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Adaptive variational multiscale methods based on a posteriori error estimation: Duality techniques for elliptic problems

Mats G. Larson [*]   Axel Målqvist [†]

May 18, 2004

Abstract

The variational multiscale method (VMM) provides a general framework for construction of multiscale finite element methods. In this paper we propose a method for parallel solution of the fine scale problem based on localized Dirichlet problems which are solved numerically. Next we present a posteriori error representation formulas for VMM which relates the error in linear functionals to the discretization errors, resolution and size of patches in the localized problems, in the fine scale approximation. These formulas are derived by using duality techniques. Based on the a posteriori error representation formula we propose an adaptive VMM with automatic tuning of the critical parameters. We primary study elliptic second order partial differential equations with highly oscillating coefficients or localized singularities.

1 Introduction

Many problems in science and engineering involve models of physical systems on many scales. For instance, models of materials with microstructure such as composites and flow in porous media. In such problems it is in general not feasible to seek for a numerical solution which resolves all scales. Instead we may seek to develop algorithms based on a suitable combination with a global problem capturing the main features of the solution and localized problems which resolves the fine scales. Since the fine scale problems are localized the computation on the fine scales is parallel in nature.

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Previous work. The Variational Multiscale Method (VMM) is a general framework for derivation of basic multiscale method in a variational context, see Hughes [7] and [9]. The basic idea is to decompose the solution into fine and coarse scale contributions, solve the fine scale equation in terms of the residual of the coarse scale solution, and finally eliminate the fine scale solution from the coarse scale equation. This procedure leads to a modified coarse scale equation where the modification accounts for the effect of fine scale behavior on the coarse scales. In practice it is necessary to approximate the fine scale equation to make the method realistic. In several works various ways of analytical modeling are investigated often based on bubbles or element Green's functions, see Oberai and Pinsky, [11] and Arbogast [1]. In [6] Hou and Wu present a different approach. Here the fine scale equations are solved numerically on a finer mesh. The fine scale equations are solved inside coarse elements and are thus totally decoupled.

New contributions. In this work we present a simple technique for numerical approximation of the fine scale equation in the variational multiscale method. The basic idea is to split the fine scale residual into localized contributions using a partition of unity and solving corresponding decoupled localized problems on patches with homogeneous Dirichlet boundary conditions. The fine scale solution is approximated by the sum $U_f = \sum_i U_{f,i}$ of the solutions $U_{f,i}$ to the localized problems. The accuracy of U_f depends on the fine scale mesh size h and the size of the patches. We note that the fine scale computation is naturally parallel.

To optimize performance we seek to construct an adaptive algorithm for automatic control of the coarse mesh size H, the fine mesh size h, and the size of patches. Our algorithm is based on the following a posteriori estimate of the error $e = u - U_c - U_f$ for the Poisson equation with variable coefficients a:

$$(e, \psi) = \sum_{i \in \mathcal{C}} (\varphi_i R(U_c), \phi_f) + \sum_{i \in \mathcal{F}} \left((\varphi_i R(U_c), \phi_f)_{\omega_i} - a(U_{f,i}, \phi_f)_{\omega_i} \right), \tag{1.1}$$

where $\psi \in H^{-1}(\Omega)$, $\mathcal{C}$ refers to nodes where no local problems have been solved, $\mathcal{F}$ to nodes where local problems are solved, U_c is the coarse scale solution, $U = U_c + U_f$, $R(U) = f + \nabla \cdot a \nabla U$ is the residual, and ϕ_f is the fine scale part of a dual solution driven by ψ.

If no fine scale equations are solved only we obtain the first term in the estimate. The second term relates the fine scale mesh parameter h to the patch size ω_i on which the local problems are solved. We have derived a similar estimate for the error in energy norm, see [10].

The framework is fairly general and may be extended to other types of multiscale methods, for instance, based on localized Neumann problems.

Outline. First we introduce the model problem and the variational multiscale formulation of this problem, we also discuss the split of the coarse and fine scale spaces. In the following section we present a posteriori estimates of the error. These results leads to an adaptive algorithm. We present numerical results and finally we present concluding remarks and suggestions on future work.

