Dynamic Computational Subgrid Modeling I

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Abstract

In this paper we propose and study a subgrid model for linear convection-diffusion-reaction problems with fractal rough coefficients. The subgrid model is based on extrapolation of a modeling residual from coarser scales using a computed solution on a finest scale 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 scale less than $h/4$.

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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 first paper in this series, and it is focused on modeling only, assuming the computational errors can be made neglible compared to the modeling errors by computing on a very fine computational mesh. In a continuation of this study [10] the model problem in two dimensions is considered, the balancing of numerical errors and modeling errors is discussed, and an adaptive algorithm is presented.

An outline of this paper is as follows: In Section 2 the linear convection-diffusion-reaction model problem is introduced and different approaches to the subgrid modeling problem is discussed. In Section 3 the basic features of *Multiresolution Analysis* (MRA) using the Haar basis is recalled, which is used to motivate an Ansatz on the form of the subgrid model, which is then used to extrapolate an approximation to the subgrid model. In Sections 6-8 simplified forms of the model problem with zero diffusion are studied, and it is shown that in these cases the solution inherits the fractal structure of the coefficients, and thus extrapolation is possible. In Section 9 the extension to non-zero diffusion is studied, and in Section 10 error estimates for the modeling errors are presented. The results of some numerical experiments with subgrid modeling are presented along the lines.

2 Problem formulation

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

$$Lu(x) \equiv -D(\epsilon(x)Du(x)) + \beta(x)Du(x) + \alpha(x)u(x) = f(x), \quad x \in I = (0,1), \quad (1)$$

together with suitable boundary conditions, where $\epsilon(x)$, $\beta(x)$ and $\alpha(x)$ are given coefficients depending on x, $f(x)$ is a given source, $D = \frac{d}{dx}$, and $u(x)$ is the solution. We assume that the coefficients ϵ, β and α are piecewise continuous, and we seek a solution $u(x)$ which is continuous on I with ϵDu continuous, and which satisfies (1) for all $x \in I$ which are not points of discontinuity of the coefficients. In the case $\epsilon = 0$, assuming that β does not vanish on I and $u(0) = 0$, the solution $u(x)$ is given by the formula

$$u(x) = \int_0^x \exp(A(y) - A(x)) \frac{f(y)}{\beta(y)} dy, \quad \text{for } x \in I, \tag{2}$$

where $A(x)$ is a primitive function of α/β (satisfying $DA = \alpha/\beta$, $A(0) = 0$). If also $\beta = 0$, then the solution is simply

$$u(x) = \frac{f(x)}{\alpha(x)}, \quad \forall x \in I,$$

assuming now that α does not vanish on I.

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 in a computation of a solution, and we denote the corresponding approximate solution by u_h. We denote by u_h the solution to the following simplified problem

$$L_h u_h(x) \equiv -D([\epsilon]^h(x) Du_h(x)) + [\beta]^h(x) Du_h(x) + [\alpha]^h(x) u_h(x) = [f]^h(x) \quad x \in I, \tag{3}$$

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 finer scales left out. The corresponding solution formula for u_h in the case $\epsilon = 0$, reads

$$u_h(x) = \int_0^x \exp(A_h(y) - A_h(x)) \frac{[f]^h(y)}{[\beta]^h(y)} dy, \quad \text{for } x \in I, \tag{4}$$

where A_h is a primitive function of $[\alpha]^h/[\beta]^h$ satisfying $A_h(0) = 0$, and $u_h(0) = 0$. We may think of u_h as an approximation of the exact solution u obtained by simplifying the model by simplifying the coefficients 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

$$L_h u = [f]^h + F_h(u), \tag{5}$$

where

$$F_h(u) = f - [f]^h - (L - L_h)u \tag{6}$$

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

$$(L_h + \tilde{L}_h)\tilde{u}_h = f, \tag{7}$$

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.

In this paper we propose methods for computing approximations of the modeling residual $F_h(u)$ using the idea of a dynamic model, in the case of the model problem (1). We show 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 $[vw]^h - [v]^h[w]^h \approx Ch^\mu$ is proposed. The two functions $C(x)$ and $\mu(x)$ are then estimated by extrapolation from computing approximations $F_H(u_h) \approx F_H(u)$ on two coarser scales H, where the solution to the simplified problem u_h is used as a substitute for the solution u to the exact problem.

3 Motivation of the Ansatz 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. 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].

3.1 The Haar MRA

In the case of the Haar basis in $L_2(I)$, with $I = [0, 1]$, the space V_0 is spanned by the scale function

$$\varphi(x) = \begin{cases} 1 & x \in I \\ 0 & x \notin I \end{cases}$$

and $V_j = \text{span}\{\varphi_{j,k}(x) = 2^{j/2}\varphi(2^j x - k)\}$. The orthogonal complement of V_j in V_{j+1} is W_j, spanned by the wavelets

$$\psi_{j,k} = 2^{j/2}\psi(2^j x - k), \quad \text{for } k = 0, 1, 2, ... < 2^j, j = 0, 1, 2, ...,$$

where the mother wavelet ψ is defined by

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

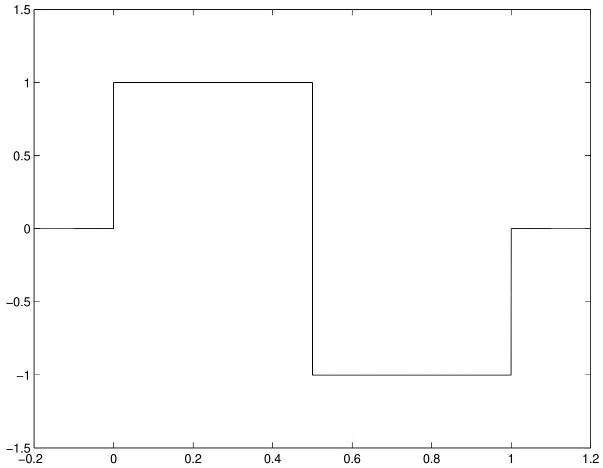

Figure 1: The "mother wavelet" $\psi(x)$.

Each $f \in L_2(I)$ has a unique decomposition

$$f = f_\varphi \varphi + \sum_{i,k} f_{i,k}\psi_{i,k} = f_\varphi + \sum_i f_i,$$

where the f_i represent the contributions on the different scales 2^{-i} corresponding to subdivisions S_i of I with mesh points $x_{i,k} = k2^{-i}$, $k = 0, 1, ..., 2^i$, and subintervals $I_{i,k} = (k2^{-i}, (k+1)2^{-i})$. The coefficients $f_{i,k}$ are given as the L_2-inner product of the function f and the corresponding Haar basis function:

$$f_{i,k} = \int_0^1 f(x)\psi_{i,k}(x)\ dx,$$

and $f_\varphi = \int_0^1 f(x)\ dx$.

3.2 The Ansatz

For $f \in L_2(I)$, where $I = [0, 1]$, we define $[f]^h$ to be the piecewise constant function on S_i, given by

$$[f]^h = f_\varphi + \sum_{j<i} f_j,$$

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 $f \in L_2(I)$ on the scale h as

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

where $x \in I$ and we extend f smoothly outside I. We denote by $\bar{f}^h$ the piecewise constant function on the scale h which coincides with f^h at the midpoints of the subintervals, and by this definition $\bar{f}^h$ is independent of the extension of f outside I. We shall use the following lemma:

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

Proof: We have

$$f = f_\varphi + \sum_j f_j \Rightarrow \bar{f}^h = \bar{f}^h_\varphi + \sum_j \bar{f}^h_j = \bar{f}^h_\varphi + \sum_{j<i} \bar{f}^h_j = f_\varphi + \sum_{j<i} f_j = [f]^h.$$

$\square$

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 then 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 $F_h(u)$ is given by

$$F_h(u) = f - [f]^h - (L - L_h)u = f - [f]^h - (\beta Du + \alpha u - [\beta]^h Du - [\alpha]^h u).$$

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

$$[F_h(u)]^h = [L_h u]^h - [Lu]^h = [\beta]^h [Du]^h - [\beta Du]^h + [\alpha]^h [u]^h - [\alpha u]^h.$$

We denote the projection $[F_h(u)]^h$ of $F_h(u)$ onto V_i by $\bar{F}_h(u)$. In the simplest situation above with $\beta = 0$, the full model is $\alpha u = f$, the approximate model is $[\alpha]^h u_h = [f]^h$, and the corresponding solutions are

$$u = f/\alpha, \quad u_h = [f]^h/[\alpha]^h.$$

The modeling residual $F_h(u)$ is given by

$$F_h(u) = f - [f]^h - (\alpha u - [\alpha]^h u),$$

and we have

$$\bar{F}_h(u) = [\alpha]^h [u]^h - [\alpha u]^h = [\alpha]^h [f/\alpha]^h - [f]^h.$$

We shall now seek to extrapolate $\bar{F}_h(u)$, and we are thus led to study in particular quantities of the form

$$E_h(v, w) = [vw]^h - [v]^h [w]^h, \tag{8}$$

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: $v, w \in L_2(I) \Rightarrow$ *For a given* x

$$E_h(v, w)(x) = \sum_{\substack{j \geq i \\ l \,:\, x \in I_{j,l}}} 2^j \; v_{j,l} w_{j,l}.$$

Proof: $v, w \in L_2(I) \Rightarrow v = \sum_j v_j, \; w = \sum_k w_k \;\Rightarrow\; vw = \sum_{j,k} v_j w_k,$

$$[v]^h = \sum_{j<i} v_j, \; [w]^h = \sum_{k<i} w_k \;\Rightarrow\; [v]^h [w]^h = \sum_{j,k \leq i} v_j w_k.$$

$$\text{Lemma 1} \;\Rightarrow\; [vw]^h = \overline{vw}^h = \overline{\sum_{j,k} v_j w_k}^h$$

$$= \sum_{j,k<i} v_j w_k + \sum_{j \geq i} v_j w_j = [v]^h [w]^h + \sum_{j \geq i} v_j w_j.$$

Finally we have for $x \in I_{j,l}$ that $v_j(x)w_j(x) = v_{j,l}\psi_{j,l}(x)\ w_{j,l}\psi_{j,l}(x) = 2^j\ v_{j,l}w_{j,l}$.

