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Multiscale Methods and Uncertainty Quantification

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Abstract
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In this thesis we consider two great challenges in computer simulations of partial differential equations: *multiscale data*, varying over multiple scales in space and time, and *data uncertainty*, due to lack of or inexact measurements.

We develop a multiscale method based on a coarse scale correction, using localized fine scale computations. We prove that the error in the solution produced by the multiscale method decays independently of the fine scale variation in the data or the computational domain. We consider the following aspects of multiscale methods: continuous and discontinuous underlying numerical methods, adaptivity, convection-diffusion problems, Petrov-Galerkin formulation, and complex geometries.

For uncertainty quantification problems we consider the estimation of p-quantiles and failure probability. We use spatial a posteriori error estimates to develop and improve variance reduction techniques for Monte Carlo methods. We improve standard Monte Carlo methods for computing p-quantiles and multilevel Monte Carlo methods for computing failure probability.

Keywords: multiscale methods, finite element method, discontinuous Galerkin, Petrov-Galerkin, a priori, a posteriori, complex geometry, uncertainty quantification, multilevel Monte Carlo, failure probability

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List of papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.

I   D. Elfverson, E. H. Georgoulis, and A. Målqvist. *An Adaptive Discontinuous Galerkin Multiscale Method for Elliptic Problems.* Multiscale Model. Simul. 11(3), 747–765 (2013).

II   D. Elfverson, E. H. Georgoulis, A. Målqvist, and D. Peterseim. *Convergence of a Discontinuous Galerkin Multiscale Method.* SIAM J. Numer. Anal. 51(6), 3351–3372 (2013).

III   D. Elfverson. *A Discontinuous Galerkin Multiscale Method for Convection-Diffusion Problems.* Available as arXiv:1509.03523 e-print (submitted).

IV   D. Elfverson, V. Ginting, and P. Henning. *On Multiscale Methods in Petrov-Galerkin Formulation.* Numer. Math. (2015).

V   D. Elfverson, M. G. Larson, and A. Målqvist. *Multiscale Methods for Problems with Complex Geometry.* Available as arXiv:1509.03991 e-print (submitted).

VI   D. Elfverson, D. J. Estep, F. Hellman, and A. Målqvist. *Uncertainty Quantification for Approximate p-Quantiles for Physical Models with Stochastic Inputs.* SIAM/ASA J. Uncertainty Quantification, 2(1), 826–850 (2014).

VII   D. Elfverson, F. Hellman, and A. Målqvist. *A Multilevel Monte Carlo Method for Computing Failure Probabilities.* Available as arXiv:1408.6856 e-print (submitted).

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Contents

1. Introduction

The focus of this thesis is twofold: we consider both partial differential equations (PDE) where the solution varies on several different scales, *multiscale problems*, and PDEs with uncertain data, *uncertainty quantification*. Modeling and simulation of this type of problems are very challenging and appear in most areas of science and engineering. A prominent example is flow in a porous medium. To apply standard one scale numerical methods and Monte Carlo (MC) simulation for multiscale and uncertainty quantification problems is in many cases intractable and in other cases impossible due to the immense cost. We will discuss how to address the difficulties in multiscale and uncertainty quantification problems separately.

Standard (one scale) numerical methods applied to multiscale problems fail to perform when the data is rough or the finest scale features of the data are not resolved by the underlying mesh. We will consider both when the coefficients and the computational domain have multiscale features. The main challenge in constructing numerical methods for multiscale problems is to reduce the computational complexity and still remain accurate. We propose a multiscale method where the coarse basis functions spanning the trial and/or test spaces are corrected using fine scale computations. Using a corrected basis the multiscale method has the same order of accuracy as a standard one scale method for smooth problems. The corrector problems are global, however the correctors decay exponentially away from the support of the coarse basis and the computation can be localized to patches. The size of the patches is chosen such that the accuracy is not affected. The corrector problems can be computed independently of each other, which makes them perfectly suited for parallel computation. The correctors can also be reused in e.g. time stepping and nonlinear iterations. For further discussion regarding numerical methods for multiscale problems see Section 3.

We consider applications where the model parameters are uncertain and random. We want to compute statistical properties of a quantity of interest of the solution of the PDE, in particular p-quantiles and failure probability. Failure probability is defined as the probability that a given functional or quantity of interest of the model solution is below some predetermined value. The estimation of p-quantiles is the inverse problem, i.e., determine the value such that a given functional of the solution is below that value with the predetermined probability p. Since we are interested in problems with high stochastic dimension, we consider sample based methods. When considering this type of problems we have two error sources: the numerical discretization of the

model and the stochastic sampling. To efficiently estimate p-quantiles or failure probability the two error sources need to be balanced. In this thesis we use spatial a posteriori error estimates within variance reductions techniques to reduce the computational cost and to balance the two error sources. For further discussion regarding failure probability see Section 4.

The main results of this thesis are the following:

- Adaptivity and convergence analysis for a Discontinuous Galerkin multiscale method.
- Multiscale methods in Petrov-Galerkin formulation.
- Extension of multiscale analysis to complex geometries.
- Improvment of Monte Carlo methods for p-quantiles and multilevel Monte Carlo method for failure probability, using selective refinement.

2. Model problem

In this chapter we present some notations, a model problem, and give a short introduction to the finite element method (FEM) and discontinuous Galerkin (DG) method.

2.1 The Poisson equation

We consider the boundary value problem

$$-\nabla \cdot A\nabla u = f \quad \text{in } D,$$
$$u = 0 \quad \text{on } \partial D, \tag{2.1}$$

where D is a spatial domain with boundary ∂D, f is an external forcing, and A is a diffusion matrix. For multiscale problems A, ∂D, and f varies over several different scales that are not necessarily resolved by the computational mesh. For uncertainty quantification $A = A(\omega)$ and $f = f(\omega)$ are realizations from a given sample space Ω. In subsurface flow the physical interpretation of A is permability, illustrated in Figure 2.1.
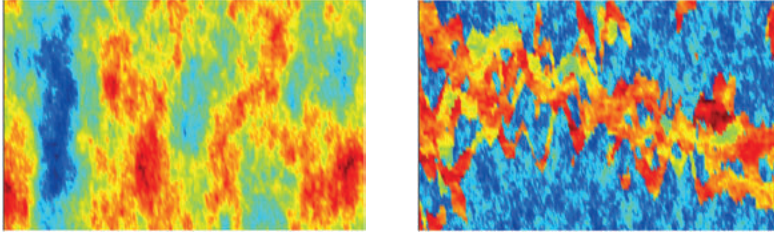
Figure 2.1. Examples of the permability in subsurface flow simulations.

