THESIS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY IN SOLID AND STRUCTURAL MECHANICS

Numerical Model Reduction and Error Control for Computational Homogenization of Transient Problems

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Cover:
Visualization of the first pressure mode (left) and the magnitude of the corresponding displacement mode (right) obtained from applying POD to solve the consolidation problem on a representative volume element with spherical inclusions.

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Abstract

Multiscale modeling is a class of methods useful for numerical simulation of mechanics, in particular, when the microstructure of a material is of importance. The main advantage is the ability to capture the overall response, and, at the same time, account for processes and structures on the underlying fine scales. The FE^2 procedure, *finite element squared*, is one standard multiscale approach in which the constitutive relation is replaced with a boundary value problem defined on an Representative Volume Element (RVE) which contains the microscale features. The procedure thus involves the solution of finite element problems on two scales: one macroscopic problem and multiple RVE problems, typically one for each quadrature point in the macroscale mesh. While the solution of the independent RVE problems can be trivially parallelized it can still be computationally impractical to solve the two-scale problem, in particular for fine macroscale meshes. It is, therefore, of interest to investigate methods for reducing the computational cost of solving the individual RVE problems, while still having control of the accuracy.

In this thesis the concept of Numerical Model Reduction (NMR) is applied for reducing the RVE problems by constructing a reduced spatial basis using Spectral Decomposition (SD) and Proper Orthogonal Decomposition. Computational homogenization of two different transient model problems have been studied: heat flow and consolidation. In both cases the RVE problem reduces to a system of ordinary differential equations, with dimension much smaller than of the finite element system.

With the reduced basis and decreased computational time comes also loss of accuracy. Thus, in order to assess results from a reduced computation, it is useful to quantify the error. This thesis focuses solely on estimation of the error stemming from the reduced basis by assuming the fully resolved finite element solution to be exact, thereby ignoring e.g. time- and space-discretization errors. For the linear model problems guaranteed, fully computable, bounds are derived for the error in (i) a constructed "energy" norm and (ii) a user-defined quantity of interest within the realm of goal-oriented error estimation. In the non-linear case approximate, fully computable, bounds are derived based on the linearized error equation.

In all cases an associated (non-physical) symmetrized variational problem in space-time is introduced as a "driver" for the estimate. From this residual-based estimates with low computational cost are obtained. In particular, no extra modes than the ones used for the reduced basis approximation are required. The performance of the estimator is demonstrated with numerical examples, and, for both the heat flow problem and the poroelastic problem, the error is overestimated by 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

All we have to decide is what to do with the time that is given to us.

Preface

The work presented in this thesis was carried out between September 2016 and May 2021 at the Division of Material and Computational Mechanics, Department of Industrial and Materials Science, Chalmers University of Technology. The research was financially supported by the Swedish Research Council (Vetenskapsrådet) grant no. 2015-05422 and grant no. 2019-05080. Some of the numerical implementations were enabled by resources provided by the Swedish National Infrastructure for Computing (SNIC) at Chalmers Centre for Computational Science and Engineering (C3SE).

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Next, I would like to thank Emil Aggestam for paving the way for this project with his master thesis work, and for letting me collaborate on the resulting publication. I would also like to thank Kristoffer Carlsson for introducing me to the Julia programming language, for collaborating on our finite element software and for our many, almost daily, discussions about programming, finite element implementation, and everything else. Thanks also to the rest of the colleagues at Chalmers for the nice working environment and for the many interesting discussions.

Finally, I would like to thank my family for their love and support and most importantly I would like to thank my wife Ronja.

Gothenburg, May 2021
Fredrik Ekre

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* **119** (2019), 38–73. 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. *International Journal for Numerical Methods in Engineering* **121** (2020), 5350–5380. DOI: 10.1002/nme.6504

Paper D F. Ekre, F. Larsson, K. Runesson, and R. Jänicke. Combining spectral and POD modes to improve error estimation of numerical model reduction for porous media. *Submitted for publication.*

Paper E F. Ekre, R. Jänicke, F. Larsson, and K. Runesson. Efficient two-scale modeling of porous media using numerical model reduction with fully computable error bounds. *Submitted for publication.*

Paper F F. Ekre, F. Larsson, K. Runesson, and R. Jänicke. Numerical Model Reduction with error estimation for computational homogenization of non-linear consolidation. *To be submitted for publication.*

The appended Papers B–F 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 an established class of methods for simulation of physical processes. The main idea behind these methods is to include effects from the microscopic level while performing simulations on the macroscopic level, all while requiring fewer computational resources compared to the alternative of fully resolving everything in a (conventional) single scale analysis. For large problems it might not even be feasible to fully resolve the microstructure. There are a number of different approaches to multiscale modeling. In this work computational homogenization using the so-called "Finite Element squared" (FE^2) technique is considered, cf. e.g. Feyel et al. [1] and Larsson et al. [2]. In the FE^2 procedure the classic constitutive relation is replaced by a boundary value problem on a Representative Volume Element (RVE) comprising the underlying microscale features. 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).

A number of different NMR techniques have been proposed for increasing the computational efficiency of multiscale methods. Reduction methods based on characteristic modes are highlighted and are widely used. The most prominent example is modal synthesis in vibration analysis, see e.g. textbooks on structural dynamics [3]. A more general method, applicable also for non-linear problems, is Proper Orthogonal Decomposition (POD), see e.g. Rousette et al. [4]. Considering multifield problems, Michel and Suquet [5] introduced Nonuniform Transformation Field Analysis (NTFA) for inelastic strain modes. NTFA together with POD was investigated by Fritzen et al. [6] for visco-elasticity. This strategy was also used by Jänicke et al. [7] for computational homogenization of poroelasticity where application of the POD basis reduces the original boundary value problem to a set of ordinary differential equations.

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. [8, 9], Boyaval [10], Ohlberger and Schindler [11], and Efendiev et al. [12, 13]. 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 [14, 15]. 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 and scope of research

The overall purpose of this research is to investigate NMR techniques and apply them to the subscale problems arising from computational homogenization of transient problems. In addition, since the NMR introduces an additional source of error, the aim is to develop methods for estimating and quantifying this error. The following tasks are identified and carried out during the Ph.D. project:

- Apply NMR to computational homogenization of a class of transient problems: heat flow and porous media.
- Develop computable guaranteed bounds for the NMR error.
- Establish a procedure for total control of the NMR error in FE^2 simulations.
- Extend the computable error estimator to goal-oriented error control in user-defined quantities of interest.
- Develop an error estimator suitable for the non-linear consolidation problem.