2 The Variational Multiscale Method

2.1 Model Problem

We study the Poisson equation with a highly oscillating coefficient a and homogeneous Dirichlet boundary conditions: find $u \in H^1_0(\Omega)$ such that

$$-\nabla \cdot a\nabla u = f \quad \text{in } \Omega, \tag{2.1}$$

where Ω is a polygonal domain in $\mathbf{R}^d$, $d = 1, 2$, or 3 with boundary Γ, $f \in H^{-1}(\Omega)$, and $a \in L^\infty(\Omega)$ such that $a(x) \geq \alpha_0 > 0$ for all $x \in \Omega$. The variational form of (2.1) reads: find $u \in \mathcal{V} = H^1_0(\Omega)$ such that

$$a(u, v) = (f, v) \quad \text{for all } v \in \mathcal{V}, \tag{2.2}$$

with the bilinear form

$$a(u, v) = (a\nabla u, \nabla v) \tag{2.3}$$

for all $u, v \in \mathcal{V}$.

2.2 The Variational Multiscale Method

We employ the variational multiscale scale formulation, proposed by Hughes see [7, 9] for an overview, and introduce a coarse and a fine scale in the problem. We choose two spaces $\mathcal{V}_c \subset \mathcal{V}$ and $\mathcal{V}_f \subset \mathcal{V}$ such that

$$\mathcal{V} = \mathcal{V}_c \oplus \mathcal{V}_f. \tag{2.4}$$

Then we may pose (2.2) in the following way: find $u_c \in \mathcal{V}_c$ and $u_f \in \mathcal{V}_f$ such that

$$\begin{aligned} a(u_c, v_c) + a(u_f, v_c) &= (f, v_c) \quad \text{for all } v_c \in \mathcal{V}_c, \\ a(u_c, v_f) + a(u_f, v_f) &= (f, v_f) \quad \text{for all } v_f \in \mathcal{V}_f. \end{aligned} \tag{2.5}$$

Introducing the residual $R : \mathcal{V} \to \mathcal{V}'$ defined by

$$(R(v), w) = (f, w) - a(v, w) \quad \text{for all } w \in \mathcal{V}, \tag{2.6}$$

the fine scale equation takes the form: find $u_f \in \mathcal{V}_f$ such that

$$a(u_f, v_f) = (R(u_c), v_f) \quad \text{for all } v_f \in \mathcal{V}_f. \tag{2.7}$$

Thus the fine scale solution is driven by the residual of the coarse scale solution. Denoting the solution u_f to (2.7) by $u_f = TR(u_c)$ we get the modified coarse scale problem

$$a(u_c, v_c) + a(TR(u_c), v_c) = (f, v_c) \quad \text{for all } v_c \in \mathcal{V}_c. \tag{2.8}$$

Here the second term on the left hand side accounts for the effects of fine scales on the coarse scales.

2.3 A VMM Based on Localized Dirichlet Problems

We introduce a partition $\mathcal{K} = \{K\}$ of the domain Ω into shape regular elements K of diameter H_K and we let $\mathcal{N}$ be the set of nodes. Further we let $\mathcal{V}_c$ be the space of continuous piecewise polynomials of degree p defined on $\mathcal{K}$.

We shall now construct an algorithm which approximates the fine scale equation by a set of decoupled localized problems. We begin by writing $u_f = \sum_{i \in \mathcal{N}} u_{f,i}$ where

$$a(u_{f,i}, v_f) = (\varphi_i R(u_c), v_f) \quad \text{for all } v_f \in \mathcal{V}_f, \tag{2.9}$$

