THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING IN SOLID AND STRUCTURAL MECHANICS

On Error-Controlled Numerical Model Reduction for Linear Transient FE^2 Analysis

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Cover:
Visualization of two spectral modes for a representative volume element with varying heat conductivity, used for microscale simulation of transient heat flow.

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Abstract

Multiscale modeling is of high interest in the engineering community due to its ability to capture the overall response, while still accounting for processes and structures on underlying fine scales. One standard approach to multiscale modeling is the so-called FE^2 procedure, where the classic constitutive relation is replaced by a boundary value problem on a Representative Volume Element (RVE) comprising the underlying microscale features. It is well realized that straight-forward use of the FE^2-strategy can be computationally intractable for a fine macroscale mesh. Therefore, it is of interest to reduce the cost of solving the individual RVE-problem(s) by introducing some kind of reduced basis, here denoted Numerical Model Reduction (NMR). However, it is important to note that the richness of the reduced basis will determine the accuracy of the solution, which calls for error control.

This thesis concerns numerical model reduction for linear transient problems in the FE^2 setting, in particular the problems of heat flow and poroelasticity. Two different reduction techniques – Spectral Decomposition and Proper Orthogonal Decomposition – are applied in order to obtain an efficient method of solving and evaluating homogenized quantities on the microscale. For the model problem of linear transient heat flow, the microscale finite element problem reduces to a set of (uncoupled) ordinary differential equations, which, obviously, can be solved more efficiently than the original fully resolved finite element problem.

For the error estimation, we focus solely on the error due to the reduced basis and ignore time- and space-discretization errors. We derive guaranteed, explicit bounds on the error in (i) a constructed "energy" norm and (ii) a user-defined quantity of interest (QoI) within the realm of goal-oriented error estimation. As a "workhorse" for the error computation, we introduce an associated (non-physical) symmetrized variational problem in space-time. We obtain low cost estimators, based on the residual, which, in particular, requires no extra modes than the ones used for the reduced basis approximation. The performance of the estimator is demonstrated with numerical examples, and, for both the heat flow problem and the poroelastic problem, we overestimate the error with an order of magnitude, which is deemed acceptable given that the estimate is fully explicit and the extra cost is negligible.

Keywords: error estimation, model reduction, computational homogenization

hello world

Preface

Acknowledgements

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Thesis

This thesis consists of an extended summary and the following appended papers:

Paper A   E. Aggestam, F. Larsson, K. Runesson, and F. Ekre. Numerical model reduction with error control in computational homogenization of transient heat flow. *Computer Methods in Applied Mechanics and Engineering* **326** (2017), 193–222. DOI: `10.1016/j.cma.2017.08.006`

Paper B   F. Ekre, F. Larsson, and K. Runesson. On error controlled numerical model reduction in FE^2-analysis of transient heat flow. *International Journal for Numerical Methods in Engineering* (2019). DOI: `10.1002/nme.6041`

Paper C   F. Ekre, F. Larsson, K. Runesson, and R. Jänicke. A posteriori error estimation for numerical model reduction in computational homogenization of porous media. *To be submitted for publication.*

The appended **Paper B** and **Paper C** were prepared in collaboration with the co-authors. The author of this thesis was responsible for the major progress of the work in the papers, i.e. took part in formulating the theory, led the planning of the papers, developed the numerical implementation, carried out the numerical simulations and prepared the manuscript. In **Paper A** the author of this thesis was responsible for the implementation and simulation of the three-dimensional numerical examples.

CONTENTS

Part I
Extended summary

1 Introduction

1.1 Background

Multiscale modeling is a well known approach for including effects from the microstructure while performing simulations on the macroscale level. The main advantage is that they usually require fewer computational resources for solving the problem. For large problems it might not even be feasible to fully resolve the microstructure with e.g. finite elements. There are a number of different approaches to multiscale modeling, e.g. Multiscale Finite Element Methods (MsFEM) and Heterogeneous Multiscale Finite Element Method (HM-FEM). Another well known approach is Variational Consistent Homogenization (VCH) and the so-called FE^2 procedure, where the classic constitutive relation is replaced by a boundary value problem on a Representative Volume Element (RVE) comprising the underlying microscale features, cf. e.g. Larsson et al. [1]. In practice this means that a full finite element problem needs to be solved in each of the quadrature points on the macroscale, and it is well-realized that straight-forward use of the FE^2-strategy can be computationally intractable for fine macroscale meshes. Therefore, it is of interest to reduce the computational cost required for solving the individual RVE-problem(s) by introducing some kind of reduced basis, here denoted Numerical Model Reduction (NMR).

Different NMR techniques for multiscale methods have been studied. Fish and coworkers [2, 3] introduced "eigendeformation reduced-order homogenization" based on the concept of Transformation Field Analysis (TFA) proposed by Dvorak and Benveniste [4]. A similar approach was proposed by Michel and Suquet [5, 6] denoted Nonuniform Transformation Field Analysis (NTFA). The NTFA approach combined with Proper Orthogonal Decomposition (POD) was investigated by Fritzen et al. [7, 8, 9, 10] for visco-elasticity and a class of standard dissipative materials. POD was also utilized by Jänicke et al. [11] for computational homogenization of poroelasticity, whereby the pore pressure plays a role similar to inelastic strains in the NTFA framework.

