Dynamic Computational Subgrid Modeling II

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May 19, 2000

Abstract

In this paper we study a subgrid model based on extrapolation of a modeling residual, in the case of a linear convection-diffusion-reaction problem $Lu = f$ in two dimensions. The solution u to the exact problem satisfies an equation $L_h u = [f]^h + F_h(u)$, where L_h is the operator used in the computation on the finest computational scale h, $[f]^h$ is the approximation of f on the scale h, and $F_h(u)$ is a modeling residual, which needs to be modeled. The subgrid modeling problem is to compute approximations of $F_h(u)$ without using finer scales than h. In this study we model $F_h(u)$ by extrapolation from coarser scales than h, where $F_h(u)$ is directly computed with the finest scale h as reference. We show in experiments that a solution with subgrid model on a scale h in most cases corresponds to a solution without subgrid model on a mesh of size less than $h/4$.

Acknowledgement

The author would like to thank his advisor Professor Claes Johnson for all helpful discussions, his inspiration, and for his encouragement throughout this work.

Contents

1 Introduction

A fundamental problem in science and engineering concerns the mathematical modeling of phenomena involving small scales. This problem arises in molecular dynamics, turbulent flow and flow in heterogeneous porous media, for example. Basic models for such phenomena, such as the Schrödinger equation or the Navier-Stokes equations, may be very accurate models of the real phenomena but may be so computationally intensive, because of the large number of degrees of freedom needed to represent the small scales, that even computers with power way beyond that presently available may be insufficient for accurate numerical solutions of the given equations. The traditional approach to get around this difficulty is to seek to find simplified models with computationally resolvable scales, whose solutions are sufficiently close to the solutions of the original full equations. Such simplified models, without the too small scales, build on mathematical modeling of the computationally unresolved scales of the full equations, which is referred to as *subgrid modeling.* To find suitable simplified models including subgrid modeling, is the central activity in modeling of turbulence, molecular dynamics and heterogeneous media.

The problem of subgrid modeling may naturally be approached by seeking to find the simplified model by suitably averaging the full equations over the resolvable scales. This was the approach in turbulence modeling taken by Reynolds a century ago, and leads to a simplified set of equations, the *Reynolds-averaged Navier-Stokes* (RANS) equations, involving the so called *Reynolds stresses.* The mean velocity field may be defined by ensemble, time, or spatial averaging, and the classical problem in turbulence modeling is to find an expression for the Reynolds stresses in terms of the resolvable scales, which is also referred to as the problem of *closure.* A large number of attempts to find solutions to the closure problem by analytical mathematical techniques have been made over the years since the time of Reynolds, but satisfactory solutions have been evasive so far. Typically in RANS models, a turbulent length scale and a turbulent time scale need to be determined. This can be done either in an *ad hoc* fashion, or by introducing additional equations determining the unknown quantities.

In a *Large Eddy Simulation* (LES) the idea is to simulate the larger scales of motion of the turbulent Navier-Stokes equations while approximating the smaller ones (for an overview see [15],[7]). By suitably averaging the Navier-Stokes equations over a certain spatial scale one obtains a simplified set of equations involving additional stresses $\tau_{ij} = \overline{u}_i\overline{u}_j - \overline{u_i u_j}$ representing the subgrid model (where $\overline{u}_i$ represents a local average of u_i and $u = (u_i)$ is the velocity), called the *subgrid scale Reynolds stresses* (SGSRS). In a LES the average is in general taken over a finer spatial scale than in RANS modeling, and since there is no averaging in time a solution to a LES is evolving with time. In a corresponding RANS simulation, the solution is smoother and in general constant in time.

The simplest subgrid scale model of turbulence is the *Smagorinsky model* [19], where the SGSRS are modeled as viscous stresses $\tau_{ij} = \nu\epsilon_{ij}(u)$, related to a certain *turbulent viscosity* (*eddy viscosity*) ν of the form $\nu = Ch^{\mu}|\epsilon(\overline{u})|$, where $C = C(x)$ and $\mu = \mu(x)$ are positive numbers in general depending on the spatial coordinate x, $h = h(x)$ represents the smallest resolvable scale at x, and $\epsilon(u) = (\epsilon_{ij}(u))$ is the strain of the velocity u. The subgrid modeling problem in this case is to find the functions $C(x)$ and $\mu(x)$. Attempts have been made to determine these functions analytically, or experimentally by finding best fit to given measured data. In both cases serious difficulties arise and the obtained simplified models do not seem to be useful over a range of problems with different data. Of course, the difficulties may stem from both the fact that the assumed form of the subgrid scale Reynolds stresses is not a reasonable one, and from the fact that the coefficients $C(x)$ and $\mu(x)$ depend on the particular problem being solved, and thus fitting the coefficients to one set of data may be of no value for other data.

In recent years, new approaches to the subgrid modeling problem have been taken based on *dynamic computational subgrid modeling*, an idea first introduced by Germano *et al.* [8]. The basic assumption here is that a particular model applies on different scales with the same value on the model parameters. Using this assumption, one seeks to find a subgrid model, for each set of data, by computing approximations of the subgrid model on coarser scales using a fine scale computed solution without subgrid model as reference, and then finally extrapolating the so obtained model to the finest computational scale, with the hope of being able to extrapolate from the finest resolvable scales to unresolvable scales. In the simplest case, this may come down to seeking to determine, for a given set of data, the coefficients $C(x)$ and $\mu(x)$ in the Smagorinsky model by best fit. In this approach, at least the dependence of the coefficients on the data may be taken into account, but still the Ansatz with a turbulent viscosity is kept. More generally, it is natural to seek to extend this approach to different forms of the Ansatz. In order for such a dynamic modeling process based on extrapolation to work, it is necessary that the underlying problem has some "scale regularity", so that the experience gained by fitting the model on a coarse scale with a fine scale solution as reference, may be extrapolated to the finer scale. It is conceivable that many problems involving a range of scales from large to small, such as fluid flow at larger Reynolds numbers, in fact does have such a regularity, once the larger scales related to the geometry of the particular problem have been resolved. The purpose of this note is to study the feasibility of the indicated dynamic computational subgrid modeling in the context of some simple model problems related to linear convection-diffusion-reaction with irregular or non-smooth coefficients with features on many scales.

The scale regularity in this case appears to be close to assuming that the coefficients have a "fractal nature" and that the solution inherits this structure to some degree.

The problem of computational mathematical modeling has two basic aspects: numerical computation and modeling. The basic idea in dynamic computational subgrid modeling is to seek to extrapolate into unresolvable scales by comparing averaged fine scale computed solutions of the original model (without subgrid modeling) on different coarser scales. To make the extrapolation possible at all, the numerical errors in the computations underlying the extrapolation have to be small enough. If the numerical errors in the fine scale computation without subgrid model are not sufficiently small, then the whole extrapolation procedure from coarser scales may be meaningless. Thus, it will be of central importance to accurately balance the errors from numerical computation and subgrid modeling. In recent years the techniques for adaptive error control based on a posteriori error estimates have been considerably advanced (see e.g. Johnson[12]). Thus, today we have techniques available that allow the desired balance of computational and modeling errors.

This is the second paper in this series. In the first paper [10], the feasibility of the dynamic computational subgrid model was investigated for some very simple one dimensional model problems related to convection-diffusion-reaction with certain non smooth "scale regular" coefficients. The subgrid model was based on extrapolation of a modeling residual, and the modeling error was studied separately by making the numerical errors neglible by computing on a very fine mesh. A priori and a posteriori error estimates for the modeling errors were also presented.

The first part of is paper is again focused on modeling only. We then introduce numerical errors, and the relation between the numerical and the modeling errors is studied. The theoretical results of [10] are extended to two dimensions, and a posteriori error estimates in terms of one modeling residual and one numerical residual are presented. In a continuation of this study the adaptive algorithm presented in this paper will be implemented, and the results will also be extended to 3 dimensional problems on unstructured meshes.

An outline of this note is as follows: In Section 2 we introduce the linear convection-diffusion-reaction model problem. We discuss different approaches to the subgrid modeling problem, and we recall the basic results of [10]. In particular, the idea of a subgrid model based on extrapolation of a modeling residual is presented. In Section 3 we recall basic features of *Multiresolution Analysis* (MRA) using the two dimensional Haar basis, which we use to motivate an Ansatz on the form of the modeling residual, which we then base the extrapolation upon. In Section 4 we present error estimates, and in Section 5 we test the method in the context of some numerical experiments in two dimensions with non smooth "scale regular" coefficients. We first consider the modeling errors separately by computing on a very fine mesh that makes the numerical errors neglible compared to the modeling errors. We then introduce numerical errors by computing on a mesh corresponding to the finest resolvable scale in the modeling problem. We conclude with some remarks in Section 6.

2 Formulation of the problem

As a model problem we consider the scalar convection-diffusion-reaction problem of the form.

$$Lu(x) = -\nabla \cdot (\epsilon(x)\nabla u(x)) + \beta(x) \cdot \nabla u(x) + \alpha(x)u(x) = f(x), \tag{1}$$

for $x \in \Omega \subset \mathbb{R}^n$, together with boundary conditions for the inflow and outflow boundaries $\partial\Omega_- = \{x \in \partial\Omega : \beta(x) \cdot n(x) < 0\}$ and $\partial\Omega_+ = \{x \in \partial\Omega : \beta(x) \cdot n(x) > 0\}$, where n is an unit outward normal from Ω. $\epsilon(x)$, $\beta(x)$, and $\alpha(x)$ are given coefficients depending on x, $f(x)$ is a given force, and $u(x)$ is the solution. We assume that the coefficients ϵ, β, and α are piecewise continuous, and we seek a weak solution u that satisfies the corresponding variational formulation of (1), and the boundary conditions in the sense of traces.