and $\{\varphi_i\}_{i \in \mathcal{N}}$ is the set of Lagrange basis functions in $\mathcal{V}_c$. Note that $\{\varphi_i\}_{i \in \mathcal{N}}$ is a partition of unity with support on the elements sharing the node i. We call the set of elements with one corner in node i a mesh star in node i and denote it S_1^i. Thus functions $u_{f,i}$ correspond to the fine scale effects created by the localized residuals $\varphi_i R(u_c)$. Introducing this expansion of u_f in the right hand side of the fine scale equation (2.5) and get: find $u_c \in \mathcal{V}_c$ and $u_f = \sum_{i \in \mathcal{N}} u_{f,i} \in \mathcal{V}_f$ such that

$$\begin{aligned} a(u_c, v_c) + a(u_f, v_c) = (f, v_c) \quad &\text{for all } v_c \in \mathcal{V}_c, \\ a(u_{f,i}, v_f) = (\varphi_i R(u_c), v_f) \quad &\text{for all } v_f \in \mathcal{V}_f \text{ and } i \in \mathcal{N}. \end{aligned} \tag{2.10}$$

We use this fact to construct a finite element method for solving (2.10) approximately in two steps.

- For each coarse node we define a patch ω_i such that $\mathrm{supp}(\varphi_i) \subset \omega_i \subset \Omega$. We denote the boundary of ω_i by $\partial\omega_i$.
- On these patches we define piecewise polynomial spaces $\mathcal{V}_f^h(\omega_i)$ with respect to a fine mesh with mesh function $h = h(x)$ defined as a piecewise constant function on the fine mesh. Functions in $\mathcal{V}_f^h(\omega_i)$ are equal to zero on $\partial\omega_i$.

The resulting method reads: find $U_c \in \mathcal{V}_c$ and $U_f = \sum_i^n U_{f,i}$ where $U_{f,i} \in \mathcal{V}_f^h(\omega_i)$ such that

$$\begin{aligned} a(U_c, v_c) + a(U_f, v_c) = (f, v_c) \quad &\text{for all } v_c \in \mathcal{V}_c, \\ a(U_{f,i}, v_f) = (\varphi_i R(U_c), v_f) \quad &\text{for all } v_f \in \mathcal{V}_f^h(\omega_i) \text{ and } i \in \mathcal{N}. \end{aligned} \tag{2.11}$$

Since the functions in the local finite element spaces $\mathcal{V}_f^h(\omega_i)$ are equal to zero on $\partial\omega_i$, U_f and therefore $U = U_c + U_f$ will be continuous.

Remark 2.1 For problems with multiscale phenomena on a part of the domain it is not necessary to solve local problems for all coarse nodes. We let $\mathcal{C} \subset \mathcal{N}$ refer to nodes where no local problems are solved and $\mathcal{F} \subset \mathcal{N}$ refer to nodes where local problems are solved. Obviously $\mathcal{C} \cup \mathcal{F} = \mathcal{N}$. We let $U_{f,i} = 0$ for $i \in \mathcal{C}$.

Remark 2.2 The choice of the subdomains ω_i is crucial for the method. We introduce a notation for extended stars of many layers of coarse elements recursively in the following way. The extended mesh star $S_L^i = \cup_{j \in S_{L-1}^i} S_1^j$ for $L > 1$. We refer to L as layers, see Figure 1.
In Figure (2) we plot solutions to localized fine scale problems $U_{f,i}$ on different patches.

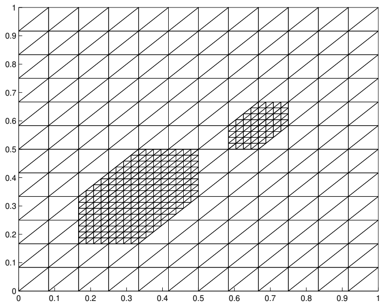

Figure 1: Two (left) and one (right) layer stars.