The scope of the work is limited by focusing on the efficiency aspect of the FE^2 procedure and using NMR to reduce the computational cost. Furthermore, the sought error control is limited to the NMR error. It is assumed that a fine underlying discretization is used such that the NMR error will be the major contribution to the total error. There are situations where a very fine mesh might be required to describe complex microstructural features or where it might be obtained from e.g. detailed voxel data, which motivates this assumption. Also, errors induced by the FE^2 procedure, e.g. homogenization errors, are neglected. Finally, for simplicity only Dirichlet boundary conditions have been considered for the RVE problem.

1.3 Structure of this thesis

This thesis consists of an of an extended summary and six appended papers. The remainder of this extended summary is structured as follows. Chapter 2 includes an overview of multiscale modeling, and in particular a description of the VCH framework for computational homogenization which has been used in this project. The FE^2 procedure is described for the two model problems of transient heat flow and transient consolidation. In particular the RVE problems are presented, which serve as the basis for the NMR. Chapter 3 includes an overview of various reduction techniques with the focus Spectral Decomposition and Proper Orthogonal Decomposition. The application of NMR to the RVE problem is described. Chapter 4 discusses estimation of the NMR introduced error. The strategy which has been developed in this project is presented. Chapter 5 includes a brief summary of the appended papers and presents the main findings. The thesis is

concluded in Chapter 6 which summarizes the results, and presents an outlook for future work.

2 FE^2 approach to multiscale modeling

Multiple methods exist for multiscale modeling with the goal of taking the microstructure of the problem into account, e.g. the Multiscale Finite Element Method (MsFEM) [16, 17], Heterogeneous Multiscale Finite Element Method [18, 8, 9], and the Variational MultiScale (VMS) method [19] and developments thereof [20, 21]. It is noted that the latter methods do not presume scale separation. In this work we adopt the procedure of computational homogenization and assume complete separation of scales between the microscale and the macroscale, cf. e.g. Feyel et al. [1], Miehe et al. [22], Geers et al. [23], and Larsson et al. [2]. The Finite Element squared (FE^2) procedure is used for solving the resulting two-scale problem and, thus, 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.

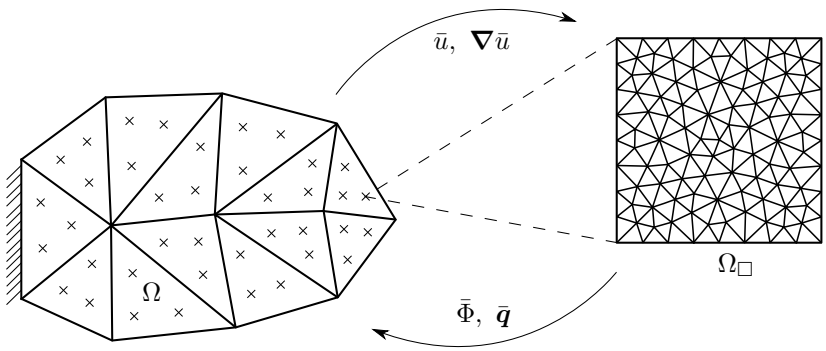

Figure 2.1: Schematic illustration of the FE^2 procedure applied to homogenization of heat flow. In each quadrature point $\bar{\boldsymbol{x}}$ of the macroscale mesh (Ω) the homogenized temperature $\bar{u}(\bar{\boldsymbol{x}}, t)$ and the gradient $\boldsymbol{\nabla}\bar{u}(\bar{\boldsymbol{x}}, t)$ are passed to the microscale ($\Omega_\square$) where the microscale problem is solved to give $\boldsymbol{u}^\mu(\bar{\boldsymbol{x}}; \boldsymbol{x}, t)$. Finally, homogenized stored heat $\bar{\Phi}(\bar{\boldsymbol{x}}; \boldsymbol{x}, t)$ and homogenized flux $\bar{\boldsymbol{q}}(\bar{\boldsymbol{x}}; \boldsymbol{x}, t)$ are passed back to the macroscale.

In an FE^2-setting it is necessary to solve one microscale problem in every 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 why 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 larger FE^2 problems.

2.1 Two-scale formulation of transient heat flow

Homogenization of transient linear heat flow is the topic of Paper A and Paper B. The weak space-time format is used as a starting point for defining the two-scale problem: find the temperature $u(\boldsymbol{x},t) \in \mathcal{U}$ such that

$$\int_I \int_\Omega \Big[vc\dot{u} + \boldsymbol{\nabla} v \cdot k \boldsymbol{\nabla} u \Big] \,\mathrm{d}\Omega \,\mathrm{d}t + \int_\Omega v(\bullet,0) c u(\bullet,0) \,\mathrm{d}\Omega = \int_I \int_{\Gamma_\mathrm{N}} v h^\mathrm{pres}(t) \,\mathrm{d}\Gamma \,\mathrm{d}t + \int_\Omega v(\bullet,0) c u_0 \,\mathrm{d}\Omega \quad \forall v \in \mathcal{V}, \quad (2.1)$$

where v is the test function, $c = c(\boldsymbol{x})$ is the volume-specific heat capacity, $k = k(\boldsymbol{x})$ is the thermal conductivity. The multiscale feature of the problem is present due to spatially fluctuating values of c and k. $\mathcal{U}$ and $\mathcal{V}$ are appropriate trial and test spaces with their exact definitions left out for brevity. The boundary conditions are defined as follows: $h(t) \coloneqq -k\boldsymbol{\nabla} u = h^\mathrm{pres}(t)$ on Γ_N and $u(t) = u^\mathrm{pres}(t)$ on Γ_D, where the full boundary $\Gamma \coloneqq \Gamma_\mathrm{N} \cup \Gamma_\mathrm{D}$ and $\Gamma_\mathrm{N} \cap \Gamma_\mathrm{D} = \varnothing$. Finally, initial conditions are $u = u_0$ in Ω at time $t = 0$.