□

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

$$v_{j,k} = \alpha\ 2^{-j(1/2+\delta)} \text{ and } w_{j,k} = \beta\ 2^{-j(1/2+\gamma)}, \tag{9}$$

where $\alpha, \beta, \delta, \gamma$ are functions of x, which corresponds to v and w having a simple fractal structure ($v_{j+1}(x) = 2^{-\delta(x)}v_j(x)$ and $w_{j+1}(x) = 2^{-\gamma(x)}w_j(x)$). In that particular situation we find that $E_h(v,w)$ has a certain form:

Corollary: *If $v, w \in L_2(I)$ with $v_{j,k} = \alpha\ 2^{-j(1/2+\delta)}$ and $w_{j,k} = \beta\ 2^{-j(1/2+\gamma)}$, where $\alpha, \beta, \delta, \gamma$ are functions of x, then for $x \in I$*

$$E_h(v,w)(x) = C(x)h^{\mu(x)},$$

where $C = \frac{\alpha\beta}{1-2^{-(\delta+\gamma)}}$ and $\mu = \delta + \gamma$.

Proof: By Lemma 2 we have for $x \in I$ that

$$\begin{aligned} E_h(v,w)(x) &= \sum_{\substack{j \geq i \\ l\,:\,x \in I_{j,l}}} 2^j\ v_{j,l}w_{j,l} = \sum_{j \geq i} 2^j\ \alpha\ 2^{-j(1/2+\delta)}\beta\ 2^{-j(1/2+\gamma)} \\ &= \sum_{j \geq i} \alpha\beta\ 2^{-j(\delta+\gamma)} = \alpha\beta\ h^{\delta+\gamma} \sum_{j \geq i} 2^{-(j-i)(\delta+\gamma)} \\ &= \alpha\beta\ h^{\delta+\gamma} \sum_{j=0} 2^{-j(\delta+\gamma)} = \frac{\alpha\beta}{1-2^{-(\delta+\gamma)}} \cdot h^{\delta+\gamma} \end{aligned}$$

□

The asymptotic behaviour of the wavelet coefficients determine the micro scale structure of a function. 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 formulate the following **Ansatz**: For given $x \in I$,

$$E_h(v,w)(x) = C(x)h^{\mu(x)}, \tag{10}$$

where $C(x)$ and $\mu(x)$ are functions independent of the cut-off h. 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 $C(x)$ and $\mu(x)$ 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 type of "scale regularity" seems to be found in, for example, the so called *inertial range* of a turbulent flow.

4 Numerics & fractal coefficients

In the next sections we are going to investigate the indicated extrapolation procedure in the context of some numerical experiments. We use a Runge-Kutta method for the initial value problems in Section 8. For the boundary value problems in Section 9 we use a standard Finite Element Method (FEM) for the diffusion dominated problems, and a Streamline Diffusion (SD) method for the convection dominated problems (see Eriksson *et. al.* [6]). In all the experiments we are going to use a cut-off scale $h = 2^{-6}$, and we compute on a subdivision of I corresponding to a scale $h/64$. We use coefficients of the type

$$\alpha(x) = 1 + \sum_{\substack{j \geq 0 \\ l\,:\,x \in I_{j,l}}} \gamma\ 2^{-j(1/2+\delta)} \psi_{j,l}(x) \equiv 1 + \alpha', \quad x \in I, \tag{11}$$

which is on the form (9) with $\alpha_{j,l} = \gamma\ 2^{-j(1/2+\delta)}$ and $\alpha_\varphi = 1$.

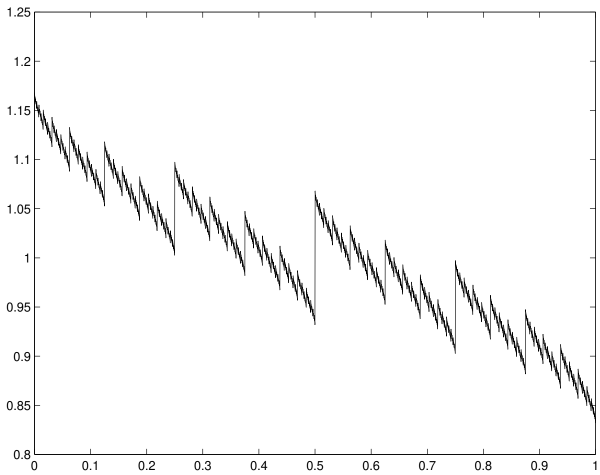

Figure 2: $\alpha(x)$ for $\gamma = 0.05$ and $\delta = 0.5$.

5 Gain-factors & mesh-factors

To measure the improvement of the corrected solution $\tilde{u}_h$ we introduce a "gain-factor" GF defined by

$$GF = \frac{\|[u - u_h]^h\|}{\|[u - \tilde{u}_h]^h\|}, \tag{12}$$

where the errors are projected onto the space V_i. We also introduce a "mesh-factor" MF_p, which measures the relative improvement in the corrected solution $\tilde{u}_h$ compared to a the improvement we get by decreasing h, defined by

$$MF_p = \frac{\|[u - u_{h/p}]^h\|}{\|[u - \tilde{u}_h]^h\|}. \tag{13}$$

The exact solution u is here approximated by a solution on the fine mesh corresponding to the scale $h/64$. We also define corresponding gain-factors and mesh-factors for the derivatives by

$$GF^D = \frac{\|[Du - Du_h]^h\|}{\|[Du - D\tilde{u}_h]^h\|}, \qquad MF_p^D = \frac{\|[Du - Du_{h/p}]^h\|}{\|[Du - D\tilde{u}_h]^h\|}. \tag{14}$$

6 The case $\epsilon(x) = \beta(x) = 0$

We first consider the problem $\alpha u = f$. We assume to start with that $f = 1$ and we consider the quantity

$$\bar{F}_h = [\alpha]^h [1/\alpha]^h - 1,$$

where α is a fractal function of the type (11). Using Lemma 2 and the fact that $\frac{1}{\alpha} = \frac{1}{1+\alpha'} \approx 1 - \alpha'$ if α' is small, that is if γ is small, we find that

$$\bar{F}_h(x) \approx \sum_{\substack{j \geq i \\ l \,:\, x \in I_{j,l}}} 2^j \, \alpha_{j,l}^2 \;=\; \gamma^2 \sum_{\substack{j \geq i \\ l \,:\, x \in I_{j,l}}} 2^{-2j\delta} \sim \gamma^2 2^{-2i\delta} \;=\; \gamma^2 h^{2\delta}, \tag{15}$$

which shows that $\bar{F}_h(x)$ is of the form $C(x)h^{\mu(x)}$ with $C(x) = \gamma^2$ and $\mu(x) = 2\delta$.

We now report the result of some numerical experiments using different values for γ and δ in (11) with γ small. We compare $\bar{F}_h$, which we here can compute directly from the data, to $\tilde{F}_h$, which is an extrapolated approximation of $\bar{F}_h$. In our first example we let $\gamma = 0.05$ and $\delta = 0.5$, and we set $H = 2h$ and $\hat{H} = 4h$. In Figure 3 we plot $\bar{F}_H$, $\bar{F}_{\hat{H}}$, $\bar{F}_h$ and $\tilde{F}_h$ for this particular case. We see that $\tilde{F}_h$ approximates $\bar{F}_h$ quite well. We have that the relative error

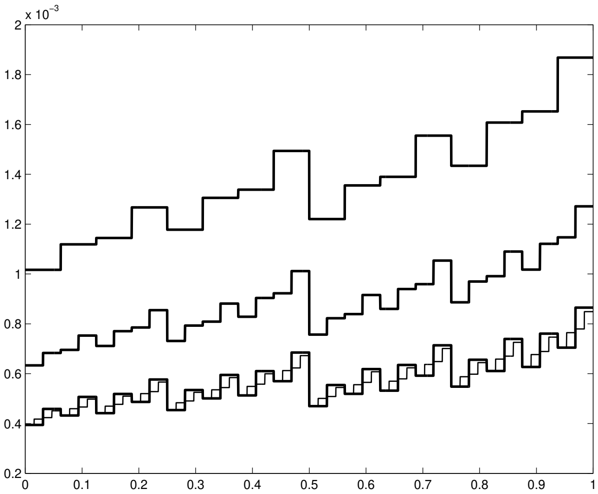

Figure 3: $\bar{F}_H$, $\bar{F}_{\hat{H}}$, $\bar{F}_h$ and $\tilde{F}_h$

γ	δ	$\|\bar{F}_h - \tilde{F}_h\| / \|\bar{F}_h\|$
0.06	0.3	$7.3 \cdot 10^{-2}$
	0.5	$3.9 \cdot 10^{-2}$
0.08	0.3	$1.0 \cdot 10^{-1}$
	0.5	$5.3 \cdot 10^{-2}$
0.1	0.3	$1.3 \cdot 10^{-1}$
	0.5	$6.9 \cdot 10^{-2}$

Table 1: $\|\bar{F}_h - \tilde{F}_h\| / \|\bar{F}_h\|$ for different γ and δ.