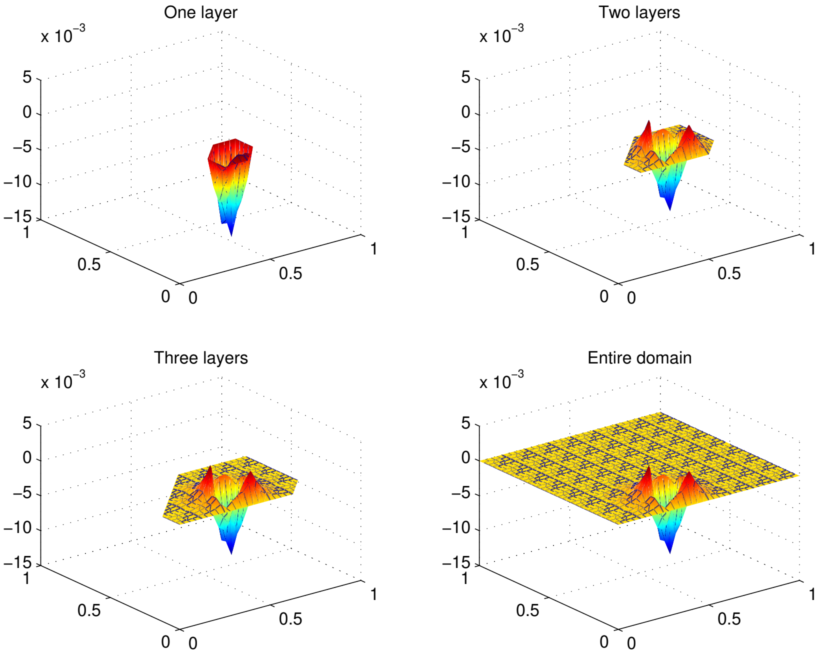

Figure 2: The fine scale solution $U_{f,i}$ for different patches.

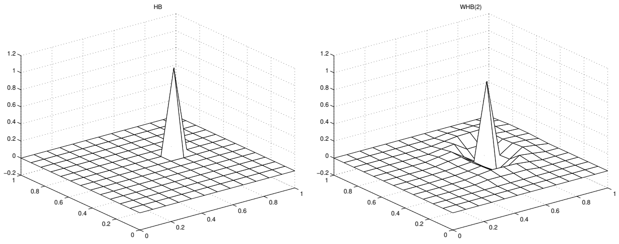

Figure 3: HB-function and WHB-function with two Jacobi iterations.

2.4 Subspaces

The choice of the fine scale space $\mathcal{V}_f$ can be done in different ways. In a paper by Aksoylu and Holst [4] three suggestions are made.

Hierarchical basis method. The first and perhaps easiest approach is to let $\mathcal{V}_f = \{v \in \mathcal{V} : v(x_j) = 0, j = \mathcal{N}\}$, where $\{x_i\}_{i\in\mathcal{N}}$ are the coarse mesh nodes. When $\mathcal{V}_f$ is discritized by the standard piecewise polynomials on the fine mesh this means that the fine scale base functions will have support on fine scale stars.

BPX preconditioner. The second approach is to let $\mathcal{V}_f$ be $L^2(\Omega)$ orthogonal to $\mathcal{V}_c$. In this case we will have global support for the fine scale base functions but for the discretized space we have rapid decay outside fine mesh stars.

Wavelet modified hierarchical basis method. The third choice is a mix of the other two. The fine scale space $\mathcal{V}_f$ is defined as an approximate $L^2(\Omega)$ orthogonal version of the Hierarchical basis method. We let $Q_c^a v \in \mathcal{V}_c$ be an approximate solution (a small number of Jacobi iterations) to

$$(Q_c^a v, w) = (v, w), \quad \text{for all } w \in \mathcal{V}_c. \tag{2.12}$$

and define the Wavelet modified hierarchical basis function associated with the hierarchical basis function φ_{HB} to be,

$$\varphi_{WHB} = (I - Q_c^a)\varphi_{HB}, \tag{2.13}$$

see Figure 3.

For an extended description of these methods see [3, 4, 2]. In this paper we focus on the WHB method.

