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Numerical Model Reduction in Computational Homogenization of Transient Heat Flow

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Micro Abstract
We present a two-scale finite element (FE^2) formulation for transient linear heat flow. For the sub-scale problem, we use spectral decomposition in order to to establish a reduced basis. We discuss a few methods to estimate the error introduced by the reduction, and in particular we aim for explicit bounds on the error in (i) energy norm and (ii) an arbitrary "quantity of interest". Numerical results confirm the validity of the computed error bounds.

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Introduction

Multiscale methods are of high interest in the engineering community due to their ability to predict the overall response, while accounting for heterogeneities on the underlying scales. One standard approach is the so-called FE^2 procedure, where the classical constitutive relation is replaced by a boundary value problem on a Representative Volume Element (RVE). In practice this means that a new finite element problem is solved in each macroscale (quadrature) point. For fine scale macroscale meshes this methods can be computationally intractable, because of the numerous RVE problems, and it is therefore of interest to reduce the computational cost. We here present a method for Numerical Model Reduction (NMR) for the solution of the RVE problems.

1 Two-scale Formulation Based on Computational Homogenization

Consider the transient heat flow problem, with linear constitutive relations, in terms of finding the temperature field $u(\boldsymbol{x}, t) \in \Omega \times [0, T]$ governed by

$$c\dot{u} - (k\boldsymbol{\nabla} u) \cdot \boldsymbol{\nabla} = 0 \qquad \text{in } \Omega \times (0, T], \tag{1a}$$

$$u = u^{\mathrm{p}}(t) \qquad \text{on } \partial\Omega \times (0, T], \tag{1b}$$

$$u = u_0(\boldsymbol{x}) \qquad \text{in } \Omega \text{ at } t = 0, \tag{1c}$$

where $c = c(\boldsymbol{x})$ is the volume-specific heat capacity and $k = k(\boldsymbol{x})$ is the thermal conductivity. We also introduced standard boundary[1] and initial conditions; prescribed temperature u^{p} on $\partial\Omega$ and $u(t = 0) = u_0(\boldsymbol{x})$. The standard weak space-time format of (1) reads: Find $u \in \mathcal{U}$ such that

$$\int_I \int_\Omega \Big[vc\dot{u} + \boldsymbol{\nabla} v \cdot k \boldsymbol{\nabla} u \Big] \,\mathrm{d}\Omega \,\mathrm{d}t + \int_\Omega [vcu]|_{t=0} \,\mathrm{d}\Omega = \int_\Omega [vcu_0]|_{t=0} \,\mathrm{d}\Omega \quad \forall v \in \mathcal{V}, \tag{2}$$

where v is the test function and where $\mathcal{U}$, $\mathcal{V}$ are appropriate trial and test spaces, respectively.

To obtain a two scale formulation of (2) we introduce (i) running averages[2] and (ii) scale-separation via first order homogenization, cf. Larsson et al. [3]. In each macroscale (quadrature)

[1]For simplicity we consider the case where the full boundary is subjected to Dirichlet boundary conditions.
[2]We introduce $\langle \bullet \rangle_\square = |\Omega_\square|^{-1} \int_{\Omega_\square} \bullet \,\mathrm{d}\Omega$ for averaging the quantity $\bullet$ over an RVE with volume $|\Omega_\square|$.

point $\bar{\boldsymbol{x}}$ we thus decompose u such that

$$u(\boldsymbol{x},t) = \underbrace{\bar{u}(\boldsymbol{x},t) + \boldsymbol{\nabla}\bar{u}(\boldsymbol{x},t)\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}]}_{=\mathcal{A}\bar{u}} + u^{\mu}(\boldsymbol{x},t), \tag{3}$$