We assume that the coefficients ϵ, β and α, and the given function f vary on a range of scales from very fine to coarse scales, and we expect the exact solution u in general to vary on a related range of scales. We denote by h the finest possible scale we allow us to use, which may be the finest possible scale in a computation of a solution, and we denote the corresponding approximate solution u_h. We assume for now that u_h is the weak solution of the following simplified problem

$$L_h u_h = -\nabla \cdot ([\epsilon]^h \nabla u_h) + [\beta]^h \cdot \nabla u_h + [\alpha]^h u_h = [f]^h, \quad x \in \Omega, \tag{2}$$

together with boundary conditions, where $[\epsilon]^h$, $[\beta]^h$, $[\alpha]^h$, and $[f]^h$ are approximations of the corresponding functions on the scale h, with the finer scales left out. We may think of u_h as an approximation of the exact solution u obtained by simplifying the model by simplifying the coefficients in the model removing scales finer than h. Typically, the coefficient $[\beta]^h$ is some local average of β on the scale h, etc. The difference $u - u_h$ thus represents a modeling error resulting from averaging the coefficients on the scale h.

2.1 Subgrid modeling

We now consider a situation where u_h is not a sufficiently good approximation of u, and we would like to improve the quality of u_h without computing using finer scales than h. The equation $Lu = f$ satisfied by the exact solution can be written in the form

$$L_h u = [f]^h + F_h(u), \tag{3}$$

where

$$F_h(u) = f - [f]^h - (L - L_h)u \tag{4}$$

acts as a *modeling residual.* The subgrid modeling problem is to model $F_h(u)$ on the scale h. There is a variety of possibilities to approach this problem. We may use $F_h(u)$ as a correction on the force and replace the model $L_h u_h = [f]^h$ by the model

$$L_h \tilde{u}_h = [f]^h + \tilde{F}_h,$$

with solution $\tilde{u}_h$, where $\tilde{F}_h$ is supposed to approximate $F_h(u)$. Alternatively, we may seek to model $L - L_h$ as a correction $\tilde{L}_h$ of the operator L_h and solve a modified problem of the form

$$(L_h + \tilde{L}_h)\tilde{u}_h = f, \tag{5}$$

where thus the correction $\tilde{L}_h$ acts as a model of $L - L_h$. In the first approach the subgrid model takes the form of a corrective force $\tilde{F}_h$ independent of $\tilde{u}_h$, and in the second approach the subgrid model also contains a correction $\tilde{L}_h \tilde{u}_h$ depending on $\tilde{u}_h$.

To find the corrected (or effective) operator is a classical problem in homogenization theory (see e.g. Bensoussan *et.al.* [2]). Analytical homogenization teqniques based on asymptotics have been used to derive effective operators, but these teqniques rely on the essential assumptions of periodicity of the coefficients, well separated scales, and an a priori knowledge of the number of scales, which may be serious restrictions. Another approach to this problem was proposed by Nielsen and Tveito [18] who studied Poisson's equation with an irregular permeability on a fine scale, where the effective (or upscaled) permeability was defined as the solution to an optimization problem, where the difference between the fine scale and the coarse scale velocity fields were minimized. Brewster and Beylkin [3] used a numerical homogenization strategy based on MRA, where the homogenized (or reduced) operator was constructed by recursively taking the equation at one scale and construct the effective equation on the next coarser scale. These ideas were then further developed by Dorobantu *et.al.* [5]. For this approach to be practical, two problems have to be solved. First, the transition between two scales has to be computationally efficient. Secondly, the form of the equations must be preserved for a recursive use of the reduction step to be possible, which is not the case in general. A great advantage when using MRA is that it does not require separation of the scales, a continuous range of scales can be handled. Hughes *et.al.* [11] used a similar idea based on a hierarchical FEM basis, where they let the linear basis functions on each element represent the coarse scales, and the bubble, edge (and face) basis functions represent the fine scales. The fine scales were then eliminated by introducing certain Green's functions related to the dual operator, which in turn had to be determined by solving a local problem on each element. In a LES, the widely used turbulent viscosity assumption is another example of a modified operator that needs to be modeled. On the other hand, in the *scale similarity model*, introduced by Bardina *et.al.* [1], and the *modified scale similarity model*, by Goutorbe *et.al.* [9] and Liu *et.al.* [13], all subgrid scale (SGS) influence on the large scales is modeled as a correction on the force.

The SGS may of course influence the larger scales in different ways. In our simple linear model problem, the SGS may typically influence each part of the operator (the convection, diffusion or reaction) or the force. One might suspect that only using a correction on the force to model the SGS may be better or worse depending on how the SGS influence the larger scales. For example, if the SGS influence only manifests itself as a modification of the viscosity, a corrective force would typically be oscillating around zero, to either increase or decrease the oscillations in the solution. In this case, modeling of the corrective force on the scale h should probably be difficult. On the other hand, using the assumption that all SGS influence should be modeled as a viscosity does not seem optimal either. In a LES the so called *mixed models*, where a scale similarity model is used together with an eddy viscosity model, have been shown to improve the stand alone scale similarity model. But this approach needs also to be applied with care since one have to make sure that the two models work together in the right way, so that each model does not try to model the SGS on its own and thereby compensate twice for the SGS effects.

2.2 Dynamic models

Germano *et.al.* [8] first introduced the concept of a *dynamic model*. The dynamic model is not a model in itself, but rather a procedure taking a subgrid model as its basis. The basic assumption is that a particular model applies on all filters used, with the same value of the parameters. One way to explain the concept is the following. Suppose a LES is done on a relatively fine grid. One could think of it as a *direct numerical simulation* (DNS), meaning a simulation of the Navier-Stokes equations on such a fine scale that all small scale phenomena are resolved without any subgrid model. One could then use the velocity field from this computation as the basis for an a priori estimate of the subgrid model parameters. This can be done at every spatial point and time step. It is then assumed that the behaviour of the smallest resolved scales of the LES is very similar to that of the subgrid scales, so that parameters so obtained can be applied in the subgrid model on the LES itself.

Hoffman *et.al.* [10] proposed a method for computing an approximation of the modeling residual $F_h(u)$ in (3) using the idea of a dynamic model, in the case of a linear convection-diffusion-reaction problem. It was shown that the filtered (local average of) $F_h(u)$ on the scale h is equal to a sum of covariances of the form $[vw]^h - [v]^h[w]^h$. Based on a Haar MRA, an Ansatz of the form $[vw]^h - [v]^h[w]^h \approx Ch^\mu$ was proposed. The two functions $C(x)$ and $\mu(x)$ were determined by extrapolation from computing approximations $F_H(u_h)$ of the modeling residual $F_H(u)$ on two coarser scales H, where the solution to the simplified problem u_h was used as a substitute for the solution u to the exact problem. A priori and a posteriori modeling error estimates for the one dimensional case were presented. Numerical experiments in one dimension were also presented, indicating that the modeling error in a corrected solution $\tilde{u}_h$ on the scale h is less than the modeling error in a non corrected solution on the scale $h/4$. In [10] only modeling errors were considered, and the numerical errors were made neglible by computing on a very fine computational mesh.

3 Extrapolation of $F_h(u)$ using MRA

The notion of Multiresolution Analysis (MRA) was introduced in the early 90's by Meyer [17] and Mallat [16] as a general framework for construction of wavelet bases. In [10] a Haar basis MRA in $L_2([0,1])$ was used to motivate an Ansatz on the form of the modeling residual $F_h(u)$, and $F_h(u)$ was then approximated using extrapolation. In this section we extend the results in [10] to two dimensions, using the Haar basis in $L_2([0,1]^2)$. Based on these results we formulate an Ansatz on $F_h(u)$, which we use to extrapolate an approximation $\tilde{F}_h$ to $F_h(u)$.

3.1 MRA

An orthonormal MRA of $L_2([0,1])$ is a decomposition of $L_2([0,1])$ into a chain of closed subspaces

$$V_0 \subset V_1 \subset ... \subset V_j \subset ...$$

such that

$$\overline{\bigcup_{j\geq 0} V_j} = L_2([0,1]).$$

Each V_j is spanned by the dilates and integer translates of one *scale function* $\varphi \in V_0$:

$$V_j = \text{span}\{\varphi_{j,k}(x) = 2^{j/2}\varphi(2^j x - k)\},$$

and the functions $\varphi_{j,k}$ form an L_2-orthonormal basis in V_j. We denote the orthogonal complement of V_j in V_{j+1} by W_j, which is generated by another orthonormal basis (the *wavelets*) $\psi_{j,k}(x) = 2^{j/2}\psi(2^j x - k)$, where $\psi \in W_0$ is called the *mother wavelet*. The space $L_2([0,1])$ can now be represented as a direct sum

$$L_2([0,1]) = V_0 \oplus W_0 \oplus ... \oplus W_j \oplus ...$$

For a more detailed presentation of the MRA concept we refer to Daubechies [4] or Louis *et.al.* [14].