$\|\bar{F}_h - \tilde{F}_h\|/\|\bar{F}_h\| = 3.2 \cdot 10^{-2}$. In Table 1 we report the relative error for some different values of γ and δ. We notice that the extrapolation works better as γ decreases, which seems natural since then the approximation (15) is more accurate. It also works better for δ large, which seems natural since then the small scale features are less significant. We also try to extrapolate $\bar{F}_h$ in the case $f \neq 1$. By a similar calculation as in (15) for f being a function of the form (11), we get

$$\begin{aligned} \bar{F}_h(x) \quad &\approx \quad \sum_{\substack{j \geq i \\ l : x \in I_{j,l}}} 2^j(\alpha_{j,l}^2 - f_{j,l}\alpha_{j,l}) \quad = \quad \sum_{j \geq i} \gamma^2 2^{-2j\delta} - \sum_{j \geq i} \gamma\gamma_f 2^{-j(\delta+\delta_f)} \\ &\sim \quad \gamma^2 2^{-2i\delta}(1 - \frac{\gamma_f}{\gamma}2^{-i(\delta_f-\delta)}) \quad = \quad \gamma^2 h^{2\delta}(1 - \frac{\gamma_f}{\gamma}h^{\delta_f-\delta}), \end{aligned} \tag{16}$$

where γ_f and δ_f are the corresponding coefficients for f. Depending on δ and δ_f, we might again use the Ansatz that $\bar{F}_h(x) \approx C(x)h^{\mu(x)}$. In Figure 4 we plot the modeling residual for some different functions f. We see that the extrapolation works well for all source terms tested, except that in the middle plot, for $f(x) = x(1-x)$, there is something strange close to where $\bar{F}_h$ change sign. We note that the fact that $\bar{F}_H$ and $\bar{F}_{\hat{H}}$ live on different scales can cause problems near where $\bar{F}_{\hat{H}}$ and $\bar{F}_H$ change signs, because $\bar{F}_H$ can be on the "wrong side" of $\bar{F}_{\hat{H}}$. This makes the extrapolation go in the wrong direction, and it might ruin the quality of the extrapolation. To avoid this problem we could for example simply let $\tilde{F}_h$ be equal to $\bar{F}_H$ whenever $\bar{F}_H$ is on the "wrong side" of $\bar{F}_{\hat{H}}$. We employ this correction and plot for $f(x) = x(1-x)$ in Figure 5. By solving

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

we get an improved solution $\tilde{u}_h$ (Figure 6), where the error $u - \tilde{u}_h$ is proportional to the difference $F_h - \tilde{F}_h$, as $u - \tilde{u}_h = (F_h - \tilde{F}_h)/[\alpha]^h$. The error in the non corrected solution u_h is proportional to F_h, since $u - u_h = F_h/[\alpha]^h$. But here, remembering that we can use $\tilde{F}_h = \bar{F}_h$ (since $\bar{F}_h$ is directly computable from the data), the simple calculation

$$\tilde{u}_h = ([f]^h + \bar{F}_h)/[\alpha]^h = ([f]^h + [\alpha]^h[u]^h - [f]^h)/[\alpha]^h = [u]^h,$$

shows that here in fact $\tilde{u}_h = [u]^h$, so $\tilde{u}_h$ is the best solution we can obtain on the scale h. Next we are going to investigate the the simplest differential equation.

7 The case $\epsilon(x) = \alpha(x) = 0$

Now we consider the problem of finding a continuous function u such that

$$\beta Du = f \quad \text{in } I, \quad u(0) = 0,$$

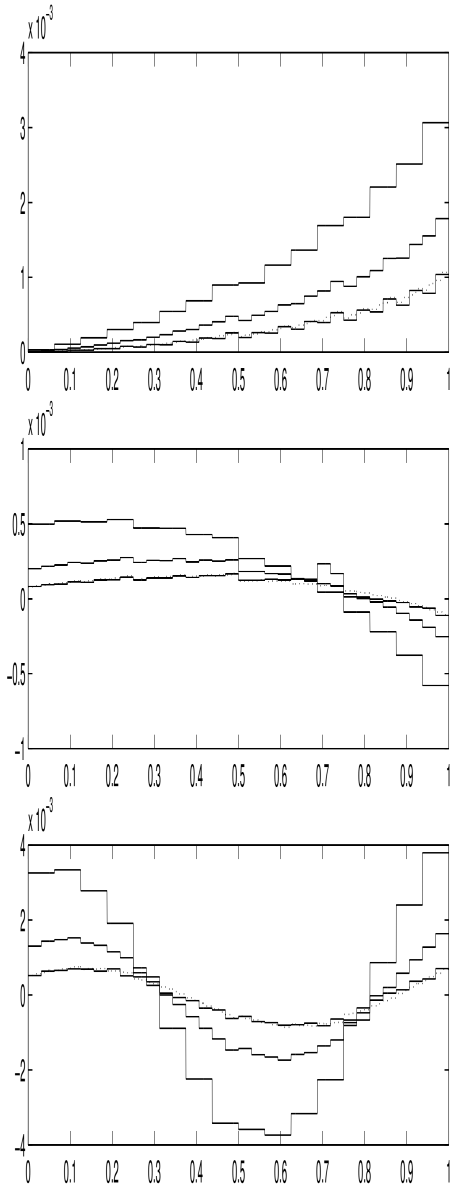

Figure 4: $f(x) = x^2$, $f(x) = x(1-x)$ and $f(x) = \sin(2\pi x)$.

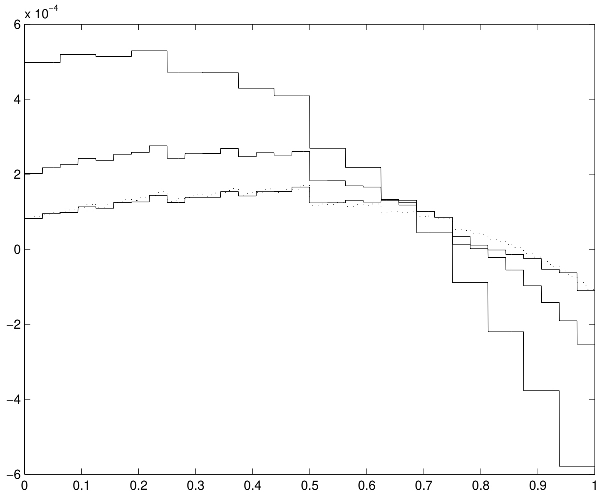

Figure 5: $f(x) = x(1-x)$

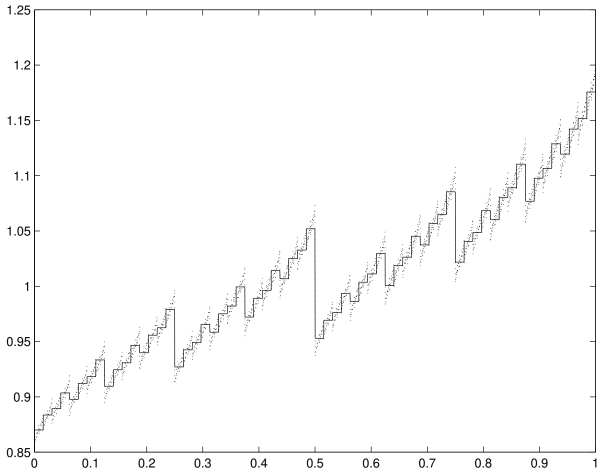

Figure 6: The corrected solution $\tilde{u}_h$.

where $Du = \frac{d}{dx}$. The solution is given by the formula

$$u(x) = \int_0^x \frac{f(y)}{\beta(y)}\, dy.$$

In this case the simplified problem takes the form

$$[\beta]^h Du_h = [f]^h \quad \text{in } I, \quad u_h(0) = 0,$$

with solution

$$u_h(x) = \int_0^x \frac{[f]^h(y)}{[\beta]^h(y)}\, dy.$$

The modeling residual is given by

$$F_h(u) = f^h - [f]^h - (\beta Du - [\beta]^h Du),$$

and

$$\bar{F}_h(u) = [\beta]^h[Du]^h - [\beta Du]^h = [\beta]^h[f/\beta]^h - [f]^h.$$

Again, $\bar{F}_h$ is computable from data. Assuming now f and β to be a fractal, extrapolation should be possible by the same reasoning as in the previous section. We then compute a corrected solution $\tilde{u}_h$ by solving

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

where $\tilde{F}_h$ is an extrapolated approximation of $\bar{F}_h$. Since we can compute $\bar{F}_h$ directly from data, and thereby let $\tilde{F}_h = \bar{F}_h$, again a simple calculation shows that $D\tilde{u}_h = [Du]^h$, but we are also interested in how good the solution $\tilde{u}_h$ is ($D\tilde{u}_h = [Du]^h \not\Rightarrow \tilde{u}_h = [u]^h$). In Table 2 we present the result of some numerical experiments for $f(x) = 1$. We extrapolate from $H = 2h$ and $\hat{H} = 4h$. We see in Table 2 that the corrected solution on h is better than a non corrected solution on $h/4$.

There is a difference in structure between the error in the solution and the error in the derivative. The error $u - u_h$ is here integrated, whereas the error $Du - Du_h$ has the same structure as in the previous section:

$$(u - u_h)(x) = \int_0^x F_h(y)/[\beta]^h(y)\ dy,$$
$$(Du - Du_h)(x) = F_h(x)/[\beta]^h(x).$$

γ	δ	GF	MF_2	MF_4
0.06	0.1	11	8.5	6.5
	0.3	2.6	1.9	1.2
0.08	0.1	13	10	7.6
	0.3	3.5	2.3	1.5
0.1	0.1	15	12	9.4
	0.3	4.3	2.9	1.9

Table 2: GF and mesh-factors for different γ and δ.