In order to obtain the pertinent two-scale problem we apply the concept of Variational Consistent Homogenization (VCH), see e.g. Larsson et al. [2]. We first 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 temperature into a homogenized field, $\bar{u}$, and a fluctuation field, u^μ. For a given RVE located at $\bar{\boldsymbol{x}}$ the temperature and the test function are decomposed as follows:

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

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

The macroscale problem is obtained by considering macroscopic test functions $\bar{v}$ (setting $v^\mu = 0$), and the microscale problems by testing each individual RVE with "fluctuation" test functions v^μ (setting $\bar{v} = 0$). We thereby seek the macroscale solution $\bar{u} \in \bar{\mathcal{U}}$ such that

$$\int_I \int_\Omega \Big[\bar{v}\dot{\bar{\Phi}} + \boldsymbol{\nabla}\bar{v} \cdot [\dot{\bar{\boldsymbol{\Phi}}} - \bar{\boldsymbol{q}}] \Big] \,\mathrm{d}\Omega \,\mathrm{d}t + \int_\Omega \Big[\bar{v}(\bullet,0)\bar{\Phi}(\bullet,0) + \boldsymbol{\nabla}\bar{v}(\bullet,0) \cdot \bar{\bar{\boldsymbol{\Phi}}}(\bullet,0) \Big] \,\mathrm{d}\Omega = \int_I \int_{\Gamma_\mathrm{N}} \bar{v}\bar{h}^\mathrm{pres} \,\mathrm{d}\Gamma \,\mathrm{d}t + \int_\Omega \Big[\bar{v}(\bullet,0)\bar{\Phi}_0 + \boldsymbol{\nabla}\bar{v}(\bullet,0) \cdot \bar{\bar{\boldsymbol{\Phi}}}_0 \Big] \,\mathrm{d}\Omega \quad \forall \bar{v} \in \bar{\mathcal{V}}, \quad (2.3)$$

where $\bar{\Phi}$ and $\bar{\boldsymbol{q}}$ are the effective stored heat and heat flux, and $\bar{\bar{\boldsymbol{\Phi}}}$ is a (non-standard) higher order storage term. Here, $\bar{\mathcal{U}}$ and $\bar{\mathcal{V}}$ are the suitably defined trial set and test space, respectively. Furthermore, $\bar{h}^\mathrm{pres}$ is the macroscopic representation of h^pres, while $\bar{\Phi}_0$ and $\bar{\bar{\boldsymbol{\Phi}}}_0$ are representations of the initial condition (u_0).

As mentioned earlier, in the FE^2 scheme, the macroscale problem and RVE problems are solved in a nested fashion. This means that for each RVE solve the macroscale

components, $\bar{u}$ and $\boldsymbol{\nabla}\bar{u}$, are constant input data. The resulting microscale problem reads as follows: for known $\bar{u}(\bar{\boldsymbol{x}}, t)$ and $\boldsymbol{\nabla}\bar{u}(\bar{\boldsymbol{x}}, t)$, find $u^\mu(\bar{\boldsymbol{x}}; \boldsymbol{x}, t) \in \mathcal{U}^\mu_\square$ such that

$$\int_I \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \Big[v^\mu c\big[\dot{\bar{u}} + \boldsymbol{\nabla}\dot{\bar{u}} \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + \dot{u}^\mu\big] + \boldsymbol{\nabla} v^\mu \cdot k\big[\boldsymbol{\nabla}\bar{u} + \boldsymbol{\nabla} u^\mu\big] \Big] \,\mathrm{d}\Omega \,\mathrm{d}t + \frac{1}{|\Omega_\square|} \int_{\Omega_\square} v^\mu(\bullet, 0) c\big[\bar{u}(\bullet, 0) + \boldsymbol{\nabla}\bar{u}(\bullet, 0) \cdot [\boldsymbol{x} - \bar{\boldsymbol{x}}] + u^\mu(\bullet, 0) - u_0\big] \,\mathrm{d}\Omega = 0 \quad \forall v^\mu \in \mathcal{V}^\mu_\square, \tag{2.4}$$

where $|\Omega_\square|$ denotes the volume of the RVE, and where $\mathcal{U}^\mu_\square$ and $\mathcal{V}^\mu_\square$ are the pertinent trial and test spaces for the RVE (with exact definitions left out for brevity, cf. e.g. Paper B). For the RVE problem we consider Dirichlet boundary conditions, i.e. $u^\mu = 0$ on $\Gamma_{\square,\mathrm{D}} = \Gamma_\square$. It is worth noting that, for the purpose of accurately predicting material behavior, Dirichlet boundary conditions are often not the best choice. Instead other types, such as Neumann boundary conditions and strong/weak periodic boundary conditions, are often used, cf. e.g. Jänicke et al. [7, 24]. In this thesis, and in the appended papers, only Dirichlet boundary conditions are considered for simplicity.

Equation (2.4) is the basic format to which the numerical model reduction is applied, cf. Chapter 3. Since the topic of this thesis is numerical model reduction of the RVE problem we leave out the details of the macroscale problem and refer to e.g. Paper B.

2.2 Two-scale formulation of transient consolidation with selective homogenization

In Papers C–F we instead consider two-scale formulation of porous media as a coupled formulation with displacement $\boldsymbol{u}$ and pressure p as unknowns. For the chosen model the weak space-time format is defined by the following problem: find $(\boldsymbol{u}, p) \in \mathcal{U} \times \mathcal{P}$, such that

$$\int_I \int_\Omega \boldsymbol{\varepsilon}[\boldsymbol{v}] : \boldsymbol{\sigma} \,\mathrm{d}\Omega \,\mathrm{d}t = \int_I \int_{\Gamma_\mathrm{N}} \boldsymbol{v} \cdot \boldsymbol{t}^\mathrm{pres} \,\mathrm{d}\Gamma \,\mathrm{d}t \quad \forall \boldsymbol{v} \in \mathcal{V}, \tag{2.5a}$$

$$\int_I \int_\Omega \Big[q\,\dot{\Phi} - \boldsymbol{\nabla} q \cdot \boldsymbol{w} \Big] \,\mathrm{d}\Omega \,\mathrm{d}t + \int_\Omega [q\Phi]|_{t=0} \,\mathrm{d}\Omega = \int_I \int_{\Gamma_\mathrm{N}} q h^\mathrm{pres} \,\mathrm{d}\Gamma \,\mathrm{d}t + \int_\Omega [q\Phi_0]|_{t=0} \,\mathrm{d}\Omega \quad \forall q \in \mathcal{Q}, \tag{2.5b}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, $\boldsymbol{\varepsilon}[\boldsymbol{u}] = [\boldsymbol{u} \otimes \boldsymbol{\nabla}]^\mathrm{s}$ is the linear strain tensor, Φ is the fluid storage function, and $\boldsymbol{w}$ the seepage velocity. The definitions of the trial and test spaces are defined are left out for brevity, refer to e.g. Paper C. For stress and fluid storage we have used linear constitutive relations

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}[\boldsymbol{u}], p) = \mathbf{E} : \boldsymbol{\varepsilon}[\boldsymbol{u}] - \alpha p \boldsymbol{I}, \tag{2.6a}$$

$$\Phi(\boldsymbol{\nabla} \cdot \boldsymbol{u}, p) = \phi + \beta p + \alpha\, \boldsymbol{\nabla} \cdot \boldsymbol{u}, \tag{2.6b}$$

where $\mathbf{E}$ is the elastic fourth order stiffness tensor, α is the Biot coefficient, β the compressibility parameter of the fluid-filled pore space, and ϕ the (initial) porosity. The seepage velocity is defined as

$$\boldsymbol{w}(\boldsymbol{\nabla}\cdot\boldsymbol{u},p) = -k(\boldsymbol{\nabla}\cdot\boldsymbol{u},p)\ \boldsymbol{\nabla}p \tag{2.7}$$

