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Abdullah Waseem, Thomas Heuzé, Laurent Stainier, V G Kouznetsova, M G D Geers. Variationally consistent computational homogenization of transient heat conduction using Craig-Bampton mode synthesis. Colloque national MECAMAT, Jan 2018, Aussois, France. hal-02279999

**HAL Id: hal-02279999**

**<https://hal.science/hal-02279999>**

Submitted on 5 Sep 2019

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# VARIATIONALLY CONSISTENT COMPUTATIONAL HOMOGENIZATION OF TRANSIENT HEAT CONDUCTION USING CRAIG-BAMPTON MODE SYNTHESIS

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**Mots-clefs :** Transient Heat Conduction, FE<sup>2</sup>, Craig-Bampton Mode Synthesis, Periodic Homogenization.

## 1 Introduction

Material with different constituents play an important role in engineering applications, especially as the demand for smaller devices are increasing and their realization by modern day fabrication technology is improving, it has become very important to correctly capture the underlying physics of these components and design them accordingly. These materials, with different constituents improve the engineering performance, are called heterogeneous materials. Different sizes, topologies and material properties make this task of correctly representing the physics more challenging. These fluctuations in properties of constituents render the coefficients of governing equations under consideration very oscillatory and makes it harder to capture the true response with some analytical or numerical tool.

Among a plethora of possible other numerical tools finite elements (FE), because of its proven robustness, is usually used to solve these governing equations. In case of such heterogeneous materials a high number of finite elements are required to solve the problem accurately. This makes the computations, even with modern day computational power, very expensive. So, effort should be made to capture this rich physics of heterogeneous materials with techniques which efficiently solve these systems with in high accuracy but with low computational cost.

Homogenization comes into play at this point. It provides the mathematical tools to represent these oscillatory coefficients with averaged/smooth coefficients, which allows to use few number of finite elements instead. Homogenization makes use of Hill-Mandel averaging conditions, which are energy consistency conditions for transferring information from micro-scale to macro-scale. Also, full separation of scales is assumed that is the length scales associated to micro-scale are very small as compared to macroscopic length scales. For low transient phenomena i.e., with low macroscopic thermal gradients and low frequency loading this assumption is valid and a steady-state response can be representative of the micro-scale physics.

However, when the phenomena is highly transient, these assumptions do not hold true for homogenization purposes. Also, the micro-scale length scales and high contrast in material properties exhibit to transient effects at micro-scale. These transient effects which should also be upscaled to the macro-scale which leads to extended Hill-Mandel conditions. In this regard, to capture the transient thermal and mechanical micro-transient effects some efforts has been made already [2, 3, 4, 5, 6]. In the context of heat conduction in [2], it is shown for the first time how to use first order computational homogenization and extended Hill-Mandel conditions for transient case.

For its mechanical counterpart in [3] used a relaxed scale separation in which the length scale of the inclusion is comparable to the size of the wavelength propagating through the material while still a long wavelength approximation is considered for the matrix. Both micro- and macro-scales are considered to be in transient regimes. [7] has extended this approach to reduce the computational cost by applying a reduction technique to eliminate the micro-scale problem by mode synthesis.

Along with all its benefits, computational homogenization for transient problems comes with a relatively high computational expense as compared to its steady-state counterpart, because at each time step for each macroscopic point a microscopic initial boundary value problem needs to be solved. In this work an effort has been made to reduce this computational cost by using the reduction technique implemented in [7]. The homogenization framework is developed according to [2] with a weak separation of scales for transient heat conduction problems.

## 2 Homogenization and reduction methodology : towards an enriched continuum.

### 2.1 Homogenization framework.

#### 2.1.1 Separation of scales.

General homogenization techniques assume complete separation of scales in which the size of a unit-cell is very small as compared to the macro-scale. This is a valid assumption for steady-state phenomena and material with small sized heterogeneities. However, in highly transient cases the size of the constituents become comparable with the macroscopic sizes and this assumption is no more valid. For weak separation of scales in heat conduction one can chose to be in the range  $t_m < T < t_i$ . Where,  $t_m$  and  $t_i$  are the matrix and inclusion characteristic diffusivity times and  $T$  is the macroscopic loading time.