The error in the corrected solution depends on the difference $F_h - \tilde{F}_h$:

$$(u - \tilde{u}_h)(x) = \int_0^x (F_h(y) - \tilde{F}_h(y))/[\beta]^h(y)\ dy,$$
$$(Du - D\tilde{u}_h)(x) = (F_h(x) - \tilde{F}_h(x))/[\beta]^h(x).$$

The error in the solution at x is equal to the integrated error from 0 to x, whereas the error in the derivative at x only depends on the value of the relevant functions at x. This means that that the effect of adding the modeling residual in the L_2-norm might be "averaged out" if γ is not great enough. The same is true for δ being too great, since then again the small scale features are not sufficiently significant ($\tilde{F}_h$ is too small). This we can see i Table 2 where GF for the corrected solution $\tilde{u}_h$ is better for γ large and δ small.

In Table 3 we also present numerical experiments for the case when $f \neq 1$ ($\gamma = 0.08$). Here, "fractal" denotes a fractal function according to (11), with $\gamma = 0.04$ and $\delta = 0.4$. Also for $f \neq 1$ the corrected solutions on h are more

$f(x)$	δ	GF	MF_2	MF_4
$x(1-x)$	0.1	16	12	9.4
	0.3	4.5	2.8	1.7
fractal	0.1	14	12	8.8
	0.3	3.7	2.6	1.7

Table 3: GF and mesh-factors for different δ ($\gamma = 0.08$).

accurate than a non corrected solution on $h/4$.

8 Initial value problems

Now we focus on the initial value problem

$$\beta Du + \alpha u = f \text{ on } I,\ u(0) = 0.$$

In this case we have

$$\begin{aligned} \bar{F}_h(u) &= [\beta]^h[Du]^h - [\beta Du]^h + [\alpha]^h[u]^h - [\alpha u]^h, \\ &= [\beta]^h[f/\beta]^h - [f]^h + [\alpha]^h[u]^h - [\beta]^h[\alpha u/\beta]^h, \end{aligned}$$

where now the solution u appears, and thus $\bar{F}_h(u)$ is not directly computable from data. Of course, using the solution formula (2) above, we can eliminate u, but at any rate global effects enter.

8.1 The case $\alpha(x) = f(x) = 1$

First we consider the case when $\alpha(x) = f(x) = 1$. Then we have

$$\bar{F}_h(u) = \Big([\beta]^h[1/\beta]^h - 1\Big) + \Big([u]^h - [\beta]^h[u/\beta]^h\Big) = \bar{F}_h^1 + \bar{F}_h^2(u).$$

Here we cannot compute $\bar{F}_h(u)$ directly from data, since $\bar{F}_h(u)$ is a function of u. Instead we use u_h as a substitute for the exact solution u. Clearly we should be able to extrapolate $\bar{F}_h^1$ by the discussion in Section 6, and $\bar{F}_h^2(u)$ is also a quantity of the form (8). We are thus led to an Ansatz of the form

$$\bar{F}_h^1(x) \approx C_1(x)h^{\mu_1(x)}, \quad \bar{F}_h^2(u)(x) \approx C_2(x)h^{\mu_2(x)},$$

where the coefficients $C_i(x)$ and $\mu_i(x)$ are computed as follows: We can extrapolate $\bar{F}_h^1$ and $\bar{F}_h^2(u)$ separately by computing the corresponding quantities $\bar{F}_H^1$, $\bar{F}_{\hat{H}}^1$ and $\bar{F}_H^2(u_h)$, $\bar{F}_{\hat{H}}^2(u_h)$. We start by computing u_h, then we compute $\bar{F}_H^1$, $\bar{F}_{\hat{H}}^1$ and $\bar{F}_H^2(u_h)$, $\bar{F}_{\hat{H}}^2(u_h)$ from which we compute the coefficients $C_1(x)$, $C_2(x)$, $\mu_1(x)$ and $\mu_2(x)$. This gives $\tilde{F}_h$ by which we can compute $\tilde{u}_h$ from the equation $[\beta]^h D\tilde{u}_h + [\alpha]^h\tilde{u}_h = [f]^h + \tilde{F}_h$.

In this section $D\tilde{u}_h \neq [Du]^h$, and we are interested in the quality of $D\tilde{u}_h$. In Table 4, we present the result of some numerical experiments. Again, we find that a corrected derivative $D\tilde{u}_h$ on the scale h is a better solution than a non corrected derivative Du_h on the scale $h/4$. In Table 5 we present the result of similar numerical experiments for the corrected solution $\tilde{u}_h$. Here we see that a corrected solution $\tilde{u}_h$ on the scale h corresponds a non corrected solution on finer scale than $h/4$ when δ is small, and a scale h_f such that $h/4 < h_f < h/2$

γ	δ	GF^D	MF_2^D	MF_4^D
0.06	0.1	3.1	2.2	1.6
	0.3	3.6	2.1	1.2
0.08	0.1	2.4	1.7	1.2
	0.3	4.5	2.6	1.5
0.1	0.1	1.9	1.5	1.0
	0.3	4.3	2.5	1.4

Table 4: GF^D and mesh-factors for the derivative $D\tilde{u}_h$.

γ	δ	GF	MF_2	MF_4
0.06	0.1	2.2	1.7	1.2
	0.3	2.2	1.2	0.63
0.08	0.1	3.1	2.2	1.6
	0.3	2.9	1.6	0.91
0.1	0.1	3.6	2.8	1.9
	0.3	2.0	1.1	0.56

Table 5: GF and mesh-factors for $\tilde{u}_h$.

when δ is larger. The dependence on γ and δ seems natural, since the equation in this section is very similar to the one considered in Section 7 (basicly it is the same equation apart from the forcing term being changed from $f(x) = 1$ to the non linear $f(x) = 1 - u(x)$), and the discussion on how the effect of adding the modeling residual in the L_2-norm might be averaged out in some cases applies also here.

8.2 The case $\beta(x) = f(x) = 1$

We now consider the problem

$$Du + \alpha u = 1 \text{ on } I, \; u(0) = 0.$$

In this case we have

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

so by the previous discussion the extrapolation of $\bar{F}_h(u)$ should be possible if α and u have a "fractal" structure. However, the result of adding the extrapolated modeling residual is not that significant in this case, there is in fact no improvement in the corrected solution $\tilde{u}_h$, and the improvement in the corrected derivative $D\tilde{u}_h$ is not as great as in the previous cases. The lack of improvement of $\tilde{u}_h$ could be explained by the connection between α and u through the solution formula (2), where the primitive function of α is integrated to get u. In Table 6 we present the result of some numerical experiments for the derivative ($H = 2h$, $\hat{H} = 4h$). We see that in this problem the quality of the corrected derivative on the scale h

γ	δ	GF^D	MF_2^D	MF_4^D
0.3	0.1	5.0	2.2	0.85
	0.3	3.2	1.2	0.45
0.5	0.1	5.0	2.2	0.85
	0.3	3.2	1.2	0.44

Table 6: GF^D and mesh-factors for $D\tilde{u}_h$.

corresponds to the quality of a non corrected derivative on a scale h_f such that $h/4 < h_f < h/2$.

8.3 The case $f(x) = 1$

Now we consider the case when both α and β are fractal test functions (not necessary the same), and $f(x) = 1$. We have

$$\bar{F}_h(u) = \Big([\beta]^h[1/\beta]^h - 1\Big) + \Big([\alpha]^h[u]^h - [\beta]^h[\alpha u/\beta]^h\Big) = \bar{F}_h^1 + \bar{F}_h^2(u),$$

where $\bar{F}_h(u)$ is split into the two parts $\bar{F}_h^1$ and $\bar{F}_h^2(u)$. The first term $\bar{F}_h^1$ is of the type described in Section 6, and by (15) we have that extrapolation is possible. The second term $\bar{F}_h^2(u)$ should be possible to extrapolate if α, β and u have a "fractal" structure. So again we are led to an Ansatz of the form

$$\bar{F}_h^1(x) \approx C_1(x)h^{\mu_1(x)}, \quad \bar{F}_h^2(u)(x) \approx C_2(x)h^{\mu_2(x)}.$$

We present the result of some numerical experiments ($H = 2h$, $\hat{H} = 4h$) in Table 7, where we find that a corrected solution $\tilde{u}_h$ on the scale h corresponds a non corrected solution on a finer scale than $h/4$ when δ is small, and a scale h_f such that $h/4 < h_f < h/2$ when δ is larger. The quality of a corrected derivative on the scale h is better than a non corrected derivative on the scale $h/4$. In Figure 7 we plot $\bar{F}_H(u_h)$, $\bar{F}_{\hat{H}}(u_h)$, $\bar{F}_h(u)$ and $\tilde{F}_h$, where we see that the extrapolation works fine.

γ_α	δ_α	γ_β	δ_β	GF	MF_2	MF_4	GF^D	MF_2^D	MF_4^D
0.5	0.3	0.08	0.1	2.2	1.6	1.1	2.5	1.8	0.93
			0.3	2.8	1.8	0.97	5.3	2.9	1.7
		0.1	0.1	2.8	2.0	1.4	2.7	1.9	1.4
			0.3	3.0	1.9	1.0	4.4	2.6	1.5
	0.5	0.08	0.1	3.0	2.1	1.4	2.8	2.0	1.3
			0.3	1.9	1.1	0.48	6.8	3.6	1.9
		0.1	0.1	2.8	2.0	1.5	2.7	1.9	1.4
			0.3	2.2	1.3	0.61	5.8	3.2	1.8

Table 7: Gain-factors and mesh-factors for $\tilde{u}_h$ and $D\tilde{u}_h$.

