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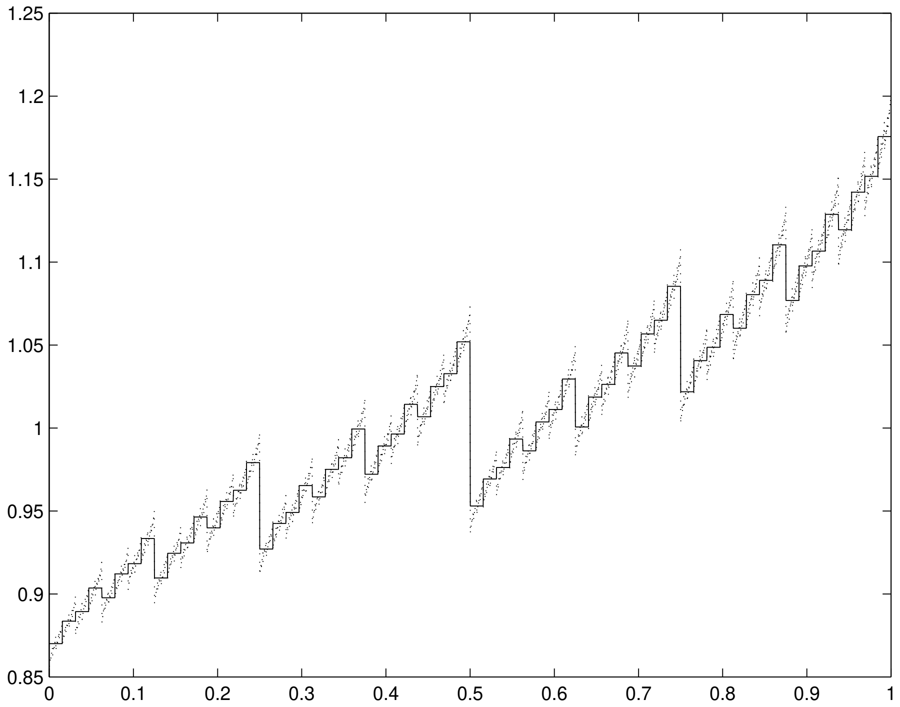

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On Dynamic Computational Subgrid Modeling

Johan Hoffman and Claes Johnson

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Abstract

In this paper we study a subgrid model based on extrapolation of a corrective force, in the case of a linear convection-diffusion problem $Lu = f$ in one dimension. The running average u^h of the exact solution u on the finest computational scale h satisfies an equation $L_h u^h = [f]^h + F_h$, where L_h is the operator used in the computation on the scale h, $[f]^h$ is the approximation of f on the scale h, and F_h acts as a corrective force, which needs to be modeled. The subgrid modeling problem is to compute approximations of F_h without using finer scales than h. In this study we model F_h by extrapolation from coarser scales than h where the corrective force is directly computed with the finest scale h as reference. We show in experiments that a corrected solution with subgrid model on scale h corresponds to a non-corrected solution on 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 involving the so called *Reynolds' stress* $\tau_{ij} = \overline{u}_i\overline{u}_j - \overline{u_i u_j}$, where $\overline{u}_i$ represents a local average of u_i and $u = (u_i)$ is the velocity, which are additional stresses representing the subgrid model. 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 of of 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 (for a survey of different approaches see Gatski *et al.*[2]).

The simplest subgrid model of turbulence is the *Smagorinsky model*, where the Reynolds' stress is modelled as a viscous stress $\tau_{ij} = \nu\epsilon_{ij}(u)$, related to a certain *turbulent viscosity* ν of the form $\nu = Ch^\mu|\epsilon(u)|$, 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 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* (first introduced by Germano *et al.*[3]). In this case one seeks to find a subgrid model for each set of data by comparing approximate solutions with different resolvable scales with the hope of being able to extrapolate from the finest resolvable scale 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 based on computed solutions on a coarse scale using a finer scale computed solution as reference, and then finally extrapolating the so obtained model to the finest computational scale. 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 very 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 on averages 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. On the other hand, 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 Johnson[4]). Thus, today we have techniques available that allow the desired balance of computational and modeling errors. In this paper we focus on modeling only, assuming the computational errors can be made neglible compared to the modeling errors without unduly raising the computational cost. We will return to the full problem including balancing of computational and modeling errors in a subsequent note.

An outline of this note is as follows: In Section 2 we introduce the linear convection-diffusion-reaction model problem. In Section 3 we recall basic features of multi scale resolution using the Haar basis. In Section 4-6 we study simplified forms of the model problem with zero diffusion and show that in these cases the solution inherits the fractal structure of the coefficients, and thus extrapolation is possible. In Section 7 we study the extension to non-zero diffusion, and in Section 8 we present error estimates. We present the results of some numerical experiments with subgrid modeling along the lines presented.

In a continuation of this study we will extend the ideas to several dimensions, including implementation of an adaptive algorithm based on error estimates of the same form as the ones presented in Section 8.

2 A model problem

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

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

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 $I = [0, 1]$ with ϵDu continuous, and which satisfy (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 $(0, 1)$ 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

$$u(x) = \frac{f(x)}{\alpha(x)}, \tag{3}$$

assuming now that α does not vanish on I.

We first assume that $\epsilon = 0$ and we assume that the coefficients 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 by u_h. We assume for now that u_h is the solution of the following simplified problem

$$L_h u_h(x) \equiv [\beta]^h(x)Du_h(x) + [\alpha]^h(x)u_h(x) = [f]^h(x) \quad \text{for } x \in I, \tag{4}$$

together with the boundary condition $u_h(0) = 0$, where $[\beta]^h$, $[\alpha]^h$, and $[f]^h$ are approximations of the corresponding functions on the scale h, with the finer scales left out. The corresponding solution formula for u_h is

$$u_h(x) = \int_0^x \exp(A_h(y) - A_h(x)) \frac{[f]^h(y)}{[\beta]^h(y)} dy \quad \text{for } x \in I, \tag{5}$$

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 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.

We consider now 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. We return below to the problem of evaluating the quality of u_h as an approximation of u using a posteriori error estimates. It is then natural to compare u_h to a running average u^h of the exact solution on the scale h instead of u itself, defined by

$$u^h(x) = h^{-1} \int_{x-h/2}^{x+h/2} u(y)\, dy, \tag{6}$$

where $x \in I$ and we extend u smoothly outside I. Taking the running average of the equation (1), we obtain

$$(\beta D u)^h + (\alpha u)^h = f^h, \tag{7}$$

which we may write in the form

$$L_h u^h = [f]^h + F_h, \tag{8}$$

where

$$F_h = F_h(u) = -(\beta D u)^h - (\alpha u)^h + [\beta]^h D u^h + [\alpha]^h u^h + f^h - [f]^h \tag{9}$$

acts as a corrective force. We conclude that the running average u^h satisfies the same equation as u_h, with a modification of the forcing term from $[f]^h$ to $[f]^h + F_h$. If the modification F_h is large and accordingly the difference $u^h - u_h$ is large, then the averaging of the coefficients had a noticeable effect, and subgrid modeling is needed.

We now seek a procedure for computing an approximation of the corrective force $F_h(u)$, in the case this quantity is not small. We shall seek such a procedure based on extrapolation from computing approximations $F_H(u_h)$ of the correction $F_H(u)$ on coarser scales H, where we thus use the computed solution u_h as a substitute for the exact solution u.

We now turn to a particular set-up convenient for analysis.

