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A posteriori optimization of parameters in stabilized methods for convection–diffusion problems – Part I

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ABSTRACT

Stabilized finite element methods for convection-dominated problems require the choice of appropriate stabilization parameters. From numerical analysis, often only their asymptotic values are known. This paper presents a general framework for optimizing stabilization parameters with respect to the minimization of a target functional. Exemplarily, this framework is applied to the SUPG finite element method and the minimization of a residual-based error estimator, an error indicator, and a functional including the crosswind derivative of the computed solution. Benefits of the basic approach are demonstrated by means of numerical results.

1. Introduction

The numerical solution of challenging problems in various engineering applications is in general not possible with standard methods that are based, e.g., on central finite differences or the Galerkin finite element method. More sophisticated schemes become necessary that are designed to tackle the special difficulties of the underlying problem.

An example, that will be considered in this paper, are scalar convection-dominated convection–diffusion equations. Solutions of these equations exhibit very fine structures, so-called layers, which cannot be resolved on meshes that are not extremely fine, at least locally. Standard discretizations lead to solutions that are globally polluted by large spurious oscillations. In practice, stabilized methods are used. These methods introduce artificial diffusion. The difficulty consists now in defining the correct amount of diffusion at the correct positions in the correct directions (anisotropic diffusion) such that numerical solutions with sharp layers and without spurious oscillations are obtained. A method that is optimal with respect to all criteria does not exist yet. Many proposed stabilized methods include so-called stabilization parameters. Often, the asymptotic choice of these parameters is known, e.g., that they should be proportional to the local mesh width. However, in practice, the proportionality factor has to be chosen. There is the experience that different choices of such factors might lead to considerably different numerical solutions. Moreover, the asymptotic choice of the stabilization parameters is based on global stability and convergence analysis. Local features of solutions, like layers, are not taken into account in this analysis.

We would like to mention a second example that demonstrates the difficulties of choosing parameters in numerical simulations – Large Eddy Simulation (LES) of turbulent flows. Turbulent flow simulations require the use of some turbulence model. An often used, so-called eddy viscosity model, is the Smagorinsky model [40]. This model is based on some insight into the physics of turbulent flows and it finally introduces a nonlinear viscosity into the discrete equations. It is rather easy to implement and very well understood from the point of view of mathematical analysis [32]. The derivation of the Smagorinsky model is based on some proportionality relations such that at the end a proportionality factor occurs. Experience shows that the use of a constant for this factor does not lead to good results. Instead, this factor has to be adapted to the local features of the turbulent flow field. An approach in this direction is the dynamic Smagorinsky model [12,33]. Despite all

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drawbacks, e.g., see [24], the dynamic Smagorinsky model is one of the most often used and most successful LES models. Nowadays, there is another approach to control the influence of the Smagorinsky model – Variational Multiscale (VMS) methods. These methods try to select appropriate scales to which this model is applied [20,15,25,26]. Turbulent flow simulations are a typical example where principal forms of models are known but the results obtained with these models depend on the correct setting of parameters. There are many more numerical methods that require the choice of parameters and for which an a posteriori choice would greatly improve the ability to use them in applications. The a posteriori choice of parameters seems to be a widely open and challenging task in scientific computing.

The idea of choosing parameters in numerical methods a posteriori is not new, the dynamic Smagorinsky model was already mentioned. In essence, this method computes two (or more) discrete solutions in different ways and the parameter choice is based on comparing them. This idea was recently carried over to scalar convection–diffusion equations in [1], based on the work from [35]. In this approach, the different solutions are computed on coarser mesh(es). On the coarser meshes, information on the respective stabilization parameters are derived which are used to update the stabilization parameters on the fine mesh. A severe drawback of this approach is that the dimension of the parameter space is not allowed to exceed the dimension of the respective test function space. Therefore, the approach cannot be applied to the optimization of stabilization parameters in discretizations with first order finite elements as considered in this paper. Moreover, the methodology seems to be only simple for a few globally constant parameters, which is explicitly not the goal of our approach. Another method which determines the stabilization parameter on the basis of two solutions was presented in [36]. In this method, the residuals and their derivatives are used to compute a characteristic length scale which enters the formula for the stabilization parameter. The computations of the stabilization parameters in [36] are restricted to convection–diffusion equations in one dimension and a generalization to more dimensions is not obvious. A method for hyperbolic conservation laws in one dimension can be found in [10]. In this paper, the streamline-diffusion stabilization parameter and an adaptively refined grid are computed a posteriori. The adaptive algorithm uses the Dual Weighted Residual (DWR) approach [2,3] with a backward-in-time dual problem. An iterative procedure based on equilibrating components of the error estimator is used to compute the stabilization parameters and the grids. This method was extended to one-dimensional nonlinear convection–diffusion–reaction equations in [18].