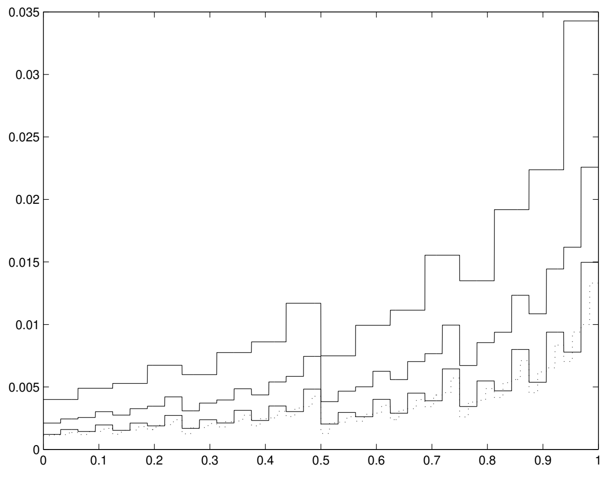

Figure 7: $\bar{F}_H(u_h)$, $\bar{F}_{\hat{H}}(u_h)$, $\bar{F}_h(u)$ and $\tilde{F}_h$

8.4 Different force terms

We conclude this section by presenting the result of some numerical experiments when $f \neq 1$. In Table 8 we present numerical results for $\gamma_\alpha = 0.5$, $\delta_\alpha = 0.3$, $\gamma_\beta = 0.1$, $\delta_\beta = 0.1$, and $H = 2h$, $\hat{H} = 4h$. We find that both the quality of the corrected solution and the corrected derivative on the scale h is better than the quality of their non corrected counterparts on the scale $h/4$. Here, "fractal" denotes a fractal test function according to (11), with $\gamma = 0.04$ and $\delta = 0.4$.

$f(x)$	GF	MF_2	MF_4	GF^D	MF_2^D	MF_4^D
x^2	2.0	1.5	1.1	1.9	1.5	1.0
$x(1-x)$	3.0	2.1	1.5	2.2	1.6	1.1
$\sin(2\pi x)$	2.8	2.0	1.4	2.7	2.1	1.4
fractal	2.6	1.9	1.2	2.0	1.4	1.1

Table 8: Gain-factors and mesh-factors for different source terms.

9 Convection-Diffusion-Reaction problems

We now consider the boundary value problem

$$-D(\epsilon Du) + \beta Du + \alpha u = f, \quad x \in I, \tag{17}$$

with a Dirichlet boundary condition $u(0) = 0$ at inflow, and a Neuman boundary condition $Du(1) = 0$ at outflow (assuming $\beta > 0$). Now we have an even more complex connection between data and solution. The simplified problem is now to find u_h such that

$$-D([\epsilon]^h Du_h) + [\beta]^h Du_h + [\alpha]^h u_h = [f]^h, \quad x \in I. \tag{18}$$

The solution to the exact problem u satisfies

$$-D([\epsilon]^h Du) + [\beta]^h Du + [\alpha]^h u = [f]^h + F_h(u), \quad x \in I, \tag{19}$$

where

$$F_h(u) = f - [f]^h - (-D(\epsilon Du) + \beta Du + \alpha u + D([\epsilon]^h Du) - [\beta]^h Du - [\alpha]^h u),$$

which gives

$$\begin{aligned}\bar{F}_h(u) &= \Big([D(\epsilon Du)]^h - [D([\epsilon]^h Du)]^h\Big) + \Big([\beta]^h [Du]^h - [\beta Du]^h\Big) \\ &+ \Big([\alpha]^h [u]^h - [\alpha u]^h\Big) = \bar{F}_h^1(u) + \bar{F}_h^2(u) + \bar{F}_h^3(u).\end{aligned}$$

As in the previous sections we make a separate Ansatz for $\bar{F}_h^1(u)$, $\bar{F}_h^2(u)$, and $\bar{F}_h^3(u)$. Using the Ansatz, we can extrapolate to obtain $\tilde{F}_h$, an approximation of $\bar{F}_h(u)$, which we use to compute the corrected solution $\tilde{u}_h$ from the equation

$$-D([\epsilon]^h D\tilde{u}_h) + [\beta]^h D\tilde{u}_h + [\alpha]^h \tilde{u}_h = [f]^h + \tilde{F}_h, \quad x \in I. \tag{20}$$

In this section we are also going to investigate the possibility to extrapolate a correction on the operator, and not only on the force.

9.1 The elliptic case with $\alpha = \beta = 0$

We now consider the case when $\beta = \alpha = 0$, that is the problem

$$-D(\epsilon Du) = f, \quad x \in I,$$

with boundary conditions $u(0) = Du(1) = 0$. Now u_h is defined to be the solution to the simplified problem

$$-D([\epsilon]^h Du_h) = [f]^h, \quad x \in I, \tag{21}$$

and the solution to the exact problem u satisfies

$$-D([\epsilon]^h Du) = [f]^h + F_h(u), \quad x \in I,$$

with the modeling residual

$$F_h(u) = f - [f]^h - (-D(\epsilon Du) - D([\epsilon]^h Du)),$$

and

$$\bar{F}_h(u) = [D(\epsilon Du)]^h - [D([\epsilon]^h Du)]^h.$$

In this case $\bar{F}_h(u)$ does not appear to be on the form (8), and consequently we cannot motivate the Ansatz on $\bar{F}_h(u)$ which we have used in the previous sections. We therefore turn to the following variational formulation of (9.1): Find $u \in V = \{v : v, Dv \in L_2(I), v(0) = 0\}$ such that

$$\int_0^1 \epsilon Du Dv \, dy = \int_0^1 fv \, dy, \quad \forall v \in V. \tag{22}$$

We have that u_h as defined in (21) satisfies

$$\int_0^1 [\epsilon]^h Du_h Dv \, dy = \int_0^1 [f]^h v \, dy, \quad \forall v \in V,$$

and the solution to the exact problem u satisfies

$$\int_0^1 [\epsilon]^h DuDv\ dy = \int_0^1 [f]^h v\ dy + \int_0^1 F_h^{\nabla}(u)Dv\ dy, \quad \forall v \in V,$$

where we have introduced a new modeling residual $F_h^{\nabla}(u)$, defined by

$$F_h^{\nabla}(u) = [\epsilon]^h Du - \epsilon Du,$$

and

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

which is of the form (8). We can therefore again use the Ansatz

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

and we expect extrapolation of $\bar{F}_h^{\nabla}(u)$ to be possible if ϵ and Du have a "fractal" structure. We denote the extrapolated approximation of $\bar{F}_h^{\nabla}(u)$ by $\tilde{F}_h^{\nabla}$ and we denote the corresponding corrected solution $\tilde{u}_h$, where $\tilde{u}_h$ is the solution to the problem

$$\int_0^1 [\epsilon]^h D\tilde{u}_h Dv\ dy = \int_0^1 [f]^h v\ dy + \int_0^1 \tilde{F}_h^{\nabla} Dv\ dy, \quad \forall v \in V.$$

In the case of Poisson's equation with an irregular diffusion coefficient and a smooth force, we might suspect that it is hard to model a correction of the diffusion operator by adding a corrective force, and we are therefore, in addition, going to model the SGS by an extrapolated correction on the operator. This we can do, for example, by defining the correction of the diffusion coefficient by

$$\epsilon_{corr}^h = -\tilde{F}_h^{\nabla}/Du_h,$$

and we denote the corresponding solution $\tilde{u}_h^{op}$, where $\tilde{u}_h^{op}$ is the solution to the problem

$$\int_0^1 ([\epsilon]^h + \epsilon_{corr}^h) D\tilde{u}_h^{op} Dv\ dy = \int_0^1 [f]^h v\ dy \quad \forall v \in V.$$

For the periodic version of this problem, with a smooth force, it is well known that the homogenized operator is obtained by using the harmonic average $[\epsilon]_{harm}^h = 1/[1/\epsilon]^h$ of ϵ, instead of the arithmetic average. We denote the corresponding solution $\tilde{u}_h^{harm}$. In Table 9 we present some numerical experiments for $f = 1$, where we compare different choices of H and $\hat{H}$. What we can see is that the

	$(H,\hat{H})$	GF	MF_2	GF^D	MF_2
$\tilde{u}_h$	$(2h,4h)$	1.1	0.79	1.1	0.73
	$(4h,8h)$	1.7	1.2	1.6	1.1
	$(8h,16h)$	3.1	2.2	2.0	1.3
$\tilde{u}_h^{op}$	$(2h,4h)$	1.1	0.79	1.1	0.73
	$(4h,8h)$	1.7	1.2	1.6	1.1
	$(8h,16h)$	3.1	2.2	2.0	1.3
$\tilde{u}_h^{harm}$		2.8	2.0	4.1	2.8

Table 9: $f = 1$ ($\gamma_\epsilon = 0.1$, $\delta_\epsilon = 0.3$).

quality of the corrected solution $\tilde{u}_h$ and the corrected derivative $D\tilde{u}_h$ improves by extrapolating further away from h, and for larger H and $\hat{H}$ the corrected solution on the scale h corresponds to a better solution than a non corrected solution on the scale $h/2$. We note that even though we loose information regarding the small scale structure of $\bar{F}_h^\nabla(u)$ when we are using large H and $\hat{H}$, we still get the best results for these cases. We may conclude that this depends on the fact that $\bar{F}_h^\nabla(u)$ is based on the derivative, and Du_h does not approximate Du well enough, and it is therefore hard to extrapolate $\bar{F}_h^\nabla(u)$ using scales close to h. On coarser scales Du_h should look more like Du, and we find that we have to use quite large H and $\hat{H}$ to get results as good as when we use the harmonic average. For the derivative we do not get as good results, even when we use very large H and $\hat{H}$. But we do not see any significant difference in these tests between extrapolating a correction on the force, or using the extrapolated modeling residual to model a correction on the operator.

When we study the same problems for an irregular force we find that using the harmonic average of ϵ is no longer optimal, and we further find that the extrapolated corrections give better results for an irregular force. In Table 10 we present results for an irregular force of the type (11) with $\gamma = 0.1$ and $\delta = 0.2$.

