29th Nordic Seminar on Computational Mechanics
NSCM-29
R. Larsson (Ed.)
2016

NUMERICAL MODEL REDUCTION WITH ERROR CONTROL FOR COMPUTATIONAL HOMOGENIZATION OF TRANSIENT HEAT FLOW

EMIL AGGESTAM*, **FREDRIK LARSSON AND KENNETH RUNESSON**

Department of Applied Mechanics
Chalmers University of Technology
Gothenburg, S-41296, Sweden
*e-mail: emil.aggestam@chalmers.se, web page: http://www.chalmers.se/am

Key words: computational homogenization, transient heat flow, numerical model reduction, error analysis.

Summary. Computational homogenization of transient heat flow is considered by analyzing the response on a representative volume element. A novel numerical model reduction strategy combined with error control is proposed.

1 INTRODUCTION

FE^2 is the technique of solving two-scale finite element problems using computational homogenization on Representative Volume Elements (RVEs) pertinent to each macroscale quadrature point. It is well realized that the straight-forward 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). One example is Fritzen and Böhlke[1]. 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[2].

Quite important, 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. (Here, we consider the full FE-solution as the exact one.) An example of error estimation due to model reduction, although not in a homogenization context and for a PGD-basis, is Ladeveze and Chamoin[3]. In this work, we consider the transient heat flow as a model problem and choose, for simplicity, to use spectral decomposition to establish the reduced basis. 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. Numerical results for a simple 1D-problem illustrate the performance and quality of the proposed error estimates.

2 COMPUTATIONAL HOMOGENIZATION

Computational homogenization is an approach used to reduce the computational cost for materials with strong micro-heterogeneity compared to direct numerical simulations of the fine-scale problem. Within each RVE, assumed to occupy the domain $\Omega_\square$, the macro-scale temperature, $\bar{u}$, and temperature gradient, $\bar{\boldsymbol{g}}$, are assumed to be given. Let u_0 be the starting temperature, T the final time and $\mathbb{H}^1(\Omega_\square)$ the appropriate Hilbert space. For each RVE, the weak format reads: Find $u(\bullet, t) \in \mathbb{U}_\square = \{v \in \mathbb{H}^1(\Omega_\square) : \; v = \bar{u} + \bar{\boldsymbol{g}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] \text{ on } \partial\Omega_\square\}$ that solves

$$\mathfrak{m}_\square(\dot{u}, \delta u) + \mathfrak{a}_\square(u, \delta u) = 0 \quad \forall \delta u \in \mathbb{U}^0_\square, \; t \in (0, T], \tag{1a}$$

$$\mathfrak{m}_\square(u(\bullet, 0), \delta u) = \mathfrak{m}_\square(u_0, \delta u) \quad \forall \delta u \in \mathbb{U}^0_\square, \tag{1b}$$

where $\mathbb{U}^0_\square = \{v \in \mathbb{H}^1(\Omega_\square) : \; v = 0 \text{ on } \partial\Omega_\square\}$ and we introduced the variational forms

$$\mathfrak{m}_\square(u, \delta u) \stackrel{\text{def}}{=} \int_{\Omega_\square} c u \delta u \, \mathrm{d}\Omega_\square, \tag{2a}$$

$$\mathfrak{a}_\square(u, \delta u) \stackrel{\text{def}}{=} \int_{\Omega_\square} k \boldsymbol{\nabla} \delta u \cdot \boldsymbol{\nabla} u \, \mathrm{d}\Omega_\square. \tag{2b}$$

The thermal conductivity, $k = k(\boldsymbol{x})$, may be strongly heterogeneous on the considered fine scale, while it is assumed that the volume-specific heat capacity, c, is a constant (for the sake of simplicity). From the solution to Equation (1), stored heat and heat flux can be calculated as

$$\bar{\Phi} = \mathfrak{m}_\square(cu, 1), \tag{3a}$$

$$\bar{\boldsymbol{q}} = -\sum_{i=1}^{N_{\mathrm{SD}}} \mathfrak{a}_\square(u, \boldsymbol{e}_i \cdot \boldsymbol{x}), \tag{3b}$$

where N_{SD} and $\boldsymbol{e}_i$ are the number of spatial dimensions and unit base vectors, respective.

3 MODEL REDUCTION

The linearity of the RVE-problem implies that the classical Spectral Decomposition method can be used. We thus compute the eigenpairs $(u_a, \lambda_a) \in \mathbb{U}^0_\square \times \mathbb{R}$ such that

$$\mathfrak{a}_\square(u_a, \delta u) = \lambda_a \mathfrak{m}_\square(u_a, \delta u) \quad \forall \delta u \in \mathbb{U}^0_\square, \quad a = 1, 2, \ldots, N, \tag{4a}$$

$$\mathfrak{m}_\square(u_a, u_b) = \delta_{ab} \quad a, b = 1, 2, \ldots, N, \tag{4b}$$

where N is the number of free spatial degrees of freedom. By using the eigenfunctions corresponding to the most significant eigenvalues, the reduced solution, u_{R}, can be obtained as $u_{\mathrm{R}}(\boldsymbol{x}, t) = \sum_{a=1}^{N_{\mathrm{R}}} u_a(\boldsymbol{x})\xi_a(t)$, where $N_{\mathrm{R}} \ll N$ is the number of used modes and ξ_a are the mode activity coefficients.