3.2 The Haar MRA in $L_2([0,1]^2)$

In the case of the two dimensional Haar basis in $L_2([0,1]^2)$, the space V_0 is spanned by the scale function

$$\Phi(x,y) = \varphi(x)\varphi(y),$$

and $V_j = \text{span}\{\Phi_{j,k}(x,y) = 2^j\Phi(2^j x - k_x, 2^j y - k_y)\}$. The orthogonal complement of V_j in V_{j+1} is $W_j = W_j^H \oplus W_j^V \oplus W_j^D$, where W_j^H, W_j^V and W_J^D are spanned by the wavelets

$$\begin{aligned}
\Psi_{i,k}^H(x,y) &= 2^j\Psi^H(2^i x - k_x, 2^i y - k_y),\\
\Psi_{i,k}^V(x,y) &= 2^j\Psi^V(2^i x - k_x, 2^i y - k_y),\\
\Psi_{i,k}^D(x,y) &= 2^j\Psi^D(2^i x - k_x, 2^i y - k_y),
\end{aligned}$$

respectively, where $j \in Z$, $k = (k_x, k_y) \in Z^2$ and

$$\begin{aligned}
\Psi^H(x,y) &= \varphi(x)\psi(y),\\
\Psi^V(x,y) &= \psi(x)\varphi(y),\\
\Psi^D(x,y) &= \psi(x)\psi(y).
\end{aligned}$$

Here ψ and φ are the one dimensional Haar mother wavelet and scale function respectively, defined by

$$\psi(x) = \begin{cases} 1 & 0 < x < 1/2 \\ -1 & 1/2 < x < 1 \\ 0 & \text{otherwise,} \end{cases}$$

$$\varphi(x) = \begin{cases} 1 & 0 < x < 1 \\ 0 & \text{otherwise.} \end{cases}$$

$$\begin{array}{|c|c|} \hline -1 & -1 \\ \hline +1 & +1 \\ \hline \end{array} \qquad \begin{array}{|c|c|} \hline +1 & -1 \\ \hline +1 & -1 \\ \hline \end{array} \qquad \begin{array}{|c|c|} \hline -1 & +1 \\ \hline +1 & -1 \\ \hline \end{array}$$

$\Psi^H(x,y)$ $\quad$ $\Psi^V(x,y)$ $\quad$ $\Psi^D(x,y)$

Each $f \in L_2([0,1]^2)$ has a unique decomposition

$$f = f_\Phi \Phi + \sum_{i,k} (f^H_{i,k}\Psi^H_{i,k} + f^V_{i,k}\Psi^V_{i,k} + f^D_{i,k}\Psi^D_{i,k}) = f_\Phi + \sum_i (f^H_i + f^V_i + f^D_i),$$

where f^H_i, f^V_i and f^D_i represent the contribution on the different scales 2^{-i} corresponding to dyadic subdivisions S_i of Ω with mesh points $x_{i,k} = k_x 2^{-i}$ and $y_{i,k} = k_y 2^{-i}$ where $k_x, k_y = 0, 1, ..., 2^i$, and subdomains $s_{i,k} = \{k_x 2^{-i} < x < (k_x + 1)2^{-i}, k_y 2^{-i} < y < (k_y + 1)2^{-i}\}$. The coefficients $f^\nu_{i,k}$ ($\nu = H, V, D$) are given as the L_2 inner product of the function f and the corresponding Haar basis function:

$$f^\nu_{i,k} = \int_\Omega f(x,y)\Psi^\nu_{i,k}(x,y)\; dxdy,$$

and $f_\Phi = \int_\Omega f(x,y)\ dxdy$.

3.3 The Ansatz

In this section we are going to formulate an Ansatz on the modeling residual $F_h(u)$, using the theory of MRA presented in the previous sections. For $f \in L_2(\Omega)$, where $\Omega = [0,1]^2$, we define $[f]^h$ to be the piecewise constant function on S_i, given by

$$[f]^h = f_\Phi + \sum_{j<i} (f_j^H + f_j^V + f_j^D),$$

where we let $h = 2^{-i}$ in the rest of this paper. Further, we recall the definition of the *running average* f^h of a function $f \in L_2(\Omega)$ on the scale h as

$$f^h(x,y) = 2^{2i} \int_{x-h/2}^{x+h/2} \int_{y-h/2}^{y+h/2} f(s,t)\ dsdt,$$

where $(x,y) \in \Omega$ and we extend f smoothly outside Ω. We denote by $\bar{f}^h$ the piecewise constant function on the scale h which coincides with f^h at the midpoints of the subdomains $s_{i,k}$. Clearly $\bar{f}^h$ is independent of the extension of f outside Ω. We shall use the following lemma:

Lemma 1: $f \in L_2(\Omega) \Rightarrow [f]^h = \bar{f}^h$.

Proof: We have

$$\begin{aligned} f &= f_\Phi + \sum_j (f_j^H + f_j^V + f_j^D) \Rightarrow \bar{f}^h = \bar{f}_\Phi^h + \overline{\sum_j (f_j^H + f_j^V + f_j^D)}^h \\ &= \bar{f}_\Phi + \overline{\sum_{j<i} (\bar{f}_j^H + \bar{f}_j^V + \bar{f}_j^D)}^h = f_\Phi + \sum_{j<i} (f_j^H + f_j^V + f_j^D) = [f]^h. \end{aligned}$$

□

We recall that V_i is the space of piecewise constant functions on S_i, and the linear mapping $L_2 \ni f \to [f]^h \in V_i$ can be identified with the L_2-projection of f onto V_i. Assuming for the moment that ϵ is constant, so that $[\epsilon]^h = \epsilon$, the modeling residual is given by

$$F_h(u) = f - [f]^h - (\beta \cdot \nabla u + \alpha u - [\beta]^h \cdot \nabla u - [\alpha]^h u).$$

From the definition we have that $[[f]^H g]^h = [f]^H [g]^h$ whenever $H \geq h$ ($H = 2^{-j}$, $h = 2^{-i}$ with $j < i$). This gives that

$$[F_h(u)]^h = [\beta]^h \cdot [\nabla u]^h - [\beta \cdot \nabla u]^h + [\alpha]^h [u]^h - [\alpha u]^h.$$

We denote the projection $[F_h(u)]^h$ of $F_h(u)$ onto V_i by $\bar{F}_h(u)$. We shall now seek to extrapolate $\bar{F}_h(u)$, and we are thus led to study in particular quantities of the form

$$E_h(v, w) = [vw]^h - [v]^h [w]^h, \tag{6}$$

for given functions v and w, which has the form of a covariance. Using the Haar basis, the covariance $E_h(v, w)$ takes a simple form:

Lemma 2: $v, w \in L_2 \Rightarrow$ *For given* $(x, y) \in \Omega$,

$$E_h(v, w)(x, y) = \sum_{\substack{j \geq i \\ l \,:\, x \in s_{j,l}}} 2^{2j} (v_j^H w_j^H + v_j^V w_j^V + v_j^D w_j^D).$$

Proof: For $v, w \in L_2$ we have

$$v = v_\Phi + \sum_j (v_j^H + v_j^V + v_j^D), \; w = w_\Phi + \sum_k (w_k^H + w_k^V + w_k^D),$$

and thus

$$\begin{aligned} vw = v_\Phi w_\Phi \;&+\; v_\Phi \sum_k (w_k^H + w_k^V + w_k^D) + w_\Phi \sum_j (v_j^H + v_j^V + v_j^D) \\ &+\; \sum_{j,k} (v_j^H + v_j^V + v_j^D)(w_k^H + w_k^V + w_k^D). \end{aligned}$$

Similarly

$$[v]^h = v_\Phi + \sum_{j<i} (v_j^H + v_j^V + v_j^D), \; [w]^h = w_\Phi + \sum_{k<i} (w_k^H + w_k^V + w_k^D),$$

and thus

$$\begin{aligned} [v]^h [w]^h = v_\Phi w_\Phi \;&+\; v_\Phi \sum_{k<i} (w_k^H + w_k^V + w_k^D) + w_\Phi \sum_{j<i} (v_j^H + v_j^V + v_j^D) \\ &+\; \sum_{j,k<i} (v_j^H + v_j^V + v_j^D)(w_k^H + w_k^V + w_k^D). \end{aligned}$$

Using Lemma 1, we obtain

$$
\begin{aligned}
&[vw]^h = \overline{vw}^h = \overline{v_\Phi w_\Phi}^h + \overline{v_\Phi \sum_k (w_k^H + w_k^V + w_k^D)}^h \\
&+ \overline{w_\Phi \sum_j (v_j^H + v_j^V + v_j^D)}^h + \overline{\sum_{j,k} (v_j^H + v_j^V + v_j^D)(w_k^H + w_k^V + w_k^D)}^h \\
&= v_\Phi w_\Phi + v_\Phi \sum_{k<i} (w_k^H + w_k^V + w_k^D) + w_\Phi \sum_{j<i} (v_j^H + v_j^V + v_j^D) \\
&+ \sum_{j,k<i} (v_j^H + v_j^V + v_j^D)(w_k^H + w_k^V + w_k^D) + \overline{\sum_{j\geq i} (v_j^H + v_j^V + v_j^D)(w_j^H + w_j^V + w_j^D)}^h \\
&= [v]^h [w]^h + \sum_{j\geq i} (v_j^H w_j^H + v_j^V w_j^V + v_j^D w_j^D).
\end{aligned}
$$