The present paper considers the Streamline-Upwind Petrov–Galerkin (SUPG) finite element method for scalar convection-dominated convection–diffusion equations introduced in [21,4]. Although a number of other stabilized finite element methods have been developed in the past decades, the SUPG method is still the standard approach. In essence, this method adds numerical diffusion in streamline direction. The amount of diffusion depends on local stabilization parameters. There are different formulae for these parameters whose asymptotics are the same, see [27] for a discussion of parameter choices. The properties of solutions obtained with the SUPG method are well known: sharp layers at the correct positions are computed, but non-negligible spurious oscillations occur in a vicinity of layers. These oscillations make the use of the SUPG method in applications difficult as they correspond in general to unphysical situations, like negative concentrations. There have been a large number of attempts to improve the SUPG method in order to get rid of these oscillations while preserving its good properties. However, none of these so-called Spurious Oscillations at Layers Diminishing (SOLD) methods turned out to be entirely successful [27,28].

To improve the solutions obtained with the SUPG method, the present paper pursues a different approach than the SOLD methods. It relies on the optimization of the stabilization parameter, however, in contrast to [1,10,18,36,35], the parameter optimization is formulated as minimization of some functional. This is a nonlinear constrained optimization problem that has to be solved iteratively. A key component of this approach consists in the efficient computation of the Fréchet derivative of the functional with respect to the stabilization parameter. This is achieved by utilizing an adjoint problem with an appropriate right-hand side. The aim of the present paper is to provide a new general framework for the optimization of parameters in stabilized methods for convection–diffusion equations and to demonstrate exemplarily the benefits of this approach. A comprehensive discussion of the choice of appropriate target functionals is postponed to the second part of this paper.

The paper is organized as follows. Section 2 presents the equation and the SUPG method. A general approach for computing the Fréchet derivative of a functional that depends on the numerical solution with respect to parameters in the numerical method is presented in Section 3. This approach is applied to the SUPG method in Section 4. Section 5 contains a proof of concept. It is demonstrated that errors to known solutions can be reduced by using as functional the error in some norm. For problems with unknown solutions, Section 6 illustrates the application of the a posteriori parameter choice based on the minimization of a residual-based a posteriori error estimator, an error indicator, and a functional that includes the crosswind derivative of the computed solution. The most important conclusions, open problems, and an outlook are presented in Section 7. Throughout the paper, standard notations are used for usual function spaces and norms, see, e.g., [6]. The notation $(\cdot,\cdot)_G$ with a set $G \subset \mathbb{R}^d,\ d = 1, 2, 3$, is used for the inner product in the space $L^2(G)$ or $L^2(G)^d$, with $(\cdot,\cdot) = (\cdot,\cdot)_\Omega$.

2. The convection–diffusion problem and its SUPG stabilization

Consider the scalar convection–diffusion problem

$$-\varepsilon\Delta u + \mathbf{b}\cdot\nabla u + cu = f \text{ in } \Omega, \quad u = u_b \text{ on } \Gamma^D, \quad \varepsilon\frac{\partial u}{\partial \mathbf{n}} = g \text{ on } \Gamma^N. \tag{1}$$

Here, $\Omega \subset \mathbb{R}^d,\ d = 2, 3$, is a bounded domain with a polyhedral Lipschitz–continuous boundary $\partial\Omega$ and Γ^D, Γ^N are disjoint and relatively open subsets of $\partial\Omega$ satisfying $\text{meas}_{d-1}(\Gamma^D) > 0$ and $\overline{\Gamma^D \cup \Gamma^N} = \partial\Omega$. Furthermore, $\mathbf{n}$ is the outward unit normal vector to $\partial\Omega$, $\varepsilon > 0$ is a constant diffusivity, $\mathbf{b} \in W^{1,\infty}(\Omega)^d$ is the flow velocity, $c \in L^\infty(\Omega)$ is the reaction coefficient, $f \in L^2(\Omega)$ is a given outer source of the unknown scalar quantity u, and $u_b \in H^{1/2}(\Gamma^D)$, $g \in L^2(\Gamma^N)$ are given functions specifying the boundary conditions. The usual assumption that

$$c - \frac{1}{2}\text{div}\mathbf{b} \geqslant c_0 \geqslant 0 \tag{2}$$

with a constant c_0 is made. Moreover, it is assumed that

$$\{\mathbf{x} \in \partial\Omega; (\mathbf{b}\cdot\mathbf{n})(\mathbf{x}) < 0\} \subset \Gamma^D, \tag{3}$$

i.e., the inflow boundary is a part of the Dirichlet boundary Γ^D.

This paper studies finite element methods for the numerical solution of (1). To this end, (1) is transformed into a variational formulation. Let $\tilde{u}_b \in H^1(\Omega)$ be an extension of u_b (i.e., the trace of $\tilde{u}_b$ equals u_b on Γ^D) and let

$$V = \{v \in H^1(\Omega); \quad v = 0 \text{ on } \Gamma^D\}.$$

Then, a weak formulation of (1) reads: Find $u \in H^1(\Omega)$ such that $u - \tilde{u}_b \in V$ and

$$a(u, v) = (f, v) + (g, v)_{\Gamma^N} \quad \forall v \in V, \tag{4}$$