#### 2.1.2 Macro-scale problem.

Without any heat generation a transient balance of energy is assumed at the macro-scale. The macroscopic temperature field  $\bar{\theta}(\bar{\mathbf{x}}, t)$  in  $\bar{\Omega}$  is the quantity of interest here. The macroscopic problem reads, find  $\bar{\theta} \in \bar{\mathcal{H}}$  :

$$\bar{\nabla} \cdot \bar{\mathbf{q}} + \dot{\bar{\epsilon}} = 0 \quad (1)$$

Here,  $\bar{\mathbf{q}}$  is the macroscopic flux,  $\bar{\epsilon}$  is the macroscopic internal energy and  $\bar{\mathcal{H}}$  is the space of admissible macroscopic temperature fields. The constitutive forms of these macroscopic quantities are unknown and will be obtained as a result of upscaling relations.

#### 2.1.3 Micro-scale problem.

Also a transient balance of energy is required at the micro-scale to account for micro-transient effects. The microscopic problem can be written as follows, find  $\theta \in \mathcal{H}$  :

$$\nabla \cdot \mathbf{q} + \dot{\epsilon} = 0 \quad (2)$$

Here,  $\mathbf{q}$ ,  $\dot{\epsilon}$  and  $\mathcal{H}$  are the microscopic flux, rate of change of internal energy and space of admissible microscopic temperature field. The constitutive models are known at this scale.

#### 2.1.4 Microscopic temperature field.

The microscopic temperature field is defined as a Taylor's expansion of macroscopic temperature at  $\bar{\mathbf{x}}$ ,

$$\theta := \bar{\theta} + \bar{\nabla} \bar{\theta} \cdot (\mathbf{x} - \bar{\mathbf{x}}) + \tilde{\theta} \quad (3)$$

Here,  $\tilde{\theta}$  is the fluctuation in  $\theta$  due to material properties and transient phenomena. It can be written as an additive decomposition of *steady-state* and *transient* temperature fluctuation fields i.e.,  $\tilde{\theta} = \theta_{ss} + \theta_{tr}$ .

#### 2.1.5 Scale transition relations.

*Downscaling relations (micro boundary conditions)* : The condition which is required while downscaling is

$$\bar{\nabla} \bar{\theta} = \langle \nabla \theta \rangle \quad (4)$$

Taking the gradient of (3) and volume averaging the result

$$\langle \nabla \theta \rangle = \bar{\nabla} \bar{\theta} + \langle \tilde{\theta} \mathbf{n} \rangle_{\partial \Omega} \quad (5)$$

This expression relates the microscopic gradient of temperature to the macroscopic gradient of temperature through the following constraint

$$\langle \tilde{\theta} \mathbf{n} \rangle_{\partial \Omega} = \mathbf{0} \quad (6)$$

Which can be satisfied using specific types of boundary conditions at the micro-scale such as 1) linear temperature boundary conditions (LT-BCs) or 2) Periodic boundary conditions (PR-BCs).

*Upscaling relations (extended Hill-Mandel conditions)* : The extended Hill-Mandel principle can be stated such as the total virtual power at the macroscopic point  $\bar{\mathbf{x}}$  should be equal to the average virtual power taken from a unit-cell associated to that macroscopic point. i.e.,

$$-\bar{\nabla} \delta \bar{\theta} \cdot \bar{\mathbf{q}} + \delta \bar{\theta} \dot{\bar{\epsilon}} = \langle -\nabla \delta \theta \cdot \mathbf{q} + \delta \theta \dot{\epsilon} \rangle \quad (7)$$

Taking left-hand-side of (7) into consideration for upscaling and substituting the variation of temperature and its gradient in it, one gets

$$-\bar{\nabla} \delta \bar{\theta} \cdot \bar{\mathbf{q}} + \delta \bar{\theta} \dot{\bar{\epsilon}} = \langle -\bar{\nabla} \delta \bar{\theta} \cdot (\mathbf{q} - (\mathbf{x} - \bar{\mathbf{x}}) \dot{\epsilon}) + \delta \bar{\theta} \dot{\epsilon} \rangle \quad (8)$$