Finally we have for $(x,y) \in s_{j,l}$ that

$$
\begin{aligned}
&v_j^H w_j^H + v_j^V w_j^V + v_j^D w_j^D = v_{j,l}^H \Psi_{j,l}^H(x,y)\ w_{j,l}^H \Psi_{j,l}^H(x,y) + v_{j,l}^V \Psi_{j,l}^V(x,y)\ w_{j,l}^V \Psi_{j,l}^V(x,y) \\
&+ v_{j,l}^D \Psi_{j,l}^D(x,y)\ w_{j,l}^D \Psi_{j,l}^D(x,y) = 2^{2j}\ (v_{j,l}^H w_{j,l}^H + v_{j,l}^V w_{j,l}^V + v_{j,l}^D w_{j,l}^D).
\end{aligned}
$$

□

Lemma 2 asserts that $E_h(v,w)$ only depends on the scales finer than h, and that there are no mixing between the scales. An interesting situation is when both v and w are "scale regular" in the sense that $v_j^\nu = \alpha_\nu 2^{-j(1+\delta_\nu)}$ and $w_j^\nu = \beta_\nu 2^{-j(1+\gamma_\nu)}$ ($\nu = H,V,D$), where $\alpha_\nu, \beta_\nu, \delta_\nu$ and γ_ν are functions of (x,y), which corresponds to v and w having a simple fractal structure ($v_{j+1}^\nu(x,y) = 2^{-\delta_\nu(x,y)} v_j^\nu(x,y)$ and $w_{j+1}^\nu(x,y) = 2^{-\gamma_\nu(x,y)} w_j^\nu(x,y)$). In that particular situation we find that $E_h(v,w)$ has a certain form:

Corollary: *If $v,w \in L_2([0,1]^2)$ with $v_{j,l}^\nu = \alpha_\nu 2^{-j(1+\delta_\nu)}$ and $w_{j,l}^\nu = \beta_\nu 2^{-j(1+\gamma_\nu)}$ ($\nu = H,V,D$), where $\alpha_\nu, \beta_\nu, \delta_\nu$ and γ_ν are functions of (x,y), then for $(x,y) \in \Omega$*

$$E_h(v,w)(x,y) = C_H(x,y) h^{\mu_H(x,y)} + C_V(x,y) h^{\mu_V(x,y)} + C_D(x,y) h^{\mu_D(x,y)},$$

where $C_\nu = \frac{\alpha_\nu \beta_\nu}{1-2^{-(\delta_\nu+\gamma_\nu)}}$ and $\mu_\nu = \delta_\nu + \gamma_\nu$.

Proof: By Lemma 2 we have

$$
\begin{aligned}
E_h(v,w)(x,y) &= \sum_{\substack{j\,\geq\,i \\ l\,:\,x\,\in\,s_{j,l}}} 2^{2j}\ (v^H_{j,l}w^H_{j,l} + v^V_{j,l}w^V_{j,l} + v^D_{j,l}w^D_{j,l}) \\
&= \sum_{j\,\geq\,i} 2^{2j}(\alpha_H 2^{-j(1+\delta_H)}\beta_H 2^{-j(1+\gamma_H)} + ... + \alpha_D 2^{-j(1+\delta_D)}\beta_D 2^{-j(1+\gamma_D)}) \\
&= \sum_{j\,\geq\,i} (\alpha_H\beta_H 2^{-j(\delta_H+\gamma_H)} + ... + \alpha_D\beta_D 2^{-j(\delta_D+\gamma_D)}) \\
&= \alpha_H\beta_H h^{\delta_H+\gamma_H} \sum_{j\,\geq\,i} 2^{-(j-i)(\delta_H+\gamma_H)} + ... + \alpha_D\beta_D h^{\delta_D+\gamma_D} \sum_{j\,\geq\,i} 2^{-(j-i)(\delta_D+\gamma_D)} \\
&= \alpha_H\beta_H h^{\delta_H+\gamma_H} \sum_{j\,=\,0} 2^{-j(\delta_H+\gamma_H)} + ... + \alpha_D\beta_D h^{\delta_D+\gamma_D} \sum_{j\,=\,0} 2^{-j(\delta_D+\gamma_D)} \\
&= \frac{\alpha_H\beta_H}{1-2^{-(\delta_H+\gamma_H)}} \cdot h^{\delta_H+\gamma_H} + ... + \frac{\alpha_D\beta_D}{1-2^{-(\delta_D+\gamma_D)}} \cdot h^{\delta_D+\gamma_D}
\end{aligned}
$$

□

Assuming that the coefficients in (1) are "scale regular" in the sense of the Corollary, and that the solution inherits this local fractal structure to some degree, we have determined the form of the covariance $E_h(v,w)$, and thereby the form of the modeling residual $\bar{F}_h(u)$, and by performing a wavelet transform (see [4],[14]) we can determine the wavelet coefficients of v and w in $E_h(v,w)$. In this paper we are not going to use the full expression for $E_h(v,w)$, instead we formulate the following **Ansatz**: For given $(x,y) \in \Omega$,

$$E_h(v,w)(x,y) \approx C(x,y)h^{\mu(x,y)}, \tag{7}$$

where $C(x,y)$ and $\mu(x,y)$ are functions independent of the cut-off h. The Corollary shows that this is, for example, the situation when the coefficients in one of the directions $\nu = H,V,D$ locally dominates. If $E_h(v,w)$ has this form, then extrapolation of $E_h(v,w)$ will be possible from knowledge of $E_H(v,w)$ and $E_{\hat{H}}(v,w)$ with $h < H < \hat{H}$, from which the coefficients $C(x,y)$ and $\mu(x,y)$ may be determined. Typically, we will assume that the coefficients have a local fractal structure. We then expect the solution u to inherit this structure to some degree, and we expect that extrapolation of the modeling residual $\bar{F}_h(u)$ will be possible. This seems to be a reasonable assumption in, for example, the inertial range of a turbulent flow.

3.4 Summary of the proposed subgrid model

We are going to use the assumption that the Ansatz (7) is valid for the scales close to the computational scale h (in particular for the two coarser scales $H, \hat{H}$), as well as for the subgrid scales. The proposed method can then be summarized as follows:

- Exact problem: $Lu = f$.
- Simplified problem: $L_h u_h = [f]^h$.
- The exact solution u satisfies $L_h u = [f]^h + F_h(u)$.
- $\bar{F}_h(u) = \sum_k E_h(v_k, w_k), \quad E_h(v_k, w_k) = [v_k]^h [w_k]^h - [v_k w_k]^h,$ for some v_k, w_k.
- Ansatz: $E_h(v_k, w_k)(x) \approx C_k(x) h^{\mu_k(x)}$.
- Extrapolation from $\hat{H} > H > h \;\Rightarrow\; \tilde{F}_h = \sum_k C_k h^{\mu_k}$
  (using $(\bar{F}_H(u), \bar{F}_{\hat{H}}(u)) \approx (\bar{F}_H(u_h), \bar{F}_{\hat{H}}(u_h))$)
- Simplified problem with subgrid model: $L_h \tilde{u}_h = [f]^h + \tilde{F}_h$.

In the next two sections we are going to evaluate this method, first in the context of error estimates, and then in the context of numerical experiments.

4 Error analysis

We first fix some notation for this section. We denote by $L_2(\Omega)$ the Hilbert space of all real-valued Lebesgue measurable functions defined on Ω, with norm

$$\|w\| = \left(\int_\Omega |w(x)|^2 \; dx \right)^{1/2}$$

and inner product

$$(v, w) = \int_\Omega v(x) w(x) \; dx.$$

We will also use a ρ-weighted inner product and norm, defined by

$$(v, w)_\rho = \int_\Omega \rho(x) v(x) w(x) \; dx, \quad \|w\|_\rho = \sqrt{(w, w)_\rho},$$

for $v, w \in L_2(\Omega)$, where the weight $\rho : \Omega \to \mathbb{R}_+$ is locally integrable on Ω. We define $L_{2,\rho}(\Omega)$ to be the Hilbert space of functions with the $\|\cdot\|_\rho$-norm finite. We further define $H^1(\Omega)$ to be the Hilbert space consisting of all real-valued Lebesgue measurable functions defined on Ω, with norm

$$\|w\|_{H^1} = \int_\Omega (|\nabla w(x)|^2 + w^2(x))\ dx$$

and inner product

$$(v, w)_{H^1} = \int_\Omega (\nabla v(x) \cdot \nabla w(x) + v(x)w(x))\ dx.$$

The problem $Lu = f$, with homogeneous boundary conditions $v|_{\partial\Omega_-} = \frac{\partial v}{\partial n}|_{\partial\Omega_+} = 0$, takes the following variational formulation: Find $u \in V = \{v \in H^1(\Omega) : v|_{\partial\Omega_-} = 0\}$ such that

$$a(u, v) = \mathbf{f}(v) \quad \forall v \in V, \tag{8}$$

where the bilinear form $a(u, v)$ is defined by

$$a(u, v) = (\epsilon\nabla u, \nabla v) + (\beta \cdot \nabla u, v) + (\alpha u, v),$$

and $\mathbf{f}(v) = (f, v)$. The corresponding simplified problem on the scale h consists of finding $u_h \in V$ such that

$$a_h(u_h, v) = \mathbf{f}_h(v) \quad \forall v \in V, \tag{9}$$

where

$$a_h(u_h, v) = ([\epsilon]^h \nabla u_h, \nabla v) + ([\beta]^h \cdot \nabla u_h, v) + ([\alpha]^h u, v),$$