Two function spaces which will be frequently used are $L^2(D)$ and $H^1(D)$. Both of the spaces are Hilbert spaces [2], i.e., both are complete inner product spaces with their inner products defined as

$$(u,v)_{L^2(D)} = \int_D uv \, dx \quad \text{and} \quad (u,v)_{H^1(D)} = (\nabla u, \nabla v)_{L^2(D)} + (u,v)_{L^2(D)}, \tag{2.2}$$

respectively. We will denote

$$\|v\|_{L^2(D)} = \sqrt{(v,v)_{L^2(D)}} \quad \text{and} \quad \|v\|_{H^1(D)} = \sqrt{(v,v)_{H^1(D)}}, \tag{2.3}$$

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the $L^2(D)$ and $H^1(D)$ norms induced by their inner products. Let us consider the function space $V_0 = \{v \in H^1(D) \mid v|_{\partial D} = 0\}$, i.e., all functions in $H^1(D)$ that vanishes on the boundary ∂D. The weak form of (2.1) reads: find $u \in V_0$ such that

$$a(u,v) := \int_D A\nabla u \cdot \nabla v \, \mathrm{d}x = \int_D fv \, \mathrm{d}x =: F(v) \quad \text{for all } v \in V_0. \qquad (2.4)$$

By the Lax-Milgram lemma, there exists a unique solution $u \in V_0$ to (2.4) if the bilinear form $a(\cdot,\cdot)$ is coercive and continuous and the forcing function $F(\cdot)$ is a bounded linear functional. For a bilinear form to be coercive and continuous it has to fulfill

$$a(v,v) \geq C_1 \|v\|^2_{H^1(D)}, \quad \text{and} \quad |a(v,w)| \leq C_2 \|v\|_{H^1(D)} \|w\|_{H^1(D)}, \qquad (2.5)$$

for all $v, w \in V_0$.

2.2 The finite element method

Since there typically is no closed form solution to (2.4) it needs to be approximated by a numerical method. A powerful numerical method is the FEM which has a strong mathematical foundation from functional analysis, that can be used to derive analytic error estimates/bounds [6].

The FEM seeks the solution in a finite dimensional subset $V_h \subset V$ of continuous piecewise polynomials defined on a mesh $\mathcal{T}_h$ covering the computational domain. The mesh typically consists of triangles/quadrilaterals in 2D and tetrahedras/prisms in 3D. Let $h : \Omega \to \mathbb{R}$ be a mesh-size function defined elementwise as $h|_T = \mathrm{diam}(T)$, i.e., the diameter of smallest circle containing T. The FEM approximation reads: find $u_h \in V_h$ such that

$$a(u_h, v) = F(v) \quad \text{for all } v \in V_h. \qquad (2.6)$$

For the solution u_h to be a good approximation of u, the space V_h needs to resolve the variation in A. For many realistic problems this assumption is very computationally demanding to fulfill.

There are two main classes of error estimates or bounds for the FEM, *a priori* and *a posteriori*. The a priori error bound depends on the data and smoothness of the exact solution u, i.e.,

$$\|u - u_h\| := \|A^{1/2}\nabla(u - u_h)\|_{L^2(D)} \leq Ch^{s-1} |u|_{H^s(D)}, \qquad (2.7)$$

where $h = \max_{T \in \mathcal{T}_h} h|_T$ and $H^s(D)$ is a function space containing all functions with bounded weak derivatives of total degree s in $L^2(D)$. To achieve linear convergence the smoothness constraint $u \in H^2(D)$ must be fulfilled. Higher order convergence can be obtain if both higher order polynomials are used and

the exact solution is smoother, $s > 2$. However even if $u \in H^2(D)$, $|u|_{H^2(D)}$ depends on the variation of the coefficient A and there is a pre-asymptotic regime where no convergence occur until the variations are resolved. The a posteriori error bound depends on the data and the numerical solution. Hence, a posteriori error bounds can be used in an adaptive algorithm to improve the numerical solution iteratively. For the standard FEM the a posteriori error bounds have the form

$$\||u - u_h|\|^2 \leq C \sum_{T \in \mathscr{T}_h} \left(h|_K^2 \|f + \nabla \cdot A \nabla u_h\|^2_{L^2(T)} \right.$$
$$\left. + h|_K \|v \cdot [A\nabla U]\|^2_{L^2(\partial T)} \right), \tag{2.8}$$

where $[\cdot]$ is the jump in function value and v is a unit normal on ∂T.

2.3 The discontinuous Galerkin method

An interesting alternative to the standard (conforming) FEM is the DG method. In DG methods there is no continuity constraint imposed on the approximation spaces. Instead the continuity is imposed weakly in the bilinear form, i.e., the DG method allows for jumps in the numerical solution between different elements in the mesh. The first DG method was introduced in [34] for numerical approximations of first order hyperbolic problems and analyzed in [26, 24]. For some early work for DG method for elliptic problems see [38, 8, 3]. See also [30] for some preliminary work and [18, 33, 35] for a literature review.