The reduced basis introduces a new source of errors and the richness of the basis will determine the accuracy of the solution. Strategies for quantifying this error have been developed for various multiscale methods and reduction techniques in previous work, cf. e.g. Abdulle et al. [12, 13], Boyaval [14], Ohlberger and Schindler [15], and Efendiev with coworkers [16, 17]. It is not only the accuracy of the solution itself that is important, usually the error in some other resulting quantity is also of interest. Within the realm of goal-oriented error estimation the aim is to estimate the error in terms of a user-defined quantities, cf. e.g. the work by Oden and Prudhomme [18, 19]. In the context of applying NMR for the subscale such a quantity could be e.g. the homogenized stress used for the macroscale computation.

1.2   Aim of research

The aim of this research is to develop efficient methods for multiscale modeling. In particular, the goal is to investigate NMR techniques, and apply them to the subscale problems arizing from computational homogenization, in an attempt to make the solution of complicated macroscopic problems feasible. As mentioned earlier, the use of NMR methods results in an extra source of errors. Moreover, in a nested multiscale method this error will propagate between the scales. Therefore, an important goal of the research is to develop error estimators for quantification of this error, both locally for a given subscale, and as a "global" measure on the macroscale.

1.3   Scope and limitations

The main focus of this work is to investigate error-controlled numerical model reduction in a FE^2 setting. The following major tasks are identified:

- implement an FE^2 algorithm utilizing NMR for the subscale problem(s);

- derive an error estimator to quantify the NMR error in terms of an "energy norm" and user-defined quantities of interest.

The present work is limited to transient linear problems. Linearity is an important property for the type of guaranteed error estimates that is utilized for quantification of the NMR error. The application of NMR with error control for non-linear problems is left for future research. Another important limitation is that only the NMR error is considered for the error estimation. Other types of errors, such as smoothening errors from the homogenization, and time and space discretization errors, are completely ignored.

2   FE^2 approach to multiscale modeling

There exist multiple methods for multiscale modeling with the goal of taking the microstructure of the problem into account, e.g. the Multiscale Finite Element Method (MsFEM) [20, 21] and the Heterogeneous Multiscale Finite Element Method [22, 12, 13]. It is noted that the latter method does not presume scale separation. In this work we adopt the procedure of Variationally Consistent Homogenization (VCH). We assume complete separation of scales between the microscale and the macroscale, cf. e.g. Larsson et al. [1], and adopt the Finite Element squared (FE^2) technique for solving the resulting two-scale problem. Thus, in a finite element setting, the effective properties are computed in each macroscale quadrature point by solving a boundary value problem defined on the subscale structure. Information is passed between the scales in both directions – the (current) macroscale solution is sent to the subscale (*prolongation*), the subscale problem is solved, and effective properties are sent back to the macroscale (*homogenization*). See Figure 2.1 for an illustration of the procedure.
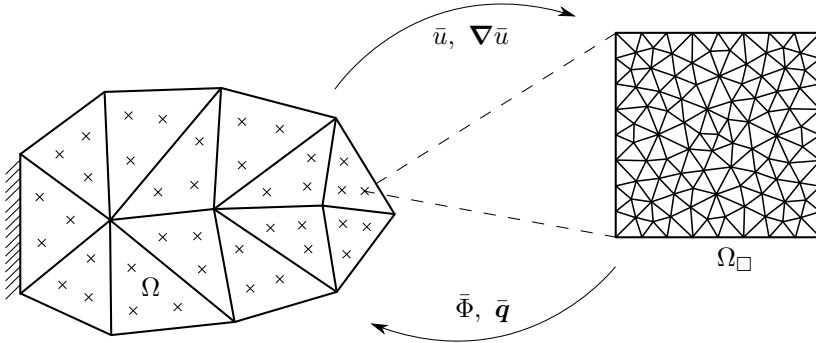
Figure 2.1: Schematic illustration of the FE^2 procedure: In each quadrature point of the macroscale mesh (Ω) the homogenized field $\bar{u}$ and the gradient $\boldsymbol{\nabla}\bar{u}$ is passed to the microscale ($\Omega_\square$) where the microscale problem is solved, and homogenized quantites (e.g. homogenized stored heat $\bar{\Phi}$ and homogenized flux $\bar{\boldsymbol{q}}$) are passed back to the macroscale.

As an example, consider the space-time weak format of linear transient heat flow[1], which was the subject of **Paper A** and **Paper B**. Find the temperature $u(\boldsymbol{x}, t) \in \mathcal{U}$ s.t.

$$\int_I \int_\Omega \Big[vc\dot{u} + \boldsymbol{\nabla}v \cdot k\boldsymbol{\nabla}u \Big]\, \mathrm{d}\Omega\, \mathrm{d}t + \int_\Omega v(\bullet, 0)cu(\bullet, 0)\, \mathrm{d}\Omega =$$
$$\int_I \int_{\Gamma_\mathrm{N}} vh^\mathrm{pres}\, \mathrm{d}\Gamma\, \mathrm{d}t + \int_\Omega v(\bullet, 0)cu_0\, \mathrm{d}\Omega \quad \forall v \in \mathcal{V}, \quad (2.1)$$

where v the test function, c the volume-specific heat capacity, k the thermal conductivity, h^pres the prescribed heat flux on part of the boundary, and u_0 the initial condition. The exact definitions of the trial and test spaces $\mathcal{U}$ and $\mathcal{V}$, are omitted for brevity.

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[1]The internal heat source is left out for brevity.