and $\mathbf{f}_h(v) = ([f]^h, v)$. In this section, we will not restrict us to the case when $[\cdot]^h$ means the truncated Haar expansion of a function. Instead we will think of $[\cdot]^h$ as being any local approximation operator on the scale h. This means in particular that $[f]^h$ might be a continuous function. The solution u to the exact problem (8) satisfies

$$a_h(u, v) = \mathcal{F}_h(v) \quad \forall v \in V, \tag{10}$$

with

$$\mathcal{F}_h(v) = ([f]^h + F_h(u), v) + (F_h^\nabla(u), \nabla v),$$

where

$$
\begin{aligned}
F_h(u) &= f - [f]^h - (\beta \cdot \nabla u + \alpha u - [\beta]^h \cdot \nabla u - [\alpha]^h u), && (11)\\
F_h^{\nabla}(u) &= [\epsilon]^h \nabla u - \epsilon \nabla u, && (12)
\end{aligned}
$$

are modeling residuals. The local averages of $F_h(u)$ and $F_h^{\nabla}(u)$ on the scale h are defined by

$$
\begin{aligned}
\bar{F}_h(u) &= [\beta]^h \cdot [\nabla u]^h - [\beta \cdot \nabla u]^h + [\alpha]^h [u]^h - [\alpha u]^h,\\
\bar{F}_h^{\nabla}(u) &= [\epsilon]^h [\nabla u]^h - [\epsilon \nabla u]^h.
\end{aligned}
$$

Above we constructed approximations $(\tilde{F}_h, \tilde{F}_h^{\nabla})$ of $(\bar{F}_h(u), \bar{F}_h^{\nabla}(u))$ by extrapolation, and we constructed a corresponding corrected solution $\tilde{u}_h$ by solving the problem

$$
a_h(\tilde{u}_h, v) = \tilde{\mathcal{F}}_h(v) \quad \forall v \in V, \tag{13}
$$

where

$$
\tilde{\mathcal{F}}_h(v) = ([f]^h + \tilde{F}_h, v) + (\tilde{F}_h^{\nabla}, \nabla v).
$$

4.1 A priori estimates of modeling errors

In the following theorems, which are extensions of the a priori modeling error estimates in [10] to two dimensions, we will for simplicity assume that $[\beta]^h$ is differentiable and satisfies $\nabla \cdot [\beta]^h = 0$. For the case when $[\beta]^h$ is the truncated Haar expansion of β, we can think of $[\beta]^h$ as being the piecewise linear function we get by linearly connecting the midpoint values of the subdomains on the scale h.

Theorem 1: *Assume that $[\beta]^h$ is differentiable with $\nabla \cdot [\beta]^h = 0$, and that $0 < c \leq [\alpha]^h$. If u and u_h are the solutions to (8) and (9) respectively, then*

$$
\|\nabla(u - u_h)\|^2_{[\epsilon]^h} + \|u - u_h\|^2 \leq C \left(\|F_h(u)\|^2 + \|F_h^{\nabla}(u)\|^2_{\frac{1}{[\epsilon]^h}} \right),
$$

$$
\|\nabla(u - \tilde{u}_h)\|^2_{[\epsilon]^h} + \|u - \tilde{u}_h\|^2 \leq C \left(\|F_h(u) - \tilde{F}_h\|^2 + \|F_h^{\nabla}(u) - \tilde{F}_h^{\nabla}\|^2_{\frac{1}{[\epsilon]^h}} \right),
$$

where $C = \max(1, \frac{1}{c})$.

Proof: We subtract (9) from (10) and write $e_h = u - u_h$. Choosing $v = e_h$, we obtain

$$\begin{aligned}&a_h(e_h, e_h) = a_h(u - u_h, e_h) = a_h(u, e_h) - a_h(u_h, e_h) = \mathcal{F}_h(e_h) - \mathbf{f}_h(e_h)\\&= (F_h(u), e_h) + (F_h^\nabla(u), \nabla e_h).\end{aligned}$$

$$\Rightarrow ([\epsilon]^h \nabla e_h, \nabla e_h) + ([\beta]^h \cdot \nabla e_h, e_h) + ([\alpha]^h e_h, e_h) = (F_h(u), e_h) + (F_h^\nabla(u), \nabla e_h).$$

We note that

$$([\beta]^h \cdot \nabla e_h, e_h) = -\frac{1}{2}(\nabla \cdot [\beta]^h e_h, e_h) = 0,$$

since $e_h|_{\partial\Omega_-} = \frac{\partial e_h}{\partial n}|_{\partial\Omega_+} = 0$ and $\nabla \cdot [\beta]^h = 0$, and conclude that

$$\|\nabla e_h\|_{[\epsilon]^h} + \|e_h\|_{[\alpha]^h} = (F_h(u), e_h) + (F_h^\nabla(u), \nabla e_h).$$

Using Cauchy-Schwartz inequality, and the inequality $2ab \leq a^2 + b^2$ $(a, b \in \mathbb{R})$, we get

$$(F_h(u), e_h) \leq \|F_h(u)\|_{\frac{1}{[\alpha]^h}} \|e_h\|_{[\alpha]^h} \leq \frac{1}{2}(\|F_h(u)\|^2_{\frac{1}{[\alpha]^h}} + \|e_h\|^2_{[\alpha]^h}).$$

Estimating $(F_h^\nabla(u), \nabla e_h)$ similarly, we get

$$\|\nabla e_h\|_{[\epsilon]^h} + \|e_h\|_{[\alpha]^h} \leq \|F_h(u)\|^2_{\frac{1}{[\alpha]^h}} + \|F_h^\nabla(u)\|^2_{\frac{1}{[\epsilon]^h}},$$

from which the desired estimate follows. For the error $u - \tilde{u}_h$ we subtract (13) from (10) and write $\tilde{e}_h = u - \tilde{u}_h$. Choosing $v = \tilde{e}_h$, we obtain

$$\begin{aligned}&a_h(\tilde{e}_h, \tilde{e}_h) = a_h(u - \tilde{u}_h, \tilde{e}_h) = a_h(u, \tilde{e}_h) - a_h(\tilde{u}_h, \tilde{e}_h) = \mathcal{F}_h(\tilde{e}_h) - \tilde{\mathcal{F}}_h(\tilde{e}_h)\\&= (F_h(u) - \tilde{F}_h, \tilde{e}_h) + (F_h^\nabla(u) - \tilde{F}_h^\nabla, \nabla \tilde{e}_h).\end{aligned}$$

from which the desired estimate follows.

$\square$

Theorem 1 indicates, for example, that if $F_h(u)$ and $F_h^\nabla(u)$ are large, then the modeling error $u - u_h$ is large and subgrid modeling is needed. On the other hand, if $F_h(u)$ and $F_h^\nabla(u)$ are both small, then the modeling error $u - u_h$ is also small and subgrid modeling is not needed. The quality of the corrected solution depends on how well we can approximate $(F_h(u), F_h^\nabla(u))$ by $(\tilde{F}_h, \tilde{F}_h^\nabla)$. We also find that the relative modeling error in u_h and $\tilde{u}_h$ is given by the relative size of $(F_h(u), F_h^\nabla(u))$ and the difference $(F_h(u), F_h^\nabla(u)) - (\tilde{F}_h, \tilde{F}_h^\nabla)$.

4.2 A posteriori error estimates

For the dynamic computational subgrid modeling teqnique to work, it is vital to control the numerical errors. First, if the numerical errors dominate, reduction of the modeling errors will not significally reduce the total error. Secondly, the quality of the approximation $F_H(u) \approx F_H(u_h)$, and thus the whole extrapolation procedure, is affected by the numerical errors in the computation of u_h. Denoting a computed solution to the simplified problem (9) by U_h, we have

$$e = u - U_h = (u - u_h) + (u_h - U_h) = e_h + E_h, \tag{14}$$

where e_h represents a modeling error and E_h a numerical error. Similarly, denoting the computed approximation of the corrected problem (13) by $\tilde{U}_h$, we have

$$\tilde{e} = u - \tilde{U}_h = (u - \tilde{u}_h) + (\tilde{u}_h - \tilde{U}_h) = \tilde{e}_h + \tilde{E}_h. \tag{15}$$

If $\|e_h\| > \|E_h\|$, then subgrid modeling may be attempted with the goal of computing a corrected solution $\tilde{U}_h$, with $\|\tilde{e}_h\| << \|e_h\|$. We now present a posteriori error estimates allowing us to estimate $\|e\|$ and $\|E_h\|$, and thereby e_h, and similarly $\|\tilde{e}\|$ and $\|\tilde{E}_h\|$, and hence $\|\tilde{e}_h\|$.

Theorem 2: *Assume that* $[\beta]^h$ *is differentiable such that* $\nabla \cdot [\beta]^h = 0$, *and that* $0 < c \leq [\alpha]^h$. *If* $E_h = u_h - U_h$ *and* $\tilde{E}_h = u_h - \tilde{U}_h$, *then*

$$\begin{aligned}
\|\nabla E_h\|^2_{[\epsilon]^h} + \|E_h\|^2 &\leq C\left(\|R_h(U_h)\|^2 + \|R_h^{\nabla}(U_h)\|^2_{\frac{1}{[\epsilon]^h}}\right), \\
\|\nabla \tilde{E}_h\|^2_{[\epsilon]^h} + \|\tilde{E}_h\|^2 &\leq C\left(\|R_h(\tilde{U}_h)\|^2 + \|R_h^{\nabla}(\tilde{U}_h)\|^2_{\frac{1}{[\epsilon]^h}}\right),
\end{aligned}$$

where $C = \max(1, \frac{1}{c})$, $R_h(w) = [f]^h - [\beta]^h \cdot \nabla w - [\alpha]^h w$, *and* $R_h^{\nabla}(w) = -[\epsilon]^h \nabla w$.