We will use the same notation for the bilinear form, energy norm, and for the discrete function spaces for the DG method as for the FEM, however, with different definitions. The approximation space for the DG method, V_h, is the space of piecewise polynomials, i.e., DG methods uses a non-conforming ansatz $V_h \not\subset V$. The DG method has a higher number of degrees of freedom than the standard (conforming) FEM, but has the advantages that non-conforming meshes can be used and that it does not suffer from stability issues for first order or convection dominated PDEs. Also, the DG method is perfectly suited for hp-adaptivity, where both the mesh size and the order of the polynomial's degree can vary over the domain, see e.g. [21]. Since the DG method seeks the solution in a space which consists of piecewise polynomials without any continuity constraints, a modified bilinear form has to be used. In the bilinear form the continuity is imposed weakly, i.e., there is a penalty which forces the jump in the approximate solution to decrease when the mesh-size decreases. Let $\mathscr{T}_h$ be a given mesh and $\mathscr{E}_h$ be the skeleton of the mesh, i.e., the set of all edges of the elements in $\mathscr{T}_h$. For two elements T^+ and T^- sharing a common edge, $e := T^+ \cap T^-$, the jump and average on e are defined as

$$\{v\} = \frac{1}{2}(v|_{T^+} + v|_{T^-}) \quad \text{and} \quad [v] = v|_{T^+} - v|_{T^-} \tag{2.9}$$

in the interior and as $\{v\} = [v] = v_T$ on the boundary. We let v_e be the unit normal pointing from T^+ to T^- and σ_e be an edge-wise constant depending on A. The bilinear form for the DG method is defined as

$$
\begin{aligned}
a(u,v) &= \sum_{T \in \mathscr{T}_h} \int_T A\nabla u \cdot \nabla v \, dx \\
&\quad - \sum_{e \in \mathscr{E}_h} \int_e \left(v_e \cdot \{A\nabla u\}[v] + v_e \cdot \{A\nabla v\}[u] - \frac{\sigma_e}{h}[u][v] \right) ds.
\end{aligned}
\tag{2.10}
$$

where σ_e is chosen large enough to make the bilinear form coercive in the standard DG energy norm, which is defined as

$$
\|v\|^2 = \left(\sum_{T \in \mathscr{T}_h} \|A^{1/2}\nabla v\|^2_{L^2(T)} + \sum_{E \in \mathscr{E}_h} \frac{\sigma_e}{h} \|[v]\|^2_{L^2(e)} \right)^{1/2}.
\tag{2.11}
$$

The DG method reads: find $u_h \in V_h$ such that

$$
a(u_h, v) = F(v) \quad \text{for all } v \in V_h.
\tag{2.12}
$$

Discontinuous Galerkin methods, as well as conforming finite element methods, perform badly when the smallest length scale of the data is not resolved. However, DG methods have the advantage in treating discontinuous coefficients, convection dominated problems, mass conservation, and flexibility of the underling mesh, all which are crucial issues in many multiscale problems, including e.g. porous media flow.

3. Multiscale problems

For *multiscale problems* standard numerical techniques fail to perform when the data is not resolved by the computational mesh [4]. A remedy for this, when the roughness is local in space, is adaptive techniques [37]. However, this is not the case for many multiscale problems. We will consider both when there are multiscale features in the coefficients and in the computational domain. In particular we consider multiscale diffusion, domains with cracks, and rough boundaries.

In the last two decades there have been a lot of research on multiscale methods treating some of these difficulties, see e.g. [20, 19, 13, 12, 9, 10, 11, 22, 23, 25, 27, 28]. Common for this these approaches is that local problems are solved on subgrid patches which resolves the data variation. The solutions to the subproblems are then used to modify a coarse scale space or equation.

We consider the local orthogonal decomposition method (LOD) first presented in [28]. See [25, 27, 23] for some preliminary work and [14, 15, 29, 32] for further development. In the LOD method the test and trial space are decomposed into coarse and fine scale subspaces using a quasi-interpolation operator. The coarse space is then corrected using fine scale information such that the corrected basis takes the fine scale behavior of the data into account. The corrected basis is constructed to be orthogonal to the kernel of the quasi-interpolation operator in the scalar product induced by the bilinear form.

3.1 Multiscale methods

In this section we will not explicitly define the function spaces and bilinear form, instead we use an abstract formulation that fits both the FEM and the DG method. We let V_H and V_h, where H, h are mesh-size functions, be the finite dimensional spaces where V_H does not and V_h does resolve the data. We assume that $V_H \subset V_h$ and $H > h$. The space V_h is referred to as the reference space and the reference solution u_h solves: find $u_h \in V_h$ such that

$$a(u_h, v) = F(v) \quad \text{for all } v \in V_h. \tag{3.1}$$

We assume u_h to be a sufficiently good approximation of u. We split the reference space V_h into a coarse and a fine scale contribution. Let $\mathscr{I}_H : L^2(\Omega) \to V_H$ be a quasi-interpolation operator onto the coarse space V_H with range$(\mathscr{I}_H) = V_H$, i.e., $V_H = \mathscr{I}_H V_h$. To simplify the analysis, we will only consider when

$\mathscr{I}_H$ is a projection, $\mathscr{I}_H^2 = \mathscr{I}_H$. The interpolation operator needs to satisfy the following local approximation and stability estimate. For any $K \in \mathscr{T}_H$ and $v \in V_h$

$$\|A^{1/2}H^{-1}(v - \mathscr{I}_H v)\|_{L^2(K)} + \|A^{1/2}\nabla \mathscr{I}_H v\|_{L^2(K)} \leq C\|v\|_{\omega_K}, \qquad (3.2)$$

holds, where $\omega_K = \mathrm{int}\{S \in \mathscr{T}_H \mid \bar{S} \cap \bar{K} \neq 0\}$ and $\|\cdot\|_{\omega_K}$ is the energy norm restricted to ω_K. We define a fine correction space to be the kernel of the interpolation operator

$$V^{\mathrm{f}} = (1 - \mathscr{I}_H)V_h = \{v \in V_h \mid \mathscr{I}_H v = 0\}. \qquad (3.3)$$