In order to obtain the pertinent two-scale problem we apply the concept of variational consistent homogenization (VCH), see e.g. Larsson et al. [1]. First, we introduce running averages over representative volume elements (RVE), with domain $\Omega_\square$ centered at macroscale coordinate $\bar{\boldsymbol{x}}$, in the weak form. Next, we assume scale separation, via first order homogenization, and decompose the field into one homogenized field, $\bar{u}$, and a fluctuation field, u^μ. For a given RVE, located at $\bar{\boldsymbol{x}}$, the field is decomposed as follows:

$$u(\bar{\boldsymbol{x}}; \boldsymbol{x}, t) = \bar{u}(\bar{\boldsymbol{x}}, t) + \boldsymbol{\nabla}\bar{u}(\bar{\boldsymbol{x}}, t) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + u^\mu(\bar{\boldsymbol{x}}; \boldsymbol{x}, t). \tag{2.2}$$

The test function v is decomposed in the same way, and we obtain the macroscale problem by considering macroscopic test functions $\bar{v}$, and the microscale problems by testing each individual RVE with "fluctuation" test functions v^μ. For the purpose of numerical model reduction we are mainly interested in the resulting subscale problem, and therefore, for the details of the macroscale problem in such a setting we refer to e.g. **Paper B**.

The resulting microscale problem reads as follows. For given macroscale input, $\bar{u}(\bar{\boldsymbol{x}}, t)$, $\boldsymbol{\nabla}\bar{u}(\bar{\boldsymbol{x}}, t)$, find $u^\mu(\bar{\boldsymbol{x}}; \boldsymbol{x}, t) \in \mathcal{U}_\square^\mu$ s.t.

$$\frac{1}{|\Omega_\square|} \int_I \int_{\Omega_\square} \left[v^\mu c \left[\dot{\bar{u}} + \boldsymbol{\nabla}\dot{\bar{u}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + \dot{u}^\mu \right] + \boldsymbol{\nabla}v^\mu \cdot k \left[\boldsymbol{\nabla}\bar{u} + \boldsymbol{\nabla}u^\mu \right] \right] \mathrm{d}\Omega \, \mathrm{d}t \; +$$
$$\frac{1}{|\Omega_\square|} \int_{\Omega_\square} v^\mu(\bullet, 0) c [\bar{u}(\bullet, 0) + \boldsymbol{\nabla}\bar{u}(\bullet, 0) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + u^\mu(\bullet, 0) - u_0] \, \mathrm{d}\Omega = 0 \quad \forall v^\mu \in \mathcal{V}_\square^\mu,$$
$$\tag{2.3}$$

where $\mathcal{U}_\square^\mu$ and $\mathcal{V}_\square^\mu$ are the pertinent trial and test spaces, with their exact definitions left out for brevity.

In a FE^2-setting it is necessary to solve one microscale problem (2.3) in each macroscale quadrature point, in general in a nested fashion. For complex macroscale structures, especially for a fine mesh in three dimensions, the number of quadrature points, and thus the number of necessary solves of the microscale problem, rapidly increases and can quickly become infeasible. This is the reason we think that numerical model reduction techniques couple well with the FE^2 method; hence, an efficient way of solving the microscale problems has the potential to reduce the necessary resources and make it possible to solve large FE^2 problems. In the subsequent chapter we discuss a couple of methods to reduce the microscale problem.

3 Numerical Model Reduction

In this section we discuss a number of ways to introduce an approximation of the fluctuation field u^μ, by using Numerical Model Reduction[2] (NMR) techniques. The aim is to reduce the cost associated with the solution of the many microscale problems in a FE^2 setting.

Many reduction techniques are based on separation of domains. Perhaps the most classical approach is to separate the time and space domains, e.g. a function $u(\boldsymbol{x}, t)$, would be approximated as

$$u(\boldsymbol{x}, t) \approx u_{\mathrm{R}}(\boldsymbol{x}, t) = \sum_a^{N_{\mathrm{R}}} \varphi_a(\boldsymbol{x}) \xi_a(t) \tag{3.1}$$

where $\varphi_a(\boldsymbol{x})$ are spatial mode functions, where $\xi_a(t)$ are time dependent "mode activity" functions, and where N_{R} is the number of mode products used in the expansion. Typically, the spatial modes are based on a finite element discretization $\mathbb{U}_{\mathrm{h}}$ with N degrees of freedom, and the goal is that $N_{\mathrm{R}} \ll N$, i.e. that the number of degrees of freedom in the reduced system is *much* smaller than in the original system. The modes thus span a space $\mathbb{U}_{\mathrm{R}}$, which is reduced compared to the original finite element space $\mathbb{U}_{\mathrm{h}}$, e.g.

$$\mathbb{U} \supset \mathbb{U}_{\mathrm{h}} \supset \mathbb{U}_{\mathrm{R}} \coloneqq \mathrm{span}\{\varphi_a(\boldsymbol{x})\}_{a=1}^{N_{\mathrm{R}}}, \tag{3.2}$$

where $\mathbb{U}$ is the continuous space, see Figure 3.1.
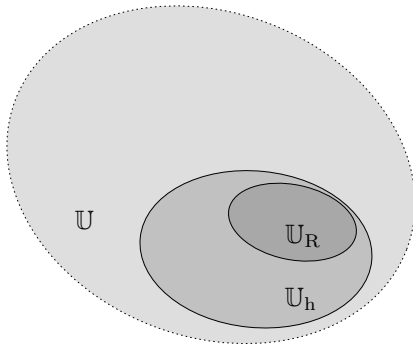
Figure 3.1: Illustration of the relation between the continuous space $\mathbb{U}$, the finite element space $\mathbb{U}_{\mathrm{h}}$ (N degrees of freedom), and the reduced space $\mathbb{U}_{\mathrm{R}}$ (N_{R} degrees of freedom) spanned by the reduced basis.