3 A Posteriori Error Estimates

3.1 The Dual Problem

To derive a posteriori error estimates of the error in a given linear functional (e, ψ) with $e = u - U$ and $\psi \in H^{-1}(\Omega)$ a given weight. We introduce the following dual problem: find

$\phi \in \mathcal{V}$ such that

$$a(v,\phi) = (v,\psi) \quad \text{for all } v \in \mathcal{V}. \tag{3.1}$$

In the VMM setting this yields: find $\phi_c \in \mathcal{V}_c$ and $\phi_f \in \mathcal{V}_f$ such that

$$\begin{aligned} a(v_c,\phi_c) + a(v_c,\phi_f) = (v_c,\psi), &\quad \text{for all } v_c \in \mathcal{V}_c, \\ a(v_f,\phi_f) + a(v_f,\phi_c) = (v_f,\psi), &\quad \text{for all } v_f \in \mathcal{V}_f. \end{aligned} \tag{3.2}$$

3.2 Error Representation Formula

We now derive an error representation formula involving both the coarse scale error $e_c = u_c - U_c$ and the fine scale error $e_f = \sum_{i\in\mathcal{N}} e_{f,i} := \sum_{i\in\mathcal{N}}(u_{f,i} - U_{f,i})$ that arises from using our finite element method (2.11).

We use the dual problem (3.2) to derive an a posteriori error estimate for a linear functional of the error $e = e_c + e_f$. If we subtract the coarse part of equation (2.11) from the coarse part of equation (2.10) we get the Galerkin orthogonality,

$$a(e_c,v_c) + a(e_f,v_c) = 0 \quad \text{for all } v_c \in \mathcal{V}_c. \tag{3.3}$$

The same argument on the fine scale equation gives for $i \in \mathcal{F}$,

$$a(e_{f,i},v_f) = (f,\varphi_i v_f) - a(e_c,\varphi_i v_f), \quad \text{for all } v_f \in \mathcal{V}_f^h(\omega_i). \tag{3.4}$$

We are now ready to state an error representation formula.

Theorem 3.1 *If $\psi \in H^{-1}(\Omega)$ then,*

$$(e,\psi) = \sum_{i\in\mathcal{C}} (\varphi_i R(U_c),\phi_f) + \sum_{i\in\mathcal{F}} \left((\varphi_i R(U_c),\phi_f)_{\omega_i} - a(U_{f,i},\phi_f)_{\omega_i} \right). \tag{3.5}$$

Proof. Starting from the definition of the dual problem and letting $v = e = u - U_c - U_f$ we get

$$\begin{aligned} (e,\psi) &= a(e,\phi) \qquad (3.6) \\ &= a(e,\phi_f) \qquad (3.7) \\ &= a(u - U_c,\phi_f) - a(U_f,\phi_f) \qquad (3.8) \\ &= (R(U_c),\phi_f) - a(U_f,\phi_f) \qquad (3.9) \\ &= (R(U_c),\phi_f) - \sum_{i\in\mathcal{F}} a(U_{f,i},\phi_f) \qquad (3.10) \\ &= \sum_{i\in\mathcal{C}} (\varphi_i R(U_c),\phi_f) + \sum_{i\in\mathcal{F}} (\varphi_i R(U_c),\phi_f) - a(U_{f,i},\phi_f). \qquad (3.11) \end{aligned}$$

which proves the theorem. □

Since equation (2.11) holds we can subtract functions $v_{f,i}^h \in \mathcal{V}_f^h(\omega_i)$ where $i \in \mathcal{F}$ from equation (3.11). For example we choose $v_{f,i}^h = \pi_{h,i}\phi_f$, where $\pi_{h,i}\phi_f$ is the Scott-Zhang interpolant of ϕ_f onto $\mathcal{V}_f^h(\omega_i)$ to get

$$\begin{aligned}(e,\psi) = &\sum_{i\in\mathcal{C}}(\varphi_i R(U_c),\phi_f) \\ &+ \sum_{i\in\mathcal{F}}\left((\varphi_i R(U_c),\phi_f - \pi_{h,i}\phi_f)_{\omega_i} - a(U_{f,i},\phi_f - \pi_{h,i}\phi_f)_{\omega_i}\right).\end{aligned} \tag{3.12}$$

Remark 3.1 Since the dual problem defined in equation (3.2) is equally hard to solve as the primal problem we need to solve it numerically as well. Normally it would not be sufficient to solve the dual problem with the same accuracy as the primal due to the Galerkin Orthogonality. However in this setting things are a bit different. Calculating ϕ_f with the same accuracy as U_f or even with lower accuracy will not result in an error equal to zero. The important thing is to only store the part of ϕ_f with support on ω_i when calculating term i in the sum of equation (3.5). The entire function ϕ_f might be hard to store in the memory of the computer.