Any function $v_h \in V_h$ can be decomposed into a coarse contribution, $v_H \in V_H$, and fine scale remainder, $v^{\mathrm{f}} \in V^{\mathrm{f}}$, i.e., $v_h = v_H + v^{\mathrm{f}}$ where $v_H = \mathscr{I}_H v_H$ and $v^{\mathrm{f}} = (1 - \mathscr{I}_H)v_h$. Choosing V_H as the coarse space the fine scale remainder v^{f} is large and oscillatory and does not decay until the variations in the data are resolved. A remedy is to correct the space V_H such that the coarse basis takes the fine scale into account. We define the corrected space by $V_H^{\mathrm{ms}} = (1+Q)V_H$ where $Q : V_H \to V^{\mathrm{f}}$ is defined as: given $v_H \in V_H$ find $Q(v_H) \in V^{\mathrm{f}}$ such that

$$a(Q(v_H), w) = -a(v_H, w) \quad \text{for all } w \in V^{\mathrm{f}}. \qquad (3.4)$$

We can write the reference space as the direct sum $V_h = V_H^{\mathrm{ms}} \oplus V^{\mathrm{f}}$. By correcting the basis functions spanning the space $V_H = \mathrm{span}\{\varphi_i\}$ we can write the corrected space as the span of corrected basis function $V_H^{\mathrm{ms}} = \mathrm{span}\{\varphi_i + Q(\varphi_i)\}$. To compute the correctors is a global computation which is as expensive as solving the original reference problem. Instead, each of the correctors of the basis φ_i are computed on localized patches

$$\begin{aligned}
\omega_i^0 &:= \mathrm{int}\left(\cup(\bar{T} \in \mathscr{T}_H \mid \bar{T} \cap \{x\} \neq \emptyset)\right) \cap \Omega, \\
\omega_i^\ell &:= \mathrm{int}\left(\cup(\bar{T} \in \mathscr{T}_H \mid \bar{T} \cap \bar{\omega}_T^{\ell-1} \neq \emptyset)\right) \cap \Omega, \quad \text{for } \ell = 1,\dots,L.
\end{aligned} \qquad (3.5)$$

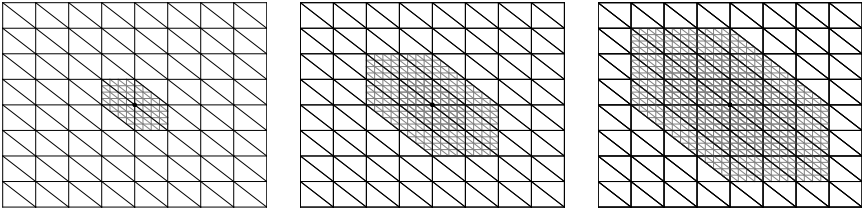See Figure 3.1 for a graphical illustration of a localized patch. Let us define

Figure 3.1. An example of 0, 1, and 2 level patches, i.e., ω_i^0, ω_i^0, and ω_i^2.

the localized corrected space by $V_H^{ms,L} = \mathrm{span}\{\varphi_i + Q^L(\varphi_i)\}$ where Q^L solves: given ϕ_i find $Q(\phi_i) \in V^{\mathrm{f}}(\omega_i^L) = \{v \in V^{\mathrm{f}}(\omega_i^L) \mid v|_{D \setminus \omega_i^L} = 0\}$ such that

$$a(Q^L(\phi_i), w) = -a(\phi_i, w) \quad \text{for all } v \in V^{\mathrm{f}}(\omega_i^L). \qquad (3.6)$$

The multiscale method posed in $V_H^{ms,L}$ reads: find $u_H^{ms,L} \in V_H^{ms,L}$ such that

$$a(u_H^{ms}, v) = F(v) \quad \text{for all } v \in V_H^{ms,L}. \tag{3.7}$$

The solution $u_H^{ms,L}$ fulfills the a priori error estimate

$$\|\|u - u_H^{ms}\|\| \leq \|\|u - u_h\|\| + CH, \tag{3.8}$$

choosing $L = \mathcal{O}(\log(H^{-1}))$, where H is the coarse mesh size and C is a constant independent of the mesh sizes h, H and the variations in A. We have that $\text{diam}(\omega_i^L) = \mathcal{O}(H \log(H^{-1}))$. See Paper II and IV for a more elaborate discussion and Paper III for a generalization toward convection-diffusion problems.

3.2 Continuous and discontinuous Galerkin method

The difference between the continuous and discontinuous Galerkin multiscale method is the choice of reference space V_h, bilinear form $a(\cdot, \cdot)$, and quasi-interpolation $\mathscr{I}_H$. The choices we make for the reference space and bilinear form are given in Section 2.2 for the FEM (continuous Galerkin) and in Section 2.3 for the DG multiscale method. The choice for the quasi-interpolation is not unique and different operators can be chosen depending on the application. Let $\mathscr{T}_H$ be the coarse mesh on which V_H is defined and $\mathscr{N}$ be the set of all vertices in $\mathscr{T}_H$.

For the continuous Galerkin method we choose $\mathscr{I}_H^{cG} : L^2(D) \to V_H$ to be defined by

$$\mathscr{I}_H^{cG} v = \sum_{x \in \mathscr{N}} (P_x v)(x) \varphi_x \tag{3.9}$$

where $P_x u \in V_H|_{\omega_x^0}$ solves

$$(P_x u, v)_{L^2(\omega_x^0)} = (u, v)_{L^2(\omega_x^0)} \quad \text{for all } v \in V_H|_{\omega_x^0}. \tag{3.10}$$

The space $V_H|_{\omega_x^0}$ is the restriction of V_H to the patch ω_x^0. See Paper V for a more elaborate discussion and Paper IV for an other choice of quasi-interpolation operator.

For the discontinuous Galerkin method we choose an elementwise L^2-projection $\mathscr{I}_H^{dG} : L^2(D) \to V_H$ defined by

$$\mathscr{I}_H^{dG} v = \sum_{T \in \mathscr{T}_H} \Pi_T v \tag{3.11}$$

where $\Pi_T u \in V_H|_T$ solves

$$(\Pi_T u, v)_{L^2(T)} = (u, v)_{L^2(T)} \quad \text{for all } v \in V_H|_T. \tag{3.12}$$

See Paper II for a more elaborate discussion.