One benefit of using an expansion like (3.1) is that the problem is reduced to that of finding a set of unknown mode functions, each of them defined in a lower dimension compared to the original function. In a numerical setting, e.g. the finite element method, it might not be feasible to solve for $u(\boldsymbol{x}, t)$ directly, but it is (hopefully) possible to solve

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[2]The terms Reduced Order Modeling (ROM) and Model Order Reduction (MOR) are also used frequently in literature. We have chosen to use the term Numerical Model Reduction (NMR) to emphasize that we are using numerical methods to reduce the numerical problem, rather than tampering with the underlying model.

for individual mode functions and construct the approximation $u_{\mathrm{R}}(\boldsymbol{x}, t)$. The quality of the approximation is dependent on the quality of the computed modes and the number of modes N_{R}. Provided that suitable mode functions have been obtained, the expansion in Eq. (3.1) reduces the original problem to a one-dimensional one, where the mode activity coefficients ξ_a are the only unknowns.

There are a number of ways to obtain suitable modes, where the "best" method is often problem dependent. For linear problems, spectral decomposition (SD) is often used, whereas a reduced base is obtained by solving the resulting generalized eigenvalue problem, e.g.

$$(\underline{K} - \lambda_i \underline{M})\underline{\varphi}_i = \underline{0}, \tag{3.3}$$

where $\underline{M}$ and $\underline{K}$ are mass- and stiffness-matrices assembled from the finite element discretization, and where λ_i and $\underline{\varphi}_i$ are eigenvalues and eigenvectors. The (truncated) series of eigenvectors span the reduced space $\mathbb{U}_{\mathrm{R}}$. Spectral Decomposition was used in **Paper A** and **Paper B** to reduce the subscale finite element problem for linear transient heatflow, reducing the problem to a set of (uncoupled) ordinary differential equations. In **Paper C** we also used spectral decomposition for a coupled problem. However, the eigenvalue problem was defined for an uncoupled version, and the resulting basis was thus thus not able to capture the coupling of the fields.

Another method for finding modes is Proper Orthogonal Decomposition (POD), also known as Karhunen-Loève decomposition or principal component analysis, see for example Rousette et al. [23]. POD is a method that extracts relevant information, the "most important" by some measure, from a dataset. In the context of finding a POD basis for the subscale problem, we collect data by performing a number of "training simulations" for the RVE, and collecting "snapshots" of the solution at different time steps. The advantage of POD over e.g. SD is that it is more flexible since the POD modes can capture, for example, nonlinearities. The disadvantage, of course, is the need for training simulations and how to verify that relevant processes have been sufficiently captured by the snapshots. In **Paper C**, POD was used to obtain a reduced basis for the model problem of poroelastic media. Following the work by Jänicke et al. [11], we were able to reduce the original finite element problem to a set of ordinary differential equations.

Another method, although not used in the present work, that has been popularized recently is Proper Generalized Decomposition (PGD), cf. e.g. Chinesta et al. [24, 25, 26] and Ladevèze et al. [27, 28]. The main advantage of the PGD method is that it can handle high-dimensional problems efficiently, by using separation of variables. As an example, a function f defined in $\mathbb{R}^N$ could be approximated as a sum of N_{R} products of mode functions defined in a lower dimension, e.g. $\mathbb{R}^1$ in the following example

$$f(x_1, x_2, \ldots, x_N) \approx \sum_a^{N_{\mathrm{R}}} X_{1,a}(x_1) X_{2,a}(x_2) \ldots X_{N,a}(x_N) \tag{3.4}$$

where $X_{i,a}$ are the mode functions, x_i, $i = 1, 2, \ldots, N_{\mathrm{R}}$ are coordinates in space, time, material parameters etc. The mode functions are computed one "layer" at a time until convergence. The resulting solution is highly parametric, and PGD is thus well suited for optimization or inverse problems, where fast evaluation is important.

When employing any of the methods mentioned above, the process can be divided into two distinct stages – usually denoted the "offline stage" and the "online stage". The offline stage includes everything that can be done in a preprocessing step and cached for later use, e.g. computing the mode functions. The online stage, where the actual problem solving is performed, can thus be made more efficient by using the precomputed quantities. Of course, this division into stages only makes sense if the precomputed quantities actually makes the overall computation more efficient, for example computing modes that can be used for every time step, or every subscale problem, in the online stage. In the case of computational homogenization it is possible to precompute modes for the subscale, and, based on these modes, precompute macroscale coefficients. These coefficients can be used for every subscale problem and for every timestep, in order to obtain an efficient way of (i) solving the subscale problem and (ii) evaluating the homogenized quantities, as demonstrated in **Papers A–C**.

4 Estimation of the NMR error

There are multiple types of error involved in the solution of a FE^2 problem, e.g. time and space discretization errors from the finite element approximation (on both scales), model errors due to prolongation and homogenization from the VCH framework, and, in the context of NMR, the error introduced by the NMR approximation, and it is of course of interest to quantify these errors.

A posteriori error estimation for finite element analysis have been discussed for many years, cf. e.g. Babuška and Rheinboldt [29, 30] for some early work on estimation of space discretization errors, and Hughes and Hulbert [31] for estimation of space-time discretization errors. The error in the solution is quite often quantified in terms of an "energy norm" associated with the problem, either globally, or locally when combined with adaptive strategies for e.g. targeted mesh refinement. However, quite often it is not only the quality of the solution itself (measured in suitable norm) that is of interest, but rather the error in some other resulting quantity. Within the realm of goal-oriented error estimation the aim is to estimate the error in terms of a predefined quantity, for example the flux or stress, cf. e.g. the work by Eriksson et al. [32], Becker and Rannacher [33], and Oden and Prudhomme [18, 19]. Parés et al. [34, 35, 36] presented guaranteed estimators in this context for discretization errors in space and time for linear parabolic problems. Several error estimators have been developed for different frameworks in the context of multiscale modeling. Chamoin and Legoll [20] developed estimators based on constitutive relation error for Multiscale Finite Element Method (MsFEM), Ohlberger [22] presented a strategy for estimating the error in the Heterogeneous Multiscale Finite Element Method (HM-FEM), and the model error from the VCH framework was quantified by, e.g., Larsson and Runesson [37, 38, 39]. Error estimators for different NMR techniques have been presented by e.g. Abdulle et al. [12, 13], Boyaval [14], Ohlberger and Schindler [15], and Efendiev and coworkers [16, 17]. An alternative procedure was introduced by Verdugo et al. [40], who developed a posteriori error estimators for the (conventional) finite element discretization error using a reduced model for the adjoint solution.