4 Adaptive Algorithm

We use the error representation formula in Theorem 3.1 to construct an adaptive algorithm. We remember the result,

$$(e,\psi) = \sum_{i\in\mathcal{C}}(\varphi_i R(U_c),\phi_f) + \sum_{i\in\mathcal{F}}\left((\varphi_i R(U_c),\phi_f)_{\omega_i} - a(U_{f,i},\phi_f)_{\omega_i}\right). \tag{4.1}$$

The first sum of the error representation formula is very similar to what we would get from using standard Galerkin on the coarse mesh. The function $\phi_f = \phi - \phi_c \sim H\nabla\phi$ which is exactly what we would expect. For the second sum we have an extra orthogonality namely that from equation (3.12). We have $\phi_f - \pi_{h,i}\phi_f \sim h\nabla\phi$ if the patches $\omega_i = \Omega$ i.e. we get the fine scale convergence. But in practice the patches are much smaller so we end up somewhere in between h and H convergence. To sum up this discussion there are three parameters of interest that need to be considered in an adaptive algorithm, H, h, and the size of the patches.

Adaptive Algorithm.

- Start with no nodes in $\mathcal{F}$.
- Calculate the primal U_c.
- Calculate the dual solution locally ϕ_f with low accuracy for all coarse nodes. (ψ_f does not need to be solved very accurately to point out the correct nodes for local calculations.)

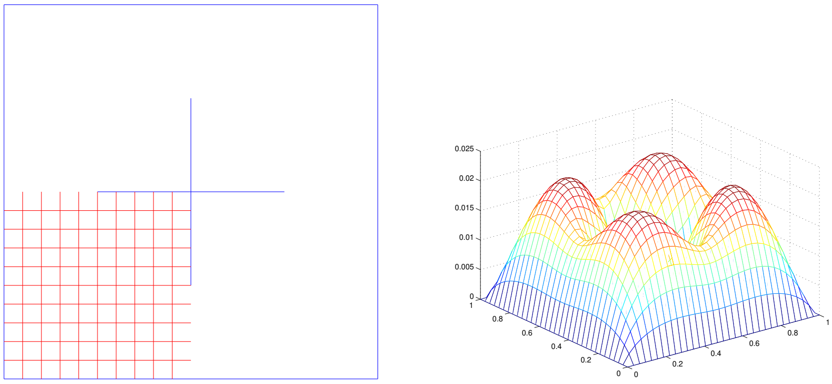

Figure 4: Geometry (left) and Reference solution (right).

- Calculate the contributions to the error for each coarse node, $C_i = (\varphi_i R(U_c), \phi_f)$.
- Solve local problems where C_i is large to get a new U_c.
- Calculate C_i and $F_i = ((\varphi_i R(U_c), \phi_f)_{\omega_i} - a(U_{f,i}, \phi_f)_{\omega_i})$, for large values in C_i solve more local problems and for large values in F_i either increase the number of layers or decrease the fine scale mesh size h for local problem i. Stop if the desired tolerance is reached or calculate a new U_c and new error indicators etc. .

5 Numerical Examples

We solve two dimensional model problems with linear base functions defined on a uniform triangular mesh.