3 Multiresolution analysis & the Haar basis

We introduce the Haar basis in $L_2(I)$, where we now restrict attention to $I = (0, 1)$, defined by the set of functions (*wavelets*)

$$\phi_{i,k} = 2^{i/2}\phi(2^i x - k), \quad \text{for } k = 0, 1, 2, ... < 2^i, i = 0, 1, 2, ..., \tag{10}$$

where (the *mother wavelet*)

$$\phi(x) = \begin{cases} 1 & 0 < x < 1/2 \\ -1 & 1/2 < x < 1 \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

Further we have (the *scale function*) $\phi_{-1} = 1$ on I and 0 elsewhere. The wavelets together with the scale function are an orthonormal basis in $L_2(I)$ (see Daubechies[1] or Louis *et al.*[5]), and each $f \in L_2(I)$ has a unique decomposition

$$f = \sum_{i,k} f_{i,k}\phi_{i,k} = \sum_i f_i, \quad f_i = \sum_k f_{i,k}\phi_{i,k}, \tag{12}$$

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:

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

For $f \in L_2(I)$ we define $[f]^h$ with $h = 2^{-i}$ to be the piecewise constant function on S_i, given by

$$[f]^h = \sum_{j \le i} f_j. \tag{13}$$

Further, we recall the definition of the *running average* $f^h(x)$ of a function $f(x) \in L_2(I)$ on the scale h as

$$f^h(x) = 2^i \int_{x-h/2}^{x+h/2} f(y)\, dy. \tag{14}$$

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. The mappings $L_2 \ni f \to \bar{f}^h \in W_h^{(0)}$ and $L_2 \ni f \to [f]^h \in W_h^{(0)}$ are both linear, where

$$W_h^{(q)} = \{v : v|_{I_{i,k}} \in \mathcal{P}^q(I_{i,k}), k = 0, 1, ..., 2^i - 1\}. \tag{15}$$

We also have that $[[f]^H g]^h = [f]^H [g]^h$ and $[[f]^h g]^H = [fg]^H$, whenever $H \geq h$ ($H = 2^{-j}$, $h = 2^{-i}$ with $j < i$). We shall use the following lemma:

Lemma 1: $[f]^h = \bar{f}^h$.

Proof: For $h = 2^{-i}$ we have

$$f = \sum_{j=-1}^{\infty} f_j \Rightarrow \bar{f}^h = \sum_{j=-1}^{\infty} \bar{f}_j^h = \sum_{j \leq i} \bar{f}_j^h = \sum_{j \leq i} f_j = [f]^h.$$

$\square$

Remark: *$[f]^h$ can also be identified with the L_2-projection of f into $W_h^{(0)}$.*

The asymptotic behaviour of the expansion coefficients $f_{i,k}$ determine the micro scale structure of f. Below we will in particular consider the case when

$$f_{i,k} = C(x) 2^{-i(1/2+\mu(x))}, \tag{16}$$

for a given $x \in I_{i,k}$, corresponding to f having a simple local fractal structure. More precisely, if (16) holds, then f is locally Hölder continuous of order $\mu(x)$ at x, cf. Daubechies[1]:

Theorem 1: *A locally integrable function f is in the Hölder space $C^{0,s}(\mathbb{R})$ if and only if there exists $C < \infty$ so that:*

$$|f_{i,k}| \leq C \; 2^{-i(1/2+s)} \quad \forall i, k.$$

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

$$u = f/\alpha, \quad u_h = [f]^h/[\alpha]^h. \tag{17}$$

The correction F_h is given by

$$F_h = [\alpha]^h u^h - (\alpha u)^h - [f]^h + f^h, \tag{18}$$

and we have

$$\bar{F}_h = [\alpha]^h [u]^h - [\alpha u]^h = [\alpha]^h [f/\alpha]^h - [f]^h, \tag{19}$$

where $\bar{F}_h$ is the piecewise constant function on the scale h that coincides with F_h at the midpoints of the intervals. We observe that $\bar{F}_h$ is independent of the extension of the functions outside the interval I. We shall now seek to extrapolate $\bar{F}_h$, and we are thus led to study in particular quantities of the form

$$E_h(v,w) = [vw]^h - [v]^h[w]^h, \tag{20}$$

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

Lemma 2: *For a given x*

$$E_h(v,w)(x) = \sum_{\substack{j\,>\,i \\ l\,:\,x\,\in\,I_{j,l}}} 2^j\, v_{j,l}w_{j,l}. \tag{21}$$

Proof: By definition $v = \sum_j v_j,\ w = \sum_k w_k \ \Rightarrow\ vw = \sum_{j,k} v_j w_k.$

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

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

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

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

□

We shall below consider situations where for a given $x \in I$,

$$E_h = E_h(v,w)(x) \approx C(x)h^{\mu(x)}, \tag{22}$$

where $C(x)$ and $\mu(x)$ are functions independent of the cut-off h. If E_h has this form, then extrapolation of E_h will be possible from knowledge of E_H and $E_{\hat{H}}$ with $h < H < \hat{H}$, from which the coefficients $C(x)$ and $\mu(x)$ may be determined. This requires the coefficients $v_{j,l}$, $w_{j,l}$ to have a related fractal structure. A basic case when this holds is obtained choosing $w = v$, with v fractal.

Typically, we will assume that the coefficients have a related fractal structure. We then expect the solution u to inherit this structure to some degree, and we expect that extrapolation of the corrective force $\bar{F}_h$ will be possible. We now consider this question in more detail starting with the case $\beta = 0$.

4 The case $\epsilon = \beta = 0$

We assume to start with that $f = 1$ and we consider the quantity

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

with

$$\alpha(x) = 1 + \sum_{j,l} \gamma\, 2^{-j(1/2+\delta)} \phi_{j,l}(x) \equiv 1 + \alpha', \quad x \in I, \tag{23}$$

which is on the form (16) with $\alpha_{j,l} = \gamma\, 2^{-j(1/2+\delta)}$ and $\alpha_{-1} = 1$.

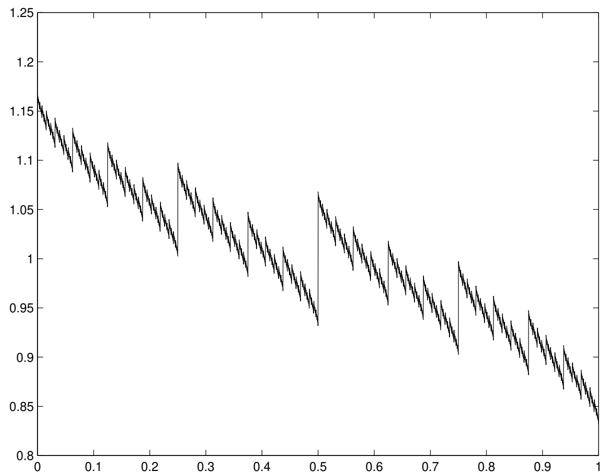

Figure 1: $\alpha(x)$ for $\gamma = 0.05$ and $\delta = 0.5$.

By Theorem 1, the function $\alpha(x)$ is Hölder continuous of order δ. 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

$$\bar{F}_h(x) \approx \sum_{\substack{j\,>\,i \\ l\,:\,x\,\in\,I_{j,l}}} 2^j\, \alpha_{j,l}^2 \;=\; \gamma^2 \sum_{\substack{j\,>\,i \\ l\,:\,x\,\in\,I_{j,l}}} 2^{-2j\delta} \sim \gamma^2 2^{-2i\delta} \;=\; \gamma^2 h^{2\delta}, \tag{24}$$

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 note that in this case $\bar{F}_h(x)$ is independent of x.