In Papers C–E we considered the case of constant permeability, i.e.

$$k(\boldsymbol{\nabla}\cdot\boldsymbol{u},p) = k_0, \tag{2.8}$$

resulting in a linear problem, and in Paper F considered a non-linear relation

$$k = k(\boldsymbol{\nabla}\cdot\boldsymbol{u},p) = \frac{1}{\alpha_0^2}(\alpha_0 + \boldsymbol{\nabla}\cdot\boldsymbol{u})^2\, k_0, \tag{2.9}$$

such that the permeability depends on the volumetric strain $\boldsymbol{\nabla}\cdot\boldsymbol{u}$, resulting in a non-linear problem. In the limit $\alpha_0 \to \infty$ the original linear case with $k = k_0$ is obtained.

In order to establish the two-scale problem we follow the same steps outlined in Section 2.1, but instead of homogenizing both fields we employ *selective* homogenization and let p be represented as a fluctuation field "living" entirely on the RVE. Thus, for an RVE located at $\bar{\boldsymbol{x}}$ the fields are decomposed as follows

$$\boldsymbol{u}(\bar{\boldsymbol{x}};\boldsymbol{x},t) = \bar{\boldsymbol{u}}(\bar{\boldsymbol{x}},t) + \bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}},t)\cdot[\boldsymbol{x}-\bar{\boldsymbol{x}}] + \boldsymbol{u}^\mu(\boldsymbol{x},t), \tag{2.10a}$$

$$p(\bar{\boldsymbol{x}};\boldsymbol{x},t) = p^\mu(\bar{\boldsymbol{x}};\boldsymbol{x},t), \tag{2.10b}$$

and similarly for the test functions $\boldsymbol{v}$ and q, respectively. The resulting macroscale problem becomes standard balance of momentum,

$$-\bar{\boldsymbol{\sigma}}\cdot\boldsymbol{\nabla} = \boldsymbol{0}, \tag{2.11}$$

on strong form, where $\bar{\boldsymbol{\sigma}}$ is the effective homogenized stress tensor.

Testing each RVE independently with $\boldsymbol{v}^\mu$ and q gives the RVE problem(s): for known $\bar{\boldsymbol{u}}(\bar{\boldsymbol{x}};\boldsymbol{x},t)$ and $\bar{\boldsymbol{\varepsilon}}(\bar{\boldsymbol{x}};\boldsymbol{x},t)$, find $(\boldsymbol{u}^\mu(\boldsymbol{x},t),\ p(\boldsymbol{x},t)) \in \mathcal{U}^\mu_\square \times \mathcal{P}^\mu_\square$ such that

$$\int_I \frac{1}{|\Omega_\square|}\int_\Omega \boldsymbol{\varepsilon}[\boldsymbol{v}^\mu] : \boldsymbol{\sigma}\,\mathrm{d}\Omega\,\mathrm{d}t = 0 \quad \forall \boldsymbol{v}^\mu \in \mathcal{V}^\mu_\square, \tag{2.12a}$$

$$\int_I \frac{1}{|\Omega_\square|}\int_\Omega \Big[q\,\dot{\Phi} - \boldsymbol{\nabla}q\cdot\boldsymbol{w}\Big]\,\mathrm{d}\Omega\,\mathrm{d}t + \frac{1}{|\Omega_\square|}\int_\Omega [q\Phi]|_{t=0}\,\mathrm{d}\Omega = \frac{1}{|\Omega_\square|}\int_\Omega [q\Phi_0]|_{t=0}\,\mathrm{d}\Omega \quad \forall q \in \mathcal{Q}^\mu_\square, \tag{2.12b}$$

where $\mathcal{U}^\mu_\square$, $\mathcal{V}^\mu_\square$, $\mathcal{P}^\mu_\square$ and $\mathcal{Q}^\mu_\square$ are appropriate trial and test spaces for the RVE (cf. Paper C). Once again we choose to consider Dirichlet boundary conditions for displacement and pressure: $\boldsymbol{u}^\mu = \boldsymbol{0}$ on $\Gamma_\square$ and $p = 0$ on $\Gamma_\square$.

The RVE problem in Equation (2.12) is the starting point for the numerical model reduction, discussed further in Chapter 3. The main differences from the case of transient heat flow, cf. Section 2.1, are the coupling of the two fields $\boldsymbol{u}^\mu$ and p, and the non-linearity that was introduced as part of Paper F.

3 Numerical Model Reduction

In a two-scale setting the computational cost of the RVE problems can be a significant bottleneck in the overall computation since the number of RVE problems scale with (i) number of timesteps, (ii) number of iterations, and (iii) the macroscale mesh density. In this section we discuss how the problem can be reduced, using Numerical Model Reduction[1] (NMR) by introducing an approximation of the fluctuation field on the RVE level.

Different NMR techniques have been studied in the context of multiscale modeling. Fish and coworkers [25, 26] introduced "eigendeformation reduced-order homogenization" based on the concept of Transformation Field Analysis (TFA) proposed by Dvorak and Benveniste [27]. A similar approach was presented by Michel and Suquet [5, 28] denoted Nonuniform Transformation Field Analysis (NTFA). The NTFA approach combined with Proper Orthogonal Decomposition (POD) was investigated by Fritzen et al. [6, 29, 30, 31] for visco-elasticity and standard dissipative materials. Jänicke et al. [7] also used POD for computational homogenization of poroelasticity, whereby the pore pressure plays a role similar to inelastic strains in the NTFA framework. Waseem et al. [32] used spectral decomposition for homogenization of transient heat flow. Another method, suitable for highly parametric problems, is Proper Generalized Decomposition (PGD), cf. e.g. Chinesta et al. [33, 34, 35] and Ladevèze et al. [36, 37]. PGD allows for further decomposition of the function to be approximated and allows for e.g. material parameters or geometric features to be parameters of the solution. A related concept is "hyperreduction" where, in addition to reducing of the number of degrees of freedom, also the cost for evaluating the residual is reduced, cf. e.g. Ryckelynck et al. [38, 39], Hernández et al. [40], and Memarnahavandi et al. [41].

