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Interacting with the subgrid world

Abstract In a number of applications, subgrid scales cannot be neglected. Sometimes, they are just a spurious by-product of a discretised scheme that lacks the necessary stability properties. In other cases, they are related to physical phenomena that actually take place on a very small scale but still have an important effect on the solution. We discuss here an attempt to recover information on the subgrid scales, by trying to simulate their effects on the computable ones.

This paper is dedicated to my friend Ron Mitchell

1 Introduction

There are essentially two types of subgrid phenomena that must be taken into account in modern numerical simulation.

One of them occurs when the discretisation lacks the necessary stability properties. This is often due to the fact that the numerical scheme does not treat in a proper way the smallest scales allowed by the computational grid. As a consequence, they appear as abnormally amplified in the final numerical results. Most types of numerical instabilities are produced in this way, as it can be easily confirmed by checking the beautiful review on numerical instabilities reported in [18]. In the last decade it has become clear that several attempts to recover stability, in these cases, could be interpreted as a way of improving the simulation of the effects of the smallest scales on the larger ones. By doing that, the small scales can be *seen* by the numerical scheme and therefore be kept under control.

A second type of subgrid phenomena is related, instead, with actual physical effects that take place on a scale which is often much smaller than the smallest one representable on the computational grid. These effects have however a strong impact on the larger scales, and cannot be neglected without jeopardizing the overall quality of the final solution.

These two situations are quite different, in nature and scale. Nevertheless it is not unreasonable to hope that some techniques that have been developed for dealing with the former class of phenomena might be adapted to deal with the latter one. In this sense, the most promising technique seems to be the use of Residual-Free Bubbles. In the following sections, we are going to summarize the general idea behind it, trying to underly its potential and its limitations. In particular we shall first present in Section 2 the basic principles of the strategy: *divide and conquer*, *static condensation* and *approximate solution*. In Section 3, as an example, we shall show how the strategy works on a simple model problem. In the final section we shall briefly discuss the possible extensions of the procedure to different problems.

2 Basic Principles

At a very general (and generic) level, the procedure can be summarized as follows. We start with a given problem, that for simplicity we assume to be linear, and in variational form:

$$\begin{cases} \text{find } u \in V \text{ such that :} \\ \\ \mathcal{L}(u,v) = (f,v), \qquad \forall v \in V. \end{cases} \tag{2.1}$$

We assume that we are given a discretised problem:

$$\begin{cases} \text{find } u_h \in V_h \text{ such that :} \\ \\ \mathcal{L}(u_h,v_h) = (f,v_h), \qquad \forall v_h \in V_h, \end{cases} \tag{2.2}$$

where $V_h \subset V$ is a finite element space, corresponding to a given decomposition $\mathcal{T}_h$ of the computational domain. We suppose, roughly speaking, that $\mathcal{T}_h$ is the finest grid we are ready to afford in the computation, in the sense that we are not ready to solve a final system having more unknowns than the dimension of V_h. Problem (2.2) is now, temporarily and artificially, augmented by considering a new subspace of V:

$$V_A := V_h + B_h, \tag{2.3}$$

where B_h is the (infinite dimensional) space of bubbles

$$B_h := \Pi_K \; B(K), \tag{2.4}$$

and, for every K in $\mathcal{T}_h$,

$$B(K) := \{v |\, v \in V, \; \text{supp}(v) \subset K\}. \tag{2.5}$$

As a typical example, if $V = H_0^1(\Omega)$, Ω being the computational domain, then $B(K) = H_0^1(K)$. The augmented problem reads now:

$$\begin{cases} \text{find } u_A \in V_A \text{ such that :} \\ \\ \mathcal{L}(u_A,v_A) = (f,v_A), \qquad \forall v_A \in V_A. \end{cases} \tag{2.6}$$

In principle, problem (2.6), although unsolvable, should be able to take into account all the small scales that *do not cross the boundaries of the elements* K. This is a severe limitation, but corresponds to a sort of **divide and conquer** principle that might, in the end, assure some feasibility to the whole procedure.

We now proceed to eliminate, at least formally, the bubble unknowns from problem (2.6). The technique that we are going to use is well known in the Engineering practice, under the name of **static condensation**. However here we apply it in a more general, infinite dimensional, case.