9.2 Constant diffusion coefficient ϵ

If the diffusion coefficient ϵ in the problem (17) is constant, then

$$\bar{F}_h(u) = \left([\beta]^h[Du]^h - [\beta Du]^h\right) + \left([\alpha]^h[u]^h - [\alpha u]^h\right). \tag{23}$$

$\bar{F}_h(u)$ consists of two parts, each of the type (8), which can be extrapolated if β, Du, and α, u respectively have a "fractal" structure. By choosing fractal test

	$(H,\hat{H})$	GF	MF_2	GF^D	MF_2
$\tilde{u}_h$	$(2h,4h)$	1.1	0.96	1.2	0.86
	$(4h,8h)$	3.2	2.8	2.5	1.8
	$(8h,16h)$	3.2	2.8	2.6	1.9
$\tilde{u}_h^{op}$	$(2h,4h)$	1.1	0.96	1.2	0.86
	$(4h,8h)$	3.2	2.8	2.5	1.8
	$(8h,16h)$	3.2	2.8	2.6	1.9
$\tilde{u}_h^{harm}$		0.86	0.74	1.2	0.89

Table 10: "Fractal" force ($\gamma = 0.1, \delta = 0.2$) and ($\gamma_\epsilon = 0.1,\ \delta_\epsilon = 0.3$).

functions α and β we expect extrapolation to work when ϵ is small, since then we have a convection dominated problem as in Section 8.

In Figure 8 we plot the two parts of $\bar{F}_h(u)$, and their extrapolated approximations for $\epsilon = 10^{-6}$ ($H = 2h$ and $\hat{H} = 4h$). We find that the extrapolation of the second part of $\bar{F}_h(u)$, based on the solution u, works fine. But in the case of the first part of $\bar{F}_h(u)$, which is based on the derivative Du, the extrapolation is not as good. This is the same problem as we met in the previous section, that is, Du_h does not approximate Du well enough. We can then either extrapolate from scales further from h, or we can avoid to base the extrapolation on the derivative at all by eliminating Du from (23) by using (17):

$$\begin{aligned}
\bar{F}_h(u) &= [\beta]^h[(f - \alpha u + \epsilon D^2 u)/\beta]^h - [f - \alpha u + \epsilon D^2 u]^h + [\alpha]^h[u]^h - [\alpha u]^h \\
&= [\beta]^h[f/\beta]^h - [f]^h + [\alpha]^h[u]^h - [\beta]^h[(\alpha u)/\beta]^h + [\beta]^h[\epsilon D^2 u/\beta]^h - [\epsilon D^2 u]^h \\
&= \bar{F}_h^1 + \bar{F}_h^2(u) + \bar{F}_h^3(u).
\end{aligned}$$

Here we recognise $\bar{F}_h^1$ and $\bar{F}_h^2(u)$ as being the same corrective forces as in Section 8, and they should be possible to extrapolate by the discussion there. This seems natural, since then if the diffusion is small the corrective force is close to the case when the diffusion is zero. Now in the case of ϵ being small, we approximate $\bar{F}_h(u) \approx \bar{F}_h^1 + \bar{F}_h^2(u)$. In Table 11 we present the result of numerical experiments for $\epsilon = 10^{-6}$ ($H = 2h$ and $\hat{H} = 4h$). We find that the quality of the corrected solution $\tilde{u}_h$ on the scale h is better than the quality of a non corrected solution on the scale $h/4$, and the same is true for the corrected derivative $D\tilde{u}_h$.

By using the extrapolated approximation of the modeling residual to correct the operator, we get similar results as when we used the modeling residual as a correction on the force, although the results are slightly worse when we correct the operator using the approximation $\bar{F}_h^3(u) \approx 0$.

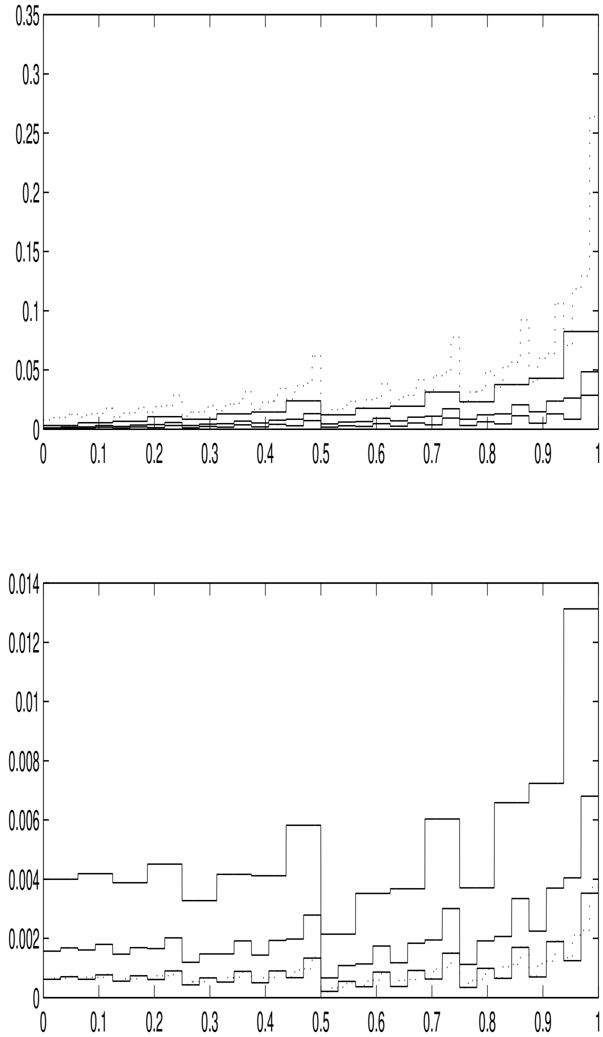

Figure 8: $\bar{F}_H(u_h)$, $\bar{F}_{\hat{H}}(u_h)$, $\bar{F}_h(u)$ and $\tilde{F}_h$ for $H = 2h$ and $\hat{H} = 4h$.

γ_α	δ_α	γ_β	δ_β	GF	MF_2	MF_4	GF^D	MF_2^D	MF_4^D
0.5	0.3	0.08	0.1	7.5	5.8	4.2	4.2	3.2	2.3
			0.3	3.4	2.3	1.4	6.3	3.7	2.3
		0.1	0.1	6.5	5.0	3.8	3.2	2.5	1.9
			0.3	3.8	2.5	1.6	5.5	4.3	2.0
	0.5	0.08	0.1	6.2	4.8	3.4	4.1	3.2	2.3
			0.3	3.1	1.9	1.2	6.9	3.8	2.2
		0.1	0.1	5.9	4.5	3.5	3.1	2.4	1.8
			0.3	3.5	2.2	1.3	5.7	3.4	1.9

Table 11: Gain-factors and mesh-factors for $\epsilon = 10^{-6}$.

9.3 The full problem

We consider the problem (17) where we now all coefficients ϵ, α and β are fractal. Following the discussion in Section 9.1 we consider the following variational formulation of (17): Find $u \in V = \{v : v, Dv \in L^2(I), v(0) = 0\}$ such that

$$\int_0^1 \epsilon DuDv\ dy + \int_0^1 \beta Duv\ dy \int_0^1 \alpha uv\ dy = \int_0^1 fv\ dy, \quad \forall v \in V. \tag{24}$$

The solution u_h to the simplified problem (18) satisfies

$$\int_0^1 [\epsilon]^h Du_h Dv\ dy + \int_0^1 [\beta]^h Du_h v\ dy \int_0^1 [\alpha]^h u_h v\ dy = \int_0^1 [f]^h v\ dy, \quad \forall v \in V,$$

and the exact solution u satisfies

$$\begin{aligned} &\int_0^1 [\epsilon]^h DuDv\ dy + \int_0^1 [\beta]^h Duv\ dy \int_0^1 [\alpha]^h uv\ dy \\ &= \int_0^1 [f]^h v\ dy + \int_0^1 F_h(u) v\ dy + \int_0^1 F_h^\nabla(u) Dv\ dy, \quad \forall v \in V, \end{aligned}$$

where the two modeling residuals $F_h(u)$ and $F_h^\nabla(u)$ are given by

$$\begin{aligned} F_h^\nabla(u) &= [\epsilon]^h Du - \epsilon Du, & (25) \\ F_h(u) &= [\beta]^h Du - \beta Du + [\alpha]^h u - \alpha u + f - [f]^h, & (26) \end{aligned}$$

and thus

$$\begin{aligned} \bar{F}_h^\nabla(u) &= [\epsilon]^h [Du]^h - [\epsilon Du]^h, \\ \bar{F}_h(u) &= \Big([\beta]^h [Du]^h - [\beta Du]^h\Big) + \Big([\alpha]^h [u]^h - [\alpha u]^h\Big) \equiv \bar{F}_h^1(u) + \bar{F}_h^2(u). \end{aligned}$$

We see that $\bar{F}_h^\nabla(u)$, $\bar{F}_h^1(u)$ and $\bar{F}_h^2(u)$ are of the form (8) and we expect extrapolation to be possible by using an Ansatz of the form

$$\bar{F}_h^1(u)(x) = C_1(x)h^{\mu_1(x)}, \quad \bar{F}_h^2(u)(x) = C_2(x)h^{\mu_2(x)}, \quad \bar{F}_h^\nabla(u)(x) = C_3(x)h^{\mu_3(x)}.$$

We obtain the improved solution $\tilde{u}_h \in V$ from the variational problem

$$\int_0^1 [\epsilon]^h D\tilde{u}_h Dv \ dy + \int_0^1 [\beta]^h D\tilde{u}_h v \ dy \int_0^1 [\alpha]^h \tilde{u}_h v \ dy$$
$$= \int_0^1 [f]^h v \ dy + \int_0^1 \tilde{F}_h v \ dy + \int_0^1 \tilde{F}_h^\nabla Dv \ dy, \quad \forall v \in V. \tag{27}$$

The relative importance of $\bar{F}_h^\nabla(u)$ compared to $\bar{F}_h(u)$ depends on the size of ϵ. If ϵ is small, then the problem is convection dominated and the results are similar to the results in Section 9.2 (by using (24) and neglecting the diffusion term). On the other hand, if the problem is diffusion dominated (ϵ large) the modeling residual $\bar{F}_h^\nabla(u)$ based on ϵ is the dominant one.