From which the macroscopic quantities can now be identified as follows, the macroscopic heat flux

$$\bar{\mathbf{q}} = \langle \mathbf{q} - \dot{\epsilon}(\mathbf{x} - \bar{\mathbf{x}}) \rangle \quad (9)$$

and the rate of change of macroscopic internal energy

$$\dot{\bar{\epsilon}} = \langle \dot{\epsilon} \rangle \quad (10)$$

The term  $\dot{\epsilon}(\mathbf{x} - \bar{\mathbf{x}})$  appearing in the macroscopic flux is the first moment of rate of change of microscopic internal energy. This term is responsible for the thermal transient effects upscaled to the macro-scale. If the size of the RVE is very small i.e.,  $(\mathbf{x} - \bar{\mathbf{x}}) \rightarrow 0$ , the transient effect will vanish and the result of classical homogenization will be recovered :  $\bar{\mathbf{q}} = \langle \mathbf{q} \rangle$ .

## 2.2 Discretization and model reduction.

### 2.2.1 Craig-Bampton reduction.

Craig-Bampton mode synthesis is a sub-structuring technique to solve large structural problems component wise. In computational homogenization, under assumptions of weak separation of scales and enforced boundary conditions, each unit-cell attached to a macroscopic point can be considered as a sub-structure. The discrete FE form of microscopic equations can be written in terms of free and prescribed nodes as follows

$$\begin{bmatrix} \underline{K}^{*pp} & \underline{K}^{*pf} \\ \underline{K}^{*fp} & \underline{K}^{*ff} \end{bmatrix} \begin{bmatrix} \tilde{\theta}^p \\ \tilde{\theta}^f \end{bmatrix} + \begin{bmatrix} \underline{C}^{*pp} & \underline{C}^{*pf} \\ \underline{C}^{*fp} & \underline{C}^{*ff} \end{bmatrix} \begin{bmatrix} \dot{\tilde{\theta}}^p \\ \dot{\tilde{\theta}}^f \end{bmatrix} = \begin{bmatrix} \tilde{q}_n^p \\ \tilde{0}^f \end{bmatrix} \quad (11)$$

*Steady-state response* : To get the steady-state response, the transient part of (11) is neglected and static-condensation should be applied to solve for the free nodes under the prescribed boundary conditions. Total steady-state response of the system can be written as

$$\begin{bmatrix} \tilde{\theta}^p \\ \tilde{\theta}_{ss}^f \end{bmatrix} = \begin{bmatrix} \underline{I}^{pp} \\ \underline{S} \end{bmatrix} \tilde{\theta}^p \quad (12)$$

here,  $\underline{S} = -(\underline{K}^{*ff})^{-1} \underline{K}^{*fp}$  and  $\underline{I}^{pp}$  is the matrix of ones of size  $(p \times p)$ . Substituting the expression for steady-state temperature in (11) and matrix multiplying leads to

$$\hat{\underline{K}} \tilde{\theta}^p + \hat{\underline{C}} \dot{\tilde{\theta}}^p = \tilde{q}_n^p \quad (13)$$

Here,  $\hat{\underline{K}} = \underline{K}^{*pp} + \underline{K}^{*pf} \underline{S}$  and  $\hat{\underline{C}} = \underline{C}^{*pp} + 2\underline{C}^{*pf} \underline{S} + \underline{S}^T \underline{C}^{*ff} \underline{S}$  are the microscopic steady-state conductivity and capacity matrices.