We now report the result of some numerical experiments using different values for γ and δ in (23) 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 $\delta = 0.5$, we set the cut off $i = 6$, and we take $H = 2h$ and $\hat{H} = 4h$. In Figure 2 we plot $\bar{F}_H(u_h)$, $\bar{F}_{\hat{H}}(u_h)$, $\bar{F}_h(u)$ and $\tilde{F}_h$ for this particular case. We see that $\tilde{F}_h$ approximates $\bar{F}_h$ well, except the fact that they live on different scales. We have $\|\bar{F}_h - \tilde{F}_h\| = 1.6 \cdot 10^{-4}$ (where $\|\cdot\|$ is the L_2-norm). In

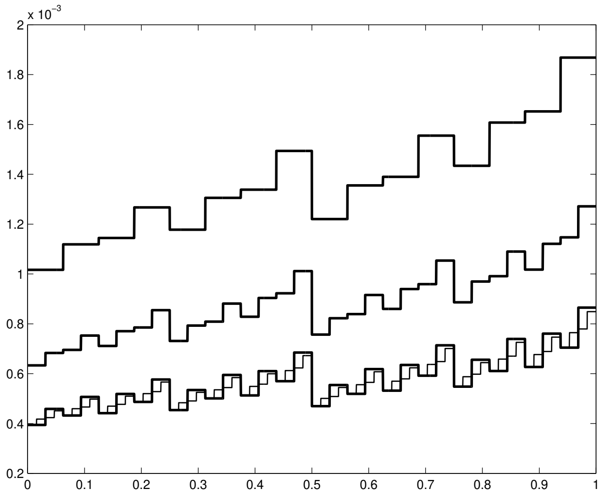

Figure 2: $\bar{F}_H$, $\bar{F}_{\hat{H}}$, $\bar{F}_h$ and $\tilde{F}_h$

γ	δ	$\|\bar{F}_h - \tilde{F}_h\|$
0.06	0.1	$3.5{\cdot}10^{-4}$
	0.3	$2.2{\cdot}10^{-5}$
	0.5	$1.4{\cdot}10^{-6}$
0.08	0.1	$3.8{\cdot}10^{-2}$
	0.3	$2.2{\cdot}10^{-3}$
	0.5	$1.6{\cdot}10^{-4}$
0.1	0.1	$5.7{\cdot}10^{-1}$
	0.3	$2.2{\cdot}10^{-2}$
	0.5	$1.5{\cdot}10^{-3}$

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

Table 1 we have computed the 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 (24) is more accurate. It also works better for δ large, which seems natural since then the small scale features is less significant. We also try to extrapolate $\bar{F}_h$ in the case $f \neq 1$. By a similar calculation as in (24) for f being a Hölder continuous function of the form (23), we get

$$\begin{aligned} \bar{F}_h(x) &\approx \sum_{\substack{j>i \\ l:x\in I_{j,l}}} 2^j\,(\alpha_{j,l}^2 - f_{j,l}\alpha_{j,l}) = \sum_{\substack{j>i \\ l:x\in I_{j,l}}} \gamma^2 2^{-2j\delta} - \sum_{\substack{j>i \\ l:x\in I_{j,l}}} \gamma\gamma_f 2^{-j(\delta+\delta_f)} \\ &\sim \gamma^2 2^{-2i\delta}(1-\frac{\gamma_f}{\gamma}2^{-i(\delta_f-\delta)}) = \gamma^2 h^{2\delta}(1-\frac{\gamma_f}{\gamma}h^{\delta_f-\delta}), \end{aligned} \tag{25}$$

where γ_f and δ_f are the corresponding coefficients for $f(x)$. We see that if δ and δ_f are sufficiently close, we might again use the Ansatz that $\bar{F}_h(x)$ is of the form $C(x)h^{\mu(x)}$. In Figure 3 we have plotted the corrective forces 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. Especially when we have non monotone source functions. Because then also u_h is not monotone, which can make $\bar{F}_{\hat{H}}$ and $\bar{F}_H$ change sign in the interval. This causes problems because near where the functions change sign $\bar{F}_H$ can be on the "wrong side" of $\bar{F}_{\hat{H}}$. This makes the extrapolation go in the wrong direction, and in some cases it damages, or totally ruins, 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 4.

As mentioned above, for the simple problem in this section we do not really need to extrapolate $\bar{F}_h$, since it is directly computable from the data. By solving

$$[\alpha]^h \tilde{u}_h = [f]^h + \tilde{F}_h, \tag{26}$$

we get an improved solution $\tilde{u}_h$ (Figure 5), where the error $u^h - \tilde{u}_h$ is proportional to the difference $F_h - \tilde{F}_h$, as $u^h - \tilde{u}_h = (F_h - \tilde{F}_h)/[\alpha]^h$. The error in the non corrected solution u_h is proportional to F_h, as $u^h - u_h = F_h/[\alpha]^h$. But, remembering that we can use $\tilde{F}_h = \bar{F}_h$, the simple calculation

$$\tilde{u}_h = ([f]^h + \bar{F}_h)/[\alpha]^h = ([f]^h + [\alpha]^h[u]^h - [f]^h)/[\alpha]^h = [u]^h, \tag{27}$$

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.

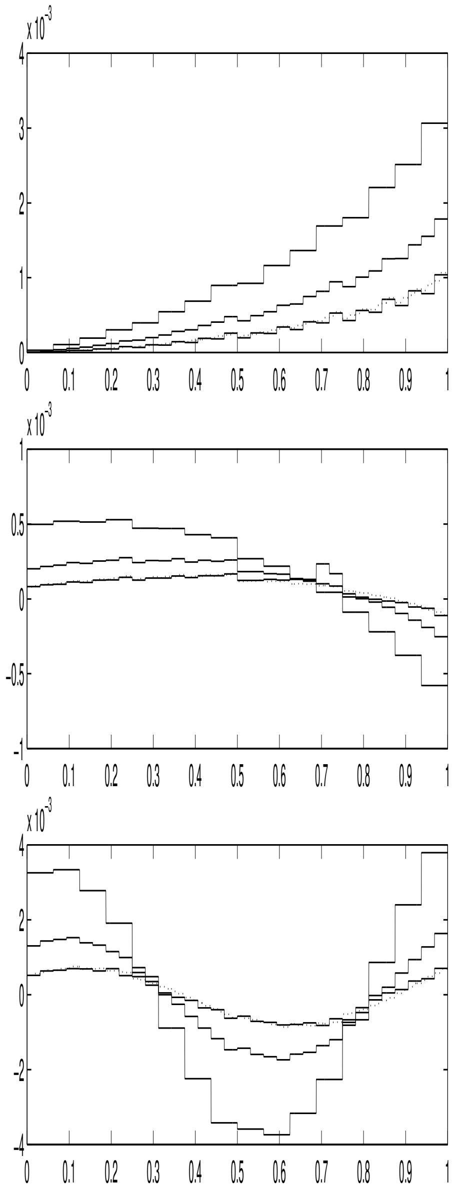

Figure 3: $f(x) = x^2$, $f(x) = x(1-x)$ and $f(x) = \sin(2\pi x)$.

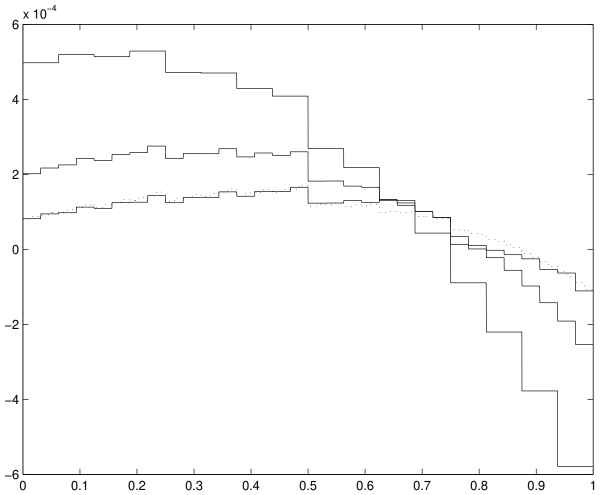

Figure 4: $f(x) = x(1-x)$

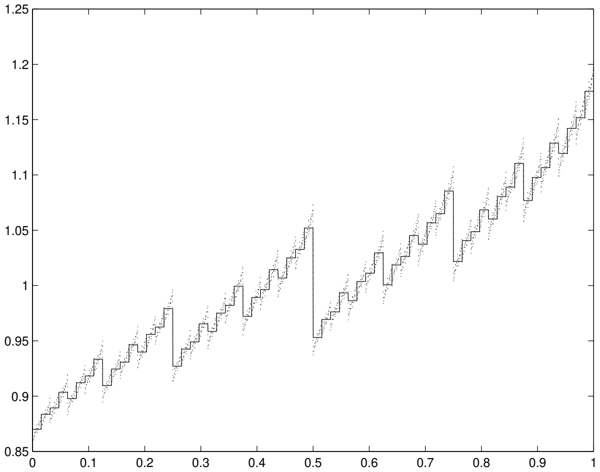

Figure 5: The corrected solution $\tilde{u}_h$.