Assuming, for simplicity, that in (2.3) we have a direct sum of subspaces of V, we can write u_A and v_A, in a unique way, as:

$$u_A = u_h + u_B, \tag{2.7}$$

and

$$v_A = v_h + v_B, \tag{2.8}$$

respectively. Inserting (2.7) into (2.6), and taking $v = v_B$ we obtain the so-called **bubble equation**:

$$\begin{cases} \text{find } u_B \in B_h \text{ such that :} \\ \\ \mathcal{L}(u_B, v_B) = -\mathcal{L}(u_h, v_B) + (f, v_B), \qquad \forall v_B \in B_h. \end{cases} \tag{2.9}$$

The bubble equation (2.9) will play a fundamental role in the following discussion. We take advantage of the split nature of the space B_h. For every element K in $\mathcal{T}_h$ we define $u_{B,K}$ as the restriction of u_B to the element K. Then, for every $\varphi \in B(K)$ we have

$$\mathcal{L}(u_B, \varphi) = (f - Lu_h, \varphi), \tag{2.10}$$

where L indicates the operator associated with the bilinear form $\mathcal{L}$. Problem (2.10) can then be written in strong form as

$$Lu_{B,K} = f - Lu_h, \tag{2.11}$$

with the associated boundary conditions. In most cases, as we have seen, $B(K)$ will be equal to $H_0^1(K)$, and the boundary conditions will be simply

$$u_{B,K} = 0 \; on \; \partial K. \tag{2.12}$$

More generally, the boundary conditions will be implicitly imposed by the two conditions $u_{B,K} \in V$ and $supp(u_{B,K}) \subset K$. We shall write the solution of (2.9) (or, in most examples, of the equivalent problem (2.11)-(2.12)) in compact form as

$$u_{B,K} = L_{B,K}^{-1}(f - Lu_h), \tag{2.13}$$

which implicitly defines the operator $L_{B,K}^{-1}$. With this notation we can write:

$$u_B = \sum_K L_{B,K}^{-1}(f - Lu_h). \tag{2.14}$$

Having made the dependence of u_B on u_h explicit in (2.14), we can go back to (2.6) and take $v_A = v_h$; inserting (2.7) and (2.14) we obtain:

$$\begin{cases} \text{find } u_h \in V_h \text{ such that :} \\ \\ \mathcal{L}(u_h, v_h) + \sum_K \mathcal{L}(L_{B,K}^{-1}(f - Lu_h), v_h) = (f, v_h), \qquad \forall v_h \in V_h. \end{cases} \tag{2.15}$$

Note that (2.15) has the same form (and the same number of unknowns) of (2.2). However, the additional term

$$\sum_K \mathcal{L}(L_{B,K}^{-1}(f - Lu_h), v_h) \tag{2.16}$$

takes now into account the effect of *some* small scales (the ones that do not cross the interelement boundaries) onto the scales that are visible on the computational grid.

The only, nonnegligible, difficulty is that, in general, (2.9) (or even the particular case of problem (2.11)-(2.12)) cannot be solved explicitly, so that the term (2.16) cannot be computed. We remark however that, in order to compute (2.16) in some approximate way, we do not need a very accurate solution of (2.9). Indeed, it is only *the effect of the small scales on the larger ones* that needs to be simulated, as comes out clearly by noting that in (2.16) the term $L_{B,K}^{-1}(f - Lu_h)$ is tested against v_h, which belongs to the coarse space. We can therefore hope that an **approximate solution** of (2.9) (or, more often, of problem (2.11)-(2.12)) can be sufficient to reproduce with reasonable accuracy the effect of the additional term (2.16). The most important aspect of the whole procedure is that such an element-by-element approximate solution can be performed in parallel, as a sort of preprocessing, and its results will then be used within the process of computing and assembling the final matrix corresponding to problem (2.15). In the next section we are going to see more practical aspects of the above discussion for a very simple model problem.