3.3 Complex domain

So far most of the work in multiscale community has been focused for treating multiscale coefficients and less on treating complex domains. However, many multiscale applications involve voids, cracks, and rough interfaces. We extend the analysis for multiscale methods when there are multiscale features in the domain that are not resolved by the mesh. For simplicity we consider the case $A = 1$ in a complex domain. Then it is only necessary to compute the corrector problems close to the complex boundary and not in the entire domain D, see Figure 3.2. In Figure 3.2 the domain boundary cuts some of the coarse elements, however this does not affect the convergence and conditioning of the multiscale method. The condition number κ of the linear system obtained
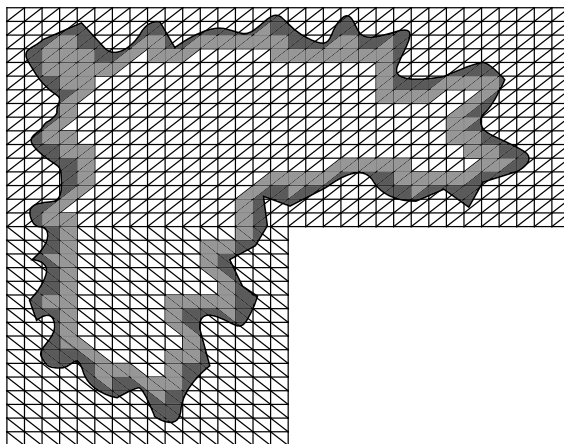

Figure 3.2. Example of complex domain embedded in a coarse mesh. The fine scale correctors only needs to be computed in the gray area. The dark Gray elements mark a 1-layer and the light gray a 2-layer patch of element round the complex boundary.

from (3.7) scales like

$$\kappa \leq CH^{-2}, \tag{3.13}$$

in the coarse mesh size H where C is a constant independent on the mesh-size and how the elements are cut by the domain boundary. See Paper V for a more elaborate discussion.

3.4 Petrov-Galerkin formulation

It is also possible to use a Petrov-Galerkin (P-G) formulation of the proposed multiscale method, i.e., using different test and trial spaces. The P-G formula-

tion reads: find $u_H^{ms,L} \in V_H^{ms,L}$ such that

$$a(u_H^{ms}, v) = F(v) \quad \text{for all } v \in V_H.\tag{3.14}$$

The P-G formulation still has the same convergence rate as the standard symmetric formulation. If global patches are used for the fine scale computations the two version are identical up to a perturbation of the right hand side,

$$a(u_H^{ms}, v) = a(u_H^{ms}, v + Q^L(v))\tag{3.15}$$

for $v \in V_H$. However, the P-G formulation can reduce the computational complexity since no communication between the correctors is needed when assembling the matrices for the corrected coarse problem, i.e., the assembling is $a(\varphi_i + Q^L(\varphi_i), \varphi_j)$ for the P-G formulation and $a(\varphi_i + Q^L(\varphi_i), \varphi_j + Q^L(\varphi_j))$ for the standard symmetric formulation. See Paper IV for a more elaborate discussion.

3.5 Adaptivity for discontinuous Galerkin multiscale method.

For porous media flow problems the permeability in the ground can vary with several orders of magnitudes over the entire domain. This motivates the use of an adaptive multiscale method to tune the method parameters in order to obtain an efficient and reliable solution. For adaptive multiscale methods, see e.g. [25, 31, 17, 1]. Given a uniform or possibly an adaptive coarse mesh $\mathcal{T}_H$, the adaptive discontinuous Galerkin multiscale method balances the error caused by truncation of the patches and the fine scale discretization error. The a posteriori error bound takes the form

$$\||u - u_H^{ms}\|| \leq C_1 \left(\sum_{S \in \mathcal{T}_h} \rho_S^2(u_H^{ms}) \right)^{1/2} + C_2 \left(\sum_{T \in \mathcal{T}_H} \rho_{\omega_T}^2(u_H^{ms}) \right)^{1/2},\tag{3.16}$$

where ρ_S^2 and $\rho_{\omega_T}^2$ are error indicators which measure the effect of the fine scale mesh size and of the truncated patches, respectively. Since using general nonconforming meshes is allowed using DG, it is easy to construct a global reference grid for the localized fine scale computations. This takes advantage of the error cancellation between different fine scale patches. See Paper I for a more elaborate discussion.

4. Uncertainty quantification

We consider PDEs with uncertain data which have high stochastic dimension. More specifically, we consider the estimation of failure probability and p-quantiles. Given some physical model

$$\mathcal{M}(\omega, u) = 0 \qquad (4.1)$$

where ω is a random parameter, let $X = X(u)$ be a quantity of interest of the model solution $u = u(\omega)$, i.e., $X : \omega \to \mathbb{R}$. The estimation of failure probability reads: given $y \in \mathbb{R}$ find $p \in [0, 1]$ such that

$$p = \Pr(X \leq y) \qquad (4.2)$$

holds. The estimation of p-quantiles is the inverse problem: given $p \in [0, 1]$ find $y \in \mathbb{R}$ such that (4.2) holds. For simplicity we will only consider failure probabilitiy here, for p-quantiles see Paper VI. Because of the high stochastic dimension we consider MC approaches using different variance reduction techniques. The curse of dimensionality does not effected MC based methods. This is a consequence of the central limit theorem which states that mean value of a sequence consisting of independent and identically distributed random variables with size n, where the random variables have mean value μ and variance σ^2, tends to the normal distribution with mean μ and variance σ^2/n, independent of the stochastic dimension [36].

The key idea is to use a posteriori error estimates/bounds to improve existing MC methods and variance reduction techniques for MC methods. We will consider the MC method and multilevel Monte Carlo method (MLMC) [16, 5, 7].