While all of the different error sources mentioned above certainly are important for FE^2 implementations, we shall in this work focus solely on the estimation of the NMR error. In practice this means that we consider a fully resolved finite element solution to be "exact", i.e. that $|u - u_{\mathrm{h}}| \approx 0$ and consequently that $|u_{\mathrm{h}} - u_{\mathrm{R}}|$ is a good approximation of $|u - u_{\mathrm{R}}|$, cf. Figure 4.1. It is obvious that the accuracy of the NMR approximation is dependent on multiple things, in particular the "quality" of the modes, i.e. how well they capture the underlying phenomena, and the number of modes N_{R} used in the expansion. As an example, in **Paper C** we used a spectral basis based on a modified version of the original problem and it was shown that this lead to a mediocre approximation since the modes completely ignored the coupling between the fields.

In order to derive the explicit residual based error estimators presented in **Papers A–C** for the NMR error we use utilize linearity of the problem. Since neither of the problems discussed in **Papers A–C** are symmetric we define an auxiliary (symmetric) problem, cf. e.g. Parés et al. [34, 35, 36]. The bilinear form of the auxiliary problem defines the norm, which is used for the estimate. Explicit bounds on the error, based on the discrete
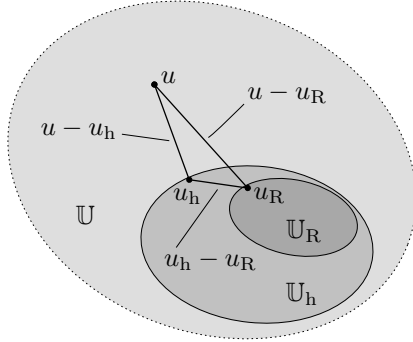
Figure 4.1: Illustration of the relation between the exact solution $u \in \mathbb{U}$, the finite element solution $u_{\mathrm{h}} \in \mathbb{U}_{\mathrm{h}}$, and the reduced solution $u_{\mathrm{R}} \in \mathbb{U}_{\mathrm{R}}$.

residual, are derived, cf. e.g. Jakobsson et al. [41]. In Figure 4.2 the typical behavior of the estimator is plotted. First, we note that a guaranteed estimator provides a bound, within which the exact error must lie. Secondly, the relation between the estimated error and the exact error determines the sharpness of the procedure. More specifically, we define the effectivity index as

$$\eta = \frac{E_{\mathrm{est}}}{E}, \tag{4.1}$$

where E_{est} and E are the estimated and exact errors, respectively. A guaranteed estimator should always result in $\eta \geq 1$, and a sharp estimator $\eta \gtrsim 1$. These properties can be investigated for examples where the exact error (i.e. the exact solution) is known.

In **Paper A** and **Paper C** the estimator is defined locally on one RVE, while in **Paper B** the estimator concerns the NMR error for the full FE^2 problem, which includes error transport between the scales. The performance of the estimator is demonstrated with numerical examples, and in general the estimator overestimates the error with an order of magnitude, i.e. $\eta \gtrsim 10$.
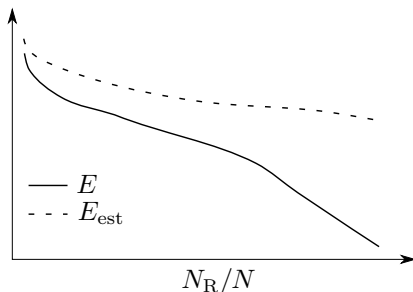

Figure 4.2: Typical behavior of the exact error E and the estimated error E_{est} as a function of number of modes N_{R} used in the approximation.

5   Summary of appended papers

Paper A: Numerical model reduction with error control in computational homogenization of transient heat flow.

Numerical Model Reduction (NMR) was exploited for solving the finite element problem on a single Representative Volume Element (RVE) that arises from computational homogenization of linear transient heat flow. In this work, since the problem is linear, an orthogonal basis for the subscale is obtained via the classical method of spectral decomposition. When employing the orthogonal base, the subscale problem reduces to a set of (uncoupled) ordinary differential equations (ODEs). The basic idea is that the basis can be truncated to N_R modes, where N_R is (much) smaller than the number of degrees of freedom (NDOFs) of the underlying finite element problem, without losing too much accuracy. Hence, the solution of the subscale problem only involves the solution of N_R ODEs. A symmetrized version of the space-time variational format was adopted for estimating the error from the model reduction in (i) energy norm and in (ii) user-defined quantities of interest. This technique, which was first developed in the context of the (non-selfadjoint) stationary diffusion-convection problem, was novel in the present context of NMR. By considering the discrete, unreduced, finite element problem as exact, we were able to obtain guaranteed bounds on the error while using only the reduced basis, and with minor additional 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. For the numerical examples that was presented, the "true error" is overestimated with a factor of 10 in the region with a low number of modes, which is considered acceptable given the efficiency of the explicit estimator, and the fact that the bounds are guaranteed.