5 The case $\epsilon = \alpha = 0$

Now we consider the problem of finding $u \in \mathcal{C}(I)$ such that

$$\beta D u = f \quad \text{in } I, \quad u(0) = 0, \tag{28}$$

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

$$u(x) = \int_0^x \frac{f(y)}{\beta(y)}\, dy. \tag{29}$$

In this case the simplified problem takes the form

$$[\beta]^h D u_h = [f]^h \quad \text{in } I, \quad u_h(0) = 0, \tag{30}$$

with solution

$$u_h(x) = \int_0^x \frac{[f]^h(y)}{[\beta]^h(y)}\, dy. \tag{31}$$

We have

$$F_h = f^h - [f]^h + [\beta]^h D u^h - (\beta D u)^h, \tag{32}$$

and thus

$$\bar{F}_h = [\beta]^h \overline{Du^h} - [\beta D u]^h = [\beta]^h [Du]^h - [\beta D u]^h = [\beta]^h [f/\beta]^h - [f], \tag{33}$$

where we used the fact that $Du^h = (Du)^h$. That is, $\bar{F}_h$ again only contains data. Now we let β be a locally Hölder continuous fractal test function of the same form as in the previous section:

$$\beta(x) = 1 + \sum_{j,l=0} \gamma\, 2^{-j(1/2+\delta)} \phi_{j,l}(x). \tag{34}$$

Extrapolation should be possible by the same reasoning as in the previous section (by the approximations (24) and (25)), and we compute the corrected solution $\tilde{u}_h$ by solving

$$[\beta]^h D\tilde{u}_h = [f]^h + \tilde{F}_h. \tag{35}$$

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 ($D\tilde{u}_h = [Du]^h \nRightarrow \tilde{u}_h = [u]^h$). To be able to measure the improvement of the corrected solution $\tilde{u}_h$ we introduce a "gain-factor" GF defined by

$$GF = \frac{\|[u]^h - [u_h]^h\|}{\|[u]^h - [\tilde{u}_h]^h\|}. \tag{36}$$

We compare this GF to a "mesh-factor" MF_p, which measures the improvement we get by refining h, defined by

$$MF_p = \frac{\|[u]^h - [u_h]^h\|}{\|[u]^h - [u_{h/p}]^h\|}, \tag{37}$$

where $\|\cdot\|$ denotes the L_2-norm. In Table 2 we present the result of some numerical experiments for $f(x) = 1$. We do our computations on the cut off level $i = 6$, and we extrapolate from $H = 2h$ and $\hat{H} = 4h$. To model the exact solution u, we have used a solution on a fine mesh 2^{-12}. We see in Table 2 that the corrected solution

γ	δ	GF	MF_2	MF_4
0.06	0.1	11	1.3	1.7
	0.3	2.6	1.4	2.2
0.08	0.1	13	1.3	1.7
	0.3	3.5	1.5	2.3
0.1	0.1	15	1.3	1.6
	0.3	4.3	1.5	2.3

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

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 $u^h - u_h$ is here integrated, whereas the error $Du^h - Du_h$ has the same structure as in the previous section:

$$(u^h - u_h)(x) = \int_0^x F_h(y)/[\beta]^h(y)\, dy, \tag{38}$$

$$(Du^h - Du_h)(x) = F_h(x)/[\beta]^h(x). \tag{39}$$

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

$$(u^h - \tilde{u}_h)(x) = \int_0^x (F_h(y) - \tilde{F}_h(y))/[\beta]^h(y)\, dy, \tag{40}$$

$$(Du^h - D\tilde{u}_h)(x) = (F_h(x) - \tilde{F}_h(x))/[\beta]^h(x). \tag{41}$$

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 the corrective force 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.

$f(x)$	δ	GF	MF_2	MF_4
$x(1-x)$	0.1	16	1.3	1.7
	0.3	4.5	1.6	2.6
$fractal$	0.1	14	1.2	1.6
	0.3	3.7	1.4	2.2

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

In Table 3 we also present numerical experiments for the case when $f \neq 1$ ($\gamma = 0.08$). Here, "$fractal$" denotes a Hölder continuous function according to (34), with $\gamma = 0.04$ and $\delta = 0.4$. Also for $f \neq 1$ the corrected solutions on h are better than the non corrected solutions on $h/4$.

6 The case $\epsilon = 0$

Now we focus on the initial value problem

$$\beta Du + \alpha u = f \text{ on } I,\ u(0) = 0. \tag{42}$$

In this case we have

$$\bar{F}_h = [\beta]^h[f/\beta]^h - [f]^h + [\alpha]^h[u]^h - [\beta]^h[\alpha u/\beta]^h, \tag{43}$$

where now the solution u appears, and thus $\bar{F}_h$ 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.

6.1 $\alpha(x) = f(x) = 1$

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

$$\bar{F}_h = \Big([\beta]^h[1/\beta]^h - 1\Big) + \Big([u]^h - [\beta]^h[u/\beta]^h\Big) = \bar{F}_h^1 + \bar{F}_h^2. \tag{44}$$

Here we cannot compute $\bar{F}_h$ directly from data, since $\bar{F}_h = \bar{F}_h(u)$. Instead we use u_h as a substitute for the exact solution u. Clearly we should be able to extrapolate the first part of F_h by the discussion in Section 4. The second part is a quantity of the form (20), and by the assumption (22) it should be possible to extrapolate if β and u have a related asymptotic structure. So each of the two parts of $\bar{F}_h$ should be possible to model as on the form $C(x)h^{\mu(x)}$, and thus we are led to an Ansatz of the form

$$\bar{F}_h^1(x) \approx C_1(x)h^{\mu_1(x)}, \quad \bar{F}_h^2(x) \approx C_2(x)h^{\mu_2(x)}. \tag{45}$$

We can extrapolate $\bar{F}_h^1$ and $\bar{F}_h^2$ separately by computing corresponding $\bar{F}_H^1(u_h)$, $\bar{F}_{\hat{H}}^1(u_h)$ and $\bar{F}_H^2(u_h)$, $\bar{F}_{\hat{H}}^2(u_h)$. We start by computing u_h, then we compute $\bar{F}_H^1(u_h)$, $\bar{F}_{\hat{H}}^1(u_h)$ and $\bar{F}_H^2(u_h)$, $\bar{F}_{\hat{H}}^2(u_h)$ from which we compute the non scale depending $C_1(x)$, $C_2(x)$, $\mu_1(x)$ 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, where we again use a solution on a fine mesh 2^{-12} as a substitute for the exact solution. Instead of comparing to the exact derivative Du we compare to $[Du]^h$, since both Du_h and $D\tilde{u}_h$ mainly live on the scale h. Again, we find that a corrected derivative $D\tilde{u}_h$ on

γ	δ	GF	MF_2	MF_4
0.06	0.1	3.1	1.4	2.0
	0.3	3.6	1.7	2.9
0.08	0.1	2.4	1.4	2.0
	0.3	4.5	1.7	3.0
0.1	0.1	1.9	1.3	1.9
	0.3	4.3	1.7	3.0

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

the scale h is a better solution than a non corrected derivative Du_h on the scale $h/4$, where the gain-factor and the mesh-factors here are defined as

$$GF = \frac{\|[Du]^h - [Du_h]^h\|}{\|[Du]^h - [D\tilde{u}_h]^h\|}, \qquad MF_p = \frac{\|[Du]^h - [Du_h]^h\|}{\|[Du]^h - [Du_{h/p}]^h\|}. \tag{46}$$

In Table 5 we present the result of similar numerical experiments for the corrected solution $\tilde{u}_h$, where we now again take the definitions (36) and (37) for the gain-factor and the mesh-factors. Here we see that a corrected solution $\tilde{u}_h$ on the

γ	δ	GF	MF_2	MF_4
0.06	0.1	2.2	1.3	1.9
	0.3	2.2	1.9	3.5
0.08	0.1	3.1	1.4	2.0
	0.3	2.9	1.8	3.2
0.1	0.1	3.6	1.3	1.9
	0.3	2.0	1.9	3.6

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

scale h corresponds a non corrected solution on finer scale than $h/4$ when δ is small, and a scale h_f such that $h/4 < h_f < h/2$ 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 5 (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 the corrective force in the L_2-norm might be averaged out in some cases applies also here.