In this thesis we consider the classical approach of separating the time and space coordinates and use a reduced spatial basis for the fluctuation fields (e.g. the temperature u^μ as in Papers A–B and displacement and pressure $(\boldsymbol{u}^\mu, p)$ as in Papers C–F). An approximation of function $u(\boldsymbol{x}, t)$, would then 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 approximated expansion. Spatial modes are usually based on a finite element discretization of the domain, e.g. $\mathbb{U}_{\mathrm{h}}$, with N degrees of freedom. The aim is, naturally, 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 spatial modes span the reduced space $\mathbb{U}_{\mathrm{R}}$, which is a subset of the original finite element space $\mathbb{U}_{\mathrm{h}}$, i.e.

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

[1] The terms Reduced Order Modeling (ROM) and Model Order Reduction (MOR) are also used frequently in the literature. We have chosen 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.

where $\mathbb{U}$ is the continuous space, see Figure 3.1. With the mode functions known, 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.

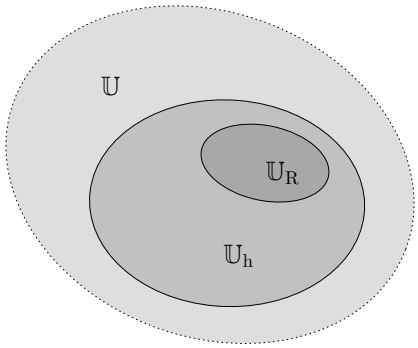

Figure 3.1: Illustration of the relation between the continuous space $\mathbb{U}$, the finite element space $\mathbb{U}_\mathrm{h}$, with N degrees of freedom, and the reduced space $\mathbb{U}_\mathrm{R}$, with N_R degrees of freedom.

The accuracy of the approximation obviously depend on the computed modes (and the number of modes). In particular, when $N_\mathrm{R} \ll N$, which is the desired case, it is important that the N_R modes are able to accurately capture the "true" solution. It thus seems natural that the process of computing the modes have an important influence on the final approximation. There are a number of ways to obtain suitable modes, where the "best" method is often problem dependent. For transient linear problems, cf. Papers A–B, Spectral Decomposition (SD) is used. The reduced basis is then based on the system mass- and stiffness matrices, $\underline{M}$ and $\underline{K}$, and solved from the generalized eigenvalue problem

$$\underline{K}\underline{\varphi}_i = \lambda_i \underline{M}\underline{\varphi}_i, \tag{3.3}$$

where λ_i and $\underline{\varphi}_i$ are eigenvalues and (discrete) eigenvectors in the finite element space $\mathbb{U}_\mathrm{h}$. 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 heat flow, reducing the problem to a set of (uncoupled) ordinary differential equations. A reduced basis based on spectral decomposition was also used for the linear, but coupled, problem in Papers C–D. In this case the generalized eigenvalue problem was similarly based on the system matrices, but the "coupling matrix" was completely ignored. The numerical examples in Papers C–D also show that the spectral base is not able to efficiently decrease the error (although, for the purpose of estimating the error it still performs well).

Proper Orthogonal Decomposition (POD), also known as Karhunen-Loève decomposition or principal component analysis, is another method for constructing a basis, see for example Rousette et al. [4]. POD is a method that extracts the "most important" (by some measure) information from a dataset. In the context of computational homogenization, and constructing a reduced basis for the RVE problem, this dataset can be collected during "training simulations" where the RVE is subjected to representative load. During

the simulation "snapshots" of the fluctuation field are then captured to build up the dataset. The advantage of POD over SD is the flexibility – it does not impose restrictions such as e.g. linearity. 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 Papers C–F, POD was used to obtain a reduced basis for the model problem of poroelastic media closely following the work by Jänicke et al. [7]. In this case the RVE problem is reduced to a set of coupled[2] ordinary differential equations.

The application of most reduced basis methods can be divided into two distinct stages which are 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 and assembling system matrices (in the case of a linear problem). The online stage, where the actual problem solving is performed, can thus be made more efficient by using the precomputed quantities. Of course, the split into an offline and an online stage only makes sense if all the preparations actually make the overall online computation more efficient. Computational homogenization is one such example since, if all RVEs have the same structure, precomputed properties can be reused by every RVE and every timestep. For linear problems (Papers A–E) the (reduced) system matrices, and macroscopic coefficients used for evaluating homogenized quantities, can be precomputed to eliminate virtually all necessary work other than solving the (small) system. For the problem of linear heat flow, the original RVE problem from Eq. (2.4) is replaced by the set of diagonalized ordinary differential equations in Eq. (3.4):

$$\begin{aligned} \dot{\xi}_a + \lambda_a \xi_a &= f_{\bar{u},a}\dot{\bar{u}} + \boldsymbol{f}_{\boldsymbol{\nabla}\bar{u},a} \cdot \boldsymbol{\nabla}\dot{\bar{u}} \\ \xi_a(0) &= \xi_{0,a} \end{aligned} \qquad a = 1, 2, \ldots, N_{\mathrm{R}} \tag{3.4}$$

where ξ_a are the unknown mode activity coefficients, where $\dot{\bar{u}}$ and $\boldsymbol{\nabla}\dot{\bar{u}}$ are inputs to the RVE, and where λ_a, $f_{\bar{u},a}$, $\boldsymbol{f}_{\boldsymbol{\nabla}\bar{u},a}$, and $\xi_{0,a}$ are quantities that can be precomputed for a given reduced basis. After solving Eq. (3.4) to obtain ξ_a the macroscopic response is evaluates as follows:

$$\bar{\Phi}(\bar{u}, \boldsymbol{\nabla}\bar{u}, \xi_a) = \bar{\Phi}_{\bar{u}}\bar{u} + \bar{\boldsymbol{\Phi}}_{\boldsymbol{\nabla}\bar{u}} \cdot \boldsymbol{\nabla}\bar{u} + \sum_{a=1}^{N_{\mathrm{R}}} \bar{\Phi}^{\mu}_{a}\xi_a, \tag{3.5a}$$

$$\bar{\bar{\boldsymbol{\Phi}}}(\bar{u}, \boldsymbol{\nabla}\bar{u}, \xi_a) = \bar{\bar{\boldsymbol{\Phi}}}_{\bar{u}}\bar{u} + \bar{\bar{\boldsymbol{\Phi}}}_{\boldsymbol{\nabla}\bar{u}} \cdot \boldsymbol{\nabla}\bar{u} + \sum_{a=1}^{N_{\mathrm{R}}} \bar{\bar{\boldsymbol{\Phi}}}^{\mu}_{a}\xi_a, \tag{3.5b}$$

$$\bar{\boldsymbol{q}}(\bar{u}, \boldsymbol{\nabla}\bar{u}, \xi_a) = \bar{\boldsymbol{q}}_{\bar{u}}\bar{u} + \bar{\boldsymbol{q}}_{\boldsymbol{\nabla}\bar{u}} \cdot \boldsymbol{\nabla}\bar{u} + \sum_{a=1}^{N_{\mathrm{R}}} \bar{\boldsymbol{q}}^{\mu}_{a}\xi_a, \tag{3.5c}$$