4 ERROR ANALYSIS

The error induced by the model reduction is estimated in (i) energy norm and (ii) an arbitrary "quantity of interest" (QoI), denoted $Q(u)$. For u being the exact solution, we thus estimate the bounds E_{est}, $E^-_{\mathrm{Q,est}}$ and $E^+_{\mathrm{Q,est}}$ such that

$$\|u - u_{\mathrm{R}}\| \leq E_{\mathrm{est}}, \tag{5a}$$

$$E^-_{\mathrm{Q,est}} \leq E_{\mathrm{Q}} \leq E^+_{\mathrm{Q,est}}, \tag{5b}$$

where $E_{\mathrm{Q}} = Q(u) - Q(u_{\mathrm{R}})$. The error estimates give guaranteed, although not necessarily sharp, bounds of the QoI by only using the reduced modes. In order to find explicit error estimates an abstract space-time formulation of the RVE-problem is considered together with a duality-based estimation of the error in a QoI and a construction of a symmetrized bilinear form in space-time.

5 RESULTS

Figure 1 shows the total RVE-solution in terms of non-dimensional temperature vs time and spatial location. Figure 2 shows the guaranteed upper and lower limit of E_{Q} along with bound of $|E_{\mathrm{Q}}|$ where $E^{\max}_{\mathrm{Q,est}} \stackrel{\mathrm{def}}{=} \max(E^+_{\mathrm{Q,est}}, -E^-_{\mathrm{Q,est}})$, for the QoI time-average stored heat.

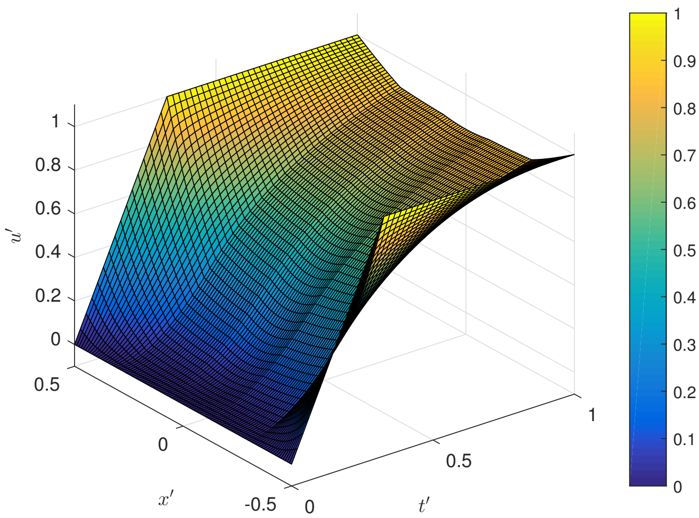

Figure 1: Total RVE-solution. $N = 100$, $N_{\mathrm{R}} = 10$, $ntsteps = 50$.

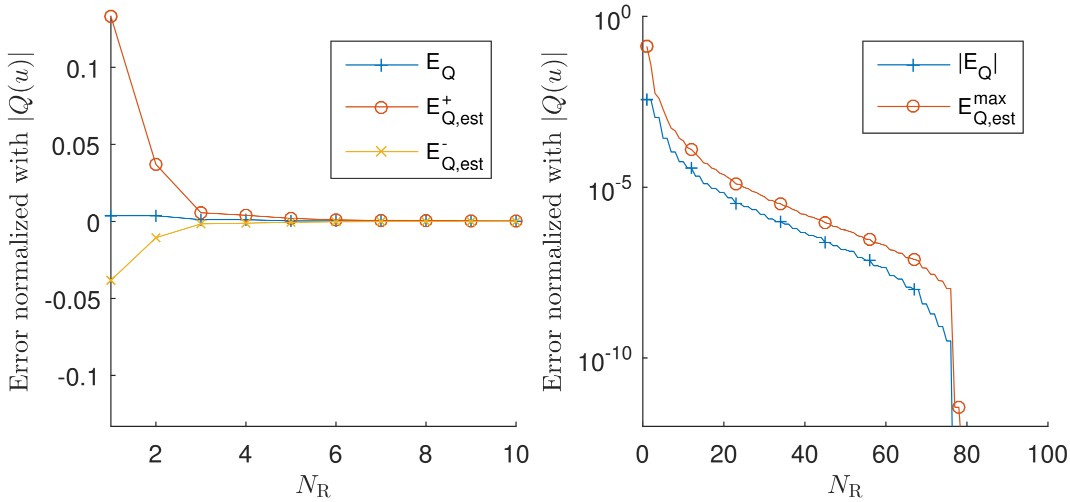

Figure 2: Error in QoI representing time-averaged stored heat vs. N_{R} for $N = 100$. Left figure: Upper and lower bounds of E_{Q}. Right figure: Bound of $|E_{\mathrm{Q}}|$.

6 CONCLUSIONS

An innovative strategy of model reduction with error control for the transient heat flow has been proposed and implemented successfully, albeit in one spatial dimension. An error analysis is performed that gives explicit (and hence also inexpensive) guaranteed bounds.

REFERENCES

[1] Fritzen, F. & Böhlke, T. Three-dimensional finite element implementation of the nonuniform transformation field analysis. *International Journal for Numerical Methods in Engineering* **84**, 803–829 (2010).

[2] Jänicke, R., Larsson, F., Runesson, K. & Steeb, H. Numerical identification of a viscoelastic substitute model for heterogeneous poroelastic media by a reduced order homogenization approach. *Computer Methods in Applied Mechanics and Engineering* **298**, 108–120 (2016).

[3] Ladevèze, P. & Chamoin, L. On the verification of model reduction methods based on the proper generalized decomposition. *Computer Methods in Applied Mechanics and Engineering* **200**, 2032–2047 (2011).