6.2 $\beta(x) = f(x) = 1$

Now we are considering the problem

$$Du + \alpha u = 1 \text{ on } I,\ u(0) = 0. \tag{47}$$

In this case we have

$$\bar{F}_h = [\alpha]^h[u]^h - [\alpha u]^h, \tag{48}$$

so by the previous discussion the extrapolation of $\bar{F}_h$ should be possible if α and u have a related asymptotic structure. However, here the result of adding the extrapolated force is not that significant, 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 motivated by the complex connection between α and u through the solution formula (2). In Table 6 we present the result of some numerical experiments for the derivative ($i = 6$, $H = 2h$, $\hat{H} = 4h$). For this problem we see that the quality of the corrected deriva-

γ	δ	GF	MF_2	MF_4
0.3	0.1	5.0	2.3	5.9
	0.3	3.2	2.6	7.1
0.5	0.1	5.0	2.3	5.9
	0.3	3.2	2.6	7.3

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

tive on the scale h corresponds to the quality of a non corrected derivative on a scale h_f such that $h/4 < h_f < h/2$, where we have used the definition (46) for GF and MF_p.

6.3 $f(x) = 1$

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

$$\bar{F}_h = \Big([\beta]^h[1/\beta]^h - 1\Big) + \Big([\alpha]^h[u]^h - [\beta]^h[\alpha u/\beta]^h\Big) = \bar{F}_h^1 + \bar{F}_h^2, \tag{49}$$

where $\bar{F}_h$ is split into the two parts $\bar{F}_h^1$ and $\bar{F}_h^2$. The first term $\bar{F}_h^1$ is of the type described in Section 4, and by (24) we have that extrapolation is possible. The second term $\bar{F}_h^2$ should be possible to extrapolate if α, β and u have a related asymptotic structure. So again we are led to an Ansatz of the form

$$\bar{F}_h^1(x) \approx C_1(x)h^{\mu_1(x)}, \quad \bar{F}_h^2(x) \approx C_2(x)h^{\mu_2(x)}. \tag{50}$$

We present the result of some numerical experiments ($i = 6$, $H = 2h$, $\hat{H} = 4h$) 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 (GF and MF_p are defined by (36) and (37)). In

γ_α	δ_α	γ_β	δ_β	GF	MF_2	MF_4
0.5	0.3	0.08	0.1	2.2	1.4	2.0
			0.3	2.8	1.6	2.9
		0.1	0.1	2.8	1.4	2.0
			0.3	3.0	1.6	2.9
	0.5	0.08	0.1	3.0	1.4	2.1
			0.3	1.9	1.7	4.0
		0.1	0.1	2.8	1.4	1.9
			0.3	2.2	1.7	3.6

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

Figure 6 we plot $\bar{F}_H(u_h)$, $\bar{F}_{\hat{H}}(u_h)$, $\bar{F}_h$ and $\tilde{F}_h$, where we see that the extrapolation works fine. In Table 8 we present the result of similar numerical experiments for

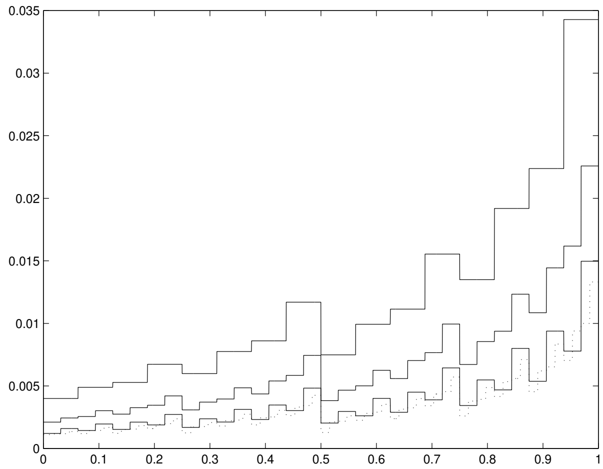

Figure 6: $\bar{F}_H(u_h)$, $\bar{F}_{\hat{H}}(u_h)$, $\bar{F}_h$ and $\tilde{F}_h$

the derivative, where we find that the quality of a corrected derivative on the scale h is better than a non corrected derivative on the scale $h/4$, where GF and MF_p are defined by (46).

γ_α	δ_α	γ_β	δ_β	GF	MF_2	MF_4
0.5	0.3	0.08	0.1	2.5	1.4	2.7
			0.3	5.3	1.8	3.1
		0.1	0.1	2.7	1.4	1.9
			0.3	4.4	1.7	3.0
	0.5	0.08	0.1	2.8	1.4	2.1
			0.3	6.8	1.9	3.5
		0.1	0.1	2.7	1.4	1.9
			0.3	5.8	1.8	3.2

Table 8: GF and mesh-factors for $D\tilde{u}_h$.

6.4 Different source terms

We conclude this section by presenting the result of some numerical experiments where $f \neq 1$. In our experiments we have $\gamma_\alpha = 0.5$, $\delta_\alpha = 0.3$, $\gamma_\beta = 0.1$, $\delta_\beta = 0.1$, the cut off $i = 6$ 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 Hölder continuous function according to (34), with $\gamma = 0.04$ and $\delta = 0.4$. GF and MF_p are defined as in (36) and (37) for $\tilde{u}_h$, and as in (46) for the derivative $D\tilde{u}_h$.

$f(x)$	GF	MF_2	MF_4
$\tilde{u}_h$			
x^2	2.0	1.3	1.9
$x(1-x)$	3.0	1.4	2.0
$\sin(2\pi x)$	2.8	1.4	2.0
$fractal$	2.6	1.4	2.1
$D\tilde{u}_h$			
x^2	1.9	1.3	1.9
$x(1-x)$	2.2	1.4	2.0
$\sin(2\pi x)$	2.7	1.3	1.9
$fractal$	2.0	1.4	1.9

Table 9: GF and mesh-factors for different source terms.