3 A model problem

We consider here, as a model problem, the classical **toy problem** of advection-dominated linear equations. From the physical point of view, we may think to the problem of the passive transport of a scalar diffusive quantity in a fluid whose velocity is known. Let then Ω be, for instance, a convex polygon, ε a positive number (= diffusion coefficient), $\mathbf{c}$ a bounded mapping from Ω to $\mathbb{R}^2$ (= velocity field) and f, say, an element of $L^2(\Omega)$ (= source term). We consider then the problem of finding u in $H_0^1(\Omega)$ such that

$$-\varepsilon\Delta u + \mathbf{c} \cdot \nabla u = f \quad in\ \Omega. \tag{3.1}$$

We can set $Lu := -\varepsilon\Delta u + \mathbf{c} \cdot \nabla u$, and

$$\mathcal{L}(u, v) := \varepsilon a(u, v) + c(u, v) \qquad \forall u, v \in H_0^1(\Omega), \tag{3.2}$$

where, in a natural way,

$$a(u, v) := \int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}x, \quad \text{and} \quad c(u, v) := \int_\Omega \mathbf{c} \cdot \nabla u \, v \, \mathrm{d}x \quad \forall u, v \in H_0^1(\Omega). \tag{3.3}$$

Assume now that we are given a decomposition $\mathcal{T}_h$ of Ω into triangles, and assume moreover that $\mathbf{c}$ and f are piecewise constant on $\mathcal{T}_h$. We take then V_h to be the space

of piecewise linear continuous functions vanishing on $\partial\Omega$, and B_h as in (2.4) with $B(K) = H^1_0(K)$ for each K. If we apply the theory of the previous section, the bubble equation (2.11) becomes, in each triangle K: find $u_{B,K}$ in $H^1_0(K)$ such that

$$-\varepsilon\Delta u_{B,K} + \mathbf{c}\cdot\nabla u_{B,K} = -(-\varepsilon\Delta u_h + \mathbf{c}\cdot\nabla u_h) + f \quad in\ K. \tag{3.4}$$

As we already pointed out, equation (3.4) is unsolvable. As we shall see in a moment, there are ways to get around this difficulty, in a more or less satisfactory way. Before discussing that, however, we want to point out the use that has to be done of its solution in the model case we have chosen. In particular, it is not difficult to check that, in the present case, we have $a(u_B, v_h) = 0$ for every $u_B \in B_h$ and for every $v_h \in V_h$. Hence the additional term (2.16) arising in (2.15) becomes

$$\mathcal{L}(u_B, v_h) = c(u_B, v_h) = \int_\Omega \mathbf{c}\cdot\nabla u_B\, v_h\,\mathrm{d}x = -\int_\Omega u_B\mathbf{c}\cdot\nabla v_h\,\mathrm{d}x, \tag{3.5}$$

with an obvious integration by parts. We also remark that the term $\mathbf{c}\cdot\nabla v_h$ is piecewise constant. Hence we see that **only the mean value** of u_B in each K will be used in the final system (2.15) for computing u_h. Moreover, still in our assumptions, we observe that the right-hand side of (3.4) is also constant in K, so that $u_{B,K}$, in each K, can be written as

$$u_{B,K} = b_K R_K, \tag{3.6}$$

where

$$R_K := -(-\varepsilon\Delta u_h + \mathbf{c}\cdot\nabla u_h) + f \tag{3.7}$$

is the *residual* in K (taking u_h as approximate solution,) and the bubble b_K is the solution of the scaled problem:

$$\begin{cases} \text{find } b_K \in H^1_0(K) \text{ such that :} \\ \\ -\varepsilon\Delta b_K + \mathbf{c}\cdot\nabla b_K = 1 \quad in\ K. \end{cases} \tag{3.8}$$

A simple computation shows that, inserting (3.6) in (3.5), the additional term (2.16) becomes

$$c(u_B, v_h) = \sum_K \frac{\int_K b_K\,\mathrm{d}x}{|K|}\int_K (\mathbf{c}\cdot\nabla u_h - f)\,\mathbf{c}\cdot\nabla v_h\,\mathrm{d}x, \tag{3.9}$$

where b_K is still the solution of (3.8), which is still unsolvable. This, as already pointed out in [11] (see also [24], [5],) corresponds to the use of the well known SUPG method (see [12], [14]) with the stabilising parameter chosen as

$$\tau_K = \frac{\int_K b_K\mathrm{d}x}{|K|}. \tag{3.10}$$

We still have to tackle the problem of getting an approximate solution of (3.8). We shall consider several possibilities. As the present model problem is by far the most deeply

studied among the various possible applications of the general technique, we shall obtain a reasonably complete overlook of the various options that can be considered also in different contexts.