*Transient response* : The transient response should be added to the steady-state solution to account for the transient effects present at the micro-scale. To calculate the transient response efficiently, spectral decomposition can be utilized, in which the solution is represented by its eigenmodes and corresponding eigen-basis i.e.,

$$\underline{\theta}_{tr}^f = \underline{\Phi} \underline{\eta} \quad (14)$$

here,  $\underline{\Phi}$  is the matrix containing the eigen-modes vectors  $\underline{\Phi}$  and  $\underline{\eta}$  is the column of modal amplitude temperature. For most of the systems, for specific loading conditions and material properties only few modes projected on the eigen-basis are enough to present the exact system with some reasonably small error. This reduces the problem from  $N$  degrees of freedom to only superposition of  $N_q$  important eigen-modes and eigen-basis ( $N_q \ll N$ ). After performing normalization using capacity matrix one gets the transient response of the unit-cell in terms of modal coordinates as follows,

$$\underline{\alpha} \underline{\eta} + \underline{\dot{\eta}} = \underline{0}^k \quad (15)$$

This gives the transient effects without any coupling to the macroscopic dynamics. The coupling can be obtained by combining the solutions of the steady-state and the transient problems.

*Linear Superposition* : To superimpose the steady-state and transient response the total microscopic response can be written in a matrix vector form as follows.

$$\begin{bmatrix} \underline{\theta}^p \\ \underline{\theta}^f \\ \underline{\theta}^f \end{bmatrix} = \begin{bmatrix} \underline{\theta}^p \\ \underline{\theta}_{tr}^f + \underline{\theta}_{ss}^f \end{bmatrix} = \begin{bmatrix} \underline{0}^{pk} & \underline{I}^{pp} \\ \underline{\Phi} & \underline{S} \end{bmatrix} \begin{bmatrix} \underline{\eta} \\ \underline{\theta}^p \end{bmatrix} \quad (16)$$

here,  $\underline{0}^{pk}$  is the matrix of zeros of size  $(p \times k)$ . substituting (16) in (11) leads to the following two equations,

$$\underline{\rho} \underline{\dot{\eta}} + \underline{\hat{K}} \underline{\theta}^p + \underline{\hat{C}} \underline{\dot{\theta}}^p = \underline{q}_n^p \quad (17)$$

which can be recognized as the total reaction flux at the prescribed boundary of the unit-cell. Here,  $\underline{\rho}$  is the coupling matrix between steady-state and transient responses and it is given by  $\underline{\rho} = \underline{S}^T \underline{C}^{*ff} \underline{\Phi} + \underline{C}^{*pf} \underline{\Phi}$ , and

$$\underline{\alpha} \underline{\eta} + \underline{\dot{\eta}} = -\underline{\rho}^T \underline{\dot{\theta}}^p \quad (18)$$

where,  $\underline{\rho}^T \underline{\dot{\theta}}^p$  is the forcing term for this modal equation.

### 2.3 Enriched Continuum

*Macroscopic flux* : The macroscopic flux given by (9) can be written only in terms of prescribed nodes on the boundary

$$\bar{q} = \frac{1}{V} (\Delta \underline{x}^p)^T \underline{q}_n^p \quad (19)$$

which after substituting the expression for temperature on the prescribed nodes at the micro-scale can be written as

$$\bar{q} = \frac{1}{V} \left[ (\Delta \underline{x}^p)^T \left( \underline{\rho} \underline{\dot{\eta}} + \underline{\hat{K}} (\underline{I}^p \bar{\theta} + \underline{\nabla} \bar{\theta} \cdot \Delta \underline{x}^p) + \underline{\hat{C}} (\underline{I}^p \dot{\bar{\theta}} + \underline{\nabla} \dot{\bar{\theta}} \cdot \Delta \underline{x}^p) \right) \right] \quad (20)$$

in compact notation

$$\bar{q} = \underline{\alpha} \underline{\dot{\eta}} + \underline{b} \bar{\theta} + \underline{B} \cdot \underline{\nabla} \bar{\theta} + \underline{c} \dot{\bar{\theta}} + \underline{C} \cdot \underline{\nabla} \dot{\bar{\theta}} \quad (21)$$

*Macroscopic internal energy* : Similarly, macroscopic internal energy can be written as

$$\dot{\bar{e}} = -\underline{d} \underline{\dot{\eta}} - \underline{e} \bar{\theta} - \underline{e} \cdot \underline{\nabla} \bar{\theta} - \underline{f} \dot{\bar{\theta}} - \underline{f} \cdot \underline{\nabla} \dot{\bar{\theta}} \quad (22)$$

Now, these constitutive expressions can be utilized in macroscopic balance of energy.