7 Extension to Convection-Diffusion-Reaction problems

We now consider the boundary value problem

$$-D(\epsilon Du) + \beta Du + \alpha u = f, \quad x \in I, \tag{51}$$

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 question is the same: Do we get a better solution by adding a corrective force $\tilde{F}_h$? The simplified problem is now to find u_h such that

$$-D([\epsilon]^h Du_h) + [\beta]^h Du_h + [\alpha]^h u_h = [f]^h, \quad x \in I. \tag{52}$$

The running average u^h of the solution satisfies

$$-D([\epsilon]^h Du^h) + [\beta]^h Du^h + [\alpha]^h u^h = [f]^h + F_h, \quad x \in I, \tag{53}$$

where

$$\begin{aligned} F_h \;\; = \;\; & -D([\epsilon]^h Du^h) + (D(\epsilon Du))^h + [\beta]^h Du^h - (\beta Du)^h \\ & +[\alpha]^h u^h - (\alpha u)^h - [f]^h + f^h, \end{aligned} \tag{54}$$

which gives

$$\begin{aligned} \bar{F}_h &= -\left(\overline{D([\epsilon]^h Du^h)} - [D(\epsilon Du)]^h\right) + \left([\beta]^h[Du]^h - [\beta Du]^h\right) + \left([\alpha]^h[u]^h - [\alpha u]^h\right) \\ &= -\left([D([\epsilon]^h Du)]^h - [D(\epsilon Du)]^h\right) + \left([\beta]^h[Du]^h - [\beta Du]^h\right) + \left([\alpha]^h[u]^h - [\alpha u]^h\right) \\ &= \bar{F}_h^1 + \bar{F}_h^2 + \bar{F}_h^3, \end{aligned} \tag{55}$$

since $Du^h = (Du)^h$ and $D([\epsilon]^h Du)^h = (D([\epsilon]^h Du))^h$. Like in the previous sections we will formulate an Ansatz for $\bar{F}_h^1$, $\bar{F}_h^2$, and $\bar{F}_h^3$. Using the Ansatz, we can extrapolate to obtain $\tilde{F}_h$, an approximation of $\bar{F}_h$, which we use to compute the corrected solution $\tilde{u}_h$ from the equation

$$-D([\epsilon]^h D\tilde{u}_h) + [\beta]^h D\tilde{u}_h + [\alpha]^h \tilde{u}_h = [f]^h + \tilde{F}_h, \quad x \in I. \tag{56}$$

7.1 Constant diffusion coefficient ϵ

If the diffusion coefficient ϵ is constant, then

$$\bar{F}_h = \left([\beta]^h[Du]^h - [\beta Du]^h\right) + \left([\alpha]^h[u]^h - [\alpha u]^h\right). \tag{57}$$

$\bar{F}_h$ consists of two parts, each of the type (20), which can be extrapolated if β and Du, and α and u respectively have a related asymptotic structure. By choosing locally Hölder continuous α and β we expect extrapolation to work when ϵ is small, since then we have a convection dominated problem as in Section 6.

In Figure 7 we plot the two parts of $\bar{F}_h$, and their extrapolated approximations for $\epsilon = 10^{-6}$ ($H = 2h$ and $\hat{H} = 4h$). We find that the extrapolation of the second part of $\bar{F}_h$, based on the solution u, works fine. But in the case of the first part of $\bar{F}_h$, which is based on the derivative Du, the extrapolation is not as good. What seems to be the problem is that Du_h does not approximate Du well enough. Therefore we would like to avoid to base the extrapolation on the derivative. We eliminate

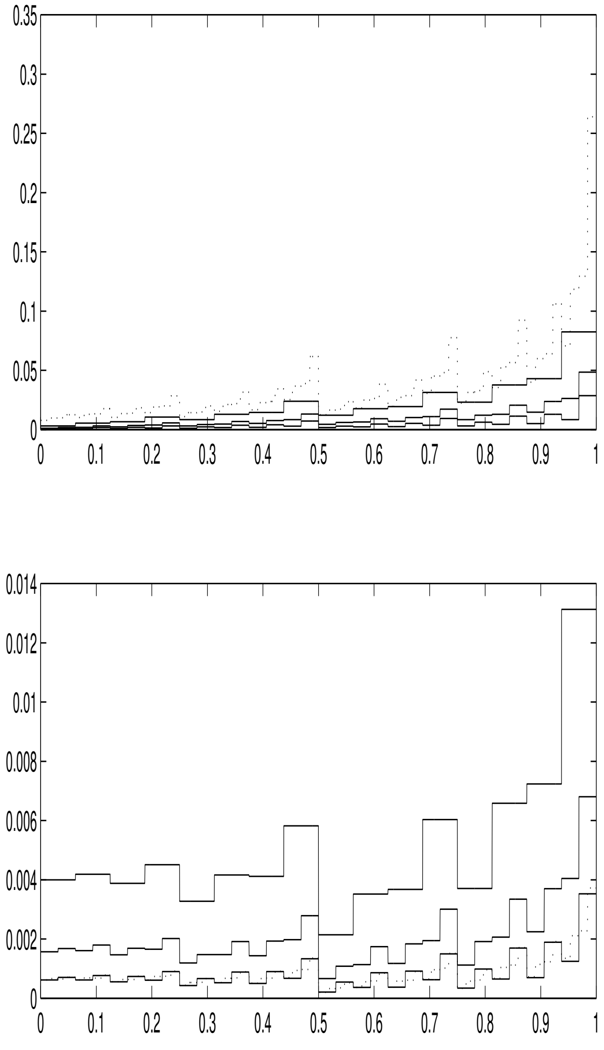

Figure 7: $\bar{F}_H(u_h)$, $\bar{F}_{\hat{H}}(u_h)$, $\bar{F}_h$ and $\tilde{F}_h$ for $H = 2h$ and $\hat{H} = 4h$.

Du from (57) by using (51):

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

Here we recognise $\bar{F}_h^1$ and $\bar{F}_h^1$ as being the same corrective forces as in Section 6, 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 $\bar{F}_h \approx \bar{F}_h^1+\bar{F}_h^2$. In Table 10 we present the result of numerical experiments for $\epsilon = 10^{-6}$ ($i = 6$, $H = 2h$ 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 $D\tilde{u}_h$. (GF and MF_p are defined by (36) and (37) for $\tilde{u}_h$, and by (46) for the derivative $D\tilde{u}_h$.)

γ_α	δ_α	γ_β	δ_β	GF	MF_2	MF_4
$\tilde{u}_h$						
0.5	0.3	0.08	0.1	7.5	1.3	1.8
			0.3	3.4	1.5	2.4
		0.1	0.1	6.5	1.3	1.7
			0.3	3.8	1.5	2.4
	0.5	0.08	0.1	6.2	1.3	1.8
			0.3	3.1	1.6	2.6
		0.1	0.1	5.9	1.3	1.7
			0.3	3.5	1.6	2.6
$D\tilde{u}_h$						
0.5	0.3	0.08	3.8	4.2	1.3	1.8
			0.3	6.3	1.7	2.8
		0.1	0.1	3.2	1.3	1.7
			0.3	5.5	1.6	2.7
	0.5	0.08	0.1	4.1	1.3	1.8
			0.3	6.9	1.8	3.1
		0.1	0.1	3.1	1.3	1.7
			0.3	5.7	1.7	3.0

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

In the diffusion dominated case, with ϵ constant, the method of adding the corrective force fails to give us an improved quality of the solution. This seems natural since the correction F_h is based only on u and Du. On the other hand, if ϵ is a locally Hölder continuous fractal function we expect the method of adding a corrective force to improve the solution. We now consider cases with variable ϵ.

7.2 Poisson's equation

We first consider the case when $\beta = \alpha = 0$,

$$-D(\epsilon Du) = f, \quad x \in I, \tag{58}$$

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

$$-D([\epsilon]^h Du_h) = [f]^h, \quad x \in I, \tag{59}$$

and the running average u^h of u satisfies

$$-D([\epsilon]^h Du^h) = [f]^h + F_h, \quad x \in I, \tag{60}$$

with

$$F_h \quad = \quad -D([\epsilon]^h Du^h) + (D(\epsilon Du))^h - [f]^h + f^h. \tag{61}$$

We have in this case $\bar{F}_h^2 = \bar{F}_h^3 = 0$, and therefore

$$\bar{F}_h = -[D([\epsilon]^h Du)]^h + [D(\epsilon Du)]^h. \tag{62}$$

In this case $\bar{F}_h$ does not appear to be on the form (20), and consequently we cannot motivate the Ansatz on $\bar{F}_h$ which we have used in the previous sections. We therefore turn to the following variational formulation of (58): Find $u \in V = \{v \in L^2(I) : v(0) = v(1) = 0\}$ such that

$$\int_0^1 \epsilon DuDv \; dy = \int_0^1 fv \; dy, \quad \forall v \in V. \tag{63}$$