In Table 12 we present the result of numerical experiments for $\epsilon_\varphi = 10^{-3}$, where both $\bar{F}_h(u)$ and $\bar{F}_h^\nabla(u)$ contributes to the correction of $\tilde{u}_h$. As in Section 9.1 we cannot avoid using the derivative as a base for the extrapolation. To compensate for the lack of accuracy of Du_h as an approximation for Du, again we extrapolate further away from h. We use $H = 4h$, $\hat{H} = 8h$ and we let $f(x) = 1$.

δ_ϵ	δ_α	δ_β	GF	MF_2	GF^D	MF_2^D
0.3	0.1	0.1	2.6	1.4	1.6	0.90
		0.3	11	5.8	1.6	0.93
	0.3	0.1	2.1	1.3	1.6	0.87
		0.3	5.1	2.8	1.8	0.94

Table 12: Gain-factors and mesh-factors ($\gamma_\epsilon = 0.1$, $\gamma_\alpha = 0.3$, $\gamma_\beta = 0.1$).

In this case a corrected solution $\tilde{u}_h$ on the scale h is better than a non corrected solution on a scale $h/2$. For the derivative the improvement is not that great. We also investigate the case when we use the modeling residuals to correct the operator instead of the force, by solving the problem

$$\int_0^1 ([\epsilon]^h + \epsilon_h^{corr}) D\tilde{u}_h^{op} Dv \ dy + \int_0^1 (\beta_h + \beta_h^{corr}) D\tilde{u}_h^{op} v \ dy$$
$$+ \int_0^1 ([\alpha]^h + \alpha_h^{corr}) \tilde{u}_h^{op} v \ dy = \int_0^1 [f]^h v \ dy, \quad \forall v \in V.$$

By using the assumptions

$$\epsilon_h^{corr} = -\tilde{F}_h^{\nabla}/Du_h \quad \beta_h^{corr} = -\tilde{F}_h^1/Du_h \quad \alpha_h^{corr} = -\tilde{F}_h^2/u_h,$$

we find that the results are more or less the same as when we let the modeling residuals act as corrective forces. Finally, in Table 13 we present the numerical results for a fractal force f, with $\gamma = 0.05$ and $\delta = 0.5$, using the extrapolated modeling residual as a correction on the force.

δ_ϵ	δ_α	δ_β	GF	MF_2	GF^D	MF_2^D
0.3	0.1	0.1	2.5	1.4	1.6	0.90
		0.3	11	5.8	1.6	0.92
	0.3	0.1	2.1	1.3	1.6	0.88
		0.3	4.8	2.7	1.8	0.94

Table 13: Fractal force, with $\gamma_\epsilon = 0.1$, $\gamma_\alpha = 0.3$, and $\gamma_\beta = 0.1$.

10 Error analysis

We now turn to the issue of developing adaptive algorithms, including quantitative error control based on a posteriori error estimates, using the extrapolation technique described above. We recall that we formally have

$$u - u_h = L_h^{-1} F_h(u), \tag{28}$$

$$u - \tilde{u}_h = L_h^{-1}(F_h(u) - \tilde{F}_h), \tag{29}$$

which shows the connection between $F_h(u)$ and $u - u_h$, and $F_h(u) - \tilde{F}_h$ and $u - \tilde{u}_h$, via the inverse L_h^{-1} of L_h. In order for $u - \tilde{u}_h$ to be smaller than $u - u_h$, that is, for $\tilde{u}_h$ to be an improvement of u_h, we anticipate that $F_h(u) - \tilde{F}_h$ should be smaller than $F_h(u)$. This means that if $F_h(u)$ is small so that u_h already is a good approximation of u, then improvement should be difficult to achieve.

In the next sections we derive explicit estimates corresponding to the abstract relations (28)-(29), and we are first going to fix some notation for this section. The space $\mathcal{C}(I)$, consisting of continuous functions on I, is equipped with the uniform norm $\|\cdot\|_\infty$, defined by

$$\|u\|_\infty = \sup_{x \in I} |u(x)|.$$

The space $L_2(I)$, consisting of Lebesgue square integrable functions, is a Hilbert space with inner product and norm defined by

$$(v, w) = \int_I v(x)w(x)\ dx, \quad \|w\| = \sqrt{(w, w)}.$$

We are also going to use the ρ-weighted inner product $(\cdot, \cdot)_\rho$ and norm, defined by

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

for $v, w \in L_2(I)$, $\rho : I \to \mathbb{R}_+$, and ρ is locally integrable in I. We define $L_{2,\rho}$ to be the Hilbert space where the norm $\|\cdot\|_\rho$ is finite.

10.1 A priori error estimates for initial value problem

For the problem without diffusion, we give two error estimates in terms of the modeling residuals, corresponding to (28)-(29).

Theorem 1: *Assume that* $0 < [\alpha]^h \leq c_0$, $0 < c_1 \leq [\beta]^h$, *and* $\epsilon = 0$, *then*

$$\|u - u_h\|_\infty \leq C\|F_h(u)\|_\infty,$$

where $C = \frac{1}{c_1}\exp(c_0/c_1)$.

Proof: We know, by the discussion above, that

$$L_h(u - u_h) = F_h(u),$$

and using the solution formula (4), we get

$$(u - u_h)(x) = \int_0^x \exp(A_h(y) - A_h(x))\frac{F_h(u)(y)}{[\beta]^h(y)}dy,$$

where $A_h(x)$ is a primitive function of $[\alpha]^h/[\beta]^h$ (satisfying $DA_h = [\alpha]^h/[\beta]^h$, $A_h(0) = 0$). We take absolute values of both sides, then we estimate the right hand side:

$$|u - u_h|(x) \leq \frac{1}{c_1}\|F_h(u)\|_\infty \int_0^1 |\exp(A_h(y) - A_h(x))|dy.$$

By the mean value theorem for $x, y \in I$

$$|A_h(x) - A_h(y)| \leq \max_{t\in I}|DA_h(t)|\ |y - x| = \max_{t\in I}\frac{[\alpha]^h(t)}{[\beta]^h(t)}\ |y - x|,$$

from which the desired result follows.

$\square$

Theorem 2: *Assume that* $0 < [\alpha]^h \leq c_0$, $0 < c_1 \leq [\beta]^h$, *and* $\epsilon = 0$, *then*

$$\|u - \tilde{u}_h\|_\infty \leq C\|F_h(u) - \tilde{F}_h\|_\infty,$$

where $C = \frac{1}{c_1}\exp(c_0/c_1)$.

Proof: We recall that

$$L_h(u - \tilde{u}_h) = F_h(u) - \tilde{F}_h,$$

and as in the proof of Theorem 1, we have

$$(u - \tilde{u}_h)(x) = \int_0^x \exp(A_h(y) - A_h(x))\frac{F_h(u)(y) - \tilde{F}_h(y)}{[\beta]^h(y)}dy,$$

from which the desired estimate follows.

$\square$

Remark: *The errors in Theorem 1-2 are also bounded in the* L_2*-norm, since* $\|w\| = (\int_0^1 w^2(y)\ dy)^{1/2} \leq (\int_0^1 \|w\|_\infty^2\ dy)^{1/2} = \|w\|_\infty$. *We can also obtain estimates in terms of* L_2*-norms by using Cauchy-Schwarz inequality.*

10.2 A priori error estimates for convection-diffusion-reaction problem

For the problem with non zero diffusion, we do not have an explicit solution formula as we had for the problem in the previous section. Instead we are going to use an energy argument to obtain error estimates. In this section, Theorem 3 and 4 corresponds to (28)-(29) when $\epsilon \neq 0$.

Theorem 3: *Assume that* $0 < c_0 \leq [\beta]^h \leq C_0$ *and* $0 < c_1 \leq [\alpha]^h$, *then*

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

where $C = \frac{1}{c_0 \min(c_1,1)\min(1,\frac{c_1}{C_0},\frac{1}{C_0})}\exp(\frac{C_0}{c_0})$.