4.1 Selective refinement

We want to estimate the probability that a quantity of interest X is below a critical value y. Let us define $Q = \mathbb{1}(X \leq y)$ where $\mathbb{1}(\text{true}) = 1$ and $\mathbb{1}(\text{false}) = 0$. Then the failure probability can be expressed as the expected value of Q, i.e., $p = \mathbb{E}[Q]$. Since the quantity of interest X is a functional of the model solution it needs to be approximated using some numerical method. We will make the following assumption on the numerical approximation X_ℓ of X. Let X_ℓ satisfy

$$|X - X_\ell| \leq \left(\frac{1}{2}\right)^\ell \quad \text{or} \quad |X - X_\ell| \leq |X_\ell - y|, \qquad (4.3)$$

for all ℓ. The approximation of Q reads

$$Q_\ell = \mathbb{1}(X_\ell \leq y).\tag{4.4}$$

The Monte Carlo estimator using selective refinement reads

$$\widehat{Q}^{MC} = \frac{1}{N} \sum_{i=1}^{N} Q_L(\omega_i)\tag{4.5}$$

where ω_i is a realization of the model data and L is fixed. Compared to a standard Monte Carlo estimator where all samples are solved to the same tolerance, the selective refinement estimator only refines samples, to the finest tolerance level, that are close to the failure, see Figure 4.1. This can significantly reduce the cost since most samples are computed on coarse model resolution and hence at smaller cost than for the standard Monte Carlo estimator. See Paper VI for a discussion towards estimating p-quantiles and Paper VII for more elaborate discussion towards failure probability.
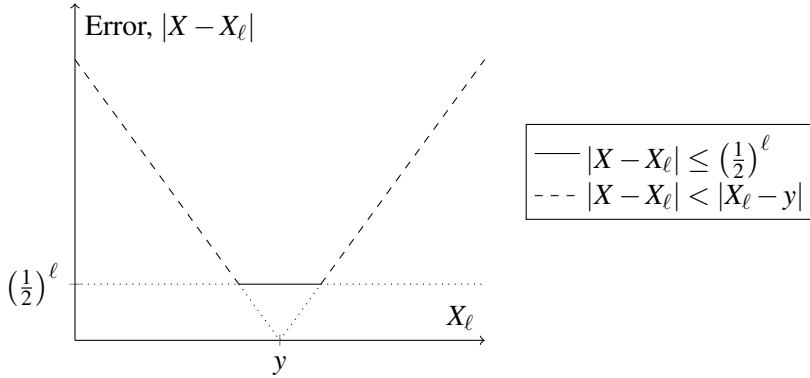

Figure 4.1. Illustration of the selective refinement condition (4.3). The numerical error is allowed to be larger far away from y.

4.2 Multilevel Monte Carlo with selective refinement

The MLMC method is a variance reduction technique that splits the estimator into different levels. On low levels many samples are used where the samples are cheap to compute and on high levels few samples are used where the samples are more expensive. The multilevel Monte Carlo estimator reads

$$\widehat{Q}^{ML} = \sum_{\ell=1}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} \left(Q_\ell(\omega_i) - Q_{\ell-1}(\omega_i)\right),\tag{4.6}$$

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where $Q_0(\omega) = 0$. Note that

$$\mathbb{E}[\widehat{Q}^{ML}] = \sum_{\ell=1}^{L} \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} (\mathbb{E}[Q_\ell(\omega_i)] - \mathbb{E}[Q_{\ell-1}(\omega_i)]) = \mathbb{E}[Q_L(\omega_i)] \qquad (4.7)$$

because of the telescopic sum. The variance of the multilevel Monte Carlo estimator is

$$\mathbb{V}[\widehat{Q}^{ML}] = \sum_{\ell=1}^{L} \frac{1}{N_\ell} \mathbb{V}[Q_\ell(\omega_i) - Q_{\ell-1}(\omega_i)]. \qquad (4.8)$$

The level dependent approximation Q_ℓ of the random variable Q satisfy

$$|\mathbb{E}[Q_\ell - Q]| \leq C_1 \left(\frac{1}{2}\right)^\ell,$$
$$\mathbb{V}[Q_\ell - Q_{\ell-1}] \leq C_2 \left(\frac{1}{2}\right)^\ell \qquad (4.9)$$

if (4.3) holds. For the root mean square error to satisfy

$$e(\widehat{Q}^{ML}) = \left(\mathbb{V}[\widehat{Q}^{ML}] + (\mathbb{E}[\widehat{Q}^{ML} - Q])^2\right)^{1/2} \leq \varepsilon, \qquad (4.10)$$

for some tolerance ε, the total cost required to compute the MLMC estimator with selective refinement is

$$\text{Cost}\left(\widehat{Q}^{ML}\right) \leq C \begin{cases} N & q < 2, \\ \text{Cost}(Q_L) & q > 2. \end{cases} \qquad (4.11)$$

where C is a generic constant independent of ε and q. The constant q typically depends on the dimension of the problem, convergence rate of the numerical approximation, and the linear solvers. This is a huge improvement compared to the standard Monte Carlo estimator which has the cost $N \cdot \text{Cost}(Q_L)$, i.e., the computational complexity for the MLMC estimator is either solving all problems att cost 1 or one problem at the highest cost. See Paper VII for a more elaborate discussion.

5. Future works

There is a rapid development in numerical techniques for both multiscale and uncertainty quantification problems. Some natural extension of the work considered in this thesis is the following.

- Combine the multiscale and uncertainty quantification algorithms. Many uncertainty quantification problems has multiscale structure.
- Use the selective refinement to create a multilevel subset simulation for rare event estimation, i.e., a small failure probabilities.
- Apply and extend the analysis to more realistic engineering problems. The numerical experiments in this thesis are based on model problems.

6. Summary of papers

6.1 Paper I

D. Elfverson, E. H. Georgoulis and A. Målqvist. *An Adaptive Discontinuous Galerkin Multiscale Method for Elliptic Problems.* Multiscale Model. Simul. 11(3), 747–765 (2013).