where $\bar{u}$ is the homogenized field, and u^{μ} the fluctuation field. The test function is decomposed similarly, e.g. $v = \bar{v} + \boldsymbol{\nabla}\bar{v}\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}] + v^{\mu}$. By only considering the homogenized test function (i.e. setting $v^{\mu}=0$) we obtain the homogenized macroscale problem: Find $\bar{u}\in\bar{\mathcal{U}}$ such that

$$A(\mathcal{A}\bar{u}+u^{\mu},\mathcal{A}\bar{v}) = L(\mathcal{A}\bar{v}) \quad \forall\bar{v}\in\bar{\mathcal{V}}, \tag{4}$$

where $\bar{\mathcal{U}}$, $\bar{\mathcal{V}}$ are appropriate function spaces for the homogenized field, and where $A(\bullet,\bullet)$ and $L(\bullet)$ are defined by

$$A(u,v) = \int_I\int_\Omega \Big[\langle vc\dot{u}\rangle_\square + \langle\boldsymbol{\nabla}v\cdot k\boldsymbol{\nabla}u\rangle_\square\Big]\,\mathrm{d}\Omega\,\mathrm{d}t + \int_\Omega\langle vcu\rangle_\square|_{t=0}\,\mathrm{d}\Omega \tag{5}$$

$$L(v) = \int_\Omega\langle vcu_0\rangle_\square|_{t=0}\,\mathrm{d}\Omega. \tag{6}$$

For each point $\bar{\boldsymbol{x}}$, we set $\bar{v}=0$ and obtain the microscale problem: Find $u^{\mu}\in\mathcal{U}^{\mu}$ such that

$$A_\square(\mathcal{A}\bar{u}+u^{\mu},v^{\mu}) = L_\square(v^{\mu}) \quad \forall v^{\mu}\in\mathcal{V}^{\mu}, \tag{7}$$

where $\mathcal{U}^{\mu}$, $\mathcal{V}^{\mu}$ are appropriate function spaces for the trial and test function of the fluctuation field and where the two RVE space-time forms are defined by

$$A_\square(u,v) = \int_I\Big[\langle vc\dot{u}\rangle_\square + \langle\boldsymbol{\nabla}v\cdot\boldsymbol{\nabla}u\rangle_\square\Big]\,\mathrm{d}t + \langle vcu\rangle_\square|_{t=0}, \tag{8}$$

$$L_\square(v) = \langle vcu_0\rangle_\square|_{t=0}. \tag{9}$$

2 Numerical Model Reduction (NMR)

With the goal of simplifying the microscale computations we will introduce Numerical Model Reduction (NMR) of the fluctuation field. We first introduce an alternative decomposition of u

$$u(\boldsymbol{x},t) = u_{\mathrm{stat}}\{\boldsymbol{x};\bar{u}(t),\boldsymbol{\nabla}\bar{u}(t)\} + u_{\mathrm{trans}}(\boldsymbol{x},t), \tag{10}$$

where u_{stat} is the stationary part, and u_{trans} the transient fluctuation part. We now introduce a reduction of u_{trans}

$$u_{\mathrm{trans}}(\boldsymbol{x},t) \approx u_{\mathrm{trans,R}}(\boldsymbol{x},t) = \sum_{a=1}^{N_{\mathrm{R}}}\varphi_a(\boldsymbol{x})\xi_a(t), \tag{11}$$

where $\{\varphi_a\}_{a=1}^{N_{\mathrm{R}}}$ are a set of linearly independent spatial modes, and ξ are time dependent "mode activity" coefficients. In this work - since this is a linear problem - we use Spectral Decomposition to compute the modes and follow closely to Aggestam et al. [1]. Hence, we obtain the modes from the generalized eigenvalue problem

$$\langle\boldsymbol{\nabla}\delta u\cdot k\boldsymbol{\nabla}\varphi_a\rangle_\square = \lambda_a\langle\delta uc\varphi_a\rangle_\square \qquad a=1,2,..,N_{\mathrm{R}}, \tag{12}$$

$$\langle\varphi_b c\varphi_a\rangle_\square = \delta_{ab} \qquad a,b=1,2,..,N_{\mathrm{R}}, \tag{13}$$

where δu is a spatial test function on the RVE.

