta_{F}}{\partial t} \quad \text{on } \omega_{F} \text{ with } \boldsymbol{q}_{F} = -k_{F} \boldsymbol{Z}_{F} \text{ and } \boldsymbol{Z}_{F} = \nabla \theta_{F}$$
$$\theta_{S} = \theta_{F} \text{ and } \boldsymbol{q}_{S} \cdot \boldsymbol{n}_{S} + \boldsymbol{q}_{F} \cdot \boldsymbol{n}_{F} = \boldsymbol{0} \text{ on } \boldsymbol{\gamma}$$

 $\mathbf{q}_i$  (i = S, F) are the thermal fluxes,  $k_i$  the thermal conductivities,  $c_i$  the thermal capacities, and  $\mathbf{n}_S = -\mathbf{n}_F$  is the outward normal to  $\omega_S$  at an interface point. The microstructure is also assumed to be periodic, i.e. the complete material can be reconstructed by periodic duplication of period l in each space dimension of a basic cell whose characteristic size is l. If L is a characteristic size of the whole structure, the scaling parameter is  $\varepsilon = l/L$ ; it is expected to be small, traducing the assumption that the scales are separated.

#### 3. Asymptotic expansion and periodic homogenization

This homogenization technique is based on the spatial description of the various fields at two scales, i.e. with two coordinate systems: one is the slow coordinates *x* at the scale of the whole structure (typically  $x \in [0, L]$ ), the other one is the fast coordinate *y*, related to the scaled microstructure cell  $\Omega$  (typically  $y \in [0, l/\varepsilon]$ ). This scaled basic cell is therefore also composed of the two phases *S* and *F* occupying the domains  $\Omega_F$  and  $\Omega_S$ ;  $\Gamma = \partial \Omega_S \cap \partial \Omega_F$  is the interface. The spatial derivative then reads  $\nabla = \frac{\partial}{\partial X} = \frac{\partial}{\partial x} + \frac{1}{\varepsilon} \frac{\partial}{\partial y}$ . In the following, we will use the notation  $\nabla_x$  and  $\nabla_y$  to denote the corresponding two gradient operators.

The temperature field  $(\theta)$  is expanded with respect to the (small) parameter  $\varepsilon$ :

$$\theta = \sum_{\alpha=0}^{\infty} \varepsilon^{\alpha} \theta_{\alpha}(\mathbf{x}, \mathbf{y}, t)$$

where all the temperature fields  $\theta_{\alpha}(x, y, t)$  are  $\Omega$ -periodic for the variable *y*.

Equating all the problem equations for the different powers of  $\varepsilon$  allows to successively provide the models for the different temperature fields [11,12].

The large contrast in material characteristics arises when the ratio between the thermal capacities or the thermal conductivities is of the order of  $\varepsilon^n$  with  $n \neq 0$ . A special case arises when the ratios between thermal conductivities is of order  $\varepsilon^2$  while the capacities are of the same order, i.e.  $\rho_F c_F \approx \rho_S c_S$  and the scaled conductivity of the *F*-phase is  $k'_F := k_F/\varepsilon^2 \approx k_S$ . In such a case, the emergent macroscopic thermal problem is of a different kind [7]. This case is usefully interpreted with characteristic times [9,13] since the characteristic macroscopic time is expected to be  $\tau_M = (C_M/k_M)(L/\pi)^2$  (if  $C_M$  and  $k_M$  are the homogenized total thermal capacity and conductivity), while their counterparts for the microscopic *S* and *F* phases are  $\tau_S = (\rho_S c_S/k_S)(l_S/\pi)^2$  and

$$au_F = rac{
ho_F c_F l_F^2}{k_F \pi^2} pprox rac{
ho_F c_F L_F^2}{k_F' \pi^2} pprox au_S / arepsilon^2 pprox au_M$$

since the characteristic lengths associated to each phase are  $l_S \approx l_F \approx l$  and  $L_S = l_S/\epsilon \approx L_F = l_F/\epsilon \approx L$ . Therefore, the transient phenomena at the micro scale for the *F*-phase may well arise at macro scale.

Details on the successive derivations of the micro and macro problems can be found in [7], and the main results are recalled in the following.