We have that u_h as defined in (59) also satisfies

$$\int_0^1 [\epsilon]^h Du_h Dv \; dy = \int_0^1 [f]^h v \; dy, \quad \forall v \in V, \tag{64}$$

and the running average u^h of u satisfies

$$\int_0^1 [\epsilon]^h Du^h Dv \; dy = \int_0^1 [f]^h v \; dy + \int_0^1 F_h^{\nabla} Dv \; dy, \quad \forall v \in V, \tag{65}$$

where

$$F_h^{\nabla} = [\epsilon]^h (Du)^h - (\epsilon Du)^h, \tag{66}$$

and therefore

$$\bar{F}_h^{\nabla} = [\epsilon]^h [Du]^h - [\epsilon Du]^h, \qquad (67)$$

which is of the form (20). We can therefore again use the Ansatz

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

and expect extrapolation of $\bar{F}_h^{\nabla}$ to work if ϵ and Du have a related asymptotic structure. We have again that $\bar{F}_h$ is based on the derivative, and again Du_h does not approximate Du as good as we would like it to. It is therefore hard to extrapolate $\bar{F}_h$. To improve the quality of the extrapolation we could use greater H and $\hat{H}$, since on coarser scales Du_h should look more like Du. On the other hand, by using greater H and $\hat{H}$ we sacrifice the information about the fine scale structure of $\bar{F}_h$. But assuming that $\bar{F}_h$ changes slowly with x, this might still be worth it. In Table 11 we present some numerical experiments for $f = 1$, and compare some different choices of H and $\hat{H}$ ($\gamma_\epsilon = 0.1$). GF and MF_2 is defined by (36) and (37) for $\tilde{u}_h$,

$(H, \hat{H})$	GF	MF_2
$\tilde{u}_h$		
($2h$,$4h$)	1.1	1.4
($4h$,$8h$)	1.7	1.4
($8h$,$16h$)	3.1	1.4
$D\tilde{u}_h$		
($2h$,$4h$)	1.1	1.5
($4h$,$8h$)	1.6	1.5
($8h$,$16h$)	2.0	1.5

Table 11: GF and MF_2 ($\gamma_\epsilon = 0.1$, $\delta_\epsilon = 0.3$) for $\tilde{u}_h$ and $D\tilde{u}_h$.

and by (46) for $D\tilde{u}_h$. What we can see is that the 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 $h/2$.

7.3 The full problem

We consider the problem (51) where we now let all coefficients ϵ, α and β be locally Hölder continuous fractal functions. Following the discussion in the previous section we consider the following variational formulation of (51): Find $u \in V = \{v \in L^2(I) : v(0) = Dv(1) = 0\}$ such that

$$\int_0^1 \epsilon Du Dv \, dy + \int_0^1 \beta Du v \, dy \int_0^1 \alpha uv \, dy = \int_0^1 fv \, dy, \quad \forall v \in V. \qquad (68)$$

The solution u_h to the simplified problem (52) satisfies

$$\int_0^1 [\epsilon]^h Du_h Dv\ dy + \int_0^1 [\beta]^h Du_h v\ dy \int_0^1 [\alpha]^h u_h v\ dy = \int_0^1 [f]^h v\ dy, \quad \forall v \in V, \quad (69)$$

and the running average u^h of u satisfies

$$\int_0^1 [\epsilon]^h Du^h Dv\ dy + \int_0^1 [\beta]^h Du^h v\ dy \int_0^1 [\alpha]^h u^h v\ dy$$
$$= \int_0^1 [f]^h v\ dy + \int_0^1 F_h v\ dy + \int_0^1 F_h^\nabla Dv\ dy, \quad \forall v \in V, \quad (70)$$

where

$$F_h^\nabla = [\epsilon]^h (Du)^h - (\epsilon Du)^h, \quad (71)$$
$$F_h = [\beta]^h (Du)^h - (\beta Du)^h + [\alpha]^h u^h - (\alpha u)^h + f^h - [f]^h, \quad (72)$$

and thus

$$\bar{F}_h^\nabla = [\epsilon]^h [Du]^h - [\epsilon Du]^h, \quad (73)$$
$$\bar{F}_h = \Big([\beta]^h [Du]^h - [\beta Du]^h\Big) + \Big([\alpha]^h [u]^h - [\alpha u]^h\Big) \equiv \bar{F}_h^1 + \bar{F}_h^2. \quad (74)$$

Both $\bar{F}_h^\nabla$, $\bar{F}_h^1$ and $\bar{F}_h^2$ are of the form (20) and we expect extrapolation to be possible by using an Ansatz of the form

$$\bar{F}_h^\nabla(x) = C_1(x) h^{\mu_1(x)}, \quad \bar{F}_h(x) = C_2(x) h^{\mu_2(x)} + C_3(x) h^{\mu_3(x)}. \quad (75)$$

We obtain the improved solution $\tilde{u}_h$ from the variational formulation

$$\int_0^1 [\epsilon]^h D\tilde{u}_h Dv\ dy + \int_0^1 [\beta]^h D\tilde{u}_h v\ dy \int_0^1 [\alpha]^h \tilde{u}_h v\ dy$$
$$= \int_0^1 [f]^h v\ dy + \int_0^1 \tilde{F}_h v\ dy + \int_0^1 \tilde{F}_h^\nabla Dv\ dy, \quad \forall v \in V. \quad (76)$$

The relative importance of $\bar{F}_h^\nabla$ compared to $\bar{F}_h$ 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 7.1, by using (58) (neglecting the diffusion term). On the other hand, if the problem is diffusion dominated (ϵ large) the corrective force $\bar{F}_h^\nabla$ based on ϵ is the dominant one.

In Table 12 we present the result of numerical experiments for $\epsilon_{-1} = 10^{-3}$, where both $\bar{F}_h$ and $\bar{F}_h^\nabla$ contributes to the correction of $\tilde{u}_h$. As in the previous section 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 $f = 1$.

In this case a corrected solution $\tilde{u}_h$ on the scale h is better than a non corrected solution on a scale h_f, such that $h/4 < h_f < h/2$ (GF and MF_p are defined by (36) and (37) for $\tilde{u}_h$, and by (46) for the derivative $D\tilde{u}_h$). For the derivative the improvement is not that great (the corrected derivative on the scale h corresponds approximately to a non corrected derivative on the scale $h/2$ for small δ_ϵ).

δ_ϵ	δ_α	δ_β	GF	MF_2	MF_4
$\tilde{u}_h$					
0.3	0.1	0.3	1.8	1.6	2.7
		0.5	2.0	1.7	2.8
	0.3	0.3	1.7	1.5	2.5
		0.5	2.0	1.6	2.6
$D\tilde{u}_h$					
0.3	0.1	0.3	1.3	1.7	2.8
		0.5	1.3	1.7	2.9
	0.3	0.3	1.4	1.6	2.6
		0.5	1.4	1.6	2.7

Table 12: GF and mesh-factors for $\tilde{u}_h$ ($\gamma_\epsilon = 0.1$, $\gamma_\alpha = 0.3$, $\gamma_\beta = 0.1$).