The obvious, and most general, way of approximating (2.9) would consist in using a Galerkin approximation: we take, for each K, a subspace B_K^* of $H_0^1(K)$ and we look for $u_B^* = \sum_K u_{B,K}^*$ such that each $u_{B,K}^* \in B_K^*$ and satisfies

$$\mathcal{L}(u_{B,K}^*, v) = -\mathcal{L}(u_h, v) + (f, v) \quad \forall v \in B_K^*, \tag{3.11}$$

where, as usual, we identify a function in B_K^* with its extension by zero on the whole Ω. In our case, this amounts to solve in each K the following approximated version of the scaled equation (3.8):

$$\begin{cases} \text{find } b_K^* \in B_K^* \text{ such that :} \\ \\ \varepsilon a(b_K^*, v) + c(b_K^*, v) = \int_K v \, \mathrm{d}x, \quad \forall v \in B_K^*. \end{cases} \tag{3.12}$$

This would then give the solution $u_{B,K}^*$ of (3.11) as $u_{B,K}^* = b_K^* R_K$, with R_K always given by (3.7). For our model problem this will correspond, in the end, to use b_K^* instead of b_K in (3.9), obtaining an SUPG method with a stabilising parameter given by

$$\tau_K = \frac{\int_K b_K^* \mathrm{d}x}{|K|}. \tag{3.13}$$

In general B_K^* will correspond to a subgrid mesh. For our particular problem, the mesh might include a suitable refinement near the outflow boundary $\partial K \setminus \partial K^-$. For a similar approach, although on a different problem, see [17].

The use of a subgrid mesh is surely the most expensive and more general way. On the other hand, one can try to use a smart cheaper choice, by using a one-dimensional subspace B_K^* of the form $B_K^* = span\{\varphi_K\}$, for a suitable choice of φ_K. In this case one can easily see that the solution of (3.12) is $b_K^* = \gamma_K \varphi_K$, with γ_K given by

$$\gamma_K = \frac{\int_K \varphi_K \, \mathrm{d}x}{\varepsilon a(\varphi_K, \varphi_K)} = \frac{\int_K \varphi_K \, \mathrm{d}x}{\varepsilon \int_K |\nabla \varphi_K|^2 \mathrm{d}x}. \tag{3.14}$$

Notice that this (as already pointed out in the early [3]) would produce again an SUPG formulation, but this time with a stabilising parameter

$$\tau_K = \frac{(\int_K \varphi_K \, \mathrm{d}x)^2}{\varepsilon |K| \int_K |\nabla \varphi_K|^2 \mathrm{d}x}, \tag{3.15}$$

corresponding (for small ε) to a huge value , unless φ_K is suitably chosen. In particular, an unrealistically blessed choice would be to take $\varphi_K = b_K$, solution of (3.8), which gives actually $u_{B,K}^* = u_{B,K}$. The need of a convenient shape for φ_K can also be traced back to the relationships between upwind methods and suitable versions of the Petrov-Galerkin method, pointed out already long time ago (see e.g. [27]). In the present

context (3.12), a realistic *ad hoc* choice for φ_K, which produces quite sensible results for all values of ε, is proposed in [9].

Another approach, proposed in [19], [20], is to choose φ_K in an arbitrary way (cubic bubble in K, or the pyramidal bubble with vertex in the barycenter of K) and add some artificial *subgrid viscosity* ε_A to (3.8), which becomes

$$-(\varepsilon+\varepsilon_A)\Delta b_K + \mathbf{c}\cdot\nabla b_K = 1 \quad in\ K. \tag{3.16}$$