Proof: We prove the theorem for the error E_h, the proof for the error $\tilde{E}_h$ is similar. We have that

$$a_h(E_h, E_h) = a_h(u_h - U_h, E_h) = a_h(u_h, E_h) - a_h(U_h, E_h) = \mathbf{f}_h(E_h) - a_h(U_h, E_h),$$

that is

$$\begin{aligned}
&([\epsilon]^h \nabla E_h, \nabla E_h) + ([\beta]^h \cdot \nabla E_h, E_h) + ([\alpha]^h E_h, E_h) \\
&= (-[\epsilon]^h \nabla U_h, \nabla E_h) + ([f]^h - [\beta]^h \cdot \nabla U_h - [\alpha]^h U_h, E_h).
\end{aligned}$$

As in the proof of Theorem 1 we use

$$([\beta]^h \cdot \nabla E_h, E_h) = -\frac{1}{2}(\nabla \cdot [\beta]^h E_h, E_h) = 0,$$

assuming $e|_{\partial\Omega_-} = \frac{\partial e}{\partial n}|_{\partial\Omega_+} = 0$ and $\nabla \cdot [\beta]^h = 0$. That gives that

$$\|\nabla E_h\|_{[\epsilon]^h} + \|E_h\|_{[\alpha]^h} = (R_h^\nabla(U_h), \nabla E_h) + (R_h(U_h), E_h),$$

from which the desired estimate follows by following the proof of Theorem 1.

□

Similarly, we can derive a posteriori error estimates for the total errors $u - U_h$ and $u - \tilde{U}_h$, in terms of a computable residual including both numerical and modeling features.

Theorem 3: *If β is differentiable such that $\nabla \cdot \beta = 0$, and $0 < c \leq \alpha$, then*

$$\|\nabla(u - U_h)\|_\epsilon^2 + \|u - U_h\|^2 \leq C\left(\|R(U_h)\|^2 + \|R^\nabla(U_h)\|_{\frac{1}{\epsilon}}^2\right),$$
$$\|\nabla(u - \tilde{U}_h)\|_\epsilon^2 + \|u - \tilde{U}_h\|^2 \leq C\left(\|R(U_h)\|^2 + \|R^\nabla(U_h)\|_{\frac{1}{\epsilon}}^2\right),$$

where $C = \max(1, \frac{1}{c})$, $R(w) = f - \beta \cdot \nabla w - \alpha w$, and $R^\nabla(w) = -\epsilon\nabla w$.

Proof: We indicate the proof for the error $e = u - U_h$, the proof for the error $u - \tilde{U}_h$ is similar. We have that

$$a(e, e) = a(u - U_h, e) = a(u, e) - a(U_h, e) = \mathbf{f}(e) - a(U_h, e),$$

from which the desired estimate follows by following the proof of Theorem 2.

□

We can rewrite the residuals $R(w)$ and $R^\nabla(w)$ as

$$R(w) = R_h(w) + F_h(w),$$
$$R^\nabla(w) = R_h^\nabla(w) + F_h^\nabla(w),$$

where $R_h(w)$ and $R_h^\nabla(w)$ are the *numerical residuals* from Theorem 2, whereas $F_h(w)$ and $F_h^\nabla(w)$ are the modeling residuals.

4.3 The adaptive algorithm

We can now, based on Theorem 5, formulate an adaptive algorithm. Given a tolerance TOL, a local meshsize h, and a norm $\|\cdot\|$, the adaptive algorithm reads:

- Compute U_h from the discretized version of (9).
- Use Theorem 3 to compute a bound for $\|u - U_h\|$.
- If $\|u - U_h\| \leq TOL$ then STOP.
- Else, compute the residuals $R_h(U_h), R_h^{\nabla}(U_h)$ and $F_h(U_h), F_h^{\nabla}(U_h)$.
- If $F_h(U_h), F_h^{\nabla}(U_h)$ are small compared to $R_h(U_h), R_h^{\nabla}(U_h)$, then refine h.
- Else, extrapolate $\tilde{F}_h$, and compute $\tilde{U}_h$ from the discretized version of (13).
- Use Theorem 3 to compute a bound for $\|u - \tilde{U}_h\|$.
- If $\|u - \tilde{U}_h\| \leq TOL$ then STOP, else refine h.

5 Numerical experiments

In this section we study the performance of the proposed subgrid model in some numerical experiments. We use coefficients that are tensor products of the one dimensional fractal functions of the form

$$\eta_{\gamma,\delta}(x) = 1 + \sum_{\substack{j \geq 0 \\ l \,:\, x \in I_{j,l}}} \gamma \; 2^{-j(1/2+\delta)} \psi_{j,l}(x), \quad x \in I = [0,1], \tag{16}$$

which are scale regular in the sense of the Corollary.

First we will use a very fine mesh (uniform quadratic with 512×512 elements) for all computations, and we will assume the numerical errors to be neglible compared to the modeling errors. We will denote by u the solution to the problem with the finest possible resolved coefficients on this mesh, and we will use u as an approximation of the exact solution to the problem in the computation of the error. To measure the relative error in u_h and $\tilde{u}_h$, projected on the scale h, we define a "gain-factor" GF, defined by

$$GF = \frac{\|[u - u_h]^h\|}{\|[u - \tilde{u}_h]^h\|}. \tag{17}$$

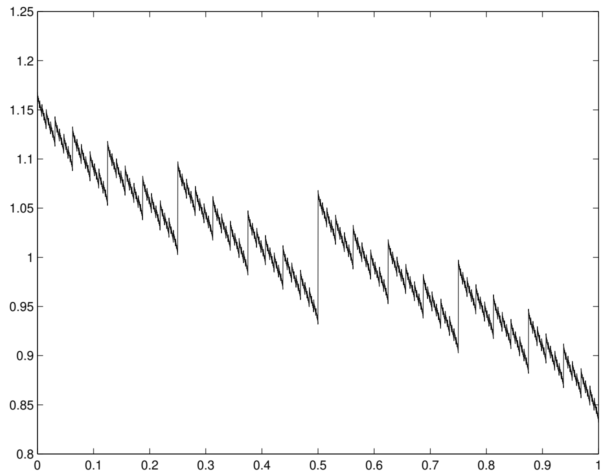


Figure 1: $\eta_{\gamma,\delta}(x)$ for $\gamma = 0.05$ and $\delta = 0.5$.

We can also relate the reduction of the modeling error we get from using the extrapolated modeling residual to the reduction of the error we get by refining the mesh, by introducing a "mesh-factor" MF_p, defined by

$$MF_p = \frac{\|[u - u_{h/p}]^h\|}{\|[u - \tilde{u}_h]^h\|}. \tag{18}$$

For example, MF_2 measures the relative improvement in $\tilde{u}_h$ compared to the improvement we get from refining the mesh uniformly once, that is, the improvement we get by using four times as many elements. In all the tests we are going to use the cut-off scale $h = 2^{-5}$.

5.1 Elliptic Equations

As a model for an elliptic problem we consider Poisson's equation

$$-\nabla \cdot (\epsilon \nabla u) = f, \tag{19}$$

with the boundary conditions $u|_{\partial\Omega_-} = \frac{\partial u}{\partial n}|_{\partial\Omega_+} = 0$, where $\partial\Omega_- = \{(x, y) : x = 0 \text{ or } y = 0\}$, $\partial\Omega_+ = \{(x, y) : x = 1 \text{ or } y = 1\}$ and n is an unit outward normal from Ω, and we formulate the corresponding variational problem: Find $u \in V = \{v \in H^1(\Omega) : v|_{\partial\Omega_-} = 0\}$ such that

$$(\epsilon \nabla u, \nabla v) = (f, v), \quad \forall v \in V.$$

The solution to the simplified equation u_h then satisfies

$$([\epsilon]^h \nabla u_h, \nabla v) = ([f]^h, v), \quad \forall v \in V,$$

and the exact solution u to (19) satisfies

$$([\epsilon]^h \nabla u, \nabla v) = ([f]^h, v) + (F_h^\nabla(u), \nabla v), \quad \forall v \in V,$$

where

$$F_h^\nabla(u) = [\epsilon]^h \nabla u - \epsilon \nabla u$$

is a modeling residual, and the projection of $F_h^\nabla(u)$ onto V_i is defined by

$$\bar{F}_h^\nabla(u) = [\epsilon]^h [\nabla u]^h - [\epsilon \nabla u]^h,$$

which is of the form (6). Here we assume that ϵ has a simple fractal structure and assuming that the solution u inherits this structure to some degree, we use the Ansatz (7) on $\bar{F}_h^\nabla(u)$: For given $(x, y) \in \Omega$,

$$\bar{F}_h^\nabla(u)(x, y) \approx C(x, y) h^{\mu(x,y)},$$

where $C, \mu : \Omega \to \mathbb{R}^2$ are independent of the cut-off h. By approximating $\bar{F}_H^\nabla(u) \approx \bar{F}_H^\nabla(u_h)$ for coarser scales H we can determine approximative C and μ. The extrapolated approximation $\tilde{F}_h^\nabla$ of $\bar{F}_h^\nabla(u)$ is then defined by

$$\tilde{F}_h^\nabla(x, y) = C(x, y) h^{\mu(x,y)},$$

and we first define $\tilde{u}_h$ to be the solution to the corrected problem

$$([\epsilon]^h \nabla \tilde{u}_h, \nabla v) = ([f]^h, v) + (\tilde{F}_h^\nabla, \nabla v), \quad \forall v \in V.$$

We define the diffusion coefficient ϵ to be the tensor product of $\eta_{\gamma,\delta}$: $\epsilon(x, y) = \eta_{\gamma,\delta}(x)\eta_{\gamma,\delta}(y)$, with $\gamma = \delta = 0.1$. For the computations we use a standard Finite Element Method (FEM) with bilinear elements. When we compute u_h and $\tilde{u}_h$ for $f(x) = 1$, and extrapolate from $H = 2h$ and $\hat{H} = 4h$, we find that $GF = 1.1$, which is not very impressive. We have $MF_2 = 0.73$, so the improvement we get by uniformly refining the mesh once is here greater than the improvement we get by correcting the equation with the extrapolated modeling residual.