where $\bar{\Phi}$, $\bar{\bar{\boldsymbol{\Phi}}}$, and $\bar{\boldsymbol{q}}$ are the storage terms and the flux pertinent to the macroscale problem, cf. Eq. (2.3), and $\bar{\Phi}_{\bar{u}}$, $\bar{\boldsymbol{\Phi}}_{\boldsymbol{\nabla}\bar{u}}$, $\bar{\Phi}^{\mu}_{a}$, $\bar{\bar{\boldsymbol{\Phi}}}_{\bar{u}}$, $\bar{\bar{\boldsymbol{\Phi}}}_{\boldsymbol{\nabla}\bar{u}}$, $\bar{\bar{\boldsymbol{\Phi}}}^{\mu}_{a}$, $\bar{\boldsymbol{q}}_{\bar{u}}$, $\bar{\boldsymbol{q}}_{\boldsymbol{\nabla}\bar{u}}$, and $\bar{\boldsymbol{q}}^{\mu}_{a}$ are all quantities that have been precomputed for the reduced basis.

Figure 3.2 shows a schematic illustration of the reduced FE^2 procedure. The macroscale problem is unchanged, but the original boundary value problem for the RVE has been

[2]For the linear problem it is possible to further transform the system into a decoupled one by performing an additional diagonalizing procedure.

replaced by an offline stage, resulting in a "database" of precomputed quantities, and an online stage involving only the solution of a small system of equations. The homogenized fields $\bar{u}$ and $\boldsymbol{\nabla}\bar{u}$ from the macroscale, together with precomputed quantities from the database (λ_a, $f_{\bar{u},a}$, $\boldsymbol{f}_{\boldsymbol{\nabla}\bar{u},a}$, and $\xi_{0,a}$) gives the fluctuation field u^μ in terms of mode coefficients ξ_a. The solution is then used together with precomputed macroscopic coefficients ($\bar{\Phi}_{\bar{u}}$, $\bar{\boldsymbol{\Phi}}_{\boldsymbol{\nabla}\bar{u}}$, $\bar{\Phi}^\mu_a$, etc) to evaluate homogenized quantities that are passed back to the macroscale.

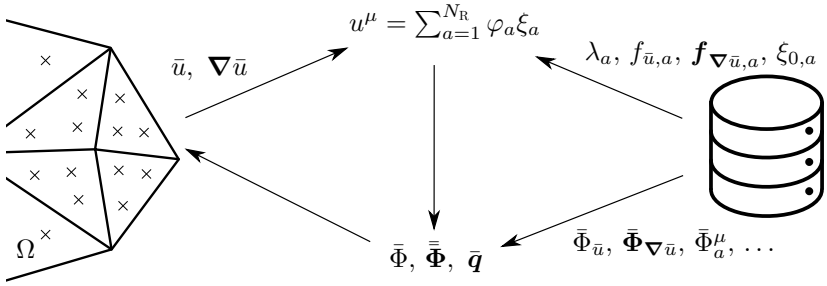

Figure 3.2: Illustration of the reduced FE^2 procedure where the RVE boundary value problem have been replaced by an offline stage, illustrated as a database of precomputed quantities, and an online stage consisting of the solution of a small system of size N_R and evaluation of homogenized quantities.

For non-linear models (Paper F) it is still necessary to perform a full online integration when assembling the local system, and when evaluating the macroscopic response. In this case the integration becomes the major contribution to the total computational cost since the cost of solving the system is negligible in comparison. For this purpose the concept of "hyperreduction" [38, 39, 40, 41] has been developed. However, this type of further reduction of the computational cost has not been considered further in the present work.

4 Estimation of the NMR error

The solution obtained from the FE^2 procedure is corrupted by errors from multiple sources such as e.g. time- and space-discretization (on both scales) and model errors introduced by the prolongation and averaging from the VCH framework. The application of NMR introduces an additional source of error when trading decreased accuracy for increased efficiency. In order to verify, and trust, the obtained solution, it is necessary to quantify and control these errors.

The error is usually measured in terms of a norm that is associated with the problem, the "energy norm", cf. e.g. Babuška and Rheinboldt [42, 43] for some early work on estimation of discretization errors in space. The error can be estimated globally, but also locally, for example element-wise, to identify areas where the error is large and, thus, finding areas where the discretization needs to be refined in an adaptive scheme. While the quality of the solution itself is certainly of interest it is quite often "secondary" quantities, e.g. quantities that are evaluated from the solution such as flux or stress, that are more important. For this purpose, goal-oriented error estimation has been developed where the aim is to control the error in predefined quantities, for example the flux on a specific boundary or the stress in a critical region of the domain. Eriksson et al. [44], Becker and Rannacher [45], and Oden and Prudhomme [14, 15] are some examples. Parés et al. [46, 47, 48] presented guaranteed goal-oriented estimators for discretization errors in space and time for linear parabolic problems. In the context of multiscale modeling Chamoin and Legoll [16] developed estimators based on constitutive relation error for Multiscale Finite Element Method (MsFEM), Ohlberger [18] presented a strategy for estimating the error for Heterogeneous Multiscale Finite Element Method (HM-FEM), and the model error from the VCH framework was quantified by, e.g., Larsson and Runesson [49, 50, 51]. Error estimators for estimating the NMR error for various reduction techniques have been presented by e.g. Abdulle et al. [8, 9], Boyaval [10], Ohlberger and Schindler [11], and Efendiev et al. [12, 13]. An alternative procedure was introduced by Verdugo et al. [52], who developed a posteriori error estimators for the (conventional) finite element discretization error using a reduced model for the adjoint solution.

As mentioned above, there are many sources of error and all of them contribute to the total error. However, the work presented in this thesis is limited to estimation of the NMR error, i.e. the error that is introduced as a result of the chosen reduction strategy. In practice this means that the fully resolved finite element solution is considered to be "exact", thereby ignoring errors from the discretization. This means that we consider $|u - u_{\mathrm{h}}| \approx 0$ and, consequently, that $|u_{\mathrm{h}} - u_{\mathrm{R}}|$ is a good approximation of $|u - u_{\mathrm{R}}|$, cf. Figure 4.1. The accuracy of the NMR approximation depends on multiple things, in particular the "quality" of the computed modes, that is, how accurately they can capture the underlying phenomena, and the number of modes N_{R} in the expansion. Papers C–D provides examples of poor accuracy stemming from a suboptimal choice of modes. In this case a spectral basis was constructed based on a modified version of the original problem, in particular the coupling between the fields was ignored, and, as the results confirm, the basis performed poorly leading to large residuals.