*Microscopic balance of energy* : Transient contribution from micro-scale can be injected in the macro-scale by solving only the reduced basis  $\eta$ .

$$\underline{\alpha} \dot{\eta} + \dot{\eta} = - \left( \underline{\rho}^T \underline{I}^p \dot{\theta} + V \underline{a}^T \cdot \nabla \dot{\theta} \right) \quad (23)$$

Energy balance (1) with constitutive relations (21) and (22) supported by the solution of (23) represent the enriched continuum at the macro-scale.

### 3 Numerical Verification

#### 3.1 Varification of CBMS model

A one-dimensional micro-scale problem is constructed with an inclusion in the center. The macroscopic loading conditions, constituents material properties and sizes were selected such that there exist significant transient effects. According to the results below CBMS performs very well as compared to FE and when the number of modes is increased, the approximated solution approaches the FE solution.

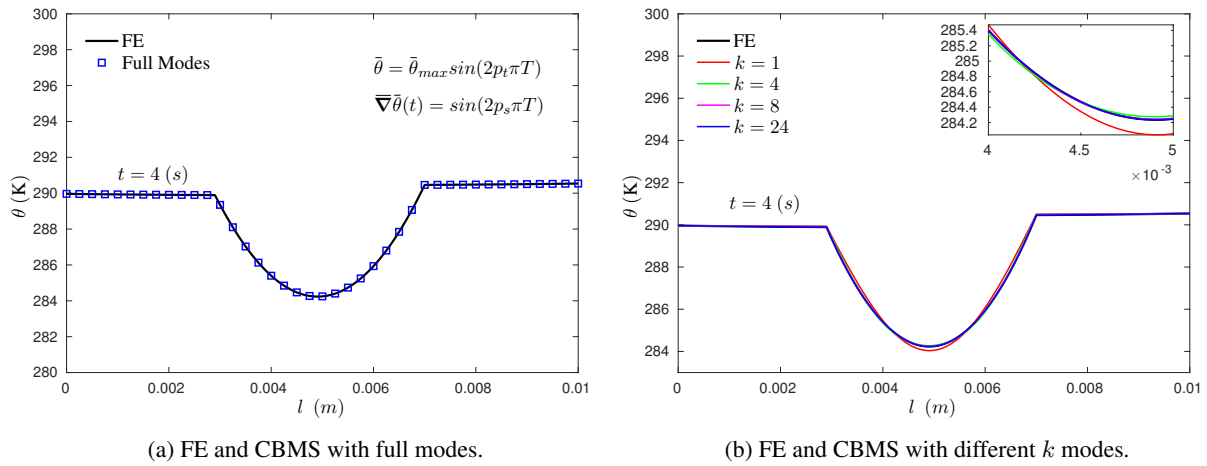


FIGURE 1 – (a) A comparison between FE solution and CBMS approximation was made at time  $t = 4$  s. The FE solution is shown in black solid line while CBMS approximated solution is shown with blue boxes plotted every 5th degree of freedom. (b) A comparison between FE solution and different number of  $k$  modes was made. The figure within zooms-in where error is largest.

#### 3.2 Comparison with quasi-static homogenization

The main advantages of the new formulation are to capture the microscopic transient and size effects, and also to perform a model reduction. No size effect is observed when a steady-state formulation [1] is used. it is plotted in dark black color shown in Fig.(2 - a). However, using current formulation as the size of the unit-cell is increased the absolute value of macroscopic flux due to transient effects is also increased.

### 4 Conclusion.

A multi-scale computational homogenization framework using Craig-Bampton's mode synthesis was developed for linear transient heat conduction with weak separation of scales. Significant computational and modeling advantages were observed as compared to [2] and [1], such as instead of solving a fully coupled system of linear equations of FE at the micro-scale now only few uncoupled equations need to be solved for modal temperatures and the transient effects are also incorporated and upscaled to the macro-scale.