Example 1. In this example we demonstrate how we can get highly improves accuracy in one part of the domain by choosing the load in the dual problem ψ equal to the indicator function for this domain. We consider the unit square with a crack in the form of a plus sign on which the solution is forced to be zero, see Figure 5 (left). We let ψ be equal to one in the lower left quadrant (marked with a thin lattice in the figure) and zero in the rest of the domain. To the right in Figure 5 we see a reference solution to the Poisson equation with $a = f = 1$ and homogeneous Dirichlet boundary conditions on this geometry. The idea is to use the adaptive algorithm to choose which areas that needs to be solved with higher accuracy. In Figure 5 we plot the dual solution, with ψ chosen as described above, to the left and the fine scale part of the dual solution to the right. After two iterations in the adaptive algorithm we see clearly that local problems have only nodes in the lower left corner. In Figure 5 the small circles refers to fine scale problems solved with two layer stars and the bigger circles refers to fine scale problems solved three layer stars. The improvement in the solution after two iteration in the adaptive algorithm is very clear. In Figure 5 we compare the standard Galerkin solution and the adaptive solution to a

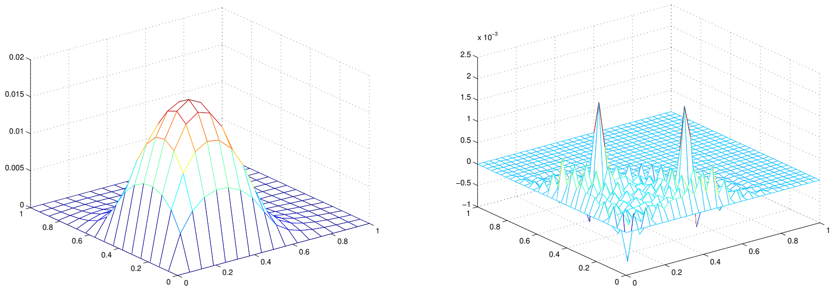

Figure 5: Dual solution (left) and fine scale part of the dual solution (right) calculated with $\psi = I_{\{0 \le x, y \le 0.5\}}$.

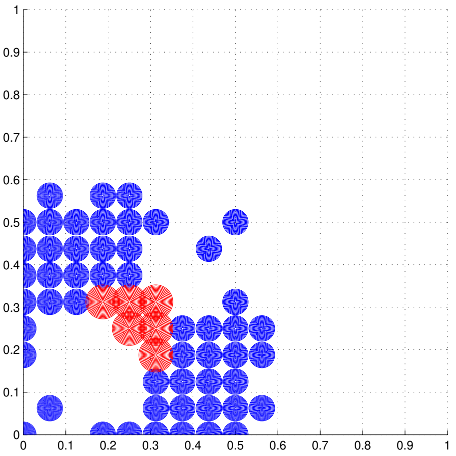

Figure 6: Local problems solved with two and three layer stars.

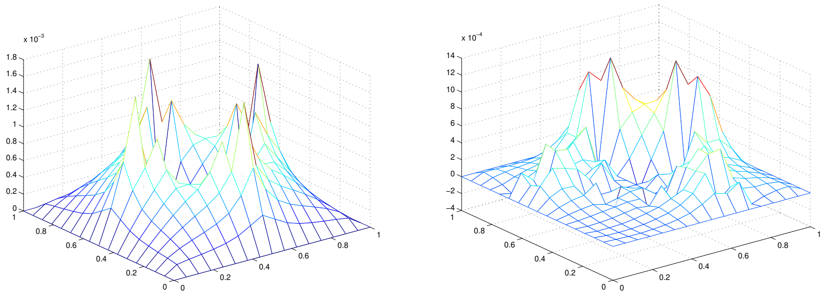

Figure 7: Galerkin error (left) and adaptive variational multiscale method error (right).