In this paper we present an adaptive discontinuous Galerkin multiscale method driven by an energy norm a posteriori error bound. In the multiscale method the problem is split into a coarse and fine scale, $V_h = V_H^{ms} \oplus V^f$. Localized fine scale problems to correct the coarse basis are solved on truncated patches of the domain and are used to construct the coarse space, V_H^{ms}. The coarse space has considerably less degrees of freedom than the fine scale reference problem. The a posteriori error bound is used within an adaptive algorithm to tune the critical parameters,

$$|||u - u_H^{ms}||| \leq C_1 \left(\sum_{S \in \mathcal{T}_h} \rho_h^2(u_H^{ms}) \right)^{1/2} + C_2 \left(\sum_{T \in \mathcal{T}_H} \rho_{\omega_T}^2(u_H^{ms}) \right)^{1/2}, \quad (6.1)$$

i.e., the error indicator of the refinement level ρ_h^2 and of the patch sizes $\rho_{\omega_T}^2$ on which the truncated fine scale problems are solved. The fine scale computations are completely parallelizable, since no communication between different processors is required when computing the basis for the multiscale space.

Contribution: The author of this thesis was main responsible for the analysis, writing, and performed all the numerical experiment. The idea was developed in close collaboration between the authors.

6.2 Paper II

D. Elfverson, E. H. Georgoulis, A. Målqvist, and D. Peterseim. *Convergence of a Discontinuous Galerkin Multiscale Method.* SIAM J. Numer. Anal. 51(6), 3351–3372 (2013).

In this paper we derive a convergence result for a discontinuous Galerkin multiscale method for second order elliptic problems. We consider a heterogeneous and highly varying diffusion matrix in $L^\infty(\Omega, \mathbb{R}_{sym}^{d \times d})$ with uniform spectral bounds without any assumption on scale separation or periodicity. The multiscale method uses a space V_H^{ms} spanned by corrected basis that is constructed by correcting a coarse basis on truncated patches. The error, due to

truncation of the corrected basis, decreases exponentially with the size of the patches. Hence, we achieve the linear convergence rate

$$|||u - u_H^{\text{ms}}||| \leq H, \tag{6.2}$$

in energy norm of the multiscale solution on a uniform mesh with mesh size H, by choosing the patch sizes to be $\mathcal{O}(H|\log H|)$. Improved convergence rate can be achieved depending on the piecewise regularity of the forcing function. Also, quadratic convergence

$$||u - u_H^{\text{ms}}||_{L^2(D)} \leq H^2, \tag{6.3}$$

in the L^2-norm is obtained for arbitrary forcing function in L^2.

Contribution: The author of this thesis was main responsible for the analysis, writing, and performed all the numerical experiment. The idea was developed in close collaboration between the authors.

6.3 Paper III

D. Elfverson. *A Discontinuous Galerkin Multiscale Method for Convection-Diffusion Problems.* Available as arXiv:1509.03523 e-print (submitted).

In this paper we consider convection-diffusion problems with rough, heterogeneous, and highly varying coefficients. We propose a generalization of the discontinuous Galerkin multiscale method presented Paper II to convection-diffusion problems. The properties of the multiscale method and the discontinuous Galerkin method allow us to better cope with multiscale features as well as interior/boundary layers in the solution. The coarse trial and test spaces are corrected using fine scale computation on localized patches of size $\mathcal{O}(H\log(H^{-1}))$, where H is the mesh size. For convection-diffusion it is better to have directed patches, i.e., increase them in the direction of the convection. Linear convergence in energy norm,

$$|||u - u_H^{\text{ms}}||| \leq H, \tag{6.4}$$

is obtain under the assumption that the ratio between the size of the convection and diffusion coefficients scales like

$$\mathcal{O}\left(\frac{\|H\mathbf{b}\|_{L^\infty(\Omega)}}{\|A^{-1}\|_{L^\infty(\Omega)}}\right) \leq 1, \tag{6.5}$$

where $\mathbf{b}$ is the convection and A is the diffusion coefficient. However the convergence rates are independent of the variation in the coefficients.

Contribution: The author of this thesis is the sole author.

6.4 Paper IV

D. Elfverson, V. Ginting, and P. Henning. *On Multiscale Methods in Petrov-Galerkin Formulation,* Numer. Math. (2015).

In this work we investigate the advantages of multiscale methods in P-G formulation in a general framework which both fit multiscale methods based on the continuous and discontinuous Galerkin method. The framework splits the high dimensional reference space into a low dimensional corrected coarse space and high dimensional corrector space. The high dimensional corrector space only contains negligible fine scale information. The corrected coarse space V_H^{ms} can then be used to obtain accurate Galerkin approximations in P-G formulation: find $u_H^{\text{ms}} \in V_H^{\text{ms}}$ such hat

$$a(u_H^{\text{ms}}, v) = F(v) \quad \text{for all } v \in V_H. \tag{6.6}$$

Thus a Petrov-Galerkin formulation preservs the convergence rate,

$$|||u - u_H^{\text{ms}}||| \leq H, \tag{6.7}$$

with only a slightly lager constant compared to original symmetric multiscale method. However, P-G method can decrease the computational complexity significantly, allowing for more efficient solution algorithms. This makes the P-G method more preferable compared to the symmetric method. We prove inf-sup stability of a P-G continuous and a discontinuous Galerkin multiscale method. As another application of the framework, we show how the Petrov-Galerkin framework can be used to construct a locally mass conservative solver for two-phase flow simulation that employs the Buckley-Leverett equation. To achieve this, we couple a Petrov-Galekin discontinuous Galerkin finite element method with an upwind scheme for a hyperbolic conservation law.

Contribution: The author of this thesis was main responsible for the analysis, writing, numerical experiments regarding the discontinuous Galerkin part of the multiscale method.

6.5 Paper V

D. Elfverson, M. G. Larson, and A. Målqvist. *Multiscale Methods for Problems with Complex Geometry.* Available as arXiv:1509.03991 e-print (submitted).

In this paper we extend the analysis for the LOD to problems on complex domains, i.e., domains with voids, cracks, and complicated boundaries. The multiscale method uses a corrected test and trial space V_H^{ms}, where correctors for the basis function are computed on truncated patches. The correctors do

only need to be computed close to the boundary. We achieve linear convergence rate

$$|||u - u_H^{\mathrm{ms}}||| \leq H, \qquad (6.8)$$

in energy norm for the multiscale solution, even if the computational mesh does not resolve the fine features of the domain D. The conditioning of the multiscale method is not affected by how the domain boundary cuts the elements in the mesh.