From Theorem 2 we know that the modeling error in $\tilde{u}_h$ depends on $F_h(u) - \tilde{F}_h$. But the error $F_h(u) - \tilde{F}_h$ consists of two components: $F_h(u) - \bar{F}_h(u)$ and $\bar{F}_h(u) - \tilde{F}_h$, where the first component is the error we get from projecting $F_h(u)$ onto V_i and the second is an extrapolation error. To compare the relative importance of the two errors we can eliminate the extrapolation error by using u instead of u_h in the

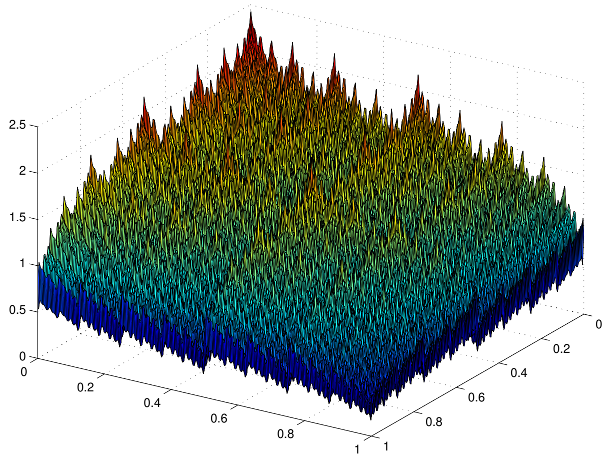


Figure 2: The fractal coefficient $\epsilon(x, y)$.

above experiment. We then get $GF = 9.9$ and $MF_2 = 7.8$, so the extrapolation error is large, and we conclude that if we can reduce the extrapolation error the total modeling error will be significally reduced. By increasing H and $\hat{H}$, we hope to reduce the extrapolation error since we anticipate that the approximations $\bar{F}_H(u) \approx \bar{F}_H(u_h)$ and $\bar{F}_{\hat{H}}(u) \approx \bar{F}_{\hat{H}}(u_h)$ should be more accurate on coarser scales H and $\hat{H}$. We find that for $(H, \hat{H}) = (4h, 8h)$ we get $GF = 1.5$ and $MF_2 = 0.99$, so now the modeling error in $\tilde{u}_h$ is the same as for one uniform mesh refinement. By increasing H and $\hat{H}$ even more we find that the modeling error is further reduced. We summarize these results in Table 1.

$(H, \hat{H})$	GF	MF_2
$(2h,4h)$	1.1	0.73
$(2h,8h)$	1.2	0.77
$(4h,8h)$	1.5	0.99
$(4h,16h)$	1.8	1.2
$(8h,16h)$	1.8	1.2

Table 1: Extrapolation level dependence, modeling errors.

Now we introduce numerical errors into the problem by computing on a uniform quadratic mesh with 32×32 elements, corresponding to the modeling scale $h = 2^{-5}$. Using the same ϵ as above and $(H, \hat{H}) = (4h, 8h)$, we get $GF = 1.7$ and $MF_2 = 1.1$. We give the results for different $(H, \hat{H})$ in Table 2.

$(H,\hat{H})$	GF	MF_2
$(2h$,$4h)$	1.2	0.78
$(2h$,$8h)$	1.3	0.84
$(4h$,$8h)$	1.7	1.1
$(4h$,$16h)$	2.1	1.3
$(8h$,$16h)$	2.1	1.3

Table 2: Extrapolation level dependence, including numerical errors.

We thus find that the subgrid model based on a corrective force works for Poisson's equation with a fractal ϵ, but to get a significant improvement in L_2-norm we have to extrapolate from coarser scales than $(H,\hat{H})=(2h,4h)$. This we also noted for the one dimensional case in [10], and one might view this result as an indication that it is hard to model a corrected diffusion operator by a correction on the force. We may therefore also try to use the extrapolated modeling residual $\tilde{F}_h^\nabla$ to model a correction on the operator. For example, we can use the assumption that

$$\epsilon_h^{corr} \approx -\tilde{F}_h^\nabla / \nabla u_h,$$

where ϵ_h^{corr} is a correction on the diffusion coefficient $[\epsilon]^h$, used in the simplified problem. That is, we now let $\tilde{u}_h$ be the solution to the problem

$$(([\epsilon]^h + \epsilon_h^{corr})\nabla u_h, \nabla v) = ([f]^h, v), \quad \forall v \in V.$$

When we test this approach we find that we get approximately the same result as when we let the modeling residual act as a correction on the force.

5.2 Hyperbolic Equations

Now we consider the problem (1) when $\epsilon << \beta$, for which the problem has a hyperbolic character. We use a Streamline Diffusion (SD) method (see Eriksson [6]) to solve the problem

$$-\epsilon\Delta u + \beta\cdot\nabla u + \alpha u = f, \tag{20}$$

with boundary conditions $u|_{\partial\Omega_-} = \frac{\partial u}{\partial n}|_{\partial\Omega_+} = 0$, where $\partial\Omega_- = \{x\in\partial\Omega:\ \beta(x)\cdot n(x)<0\}$, $\partial\Omega_+ = \{x\in\partial\Omega:\ \beta(x)\cdot n(x)>0\}$ and n is an unit outward normal from Ω. ϵ is constant such that $\epsilon << \|\beta\|$, and we have the corresponding simplified problem

$$-\epsilon\Delta u_h + [\beta]^h\cdot\nabla u_h + [\alpha]^h u_h = [f]^h,$$

with the same boundary conditions as for (20). The exact solution u to the problem (20) satisfies

$$-\epsilon\Delta u + [\beta]^h \cdot \nabla u + [\alpha]^h u = [f]^h + F_h(u),$$

where the modeling residual $F_h(u)$ projected onto V_i is given by

$$\begin{aligned}
\bar{F}_h(u) &= [\beta]^h \cdot [\nabla u]^h - [\beta \cdot \nabla u]^h + [\alpha]^h [u]^h - [\alpha u]^h \\
&= [\beta_1]^h [\frac{\partial u}{\partial x}]^h - [\beta_1 \frac{\partial u}{\partial x}]^h + [\beta_2]^h [\frac{\partial u}{\partial y}]^h - [\beta_2 \frac{\partial u}{\partial y}]^h + [\alpha]^h [u]^h - [\alpha u]^h \\
&= \bar{F}_h^1(u) + \bar{F}_h^2(u) + \bar{F}_h^3(u). \qquad (21)
\end{aligned}$$

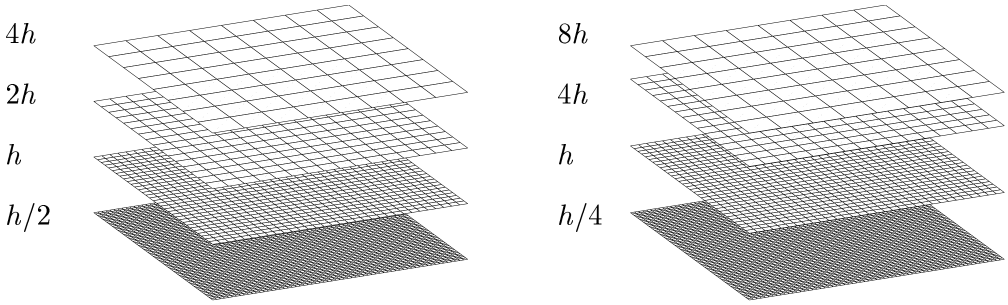
Now we let $\beta = (\beta_1, \beta_2)$, where $\beta_1(x,y) = \beta_2(x,y) = \eta_{\gamma_\beta,\delta_\beta}(x)\eta_{\gamma_\beta,\delta_\beta}(y)$, and $\alpha(x,y) = \eta_{\gamma_\alpha,\delta_\alpha}(x)\eta_{\gamma_\alpha,\delta_\alpha}(y)$. We set $\gamma_\beta = 0.2$, $\delta_\beta = 0.25$, $\gamma_\alpha = 0.3$, $\delta_\alpha = 0.08$, and $\epsilon = 10^{-3}$. Following the discussion in the previous sections, the simple fractal structure of the coefficients α and β, together with the assumption that the solution inherits this structure to some degree, motivates an Ansatz on $\bar{F}_h(u)$: For given $(x,y) \in \Omega$,

$$\bar{F}_h^k(u)(x,y) \approx C_k(x,y) h^{\mu_k(x,y)}, \quad k = 1,2,3,$$

where $C_k, \mu_k : \Omega \to \mathbb{R}$ are independent of the cut-off h. By computing approximations $\bar{F}_H^k(u) \approx \bar{F}_H^k(u_h)$ on coarser scales H and $\hat{H}$ we can independently determine (C_k, μ_k) without using more scales than if we just had to determine one set of parameters (C, μ). We denote the extrapolated approximations $\tilde{F}_h^k$, and we denote the sum $\tilde{F}_h$. We define the corrected solution $\tilde{u}_h$ to be the solution to the problem

$$-\epsilon\Delta\tilde{u}_h + [\beta]^h \cdot \nabla\tilde{u}_h + [\alpha]^h \tilde{u}_h = [f]^h + \tilde{F}_h.$$