Paper B: On error controlled numerical model reduction in FE²-analysis of transient heat flow.

Numerical model reduction was exploited for solving the nested two-scale (FE^2) problem that arises from computational homogenization of linear transient heat flow. Due to linearity, the same type of reduction technique as in **Paper A**, spectral decomposition, was used for the reduction of the underlying subscale problems. With the reduction, the computationally demanding two-scale FE^2 problem results in a "two-scale FE^1 problem", i.e. only the macroscale problem is fully resolved with finite elements, whereas the subscale problems are reduced to a set of independent ordinary differential equations. A symmetrized version of the space-time variational format of the macroscale problem was used for the error estimation, similar to the symmetrized format used in **Paper A**. The key difference for the estimator, compared to **Paper A**, is the ability to also take into account the error transport between the two scales, which was previously completely ignored. It is noted, however, that other error sources, such as time and space discretization, is still ignored. The estimate still only depends on the reduced basis used for the solution, and is explicit, resulting in a computationally efficient estimator where the extra cost is negligible compared to the cost of solving the two-scale problem. Guaranteed bounds on the NMR

error, as compared to the fully resolved finite element solution, for the two-scale problem is obtained for (i) energy norm and (ii) user-defined (macroscale) quantities of interest. The performance of the two-scale estimator was demonstrated in two examples, where the macroscale was modeled in one and two dimensions, both with three-dimensional subscale problems. The behavior of the estimate is very similar to the behavior of the subscale estimate from **Paper A**– it overestimates the "true error" with an order of magnitude for small number of modes, which is deemed acceptable given that the bounds are guaranteed and the efficiency of the error indicator.

Paper C: A posteriori error estimation for numerical model reduction in computational homogenization of porous media.

Numerical Model Reduction (NMR) was adopted for solving the microscale problem that arizes from computational homogenization of a model problem of porous media with displacement and pressure as unknown fields. A reduced basis was obtained for the pressure field using (i) Proper Orthogonal Decomposition (POD) and (ii) Spectral Decomposition (SD). This strategy has been used in previous work – the main contribution of this paper was the extension with an a posteriori estimator for assessing the error in (i) energy norm and in (ii) a given quantity of interest. A similar strategy as in **Paper A** and **Paper B** was used for the derivation of the estimator – a symmetrized format of the weak form was used in order to derive the explicit residual-based estimate. Guaranteed, explicit, bounds were derived and the performance of the error estimates was demonstrated via numerical results. A comparison between the SD basis and the POD basis was performed. As expected, the POD basis yielded a small error, and thus also a smaller estimate, but the sharpness when comparing the estimate to the exact error is poor. In contrast, the SD basis resulted in a higher error, but a sharper estimate.

6   Conclusions and outlook

In the present work we applied numerical model reduction for the subscale problems in an FE^2 setting. In particular, Spectral Decomposition and Proper Orthogonal Decomposition were used in order to define a reduced solution space and, thereby, obtain efficient methods for solving the subscale problems and evaluating the homogenized quantities that are needed for the macroscale. We derived an explicit, residual-based, estimator for estimating the NMR error in both the energy norm and user-defined linear quantities of interest.

As an outlook for further development, it is of interest to also include other error sources in the estimate. In particular, both time and space discretization errors, and model errors due to homogenization, were completely neglected so far. In this work we only considered Dirichlet type of boundary conditions for the subscale problems. However, this type of boundary conditions is not always the best choice, and it would be interesting to further develop the reduction strategy, and the error estimator, to also handle other types, such as Neumann or periodic boundary conditions. Finally, the present work is limited to linear problems. It would be interesting to investigate NMR for nonlinear problems further, and, in particular, derive an estimator with the capability to obtain guaranteed or approximate bounds on the NMR error.

References

[1] F. Larsson, K. Runesson, and F. Su. Variationally Consistent Computational Homogenization of Transient Heat Flow. en. *International Journal for Numerical Methods in Engineering* **81**.13 (2010), 1659–1686. ISSN: 1097-0207. DOI: 10.1002/nme.2747.

[2] J. Fish and Z. Yuan. Multiscale Enrichment Based on Partition of Unity for Nonperiodic Fields and Nonlinear Problems. en. *Computational Mechanics* **40**.2 (July 2007), 249–259. ISSN: 1432-0924. DOI: 10.1007/s00466-006-0095-0.

[3] C. Oskay and J. Fish. On Calibration and Validation of Eigendeformation-Based Multiscale Models for Failure Analysis of Heterogeneous Systems. en. *Computational Mechanics* **42**.2 (July 2008), 181–195. ISSN: 1432-0924. DOI: 10.1007/s00466-007-0197-3.

[4] Dvorak George J. and Benveniste Yakov. On Transformation Strains and Uniform Fields in Multiphase Elastic Media. *Proceedings of the Royal Society of London. Series A: Mathematical and Physical Sciences* **437**.1900 (May 1992), 291–310. DOI: 10.1098/rspa.1992.0062.

[5] J. C. Michel and P. Suquet. Nonuniform Transformation Field Analysis. *International Journal of Solids and Structures*. Special Issue in Honor of George J. Dvorak **40**.25 (Dec. 2003), 6937–6955. ISSN: 0020-7683. DOI: 10.1016/S0020-7683(03)00346-9.

[6] J. C. Michel and P. Suquet. Computational Analysis of Nonlinear Composite Structures Using the Nonuniform Transformation Field Analysis. *Computer Methods in Applied Mechanics and Engineering*. Advances in Computational Plasticity **193**.48 (Dec. 2004), 5477–5502. ISSN: 0045-7825. DOI: 10.1016/j.cma.2003.12.071.