As pointed out in [7], if one approximates (3.16) with a one degree of freedom subspace $B_K^* = span\{\varphi_K\}$, the corresponding approximate solution has again the form $b_K^* = \gamma_K\varphi_K$, but now γ_K is given by

$$\gamma_K = \frac{\int_K \varphi_K\,\mathrm{d}x}{(\varepsilon+\varepsilon_A)\int_K |\nabla\varphi_K|^2\mathrm{d}x}, \tag{3.17}$$

and the corresponding τ_K becomes

$$\tau_K = \frac{(\int_K \varphi_K\,\mathrm{d}x)^2}{(\varepsilon+\varepsilon_A)|K|\int_K |\nabla\varphi_K|^2\mathrm{d}x}, \tag{3.18}$$

leaving us with the crucial problem of the choice of ε_A. For some heuristic attempt to get a sensible choice for ε_A, see [7]. It is interesting, and somehow surprising, that the stabilising effect of the procedure is minor for a big subgrid viscosity ε_A, and much bigger for a small subgrid viscosity, as shown by (3.18).

Another possibility (more specially tailored for the present model problem) to obtain a satisfactory approximate solution of (3.8) is to consider the associated *limit problem*: find $\tilde{b}_K$ in, say, $H^1(K)$, such that:

$$\begin{cases} \mathbf{c}\cdot\nabla\tilde{b}_K = 1 \quad in\ K, \\ \\ \tilde{b}_K = 0 \quad on\ \partial K^- = \{x\in\partial K\ such\ that\ \mathbf{c}\cdot\mathbf{n}_K < 0\}, \end{cases} \tag{3.19}$$

where $\mathbf{n}_K$ is the outward normal to K. It is easy to check that the difference between the integral of b_K and the integral of $\tilde{b}_K$ is $O(\varepsilon)$ for $\varepsilon\to 0$. On the other hand, the solution of (3.19) is elementary, and can be computed with paper and pencil. Hence, in practice, one substitutes $\tilde{b}_K$ in place of b_K in (3.9), obtaining an SUPG method with a stabilising parameter given by

$$\tau_K = \frac{\int_K \tilde{b}_K\mathrm{d}x}{|K|}. \tag{3.20}$$

This is essentially the approach proposed in [11], and gives quite reasonable answers even for ε only moderately small.

To conclude our little discussion on the model problem (3.1), we summarize the possible choices to get an approximate solution of (3.4) (or of its scaled version (3.8).)

We can use a Galerkin subgrid method, with a fine enough (or smart enough) grid. We can use a one-dimensional Galerkin method with a smart choice of the one-dimensional subspace, or we can use a plain one dimensional subspace and add a smart artificial subgrid viscosity. Finally, we can solve a *reduced equation* (3.19) by hand. All of these approaches will produce in the end an SUPG method, with different values of the stabilising parameter.

We also note that similar procedures can also be adapted and applied, with minor additional complications, to the cases in which the original finite element space V_h is made, say, of piecewise polynomials of degree $k > 1$. The practical aspects of such an extension will become clearer in the next section. We just mention here that, for higher order polynomials, we obtain variants of SUPG that do not coincide with it anymore, and whose stabilising effect has still to be tested in practice.

Finally, we point out that, from the theoretical point of view, the convergence analysis developed for SUPG methods clearly applies to the case of our model problem (3.1), if V_h is made of piecewise linear functions (that is for $k = 1$.) However, recently, an independent analysis has been carried out starting directly from the formulation (2.15) (see [8]). This type of analysis can also be extended to the case of higher order polynomials. In particular, error estimates of usual type, for $k > 1$, have been obtained for $\varepsilon|u - u_h|_1^2$ and for $\mathbf{c} \cdot (u - u_h)$ in a weighted L^2-norm in [10]. By *usual type* we mean here error estimates that are half an order suboptimal: see [26], [21], [28]. More recently, global L^2-error estimates and local H^1-error estimates have been obtained, for the formulation (2.15), in [29].

4 Extensions to other problems

Having the example of Section 3 in mind, we now go back to the more general level of Section 2, for a brief discussion on possible applications to different problems. It is clear, from the above section, that all the viable strategies make use of the split nature of the bubble equation (2.9). This is the crucial point of the *divide and conquer* strategy, essentially contained in assumption (2.5). Splitting (2.9) among the subdomains, its *approximate solution* can be done in parallel. However, in order to perform the *static condensation*, one has to be able to substitute u_B (or, actually, its approximation) as a function of the original (and final) unknown u_h in (2.15). For this, we proceed in the following way: as a first step we identify, in each K, the smallest linear space that contains all possible residuals, namely

$$R_h^K := span\{f_{|K}, Lv_{h|K},\ v_h \in V_h\}. \tag{4.1}$$

In many cases, $f_{|K}$ can be approximated, without major loss of information, by means of elements of the space $(LV_h)_{|K}$, that can therefore be used in place of R_h^K. In the previous section, this was the space of constants on K.

