Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 326 (2017) 193–222
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Numerical model reduction with error control in computational homogenization of transient heat flow

Emil Aggestam*, Fredrik Larsson, Kenneth Runesson, Fredrik Ekre

Department of Applied Mechanics, Chalmers University of Technology, Gothenburg, S-41296, Sweden

Received 18 November 2016; received in revised form 3 July 2017; accepted 8 August 2017
Available online 14 August 2017

Abstract

Numerical Model Reduction (NMR) is exploited for solving the finite element problem on a Representative Volume Element (RVE) that arises from the computational homogenization of a model problem of transient heat flow. Since the problem is linear, an orthogonal basis is obtained via the classical method of spectral decomposition. A symmetrized version of the space–time variational format is adopted for estimating the error from the model reduction in (i) energy norm and in (ii) given Quantities of Interest. This technique, which was recently developed in the context of the (non-selfadjoint) stationary diffusion–convection problem, is novel in the present context of NMR. By considering the discrete, unreduced, model as exact, we are able to obtain guaranteed bounds on the error while using only the reduced basis and with minor computational effort. The performance of the error estimates is demonstrated via numerical results, where the subscale is modeled in both one and three spatial dimensions.

Keywords: Model reduction; Error control; Computational homogenization; Transient

1. Introduction

Computational homogenization is a well-established approach in material modeling with the purpose to account for strong micro-heterogeneity in an approximate, yet “sufficiently accurate”, fashion while reducing the computational cost as compared to Direct Numerical Simulation (DNS) of the fine-scale problem. When the intrinsic material properties are nonlinear and/or the subscale problem is inherently transient, it is necessary to resort to nested macro-subscale computations (Finite Element squared, FE^2), whereby the subscale computations are carried out on a so called Representative Volume Element (RVE) in each “quadrature point” in the macroscale domain (possibly within a given timestep). Clearly, the purpose is to obtain macroscale properties of engineering interest; hence, whether it is possible to avoid resolution via DNS of the fine-scale problem and accept the homogenized solution can only be assessed via some sort of goal-oriented error quantification.

* Corresponding author.
E-mail address: emil.aggestam@chalmers.se (E. Aggestam).

http://dx.doi.org/10.1016/j.cma.2017.08.006

However, it is widely realized that straight-forward application of the FE^2-strategy can be computationally intractable for a fine macroscale mesh, particularly in 3D. Therefore, there is significant interest in reducing the cost of solving the individual RVE-problem(s) by introducing some kind of reduced basis, here denoted Numerical Model Reduction (NMR). In particular, we note strategies that are based on the superposition of "modes" that are characteristic for the RVE-solution fields. In the case of subscale small strain (visco)plasticity, various attempts have been made to approximate the inelastic strain field by a reduced basis, so called "inelastic modes"; one of the early proposals being the so called "eigendeformation-based reduced order homogenization" technique by Fish and coworkers, [1,2], which in its turn relies on the Transformation Field Analysis (TFA) that was originally proposed by Dvorak and Benveniste [3]. A similar approach, coined Nonuniform Transformation Field Analysis (NTFA), was proposed by Michel and Suquet [4,5]. Recent developments are by Fritzen and coworkers [6,7], who extended the idea further within the framework of Proper Orthogonal Decomposition (POD) and applied it to visco-elasticity and, more generally, to a (sub)class of Standard Dissipative Materials. Hernández et al. [8] proposed a reduced method based on POD and reduced sampling (quadrature) in a similar framework. Reduced order modeling in the context of the multiscale finite element model was considered by Nguyen [9]. Moreover, for a class of coupled problems an additional "bonus" is that it is possible to reduce the macroscale problem to that of a single-phase, whereby the "mode coefficients" play the role of classical internal variables, e.g. Jänicke et al. [10]. In other words, the character of homogenization problem changes such that the resulting macroscopic equations represent a single-phase poro-viscoelastic material. Efendiev et al. [11] proposed a reduction basis from Spectral Decomposition in the context of porous media flow.

Quite importantly, however, is the obvious fact that the richness of the reduced basis will determine the accuracy of the RVE-solution, which calls for error control. An example of error estimation due to model reduction, although not in a homogenization context and for a PGD-basis, is Ladeveze and Chamoin [12]. PGD for homogenization of non-linear problems was considered by Cremonesi et al. [13]. Error estimators for POD-type reduction techniques have been developed by, e.g., Abdulle and Bai [14] for the heterogeneous multiscale method, Boyaval [15] and Paladim [16] for numerical homogenization, Ohlberger and Schindler [17] for the multiscale finite element method, and Kerfriden et al. [18] for projection-based reduced order modeling. Control of discretization errors (without model reduction) is discussed by, e.g., Jhurani and Demkowicz [19] and Larsson and Runesson [20].

In this paper, we consider the transient heat conduction as a model problem and choose, for simplicity, to use Spectral Decomposition to establish the reduced basis. (We consider the standard FE-solution in space–time as the exact one, i.e. we disregard any discretization error and consider only the error induced by the NMR strategy.) For this particular choice of basis, we discuss a few strategies to estimate the "solution error" without computing additional basis functions (modes). In particular, we aim for guaranteed, explicit bounds on the error in (i) energy norm and (ii) an arbitrary "quantity of interest" (QoI) within the realm of goal-oriented error estimation. It is noted that the QoI is generally defined in space–time to achieve maximal generality. As a "workhorse" for the error computation, that requires negligible additional cost, we thereby introduce an associated (non-physical) symmetrized variational problem in space–time and use ideas previously put forward by Parés et al. [21–23]. Furthermore, explicit bounds are obtained utilizing the discrete residual, cf. Jacobsson et al. [24] who developed bounds for Component Modal Synthesis (CMS) for static elasticity.

Throughout this paper, meager type is used to denote scalars, whereas bold type is used to denote vectors and (higher order) tensors. Scalar product (single contraction) is denoted by $\cdot$. For example, if $\boldsymbol{a}, \boldsymbol{b}$ are vectors and $\boldsymbol{A}$ is a second order tensor, we have $\boldsymbol{a} \cdot \boldsymbol{b} = a_i b_i$, $(\boldsymbol{A} \cdot \boldsymbol{b})_i = A_{ij} b_j$, where the Einstein summation convention is used.

As to homogenization in the spatial domain, volume averaging of an intensive field $\diamond$ is denoted

$$\langle \diamond \rangle_\square \overset{\text{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \diamond \, \mathrm{d}\Omega, \tag{1}$$

where $\Omega_\square$ is the domain occupied by the RVE. The macroscale representation of $\diamond$ is denoted $\bar{\diamond}$, and frequently it holds that $\bar{\diamond} = \langle \diamond \rangle_\square$.

The paper is organized as follows: Section 2 gives a review of computational homogenization as applied to the chosen transient model problem and introduces the concept of Numerical Model Reduction (NMR). Section 3 describes how to estimate the error from NMR. The error estimation is carried out both in the classical energy norm and in a relevant Quantity of Interest, e.g. time-averaged flux. Section 4 presents the numerical results that verify the performance of NMR and the quality of the derived explicit error estimates. The RVE is modeled in both one and three spatial dimensions. Finally, Section 5 concludes the paper with a summary and an outlook to future work.