[7] F. Fritzen and T. Böhlke. Reduced Basis Homogenization of Viscoelastic Composites. *Composites Science and Technology* **76** (Mar. 2013), 84–91. ISSN: 0266-3538. DOI: 10.1016/j.compscitech.2012.12.012.

[8] F. Fritzen and M. Leuschner. Reduced Basis Hybrid Computational Homogenization Based on a Mixed Incremental Formulation. *Computer Methods in Applied Mechanics and Engineering* **260** (June 2013), 143–154. ISSN: 0045-7825. DOI: 10.1016/j.cma.2013.03.007.

[9] F. Fritzen, M. Hodapp, and M. Leuschner. GPU Accelerated Computational Homogenization Based on a Variational Approach in a Reduced Basis Framework. *Computer Methods in Applied Mechanics and Engineering* **278** (Aug. 2014), 186–217. ISSN: 0045-7825. DOI: 10.1016/j.cma.2014.05.006.

[10] F. Fritzen and M. Leuschner. Nonlinear Reduced Order Homogenization of Materials Including Cohesive Interfaces. en. *Computational Mechanics* **56**.1 (July 2015), 131–151. ISSN: 1432-0924. DOI: 10.1007/s00466-015-1163-0.

[11] R. Jänicke, F. Larsson, K. Runesson, and H. Steeb. 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** (Jan. 2016), 108–120. ISSN: 0045-7825. DOI: 10.1016/j.cma.2015.09.024.

[12] A. Abdulle and Y. Bai. Adaptive Reduced Basis Finite Element Heterogeneous Multiscale Method. *Computer Methods in Applied Mechanics and Engineering* **257** (Apr. 2013), 203–220. ISSN: 0045-7825. DOI: 10.1016/j.cma.2013.01.002.

[13] A. Abdulle, Y. Bai, and G. Vilmart. *Reduced Basis Finite Element Heterogeneous Multiscale Method for Quasilinear Elliptic Homogenization Problems*. July 2014. DOI: 10.3934/dcdss.2015.8.91.

[14] S. Boyaval. Reduced-Basis Approach for Homogenization beyond the Periodic Setting. *Multiscale Modeling & Simulation* **7**.1 (Jan. 2008), 466–494. ISSN: 1540-3459. DOI: 10.1137/070688791.

[15] M. Ohlberger and F. Schindler. Error Control for the Localized Reduced Basis Multiscale Method with Adaptive On-Line Enrichment. *SIAM Journal on Scientific Computing* **37**.6 (Jan. 2015), A2865–A2895. ISSN: 1064-8275. DOI: 10.1137/151003660.

[16] Y. Efendiev, J. Galvis, and F. Thomines. A Systematic Coarse-Scale Model Reduction Technique for Parameter-Dependent Flows in Highly Heterogeneous Media and Its Applications. *Multiscale Modeling & Simulation* **10**.4 (Jan. 2012), 1317–1343. ISSN: 1540-3459. DOI: 10.1137/110853030.

[17] Y. Efendiev, J. Galvis, and E. Gildin. Local–Global Multiscale Model Reduction for Flows in High-Contrast Heterogeneous Media. *Journal of Computational Physics* **231**.24 (Oct. 2012), 8100–8113. ISSN: 0021-9991. DOI: 10.1016/j.jcp.2012.07.032.

[18] S. Prudhomme and J. T. Oden. On Goal-Oriented Error Estimation for Elliptic Problems: Application to the Control of Pointwise Errors. *Computer Methods in Applied Mechanics and Engineering* **176**.1 (July 1999), 313–331. ISSN: 0045-7825. DOI: 10.1016/S0045-7825(98)00343-0.

[19]   J. T. Oden and S. Prudhomme. Goal-Oriented Error Estimation and Adaptivity for the Finite Element Method. *Computers & Mathematics with Applications* **41**.5 (Mar. 2001), 735–756. ISSN: 0898-1221. DOI: 10.1016/S0898-1221(00)00317-5.

[20]   L. Chamoin and F. Legoll. A Posteriori Error Estimation and Adaptive Strategy for the Control of MsFEM Computations. *Computer Methods in Applied Mechanics and Engineering* **336** (July 2018), 1–38. ISSN: 0045-7825. DOI: 10.1016/j.cma.2018.02.016.

[21]   Y. Efendiev and T. Hou. Multiscale Finite Element Methods for Porous Media Flows and Their Applications. *Applied Numerical Mathematics*. Special Issue for the International Conference on Scientific Computing **57**.5 (May 1, 2007), 577–596. ISSN: 0168-9274. DOI: 10.1016/j.apnum.2006.07.009.

[22]   M. Ohlberger. A Posteriori Error Estimates for the Heterogeneous Multiscale Finite Element Method for Elliptic Homogenization Problems. *Multiscale Modeling & Simulation* **4**.1 (Jan. 2005), 88–114. ISSN: 1540-3459. DOI: 10.1137/040605229.

[23]   S. Roussette, J. C. Michel, and P. Suquet. Nonuniform Transformation Field Analysis of Elastic–Viscoplastic Composites. *Composites Science and Technology*. Mechanical Response of Fibre Reinforced Composites **69**.1 (Jan. 2009), 22–27. ISSN: 0266-3538. DOI: 10.1016/j.compscitech.2007.10.032.

[24]   F. Chinesta, A. Ammar, and E. Cueto. Recent Advances and New Challenges in the Use of the Proper Generalized Decomposition for Solving Multidimensional Models. *Arch Computat Methods Eng* **17**.4 (Dec. 1, 2010), 327–350. ISSN: 1886-1784. DOI: 10.1007/s11831-010-9049-y.