In Papers A–F we have derived a posteriori, residual based, error estimators for the

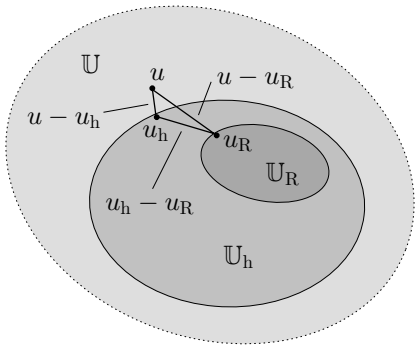

Figure 4.1: Illustration of the relation between the exact solution $u \in \mathbb{U}$, the finite element solution $u_{\mathrm{h}} \in \mathbb{U}_{\mathrm{h}}$, and the reduced solution $u_{\mathrm{R}} \in \mathbb{U}_{\mathrm{R}}$.

NMR error in the RVE solution which are explicit and fully computable. In Paper B the error transport between the scales where also considered to give an estimate of the NMR error for the full FE^2 problem. For the (linear) problems presented in Papers A–E the estimators provide guaranteed bounds of the NMR error in terms of both an associated energy norm an in terms of predefined quantities of interest. The estimates are based on a symmetric auxiliary problem, cf. e.g. Parés et al. [46, 47, 48] and a corresponding auxiliary error equation. The auxiliary form is defined such that it defines an "energy norm" associated with the problem, and, through the auxiliary error, provides a bound on the true error, i.e. $\|e\| \leq \|\hat{e}\|$ where e is the exact error and $\hat{e}$ is the auxiliary error representation. An explicit estimate of the (discrete) residual is derived, cf. e.g. Jakobsson et al. [53] which in turn provides an estimate of the auxiliary error, e.g. $\|e\| \leq \|\hat{e}\| \leq E_{\mathrm{est}}$ where E_{est} is the estimate of the residual. A similar strategy is used for the non-linear problem considered in Paper F. In this case the estimate is based on the linearized error equation, and the auxiliary form provides only an approximate bound on the true error.

The overall strategy can, without going into specifics, be summarized with the following "building blocks":

- Definition of error equation for error $e = u - u_{\mathrm{R}}$:

$$A(e, v) = R(v), \tag{4.1}$$

  where $A(\bullet, \bullet)$ is the weak space-time form of the problem, and $R(\bullet)$ the residual.

- Definition of an auxiliary bilinear and symmetric form $\hat{A}$ such that

$$\|\bullet\| \coloneqq \sqrt{\hat{A}(\bullet, \bullet)}, \quad \hat{A}(\bullet, \bullet) \leq A(\bullet, \bullet). \tag{4.2}$$

  where $\hat{A}(\bullet, \bullet)$ defines the auxiliary symmetric space-time format.

- Definition of auxiliary error equation for auxiliary error representation $\hat{e}$:

$$\hat{A}(\hat{e}, v) = R(v). \tag{4.3}$$

- Combining error equations and the bound given by $\hat{A}(\bullet, \bullet)$ for obtaining the bound $\|e\| \leq \|\hat{e}\|$:

$$\|e\| = \hat{A}(e, e) \leq A(e, e) = R(e) = \hat{A}(\hat{e}, e) \leq \|\hat{e}\|\|e\|. \tag{4.4}$$

- Estimation of the residual:

$$|R(\hat{e})| \leq E_{\text{est}}\|\hat{e}\|, \tag{4.5}$$

  where E_{est} is the final energy norm estimate, i.e.

$$\|e\| \leq \|\hat{e}\| \leq E_{\text{est}}. \tag{4.6}$$

The typical behavior of the estimator is illustrated in Figure 4.2 as a function of the number of modes used in the reduction. 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 an effectivity index

$$\eta = \frac{E_{\text{est}}}{E}, \tag{4.7}$$

where E_{est} and E are the estimated and exact errors, respectively, such that a guaranteed estimator should always result in $\eta \geq 1$, and a sharp estimator $\eta \gtrsim 1$. The same behavior is encountered in all the examples, in particular the behavior of the effectivity index: for low number of modes the estimator is "sharp", overestimating the error with an order of magnitude, but as the number of modes increase the estimator quickly deteriorates.

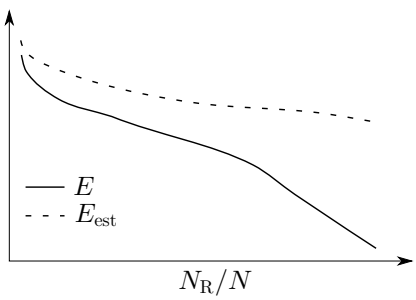

Figure 4.2: Typical behavior of the exact error E and the estimated error E_{est} as a function of number of modes N_{R} used in the approximation.

For estimating the error in terms of user-defined quantities of interest the following additional steps were used:

- Definition of the exact and reduced dual problems:

$$A^\star(u^\star, v) = Q(v), \quad A^\star(u^\star_{\text{R}}, v) = Q(v), \tag{4.8}$$

  where Q is a linear output functional for measuring user-defined quantities.

- Definition of dual error equation for dual error $e^\star$:

$$A^\star(e^\star, v) = R^\star(v). \tag{4.9}$$

- Definition of auxiliary dual error equation for auxiliary dual error representation $\hat{e}^\star$:

$$\hat{A}(\hat{e}^\star, v) = R^\star(v). \tag{4.10}$$

- Linear combination of the auxiliary primal and dual error representations for obtaining upper (E_{Q}^+) and lower (E_{Q}^-) estimates on $Q(e)$, i.e. the error in the quantity of interest:

$$E_{\mathrm{Q}}^- \leq Q(e) \leq E_{\mathrm{Q}}^+. \tag{4.11}$$

The behavior of the goal oriented estimator is very similar to the estimator for the energy norm of the error. For a small number of modes the sharpness is acceptable and the estimated error overestimates the true error with an order of magnitude.

5 Summary of appended papers

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

Numerical Model Reduction (NMR) is exploited for solving the finite element problem on a single Representative Volume Element (RVE) that arises from computational homogenization of linear transient heat flow. 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-self adjoint) stationary diffusion-convection problem, is novel in the present context of NMR. By considering the discrete, unreduced, finite element problem as exact, we are 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 are 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 FE^2-analysis of transient heat flow.