First we consider only modeling errors, making the numerical errors neglible compared to the modeling errors by computing on the fine mesh. We use the cut-off $h = 2^{-5} \approx \sqrt{\epsilon}$, and when extrapolating from $(H, \hat{H}) = (2h, 4h)$ we get $GF = 1.9$ and $MF_2 = 1.7$. This means that the modeling error in the corrected solution $\tilde{u}_h$ is less than the modeling error in a non corrected solution on a uniformly refined mesh, so $\tilde{u}_h$ corresponds to an "extrapolation of u_h beyond the unresolved scale $h/2$".



We decompose $F_h(u) - \tilde{F}_h$ into $(F_h(u) - \bar{F}_h(u)) + (\bar{F}_h(u) - \tilde{F}_h)$, where the first component is the error we get from projecting $F_h(u)$ onto V_i and the second is an extrapolation error. By eliminating the extrapolation error, by using $\bar{F}_h(u)$ instead of $\bar{F}_h(u_h)$, we find that also for this hyperbolic problem the extrapolation error is significant.

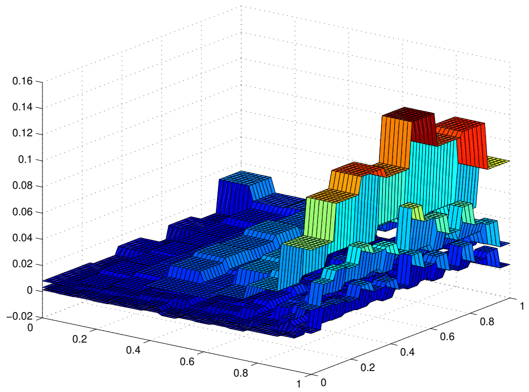


Figure 3: $\bar{F}^1_{\hat{H}}(u_h)$, $\bar{F}^1_{H}(u_h)$ and $\tilde{F}^1_h$.

By comparing the error $\bar{F}^1_h(u) - \tilde{F}^1_h$ and $\bar{F}^2_h(u) - \tilde{F}^2_h$ to the error $\bar{F}^3_h(u) - \tilde{F}^3_h$, we find that the errors in the corrective forces that are based on ∇u are a lot more significant than the error in the corrective force that is based on u. This was also observed for the one dimensional problem in [10], and we note that in LES the SGSRS $\tau_{ij} = \overline{u}_i\overline{u}_j - \overline{u_i u_j}$ is expressed in the computed variables $\overline{u}_i$, which should be an advantage for modeling purposes. In Figure 3 we have plotted $\bar{F}^1_{\hat{H}}(u_h)$, $\bar{F}^1_H(u_h)$ and $\tilde{F}^1_h$, and in Figure 4 the extrapolated modeling residual $\tilde{F}_h$ is plotted, where we have extrapolated from scales $2h$ and $4h$.

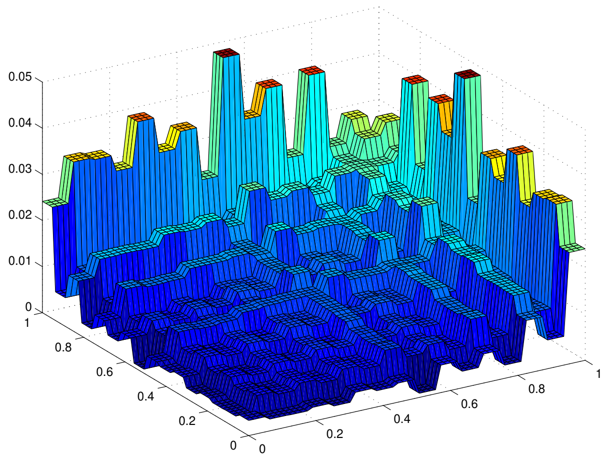


Figure 4: The extrapolated modeling residual $\tilde{F}_h$.

In [10], two ways to reduce the extrapolation error were suggested. One is to extrapolate from coarser scales than $H = 2h$ and $\hat{H} = 4h$. In this case we assume that the loss of accuracy we get from using coarser scales is dominated by the gain we get from the fact that ∇u_h better resembles ∇u on the coarser scales, and we further assume that the scale regularity of the problem is similar on the scale $\hat{H}$. By extrapolating from $H = 4h$ and $\hat{H} = 8h$ we get $GF = 7.5$ and $MF_4 = 2.3$, so now $\tilde{u}_h$ corresponds to an "extrapolation of u_h beyond the unresolved scale $h/4$".

For the special cases when $\beta = (\beta_1, 0)$ or $\beta = (0, \beta_2)$ we can avoid to base the computation of the corrective force on ∇u at all. In the problem (20), with $\beta = (\beta_1, 0)$, we can eliminate ∇u from (21) by using (20) and neglecting the terms including ϵ,

$$\begin{aligned}
\bar{F}_h(u) &= [\beta_1]^h[\frac{\partial u}{\partial x}]^h - [\beta_1\frac{\partial u}{\partial x}]^h + [\alpha]^h[u]^h - [\alpha u]^h \\
&= [\beta_1]^h[\frac{1}{\beta_1}(f - \alpha u + \epsilon\Delta u)]^h - [f - \alpha u + \epsilon\Delta u]^h + [\alpha]^h[u]^h - [\alpha u]^h \\
&\approx [\beta_1]^h[f/\beta_1]^h - [f]^h + [\alpha]^h[u]^h - [\beta_1]^h[(\alpha u)/\beta_1]^h.
\end{aligned}$$

But this method is, as we remarked, only applicable when $\beta = (\beta_1, 0)$ or $\beta = (0, \beta_2)$, and ϵ has to be small enough, so that the approximation of neglecting the terms involving ϵ is justified.

We then introduce numerical errors by computing on a quadratic mesh with 32×32 elements, corresponding to the cut-off scale $h = 2^{-5}$ ($h \approx \sqrt{\epsilon}$). By extrapolating from $H = 2h$ and $\hat{H} = 4h$ we get $GF = 1.6$ and $MF_2 = 0.91$, so the modeling error in the corrected solution approximately corresponds the modeling error in a non corrected solution on the scale $h/2$. We find that by extrapolating from greater H and $\hat{H}$, up to a certain level, we further reduce the error in $\tilde{u}_h$ (this is summarized in Table 3).

error	$(H, \hat{H})$	GF	MF_2	MF_4
modeling	$(2h,4h)$	2.1	1.2	0.65
	$(2h,8h)$	2.4	1.4	0.75
	$(4h,8h)$	7.5	4.5	2.3
	$(4h,16h)$	7.2	4.3	2.2
	$(8h,16h)$	1.1	0.63	0.33
modeling + numerical	$(2h,4h)$	1.6	0.91	0.47
	$(2h,8h)$	1.8	1.0	0.52
	$(4h,8h)$	3.9	2.2	1.1
	$(4h,16h)$	5.5	3.1	1.6
	$(8h,16h)$	1.4	0.79	0.40

Table 3: Extrapolation level dependence, with and without numerical errors.

6 Conclusions

In this paper we have investigated the feasibility of extrapolating a modeling residual to model the subgrid scales, in the case of a convection-diffusion-reaction problem with features on a range of scales in two dimensions. We assumed some "scale regularity" in the coefficients, and for this case we motivated an Ansatz on the modeling residual by using a Haar MRA. We then showed that it was possible to compute the modeling residual on coarse scales with a fine scale computed solution without subgrid model as a reference, and then extrapolate the modeling residual to the computational scale. We presented a priori and a posteriori error estimates for the corrected and the non corrected solutions, both for the numerical and the modeling errors. We showed in numerical experiments for the hyperbolic model problem that by extrapolating from $2h$ and $4h$, where h is the computational scale, the sum of the numerical and modeling errors in the corrected solution typically corresponded to a non corrected solution on the scale $h/2$, and by extrapolating from $4h$ and $8h$ the corrected solution corresponded to a non corrected solution on the scale $h/4$. For the elliptic problem, extrapolating from $4h$ and $8h$ typically corresponded to a non corrected solution on the scale $h/2$.

It was further noted that the extrapolation procedure was more efficient when the corrective force was based on the computed solution, and not on the gradient of the computed solution. This is e.g. the case for the SGSRS in LES, and in a continuation of this work we will test these ideas in a LES setting.

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