[25]   F. Chinesta, P. Ladeveze, and E. Cueto. A Short Review on Model Order Reduction Based on Proper Generalized Decomposition. *Arch Computat Methods Eng* **18**.4 (Oct. 11, 2011), 395. ISSN: 1886-1784. DOI: 10.1007/s11831-011-9064-7.

[26]   F. Chinesta, R. Keunings, and A. Leygue. *The Proper Generalized Decomposition for Advanced Numerical Simulations: A Primer*. Springer Science & Business Media, Oct. 8, 2013. 127 pp. ISBN: 978-3-319-02865-1.

[27]   P. Ladevèze, J.-C. Passieux, and D. Néron. The LATIN Multiscale Computational Method and the Proper Generalized Decomposition. *Computer Methods in Applied Mechanics and Engineering*. Multiscale Models and Mathematical Aspects in Solid and Fluid Mechanics **199**.21 (Apr. 1, 2010), 1287–1296. ISSN: 0045-7825. DOI: 10.1016/j.cma.2009.06.023.

[28]   P. Ladevèze and L. Chamoin. On the Verification of Model Reduction Methods Based on the Proper Generalized Decomposition. *Computer Methods in Applied Mechanics and Engineering* **200**.23 (June 2011), 2032–2047. ISSN: 0045-7825. DOI: 10.1016/j.cma.2011.02.019.

[29]   I. Babuvška and W. Rheinboldt. Error Estimates for Adaptive Finite Element Computations. *SIAM Journal on Numerical Analysis* **15**.4 (Aug. 1978), 736–754. ISSN: 0036-1429. DOI: 10.1137/0715049.

[30]   I. Babuška and W. C. Rheinboldt. A-Posteriori Error Estimates for the Finite Element Method. en. *International Journal for Numerical Methods in Engineering* **12**.10 (1978), 1597–1615. ISSN: 1097-0207. DOI: 10.1002/nme.1620121010.

[31]   T. J. R. Hughes and G. M. Hulbert. Space-Time Finite Element Methods for Elastodynamics: Formulations and Error Estimates. *Computer Methods in Applied Mechanics and Engineering* **66**.3 (Feb. 1988), 339–363. ISSN: 0045-7825. DOI: 10.1016/0045-7825(88)90006-0.

[32]   K. Eriksson, D. Estep, P. Hansbo, and C. Johnson. Introduction to Adaptive Methods for Differential Equations. *Acta Numerica* **4** (Jan. 1995), 105–158. ISSN: 1474-0508, 0962-4929. DOI: 10.1017/S0962492900002531.

[33]   R. Becker and R. Rannacher. A Feed-Back Approach to Error Control in Finite Element Methods: Basic Analysis and Examples (1996).

[34]   N. Parés, P. Díez, and A. Huerta. Exact Bounds for Linear Outputs of the Advection-Diffusion-Reaction Equation Using Flux-Free Error Estimates. *SIAM Journal on Scientific Computing* **31**.4 (Jan. 2009), 3064–3089. ISSN: 1064-8275. DOI: 10.1137/080724356.

[35]   N. Parés, P. Díez, and A. Huerta. Bounds of Functional Outputs for Parabolic Problems. Part I: Exact Bounds of the Discontinuous Galerkin Time Discretization. *Computer Methods in Applied Mechanics and Engineering*. Computational Methods in Fluid–Structure Interaction **197**.19 (Mar. 15, 2008), 1641–1660. ISSN: 0045-7825. DOI: 10.1016/j.cma.2007.08.025.

[36]   N. Parés, P. Díez, and A. Huerta. Bounds of Functional Outputs for Parabolic Problems. Part II: Bounds of the Exact Solution. *Computer Methods in Applied Mechanics and Engineering*. Computational Methods in Fluid–Structure Interaction **197**.19 (Mar. 15, 2008), 1661–1679. ISSN: 0045-7825. DOI: 10.1016/j.cma.2007.08.024.

[37]   F. Larsson and K. Runesson. RVE Computations with Error Control and Adaptivity: The Power of Duality. en. *Computational Mechanics* **39**.5 (Apr. 2007), 647–661. ISSN: 1432-0924. DOI: `10.1007/s00466-006-0108-z`.

[38]   F. Larsson and K. Runesson. Adaptive Bridging of Scales in Continuum Modeling Based on Error Control. English. *International Journal for Multiscale Computational Engineering* **6**.4 (2008). ISSN: 1543-1649, 1940-4352. DOI: `10.1615/IntJMultCompEng.v6.i4.80`.

[39]   F. Larsson and K. Runesson. On Two-Scale Adaptive FE Analysis of Micro-Heterogeneous Media with Seamless Scale-Bridging. *Computer Methods in Applied Mechanics and Engineering*. Special Issue on Modeling Error Estimation and Adaptive Modeling **200**.37 (Sept. 2011), 2662–2674. ISSN: 0045-7825. DOI: `10.1016/j.cma.2010.10.012`.

[40]   F. Verdugo, N. Parés, and P. Díez. Goal-Oriented Space-Time Adaptivity for Transient Dynamics Using a Modal Description of the Adjoint Solution. *Comput Mech* **54**.2 (Aug. 1, 2014), 331–352. ISSN: 1432-0924. DOI: `10.1007/s00466-014-0988-2`.

[41]   H. Jakobsson, F. Bengzon, and M. G. Larson. Adaptive Component Mode Synthesis in Linear Elasticity. en. *International Journal for Numerical Methods in Engineering* **86**.7 (2011), 829–844. ISSN: 1097-0207. DOI: `10.1002/nme.3078`.