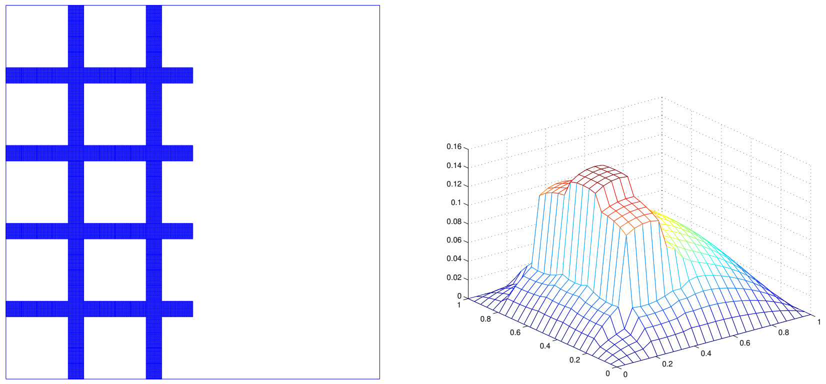

Figure 8: The coefficient $a = 1$ on the white parts and $a = 0.05$ on the lattice (left) and reference solution on this geometry (right).

reference solution. We see how the error in the lower left quadrant is much smaller but the error in the rest of the domain is very similar to the standard Galerkin error.

Example 2. Next we turn our attention to a model problem with oscillating coefficient a in a part of the domain, see Figure 5. In this example we choose $f = \psi = 1$ which makes the primal and the dual equivalent. In Figure 5 we note that the adaptive algorithm automatically picks nodes in the left part of the domain for local problems to increase accuracy. In the first example we want to refine a certain part of the domain and therefore we choose ψ in order to do so, here we want good accuracy on the whole domain and the adaptive algorithm chooses where to refine automatically. Again we compare standard Galerkin and our solution to a reference solution calculated on a finer mesh. The result can be seen in Figure 5. Again we see a nice improvement compared to the standard Galerkin error. The choice $\psi = 1$ indicates control of the mean of the error over the domain.

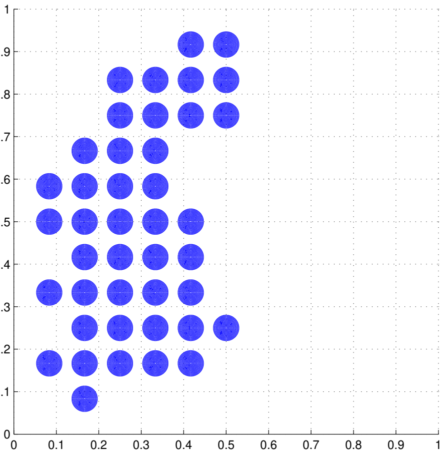

Figure 9: The dots marks coarse nodes where local problems have been solved.

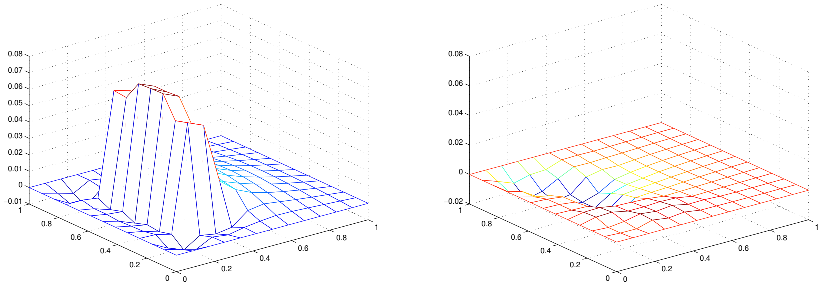

Figure 10: Standard Galerkin error (left) and the error using adaptivity (right).

6 Conclusions and Future Work

We have presented a method for parallel solution of the fine scale equations in the variational multiscale method based on solution of localized Dirichlet problems on patches and developed an a posteriori error analysis for the method. Based on the estimates we design a basic adaptive algorithm for automatic tuning of the critical parameters: resolution and size of patches in the fine scale problems. It is also possible to decide whether a fine scale computation is necessary or not and thus the proposed scheme may be combined with a standard adaptive algorithm on the coarse scales. The method is thus very general in nature and may be applied to any problem where adaptivity is needed.

In this paper we have focused on two scales in two spatial dimensions. A natural extension would be to solve three dimensional problems with multiple scales. It is also natural to extend this theory to other equations modeling for instance flow and materials. We also intend to study non-linear and time dependent equations using this approach.

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