The result of introducing (11) in the microscale problem (7) is a set of N_{R} ordinary differential equations

$$\left.\begin{aligned}\dot{\xi}_a + \lambda_a\xi_a &= f_a(t;\dot{\bar{u}},\boldsymbol{\nabla}\dot{\bar{u}})\\ \xi_a(0) &= \xi_{a,0}\end{aligned}\right\} \qquad a=1,2,..,N_{\mathrm{R}}, \tag{14}$$

which can be solved in an efficient manner. When the mode coefficients are solved for the effective response can be evaluated and used for the macroscale computation.

3 Estimation of NMR Error

It is of interest to estimate the introduced solution error. Here we will focus solely on the error due to NMR and ignore other error sources (such as time and space discretization). We define the (two-scale) error as

$$(\bar{e}, e^{\mu}) = (\bar{u} - \bar{u}_{\mathrm{R}}, u^{\mu} - u^{\mu}_{\mathrm{R}}), \tag{15}$$

where u is the exact solution and u_{R} the solution to the reduced problem. We define a corresponding error equation, given by

$$A(e, v) = L(v) - A(u_{\mathrm{R}}, v) = R(v). \tag{16}$$

In order to define a norm, we introduce the symmetric form A^{s}, cf. Parés et al. [4], as

$$A^{\mathrm{s}}(u, v) = \frac{1}{2}[A(u, v) + A(v, u)] = \int_I \int_\Omega \langle \boldsymbol{\nabla} v \cdot k \boldsymbol{\nabla} u \rangle_\square \,\mathrm{d}\Omega \,\mathrm{d}t + \frac{1}{2} \int_\Omega \Big[\langle vcu \rangle_\square|_{t=0} + \langle vcu \rangle_\square|_{t=T} \Big] \,\mathrm{d}\Omega. \tag{17}$$

We now define the norm of the error

$$\|e\|^2 = A^{\mathrm{s}}(e, e), \tag{18}$$

and by using Cauchy-Schwartz inequality we obtain the upper bound $\|e\| \leq \|e^{\mathrm{s}}\|$ where e^{s} solves the symmetric error equation

$$A^{\mathrm{s}}(e^{\mathrm{s}}, v) = R(v) \quad \forall v \in \mathcal{V}. \tag{19}$$

Utilizing that the symmetrized error equation (19) is localizable in time, and using properties of the reduction technique, (in particular orthogonality,) we can obtain the explicit error estimate, cf. Jakobsson et al. [2],

$$\|e\|^2 \leq \|e^{\mathrm{s}}\|^2 \leq \int_I \left[\frac{1+\gamma}{\lambda_{N_{\mathrm{R}}}} \int_\Omega \langle c(\Pi_{\mathrm{C}} \dot{u}_{\mathrm{stat,R}})^2 \rangle_\square \,\mathrm{d}\Omega \right] \mathrm{d}t + 4 \int_\Omega \langle c(\Pi_{\mathrm{C}}[u_0 - u_{\mathrm{stat,R}}(0)])^2 \rangle_\square \,\mathrm{d}\Omega, \tag{20}$$

where $\Pi_{\mathrm{C}} v = v - \Pi_{\mathrm{R}} v$ and $\Pi_{\mathrm{R}} v$ is the projection of v on to the reduced space. The constant γ connects the alternative decomposition (10) to the standard decomposition (3). We note, in particular, that the estimates do not (explicitly) depend on the microscale solution, and that no extra modes are needed for estimating the error.