Proof: First we subtract (18) from (19), where we set $e = u - u_h$. Then we multiply both sides with e and integrate from 0 to $x_{i,k}$. By using partial integration and rewriting eDe as $\frac{1}{2}De^2$, we get:

$$2\int_0^{x_{i,k}} [\epsilon]^h (De)^2\ dy + \int_0^{x_{i,k}} [\beta]^h De^2\ dy + 2\int_0^{x_{i,k}} [\alpha]^h e^2\ dy$$
$$= 2\int_0^{x_{i,k}} F_h(u)e\ dy + 2\int_0^{x_{i,k}} F_h^{\nabla}(u)De\ dy,$$

where $F_h^{\nabla}(u)$ and $F_h(u)$ are defined by (25) and (26). Since $[\beta]^h$ is constant on each interval $I_{i,l}$ we have

$$\int_0^{x_{i,k}} [\beta]^h De^2\ dy = \sum_{l=1}^{k-1}\int_{I_{i,l}} [\beta]^h De^2\ dy = [\beta]^h(x_{i,k}^-)e^2(x_{i,k}) - \sum_{l=1}^{k-1} e^2(x_{i,l})|[\beta]^h|_l,$$

where $|[\beta]^h|_l = [\beta]^h(x_{i,l}^+) - [\beta]^h(x_{i,l}^-)$ is the jump in $[\beta]^h$ at $x_{i,l}$. This gives

$$2\int_0^{x_{i,k}} [\epsilon]^h (De)^2\ dy + 2\int_0^{x_{i,k}} [\alpha]^h e^2\ dy + [\beta]^h(x_{i,k}^-)e^2(x_{i,k})$$
$$= 2\int_0^{x_{i,k}} F_h(u)e\ dy + 2\int_0^{x_{i,k}} F_h^{\nabla}(u)De\ dy + \sum_{l=1}^{k-1} e^2(x_{i,l})|[\beta]|_l.$$

Now we can split the first integral in the right hand side by using Cauchy-Schwarz inequality, and the inequality $2ab \le a^2 + b^2$ $(a, b \in \mathbb{R})$:

$$2\int_0^{x_{i,k}} F_h(u)e\ dy \le 2(\int_0^{x_{i,k}} \frac{F_h^2(u)}{[\alpha]^h}\ dy)^{1/2}(\int_0^{x_{i,k}} [\alpha]^h e^2\ dy)^{1/2}$$
$$\le \int_0^{x_{i,k}} \frac{F_h^2(u)}{[\alpha]^h}\ dy + \int_0^{x_{i,k}} [\alpha]^h e^2\ dy.$$

Then we move the second of these new integrals to the left hand side. By the same operations on the second integral we get:

$$\int_0^{x_{i,k}} [\epsilon]^h (De)^2\ dy + \int_0^{x_{i,k}} [\alpha]^h e^2\ dy + [\beta]^h(x_{i,k}^-)e^2(x_{i,k})$$
$$= \int_0^{x_{i,k}} \frac{F_h^2(u)}{[\alpha]^h}\ dy + \int_0^{x_{i,k}} \frac{(F_h^{\nabla}(u))^2}{[\epsilon]^h}\ dy + \sum_{l=1}^{k-1} e^2(x_{i,l})|[\beta]^h|_l.$$

We divide the equation by $[\beta]^h(x_{i,k}^-)$ and use that $0 < c_0 \leq [\beta]^h$. By then using Grönwall's lemma we get

$$\frac{1}{[\beta]^h(x_{i,k}^-)}\int_0^{x_{i,k}}[\epsilon]^h(De)^2\ dy + \frac{1}{[\beta]^h(x_{i,k}^-)}\int_0^{x_{i,k}}[\alpha]^h e^2\ dy + e^2(x_{i,k})$$
$$\leq \frac{1}{c_0}(\int_0^{x_{i,k}}\frac{F_h^2(u)}{[\alpha]^h}\ dy + \int_0^{x_{i,k}}\frac{(F_h^\nabla)^2(u)}{[\epsilon]^h}\ dy)\exp\left(\frac{1}{c_0}\sum_{l=1}^{k-1}|[\beta]^h|_l\right).$$

This is true for all $x_{i,k} \in I$, in particular it is true for $x_{i,k} = x_{i,2^i} = 1$. If we then use the given bounds on $[\alpha]^h$ and $[\beta]^h$ we get

$$\frac{1}{C_0}\int_0^1[\epsilon]^h(De)^2\ dy + \frac{1}{C_0}\int_0^1 c_1 e^2\ dy + e^2(1)$$
$$\leq \frac{1}{c_0}(\int_0^1\frac{F_h^2(u)}{c_1}\ dy + \int_0^1\frac{(F_h^\nabla(u)}{[\epsilon]^h}\ dy)\exp\left(\frac{1}{c_0}\sum_{l=1}^{2^i-1}|[\beta]^h|_l\right).$$

But now we observe that

$$\sum_{l=1}^{2^i-1}|[\beta]^h|_l = [\beta]^h(1),$$

from which the desired estimate follows.

$\square$

Theorem 4: *Assume that* $0 < c_0 \leq [\beta]^h \leq C_0$ *and* $0 < c_1 \leq [\alpha]^h$, *then*

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

where $C = \frac{1}{c_0\min(c_1,1)\min(1,\frac{c_1}{C_0},\frac{1}{C_0})}\exp(\frac{C_0}{c_0})$.

Proof: If we subtract (20) from (18) and set $e = u - \tilde{u}_h$, then multiply both sides by e and integrate from 0 to $x_{i,k}$, we get

$$2\int_0^{x_{i,k}}[\epsilon]^h(De)^2\ dy + \int_0^{x_{i,k}}[\beta]^h De^2\ dy + 2\int_0^{x_{i,k}}[\alpha]^h e^2\ dy$$
$$= 2\int_0^{x_{i,k}}(F_h(u) - \tilde{F}_h)e\ dy + 2\int_0^{x_{i,k}}(F_h^\nabla(u) - \tilde{F}_h^\nabla)De\ dy.$$

Then by following the proof of Theorem 3, the desired estimate follows.

□

10.3 A posteriori error estimates

To derive a posteriori error estimates we consider the following dual problem for φ related to the problem (17):

$$L^*\varphi = -D(\epsilon D\varphi) - D(\beta\varphi) + \alpha\varphi = \Psi, \quad x \in I, \tag{30}$$

with $\varphi(1) = D\varphi(0) = 0$. We obtain strong stability estimates for φ in terms of Ψ by first multiplying (30) by φ and integrate from 0 to $x_{i,k}$, and then use partial integration to get

$$2\int_0^{x_{i,k}} \epsilon(D\varphi)^2\, dy + \int_0^{x_{i,k}} \beta D\varphi^2\, dy + 2\int_0^{x_{i,k}} \alpha\varphi^2\, dy = 2\int_0^{x_{i,k}} \Psi\varphi\, dy.$$

Then we mimic the proof of Theorem 3, to obtain the following estimate for the solution to the dual problem (30):

$$\|\varphi\|^2 + \|D\varphi\|_\epsilon^2 + \varphi^2(1) \le C\|\Psi\|^2,$$

where C is the same constant as in Theorem 3. By taking the L_2-inner product of e and Ψ, where we let e denote either the error $u - u_h$ or the error $u - \tilde{u}_h$, we get

$$(e, \Psi) = (e, L^*\varphi) = (Le, \varphi) = (R, \varphi),$$

where R denotes the residual $R = R(u_h) = f - Lu_h$ or the residual $R = R(\tilde{u}_h) = f - L\tilde{u}_h$ respectively. But we have that

$$\begin{aligned} R(u_h) &= f - Lu_h = f - (L_h u_h + Lu_h - L_h u_h) = f - ([f]^h + Lu_h - L_h u_h) \\ &= f - [f]^h - (L - L_h)u_h = F_h(u_h), \\ R(\tilde{u}_h) &= f - L\tilde{u}_h = f - (L_h\tilde{u}_h + L\tilde{u}_h - L_h\tilde{u}_h) = f - ([f]^h + \tilde{F}_h + L\tilde{u}_h - L_h\tilde{u}_h) \\ &= f - [f]^h - (L - L_h)\tilde{u}_h - \tilde{F}_h = F_h(\tilde{u}_h) - \tilde{F}_h, \end{aligned}$$

which shows a natural connection between the modeling residual and the total residual, since we have neglected the numerical errors in this paper.

Now if we let $\Psi = \chi_{[x-h/2, x+h/2]}$ (where χ_I denotes the characteristic function for the interval I) we get a local error representation for e^h at x. And if we want to get a bound on $\|[e]^h\|$, we choose $\Psi = [e]^h$ and remember that $[e]^h$ can be identified with the L_2-projection of e onto V_i, and therefore $(e, [e]^h) = ([e]^h, [e]^h) = \|[e]^h\|^2$. So we get that

$$\|[e]^h\|^2 = (R, \varphi),$$

where φ solves the problem (30) with $\Psi = [e]^h$. We sum up the above discussion in a final theorem:

Theorem 5: *We have the following a posteriori error estimates:*

$$\begin{aligned} \|[u - u_h]^h\|^2 &= (F_h(u_h), \varphi), \\ \|[u - \tilde{u}_h]^h\|^2 &= (F_h(\tilde{u}_h) - \tilde{F}_h, \varphi), \end{aligned}$$

where φ is the solution to the problem (30) with $\Psi = [u]^h - [u_h]^h$ and $\Psi = [u]^h - [\tilde{u}_h]^h$ respectively. We have also the following local error representations:

$$\begin{aligned} (u - u_h)^h(x) &= (F_h(u_h), \varphi), \\ (u - \tilde{u}_h)^h(x) &= (F_h(\tilde{u}_h) - \tilde{F}_h, \varphi), \end{aligned}$$

where φ now is the solution to the problem (30) with $\Psi = \chi_{[x-h/2, x+h/2]}$.

11 Conclusions

In this paper we have investigated the performance of a subgrid model based on extrapolation of a modeling residual, in the case of a one dimensional convection-diffusion-reaction problem with rough coefficients with features on a range of scales. Assuming a certain "scale regularity" of the coefficients, and by using a Haar Multiresolution Analysis, we motivated an Ansatz on the modeling residual of the form Ch^μ, where h is the mesh size and $C = C(x)$ and $\mu = \mu(x)$ coefficients to be determined. We then showed that it was possible to determine the subgrid model on coarse scales with a fine scale computed solution without subgrid model as a reference, and then extrapolate the subgrid model to the computational scale. We presented a priori and a posteriori modeling error estimates for the corrected and the non corrected solutions. We showed in numerical experiments that by extrapolating from $2h$ and $4h$, where h is the computational scale, the modeling errors in the corrected solution were typically less than in a non corrected solution on the scale $h/4$. For Poisson's equation, extrapolating from $4h$ and $8h$ typically was better than a non corrected solution on the scale $h/2$. We did not note any difference in the results when we used the modeling residual as a correction on the force, or when we used it as a correction on the operator. It was further noted that the extrapolation procedure was more effective when the extrapolation was based on the computed solution u_h itself, and not on the derivative Du_h.

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