#### 3.1. Macroscopic property of $\theta_{S0}$

The first result for the *S*-phase is that the temperature at order 0, i.e. multiplied by  $\varepsilon^0$ , does not depend on the fast variable:

$$\theta_{\rm SO} = \theta_{\rm SO}(x,t)$$

it is therefore a macroscopic temperature field, and its gradient with respect to the fast variable y is null. Its gradient with respect to the slow variable x is a macroscopic temperature gradient

$$\mathbf{Z}_{S0}(\mathbf{x},t) = \nabla_{\mathbf{x}}\theta_{S0}$$

### 3.2. Localization property of $\theta_{S1}$

The next order equations give the problem that  $\theta_{s1}$  should satisfy:

$$\begin{aligned} \nabla_{y} \cdot \boldsymbol{q}_{S0} &= 0 \quad \text{with} \quad \boldsymbol{q}_{S0} = -k_{S}(\boldsymbol{Z}_{S0} + \nabla_{y}\theta_{S1}) \quad \text{in } \Omega_{S} \\ \boldsymbol{q}_{S0} \cdot \boldsymbol{n}_{S} &= 0 \quad \text{on } \Gamma \\ \theta_{S1} \text{ is } \Omega \text{-periodic} \end{aligned}$$

It is a steady-state thermal problem whose variational formulation is

$$\int_{\Omega_{\rm S}} \nabla_{\rm y} \theta^{\star} \cdot k_{\rm S} \nabla_{\rm y} \theta_{\rm S1} d\Omega = - \int_{\Omega_{\rm S}} \nabla_{\rm y} \theta^{\star} \cdot k_{\rm S} \mathbf{Z}_{\rm S0} d\Omega \tag{1}$$

for all  $\Omega$ -periodic test functions  $\theta^{\star}(y)$ . It is usually discretized with finite elements, and its solution is linear with respect to the macroscopic loading  $Z_{50}$ . Therefore this solution, and its gradient  $Z_{51} = \nabla_y \theta_{51}$  can be expressed using a linear operator which is a characteristic of the *S*-microstructure. For instance,

$$\boldsymbol{Z}_{S1}(\boldsymbol{x},\boldsymbol{y},t) = -\boldsymbol{L}_{S}(\boldsymbol{y})\boldsymbol{Z}_{S0}(\boldsymbol{x},t)$$

The numerical determination of  $L_s$  requires: (i) as many resolutions of the previous linear micro problem (1) on  $\Omega_s$  as there are independent components in  $Z_{s0}$ , i.e. 2 for 2D problems, and 3 for 3D problems, and (ii) the storage of the same number of temperature gradient fields on  $\Omega_s$  (the columns of the matrix  $L_s$ ).

This operator is a localization operator for the temperature gradient. Indeed, it allows to recover the first two terms of the full temperature gradient, obtained from the asymptotic expansion of  $\theta_s$ , once the macroscopic gradient is known:

$$\mathbf{Z}_{S} \approx \mathbf{Z}_{S0}(x,t) + \mathbf{Z}_{S1}(x,y,t) = (\mathbf{1} - \mathbf{L}_{S})\mathbf{Z}_{S0}$$
  
and of the thermal flux

$$\boldsymbol{q}_{\mathrm{S}} = -k_{\mathrm{S}}\boldsymbol{Z}_{\mathrm{S}} \approx \boldsymbol{q}_{\mathrm{SO}} = -k_{\mathrm{S}}(\boldsymbol{1} - \boldsymbol{L}_{\mathrm{S}})\boldsymbol{Z}_{\mathrm{SO}}$$

#### 3.3. Problem to solve for $\theta_{F0}$

The zero-order terms for the *F*-phase provide the following problem:

$$\rho_F c_F \theta_{F0} = -\nabla_y \cdot \boldsymbol{q}_{F1} \quad \text{with} \quad \boldsymbol{q}_{F1} = -k'_F \nabla_y \theta_{F0} \quad \text{in } \Omega_F \\
\theta_{F0} = \theta_{S0} \quad \text{on } \Gamma \\
\theta_{F0} \text{ is } \Omega\text{-periodic}$$

This problem couples the micro and the macro scales due to the fact that  $\theta_{F0}$  still depends on the *y* coordinate, and due to the presence of the  $\theta_{S0}(x,t)$  term as a boundary condition on  $\Gamma$ . On the *F*-cell, this term is uniform due to the scale separation. A change in variable may be useful: if we denote

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