4 Goal Oriented Error Estimation

It is also of interest to estimate the error in pre-determined Quantities of Interest (QoI). To this end we define a general linear functional to represent the QoI

$$L^\star(u) = \int_I \int_\Omega \Big[\langle ucX \rangle_\square + \langle \boldsymbol{\nabla} u \cdot k \boldsymbol{\nabla} Y \rangle_\square \Big] \,\mathrm{d}\Omega \,\mathrm{d}t + \int_\Omega \langle ucZ \rangle_\square|_T \,\mathrm{d}\Omega, \tag{21}$$

where X, Y, Z are a priori chosen functions which can be adapted for different QoI. We also define $E_{\mathrm{QoI}} = L^\star(e)$ as the error in the QoI. To estimate the NMR error, E_{QoI}, we introduce the dual problem: Find the dual solution $u^\star \in \mathcal{U}^\star$ such that

$$A(v, u^\star) = L^\star(v) \quad \forall v \in \mathcal{V}^\star \tag{22}$$

where $\mathcal{U}^\star$, $\mathcal{V}^\star$ are suitable function spaces. We finally use the parallelogram law to set up the following upper and lower bounds

$$E^-_{\mathrm{QoI}} < E_{\mathrm{QoI}} < E^+_{\mathrm{QoI}}, \tag{23}$$

where E^-_{QoI}, E^+_{QoI} can be obtained explicitly in terms of the reduced solutions, u_{R} and $u^\star_{\mathrm{R}}$.

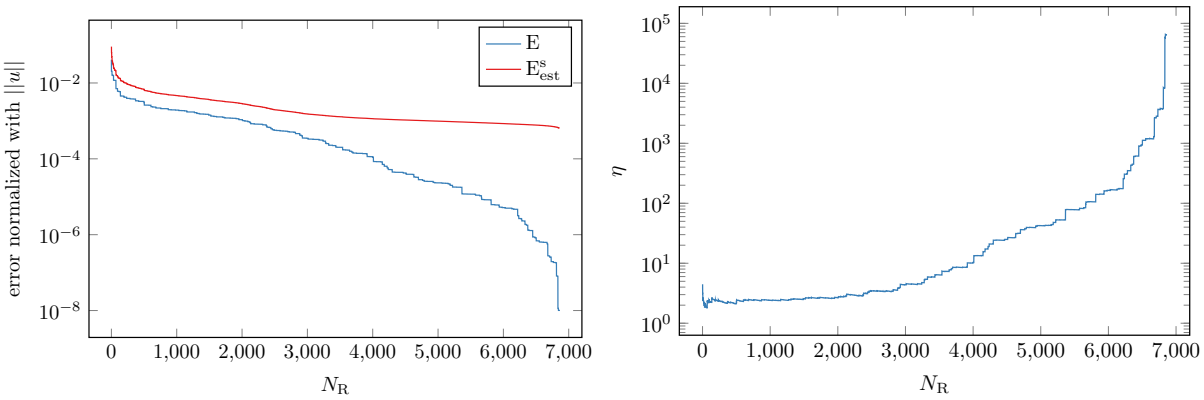

Figure 1. Left: Exact (E) and estimated (E^s_{est}) energy norm of the error. Right: Corresponding effectivity index $\eta = E^s_{est}/E$.

5 Numerical Example

We consider a simple two-scale problem as an example. The macroscale problem is a 1D heat flow through a wall with instantaneous heat increase at one boundary, and the microscale problem is a 3D RVE with a spherical inclusion. The inclusion has 5 times lower heat conductivity compared to the surrounding material. In Figure 1 the exact and estimated error is plotted together with the corresponding effectivity index. We note that the error estimation performs well in the region where $N_R <\approx 0.4N$.

Conclusions and Future Extensions

In this work we have presented a NMR approach to multiscale modeling. We obtain guaranteed bounds of the error at very low cost. It is important to note that the method is limited to linear problems; for non-linear problems it is necessary to resort to other model reduction techniques, such as Proper Orthogonal Decomposition. This will also mean that we abandon guaranteed bounds, and will instead aim for good approximations of the resulting error.

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