Numerical model reduction is 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, is 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 is 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 is demonstrated in two examples, where the macroscale is 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) is adopted for solving the microscale problem that arises from computational homogenization of a model problem of porous media, with displacement and pressure as unknown fields. A reduced basis is obtained for the pressure field using (i) Proper Orthogonal Decomposition (POD) and (ii) Spectral Decomposition (SD). By using the NTFA framework, corresponding displacement modes can be precomputed at an offline stage. A similar strategy as in Paper A and Paper B is used for the derivation of energy norm and goal oriented error estimators – a symmetrized format of the weak form is used in order to derive the explicit residual-based estimates. Guaranteed, explicit, bounds are derived and the performance of the error estimates is demonstrated via numerical results. A comparison between the SD basis and the POD basis is performed. As expected, the POD basis yields 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 results in a higher error, but a sharper estimate.

Paper D: Combining spectral and POD modes to improve error estimation of numerical model reduction for porous media.

Spectral decomposition and Proper Orthogonal Decomposition is used to reduce the computational cost of solving the RVE problem pertinent to computational homogenization of porous media. This work directly continues upon Paper C with the extension of *combined* reduced basis consisting of both spectral modes and POD modes. It was noted in Paper C that a spectral basis resulted in a high error, but the resulting error estimator was sharp. In contrast, a POD basis resulted in a low error, but the error estimator was not as sharp compared to the spectral base, prompting the idea of constructing a combined basis. Numerical examples are presented for two three-dimensional RVEs with different microstructures. The results suggests that a combined basis can give a lower value of the computed error bound for the same number of reduced modes. Since this is the measure that can be assessed in a stopping criteria in, e.g., an adaptive algorithm, the combined basis can be considered the most efficient one. However, the performance highly depends on the eigenvalue spectrum from the spectral basis and, hence, the microstructure.

Paper E: Efficient two-scale modeling of porous media using numerical model reduction with fully computable error bounds.

The microscale problem arising from computational homogenization of linear transient

porous media is solved by adopting the concept of NMR. Homogenization is performed for both the displacement and pressure, in contrast to Papers C–D where selective homogenization was used, and weak periodic boundary conditions are used for the RVE problem. A numerical example concerning a three-dimensional RVE with randomly distributed inclusions is presented. The estimator from Papers C–D, although still applicable only for Dirichlet boundary conditions, is used for estimating the error in the homogenized stress.

Paper F: Numerical model reduction with error estimation for computational homogenization of non-linear consolidation.

Numerical model reduction is adopted for solving the non-linear microscale problem that arises from computational homogenization of non-linear porous media. More specifically, we consider the case of deformation-dependent permeability. Proper Orthogonal Decomposition is used for creating a reduced spatial basis for the pressure and displacement following the work in Papers C–E. An explicitly, fully computable, a posteriori error estimator that approximates the NMR error is derived based on the linearized error equation. A bilinear symmetric auxiliary form is presented that *approximately* bounds the exact error from above. The auxiliary form is defined and motivated by the fact that it in the "linear limit" strictly bounds the error. This is in contrast to the work presented in previous papers, Papers A–E, where the corresponding bound is strict. Numerical results are presented for a three-dimensional RVE with random microstructure applied to transient macroscopic loading. The results indicate that, for the chosen loading, the estimator overestimates the error by one order of magnitude for close to linear loads, and slightly more as the non-linearity (and the error) is increased by an increased amplitude of the macroscale loading.

6 Conclusions and outlook

In this thesis methods for reducing the computational cost for solving RVE problems using NMR has been presented. Two different strategies for constructing a reduced basis were considered: in Papers A–B Spectral Decomposition was used for transient heat flow, and in Papers C–F Proper Orthogonal Decomposition was used for the problem of transient consolidation. In both cases the RVE problem was reduced from a full finite element problem to a (small) set of ordinary differential equations that could be solved efficiently.

In addition to the NMR formulation, low cost, fully computable, estimators for quantifying the NMR error have been proposed. For linear problems (Papers A–E), a strategy for obtaining guaranteed bounds on the error in terms of an energy norm, and also in terms of user-defined quantities, such as fluxes or stresses, was presented. In Paper A and Papers C–E the estimator was derived for estimation of the error local on one RVE. In Paper B, the full FE^2 problem was considered. For this case an estimator for the total error, taking into account also the error propagation between the two scales, was presented. The performance of the estimators was demonstrated in a number of numerical simulations. The examples show that even when using just a few modes in the approximation, i.e. when $N_R \ll N$, the error is small. In this region the estimated error overestimates the true error with one or two orders of magnitude. As the number of modes increase the usefulness of the estimator also deteriorates. This behavior was observed for both the heat flow problem and the porous media problem, and for error estimation in terms of energy norm as well as user-defined quantities of interest.

One interesting finding from Paper C was that the the POD basis performed well w.r.t. reducing the *actual* error, but worse in terms of the *estimated* error. On the contrary, the spectral basis performed poorly in terms of reducing the actual error, but performed better in terms of the sharpness of the estimator. The idea of a combined basis, using modes from both spectral decomposition and POD, was developed in Paper D where it was shown that it is possible to combine modes in order to obtain a lower error bound than for using any of the individual basis alone.

In Paper F we considered a non-linear formulation of consolidation using POD reduction for the RVE problem. An estimator for the error in terms of a suitably defined energy norm was presented. In this case the estimate was based on the linearized error equation that results in an approximate, instead of guaranteed, bound of the NMR error. Numerical examples demonstrated the effectiveness of the estimator. Similarly as for the linear problems, the effectivity of the estimate is best in the region of $N_R \ll N$.

A logical next step for further development is to extend the estimator for the non-linear poroelasticity problem to goal-oriented error estimation.

Since we in this work focused solely on the NMR error, it is also of interest to further develop the estimators to handle other sources of error, such as time- and space-discretization errors, and model errors due to homogenization. This would give a more complete picture in the sense of estimating the total error without, as was done in this work, assuming that the NMR error is the major contributor. Another interesting extension is adaptivity, where the estimators developed in this work can be applied in an adaptive FE^2-scheme. The estimate would then serve as an indicator for which areas, or which RVEs, that need to be refined using more modes.

In this work only Dirichlet type of boundary conditions for the subscale problems were implemented. Although this choice simplifies the formulation of the estimate, it is not necessarily the best one. For completeness, it would be interesting to apply the reduction strategy, and the error estimator, to Neumann and periodic boundary conditions.

For a non-linear problem the cost of integration becomes significant compared to the cost of solving the reduced system. To this end it could be useful to apply hyperreduction, while adjusting the estimator accordingly, to further speed up the simulations.

Finally, the developed strategy can be adopted for other engineering applications than those studied in this thesis. The results for poroelasticity are directly transferable to other problems such as, e.g., thermoelasticity or the chemo-mechanically coupled problem. The procedure developed for the non-linear problem should be investigated for other important applications of non-linear transient character, accounting for e.g. inelastic deformations.

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