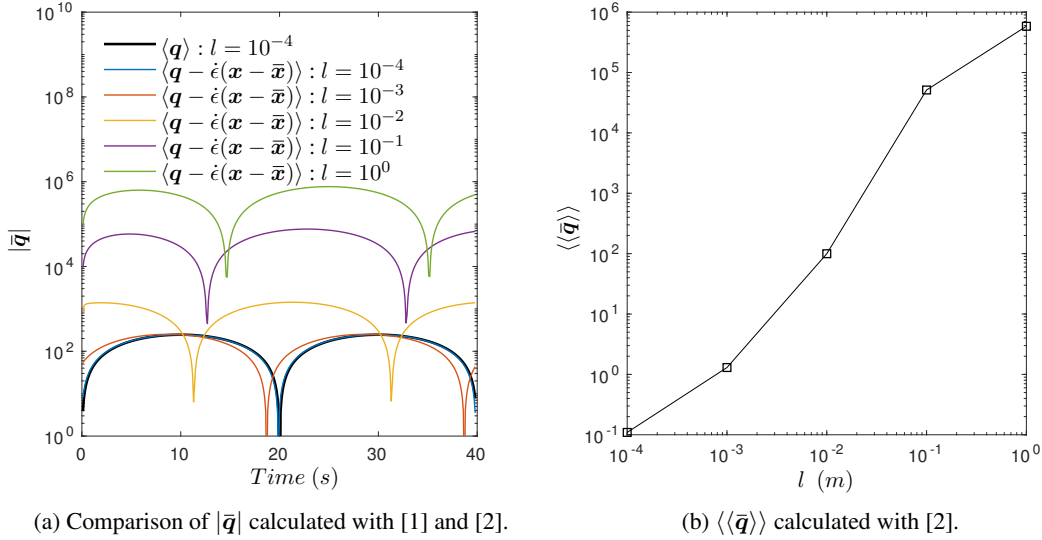


FIGURE 2 – (a) Time evolution of  $|\bar{q}|$  with [1] and [2] cases. (b) Time averaged macroscopic flux  $\bar{q}$  defined as  $\langle\langle \bar{q} \rangle\rangle = \frac{1}{T} \int_T \bar{q} dt$ .

## Références

- [1] Özdemir, I and Brekelmans, WAM and Geers, MGD Computational homogenization for heat conduction in heterogeneous solids. *International Journal for Numerical Methods in Engineering*, 73 :185–204, 2008
- [2] Larsson, Fredrik and Runesson, Kenneth and Su, Fang Variationally consistent computational homogenization of transient heat flow. *International Journal for Numerical Methods in Engineering*, 81 :1659–1686, 2010
- [3] Pham, Kim and Kouznetsova, Varvara G and Geers, Marc GD Transient computational homogenization for heterogeneous materials under dynamic excitation *Journal of the Mechanics and Physics of Solids*, 61 :2125–2146, 2013
- [4] de Souza Neto, EA and Blanco, PJ and Sánchez, PJ and Feijóo, RA An RVE-based multiscale theory of solids with micro-scale inertia and body force effects. *Mechanics of Materials*, 80 :136–144, 2015
- [5] Ramos, Gustavo Roberto and Santos, Tiago and Rossi, Rodrigo An extension of the Hill-Mandel principle for transient heat conduction in heterogeneous media with heat generation incorporating finite RVE thermal inertia effects. *International Journal for Numerical Methods in Engineering*, 111 :1097–0207, 2017
- [6] Matine, A and Boyard, N and Legrain, G and Jarny, Y and Cartraud, Patrice Transient heat conduction within periodic heterogeneous media : A space-time homogenization approach. *International Journal of Thermal Sciences*, 92 :217–229, 2015.
- [7] Sridhar, Ashwin and Kouznetsova, Varvara G and Geers, Marc GD. Homogenization of locally resonant acoustic metamaterials towards an emergent enriched continuum. *Computational Mechanics*, 57 :423–435, 2016.