The second step is then to choose, for each K, a basis $\{g_K^i\}_{\{i=1,..,N_K\}}$ of the space R_h^K. Clearly, N_K denotes the dimension of such space. Then, for each $i = 1, .., N_K$,

we seek an approximate solution of the local problem:

$$\begin{cases} \text{find } \psi_K^i \in H_0^1(K) \text{ such that :} \\ \\ \mathcal{L}(\psi_K^i, v) = (g_K^i, v) \quad \forall v \in H_0^1(K). \end{cases} \tag{4.2}$$

In the example of the previous section, there was just one function g_K^i, namely the constant 1 appearing in (3.8), and the corresponding function ψ_K^i was denoted by b_K.

The most general and widely applicable strategy in order to obtain an approximate solution of (4.2) consists, as we have seen, in the use of a Galerkin approximation, corresponding to a suitable choice of $B_K^* \subset H_0^1(K)$. Then one can solve N_K problems of the type:

$$\begin{cases} \text{find } \psi_K^{*,i} \in B_K^* \text{ such that :} \\ \\ \mathcal{L}(\psi_K^{*,i}, v) = (g_K^i, v) \quad \forall v \in B_K^*. \end{cases} \tag{4.3}$$

The technique has been successfully applied to advection dominated flows, in cases more complex than the one of the previous Section. See e.g. [17]. For an application of this technique to the Helmholtz equation see for instance [15], [16].

On more special classes of problems one might also think to extend some of the *tricks* of the previous Section. For instance, the use of the limit problem (3.19) can surely be adapted to advection diffusion problems with a more general choice of V_h. See e.g. [6].

On the other hand, for singularly perturbed problems where some artificial viscosity (or similar regularization) is usually employed, the idea of using only a kind of *subgrid viscosity* (or subgrid regularization,) as in (3.16), is surely appealing for its simplicity and rather wide range of applicability. However, as we have seen, the choice of the subgrid artificial viscosity ε_A appears to be crucial, and requires deeper investigations.

Another possible interesting area where these ideas can be applied is the solution of elliptic problems with rough coefficients. Consider for instance the problem of finding $u \in H_0^1(\Omega)$ such that

$$-\sum_{i,j=1,2} \frac{\partial}{\partial x_j}(a_{i,j}(\mathbf{x}) \frac{\partial u}{\partial x_i}) = f \quad in\ \Omega, \tag{4.4}$$

where we assume that the matrix $a_{i,j}$ satisfies the usual uniform strong ellipticity conditions, but has jumps within Ω, on a scale that is only affordable when solving local problems in parallel. Problems of this type arise for instance in petroleum engineering, but the range of possible applications is clearly much wider. Notice that writing (4.4) in mixed form (see e.g. [4]) the space V, in the notation of the Section 2, becomes $H(\mathrm{div};\Omega) \times L^2(\Omega)$. It is interesting to see that the present general strategy, in this case, gives back the upscaling method of [1], [2]. The mixed formulation, within this approach, seems to be particularly appealing. Indeed, for an element (σ, u) in $H(\mathrm{div};\Omega) \times L^2(\Omega)$, the condition $supp((\sigma, u)) \subset K$ only requires $\sigma \cdot \mathbf{n}_K = 0$ on ∂K.

Notice that a conventional variational formulation would use $V = H_0^1(\Omega)$, forcing the elements of the bubble space to satisfy $u = 0$ on ∂K, which looks as a more severe limitation. It would be interesting however to compare the two approaches on some practical problems. Similarly, the relations of these approaches with the one of Hou (see e.g. [22], [23]) are surely worth investigating.

The application of the paradigm "divide and conquer/ static condensation/ approximate solution" to some nonlinear problems is currently under investigation. The obvious choice would be to apply it to the various linearized problems in an iterative procedure, but in particular cases the structure of the nonlinearity might suggest a better strategy.

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