8 Error analysis

We now turn to the issue of developing adaptive algorithms using the extrapolation technique described above and including also quantitative error control based on a posteriori error estimates. We recall that we consider a linear model problem

$$Lu = f, \tag{77}$$

including boundary conditions, and define u_h to be the solution of a simplified problem

$$L_h u_h = [f]^h. \tag{78}$$

The running average u^h satisfies

$$L_h u^h = [f]^h + F_h, \tag{79}$$

with F_h a corrective force. We seek to compute an approximation $\tilde{F}_h$ to F_h by extrapolation and construct a corresponding corrected solution $\tilde{u}_h$ by solving

$$L_h \tilde{u}_h = [f]^h + \tilde{F}_h. \tag{80}$$

We have formally

$$u^h - u_h = L_h^{-1} F_h, \tag{81}$$

$$u^h - \tilde{u}_h = L_h^{-1}(F_h - \tilde{F}_h), \tag{82}$$

which shows the connection between F_h and $u^h - u_h$, and $F_h - \tilde{F}_h$ and $u^h - \tilde{u}_h$, via the inverse L_h^{-1} of L_h. In order for $u^h - \tilde{u}_h$ to be smaller than $u^h - u_h$, that is, for $\tilde{u}_h$ to be an improvement of u_h, we anticipate that $F_h - \tilde{F}_h$ should be smaller than F_h. This means that if F_h is small so that u_h already is a good approximation of u, then improvement should be difficult to achieve. By a similar argument, we obtain the following error representations, where the error is estimated in terms of computable residuals:

$$[u]^h - [u_h]^h = [L^{-1}R(u_h)]^h, \tag{83}$$
$$[u]^h - [\tilde{u}_h]^h = [L^{-1}R(\tilde{u}_h)]^h, \tag{84}$$

where $R(w) = f - Lw$. In the next three sections we derive explicit estimates corresponding to the abstract relations (81)-(84).

8.1 Diffusion coefficient $\epsilon = 0$

For the problem in Section 6, without diffusion, we give two error estimates in terms of the corrective forces. Theorem 2 and 3 corresponds to (81)-(82), where $\|\cdot\|_\infty$ denotes the uniform norm on $I = (0,1)$.

Theorem 2: *Let $h = 2^{-i}$ and assume $0 < [\alpha]^h \le c_0$ and $0 < c_1 \le [\beta]^h$. If u^h and u_h are defined as in Section 6, then*

$$\|u^h - u_h\|_\infty \le C\|F_h\|_\infty, \tag{85}$$

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

Proof: We know, by the discussion in the previous section, that

$$L_h(u^h - u_h) = F_h, \tag{86}$$

and using the solution formula (5) in Section 2, we get

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

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:

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

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

$$|A_h(x) - A_h(y)| \le \max_{t\in I}|DA_h(t)|\ |y - x| = \max_{t\in I}\frac{[\alpha]^h(t)}{[\beta]^h(t)}\ |y - x|, \tag{87}$$

from which the desired result follows.

□

Theorem 3: *Let* $h = 2^{-i}$ *and assume* $0 < [\alpha]^h \leq c_0$ *and* $0 < c_1 \leq [\beta]^h$*. If* u^h *and* $\tilde{u}_h$ *are defined as in Section 6, then*

$$\|u^h - \tilde{u}_h\|_\infty \leq C\|F_h - \tilde{F}_h\|_\infty, \tag{88}$$

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

Proof: We recall that

$$L_h(u^h - \tilde{u}_h) = F_h - \tilde{F}_h, \tag{89}$$

and as in the proof of Theorem 2, we have

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

from which the desired estimate follows.

□

Remark: *The errors in Theorem 2-3 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.*

8.2 Full Convection-Diffusion-Reaction problem

For the problem in Section 7, with non zero diffusion, we do not have an explicit solution formula as we had for the problem in Section 6. Instead we are going to use an energy argument to obtain error estimates. In this section, Theorem 4 and 5 corresponds to (81)-(82) when $\epsilon \neq 0$.

Theorem 4: *Let* $h = 2^{-i}$ *and assume that* $0 < c_0 \leq [\beta]^h \leq C_0$*,* $0 < c_1 \leq [\alpha]^h$ *and* $0 < c_2 \leq [\epsilon]^h$*. If* u_h *and* u^h *are defined as in Section 7, then*

$$\begin{aligned}&\int_0^1 (D(u^h - u_h))^2\,dy + \int_0^1 (u^h - u_h)^2\,dy + (u^h - u_h)^2(1)\\ &\leq C(\|F_h\|^2 + \|F_h^\nabla\|^2),\end{aligned} \tag{90}$$

where $C = \frac{1}{c_0 \min(c_1,c_2)\min(1,\frac{c_1}{C_0},\frac{c_2}{C_0})}\exp(\frac{C_0}{c_0})$.

Proof: First we subtract (52) from (53), where we set $e = u^h - u_h$. 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:

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

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

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

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

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

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

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

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

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

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 also use the given bounds on $[\alpha]^h$, $[\beta]^h$ and $[\epsilon]^h$ we get

$$\frac{1}{C_0}\int_0^1 c_2(De)^2\,dy + \frac{1}{C_0}\int_0^1 c_1 e^2\,dy + e^2(1)$$
$$\leq \frac{1}{c_0}(\int_0^1 \frac{F_h^2}{c_1}\,dy + \int_0^1 \frac{(F_h^\nabla)^2}{c_2}\,dy)\exp\left(\frac{1}{c_0}\sum_{l=1}^{2^i-1}|[\beta]^h|_l\right).$$

But now we observe that

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

from which the desired estimate follows.

□

Theorem 5: *Let $h = 2^{-i}$ and assume that $0 < c_0 \leq [\beta]^h \leq C_0$, $0 < c_1 \leq [\alpha]^h$ and $0 < c_2 \leq [\epsilon]^h$. If u^h and $\tilde{u}_h$ are defined as in Section 7, then*

$$\int_0^1 (D(u^h - \tilde{u}_h))^2\,dy + \int_0^1 (u^h - \tilde{u}_h)^2\,dy + (u^h - \tilde{u}_h)^2(1)$$
$$\leq C(\|F_h - \tilde{F}_h\|^2 + \|F_h^\nabla - \tilde{F}_h^\nabla\|^2), \tag{91}$$

where $C = \frac{1}{c_0\min(c_1,c_2)\min(1,\frac{c_1}{C_0},\frac{c_2}{C_0})}\exp(\frac{C_0}{c_0})$.

Proof: If we subtract (56) from (52) and set $e = u^h - \tilde{u}_h$, then multiply both sides by e and integrate from 0 to $x_{i,k}$, we get

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

Then by following the proof of Theorem 4, the desired estimate follows.

□

8.3 A posteriori error estimates

To derive a posteriori error estimates we consider the following dual problem for φ related to the problem (51):

$$L^*\varphi = -D(\epsilon D\varphi) - D(\beta\varphi) + \alpha\varphi = \Psi,\ \ x \in I, \tag{92}$$

with $\varphi(0) = D\varphi(1) = 0$. We obtain strong stability estimates for φ in terms of Ψ by first multiplying (92) 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 4, to obtain the following estimate for the solution to the dual problem (92):

$$\|\varphi\|^2 + \|D\varphi\|^2 + \varphi^2(1) \le C\|\Psi\|^2, \tag{93}$$

where C is the same constant as in Theorem 4. By taking the 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. 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 into $W_h^{(0)}$, and therefore $(e, [e]^h) = ([e]^h, [e]^h) = \|[e]^h\|^2$. So we get that

$$\|[e]^h\|^2 = (R, \varphi), \tag{94}$$

where φ solves the problem (92) with $\Psi = [e]^h$. We sum up the above discussion in a final theorem:

Theorem 6: *If u^h, u_h and $\tilde{u}_h$ are defined as in Section 7, then*

$$\begin{aligned} \|[u]^h - [u_h]^h\|^2 &= (R(u_h), \varphi), \\ \|[u]^h - [\tilde{u}_h]^h\|^2 &= (R(\tilde{u}_h), \varphi), \end{aligned} \tag{95}$$

where $R(w) = f - Lw$, and φ is the solution to the problem (92) with $\Psi = [u]^h - [u_h]^h$ and $\Psi = [u]^h - [\tilde{u}_h]^h$ respectively.

We also have the following local error representation:

$$\begin{aligned} (u^h - u_h)(x) &= (R(u_h), \varphi), \\ (u^h - \tilde{u}_h)(x) &= (R(\tilde{u}_h), \varphi), \end{aligned} \tag{96}$$

where φ now is the solution to the problem (92) with $\Psi = \chi_{[x-h/2,x+h/2]}$.

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