Contribution: The author of this thesis was main responsible for the analysis, writing, and performed all the numerical experiments. The idea was developed in close collaboration between the authors.

6.6 Paper VI

D. Elfverson, D. J. Estep, F. Hellman, and A. Målqvist. *Uncertainty Quantification for Approximate p-Quantiles for Physical Models with Stochastic Inputs.* SIAM/ASA J. Uncertainty Quantification, 2(1), 826–850 (2014).

In this paper we consider the estimation of p-quantiles for a given functional evaluated on numerical solutions of a deterministic model in which model input is subject to stochastic variation. We derive upper and lower bounding estimators of the p-quantile, i.e., given p and $0 < \beta < 1$ find the computational bounds y^- and y^+ such that

$$\Pr(y \in [y^-, y^+]) > 1 - \beta. \qquad (6.9)$$

The main idea is to perform an a posteriori error analysis for the p-quantile estimators that takes into account the effects of both the stochastic sampling error and the deterministic numerical solution error. We propose a selective refinement algorithm for computing an estimate of the p-quantile with a desired accuracy in a computationally efficient fashion. In the selective refinement only samples that can effect the p-quantile are refined, i.e., different samples are solved to different accuracy. Only a relatively small subset of samples significantly affects the accuracy of a p-quantile estimator and need to be solved to full accuracy. The algorithm leads to significant computational gain. For instance, if the numerical model is a first order discretization of a partial differential equation with spatial dimension greater than one, the reduction in computational work (compared to standard Monte Carlo using n samples) is asymptotically proportional to $n^{1/2}$.

Contribution: The author of this thesis did the writing and performed the numerical experiment in close collaboration with the third author. The analysis was done in close collaboration with the author of this thesis, the third, and the fourth author. The idea was developed in close collaboration between all the authors.

6.7 Paper VII

D. Elfverson, F. Hellman, and A. Målqvist. *A Multilevel Monte Carlo method for Computing Failure Probabilities.* Available as arXiv:1408.6856 e-print (submitted).

In this paper we propose and analyze a method for computing failure probabilities of systems modeled as numerical deterministic models (e.g., PDEs) with uncertain input data. Failure probability is defined as the probability that a functional of the solution to the model is below some critical value, i.e., given y find p such that

$$p = \Pr(X < y) \tag{6.10}$$

where X is a quantity of interest. By combining selective refinement with a multilevel Monte Carlo method we develop a method which reduces computational cost without loss of accuracy compared to the standard multilevel Monte Carlo method. We prove how the computational cost of the method relates to the root mean square error of the failure probability and is asymptotically proportional to solving a single accurate realization of the numerical model (independent of the number of samples) or a standard Monte Carlo method where all samples have cost 1 (independent of the numerical cost) which is the optimal rate.

Contribution: The author of this thesis did the analysis, writing, and performed the numerical experiment in close collaboration with the second author. The idea was developed in close collaboration between the authors.

7. Summary in Swedish

I denna avhandling fokuserar vi både på partiella differentialekvationer med data som varierar över flera olika skalor i rummet, *multiskalproblem*, samt som har osäkerhet i datat, *osäkerhetskvantifiering*. Modellering och simulering av denna typ av problem är mycket utmanande och förekommer i de flesta områden inom vetenskap och teknik. Några exempel är flöden i porösa medier och kompositmaterial. Vanliga numeriska metoder, t.ex enskaliga numeriska metoder samt Monte Carlo simuleringar för multiskal och osäkerhetkvantifieringsproblem är i många fall olämpliga och i andra fall omöjligt att använda på grund av deras höga kostnad. I denna avhandling behandlar vi problemen som dyker upp i multiskal- och osäkerhetskvantifieringsproblem separat.

Standardmetoderna för numeriska beräkningar fungerar dåligt för multiskalproblem när man har snabbt varierande data och när den finskaliga informationen i data inte löses upp av beräkningsnätet. Vi behandlar problem där både koefficienterna och beräkningsdomänen har multiskalstruktur. Den huvudsakliga utmaningen i att konstruera numeriska metoder för multiskalproblem är att minska beräkningskomplexiteten utan att förlora noggrannhet i lösningen. Vi utvecklar en multiskalmetod där grova basfunktioner som spänner upp lösningen korrigeras med hjälp av lokaliserade finskaliga beräkningar. Lösningen för multiskalmetoden har samma konvergenshastighet som standard metoderna har för problem utan multiskaldata. De finskaliga korrektionsproblemen avtar exponentiell bort från stödet av den ursprungliga basfunktionen och beräkningarna kan därför lokaliseras till små områden. Storleken av beräkningsområderna kan väljas så att konvergensen för multiskalmetoden inte påverkas. Korrektionsproblemen kan lösas helt oberoende av varandra, vilket gör metoden perfekt lämpad för parallella beräkning. Det är också möjligt att återanvända de finskaliga beräkningarna i t.ex. tidsstegning och icke-linjära iterationer.

I osäkerhetkvantifiering fokuserar vi på tillämpningar där modellparametrarna beror på stokastiska variationer. Vi vill beräkna statistiska egenskaper hos en kvantitet av lösningen till modellen, mer exakt så vill vi beräkna p-kvantiler och felsannolikheter. Felsannolikheter definieras som sannolikheten att en given kvantiteten av lösningen till modellen är mindre än något kritiskt värde. Uppskattningen av p-kvantiler är det inversa problemet, dvs bestäm värdet så att en givna kvantiteten av lösningen är större eller mindre än ett givet värde med sannolikhet p. Beräkningar av den här typen av problem har två felkällor, ett numeriskt fel från diskretiseringen av modellen och ett statistiskt fel från ett ändligt antal stickprov. För att uppskatta p-kvantiler eller

felsannolikheter effektivt så måste de båda felkällorna balanseras. Vi utvecklar tekniker för att uppskatta/beräkna det nummeriska felet tillammans med existerande variansreducerande metoder för att minska beräkningskostnaden samt för att balansera de båda felkällorna.

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