Adaptive computation of parameters in stabilized methods for convection-diffusion problems

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Abstract Stabilized finite element methods for convection-dominated problems contain parameters whose optimal choice is usually not known. This paper presents techniques for computing stabilization parameters in an adaptive way by minimizing a target functional characterizing the quality of the approximate solution. This leads to a constrained nonlinear optimization problem. Numerical results obtained for various target functionals are presented. They demonstrate that a posteriori optimization of parameters can significantly improve the quality of solutions obtained using stabilized methods.

1 Introduction

This paper is devoted to the numerical solution of a steady scalar convection-diffusion equation

$$-\varepsilon\,\Delta\,u+\mathbf{b}\cdot\nabla u+c\,u=f \quad \text{in } \Omega\,, \qquad u=u_b \quad \text{on } \partial\Omega \tag{1}$$

by means of the finite element method. In (1), $\Omega\subset\mathbb{R}^d$, $d=2,3$, is a bounded domain with a polygonal (resp. polyhedral) Lipschitz-continuous boundary $\partial\Omega$, $\varepsilon>0$ is constant, $\mathbf{b}\in W^{1,\infty}(\Omega)^d$, $c\in L^\infty(\Omega)$, $f\in L^2(\Omega)$, and $u_b\in H^{1/2}(\partial\Omega)$. The Dirichlet boundary condition is used for the sake of simplicity only. In the numerical

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computations presented in this paper also more general boundary conditions were used.

Problem (1) is a simple model problem for convection-diffusion effects appearing in many more complicated applications. Therefore, it is important to be able to solve this problem numerically in a satisfactory way. However, this is by no means easy if convection dominates diffusion, i.e., $\varepsilon \ll |\mathbf{b}|$, since then the solution of (1) contains so-called layers, which are narrow regions where the solution changes abruptly. It is well known that the standard Galerkin finite element method provides approximate solutions that are globally polluted by spurious oscillations unless the computational mesh is sufficiently fine, i.e., $\varepsilon \gtrsim |\mathbf{b}|\,h$ where h is the mesh parameter.

To suppress the spurious oscillations, there are basically two options. Either one can use a layer-adapted mesh (e.g., a piecewise uniform mesh or a mesh obtained by an anisotropic adaptive refinement strategy) or one can consider a relatively coarse mesh and employ a modification of the standard discretization. There are various modifications that can be found in the literature: special discretizations of the convective term (upwinding), introduction of additional terms (stabilization) or manipulations at the algebraic level (e.g., FEMTVD schemes). In this paper, we shall be interested in stabilization techniques applied on relatively coarse meshes.

A common feature of stabilized finite element methods is that they contain parameters whose values significantly influence the quality of the approximate solution but whose optimal choice is usually not known. The aim of the present paper is to describe techniques that make it possible to compute stabilization parameters in an adaptive way by minimizing a functional characterizing the quality of the approximate solution. This leads to a constrained nonlinear optimization problem. The paper is a continuation of our previous work published in [3] where basic ideas of the optimization of stabilization parameters were presented.

The plan of the paper is as follows. In the next two sections we discuss linear and nonlinear stabilization approaches for finite element discretizations of (1). Then, in Section 4, we describe our approach of parameter optimization and explain how the Fréchet derivative of the target functional can be computed in an efficient way. Finally, in Section 5, we construct several target functionals and illustrate their properties by means of numerical results.

2 Linear stabilized methods

Let W_h be a finite element space approximating the space $H^1(\Omega)$ and set $V_h := W_h \cap H^1_0(\Omega)$. Let $u_{bh} \in W_h$ be a function whose trace approximates the function u_b. The simplest finite element discretization of (1) is the Galerkin method that reads: Find $u_h \in W_h$ such that $u_h = u_{bh}$ on $\partial\Omega$ and

$$a(u_h, v_h) = (f, v_h) \qquad \forall\, v_h \in V_h\,,$$

where $a(u,v) = \varepsilon\,(\nabla u, \nabla v) + (\mathbf{b}\cdot\nabla u, v) + (c\,u, v)$ and $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$ or $L^2(\Omega)^d$. As we mentioned in the introduction, the Galerkin discretization is not appropriate if convection dominates diffusion and, as a remedy, a stabilization of the Galerkin method will be considered.

A stabilized finite element method for the numerical solution of (1) can be obtain from the Galerkin method by adding a stabilization term. We shall consider methods that read: Find $u_h \in W_h$ such that $u_h = u_{bh}$ on $\partial\Omega$ and

$$a(u_h, v_h) + \sum_{K\in\mathscr{T}_h} \tau_K\, s_K(u_h, v_h) = (f, v_h) \qquad \forall\, v_h \in V_h\,.$$

Here $\mathscr{T}_h$ is the triangulation used for constructing the finite element space W_h, τ_K is a nonnegative stabilization parameter, and s_K is a local form whose arguments are functions defined on the set $K \in \mathscr{T}_h$. The form s_K is always linear in the second argument and, if $f = 0$, it is also linear in the first argument. There are examples of s_K which are bilinear for any f. The parameter τ_K determines the artificial diffusion added by the stabilization term and it should be not 'too small' to remove oscillations but also not 'too large' to avoid excessive smearing. Consequently, it is very difficult to find appropriate values of τ_K a priori.

One of the most popular finite element approaches for convection-dominated problems is the SUPG method for which

$$s_K(u,v) = (\mathscr{L}_h u - f, \mathbf{b}\cdot\nabla v)_K$$

with the differential operator $\mathscr{L}_h = -\Delta_h + \mathbf{b}\cdot\nabla + c$ where the subscript h indicates that the Laplace operator is applied elementwise. The stabilization parameter is often defined by

$$\tau_K = \frac{h_K}{2\,|\mathbf{b}|}\left(\coth \mathrm{Pe}_K - \frac{1}{\mathrm{Pe}_K}\right) \quad \text{with} \quad \mathrm{Pe}_K = \frac{|\mathbf{b}|\,h_K}{2\,\varepsilon}\,, \tag{2}$$

where h_K is the diameter of K in the direction of $\mathbf{b}$.

3 Nonlinear stabilized methods

Since solutions of linear stabilized methods usually possess spurious oscillations in layer regions, the so-called SOLD (spurious oscillations at layers diminishing) methods have been developed. These methods add an additional stabilization term to the left-hand side of a linear stabilized method. Typical examples of this term are $(\widetilde{\varepsilon}\,\nabla u_h, \nabla v_h)$ adding isotropic artificial diffusion and $(\widetilde{\varepsilon}\,P\,\nabla u_h, P\,\nabla v_h)$ with the orthogonal projection P onto the plane orthogonal to $\mathbf{b}$, adding crosswind artificial diffusion. The parameter $\widetilde{\varepsilon}$ usually depends on the unknown approximate solution u_h and hence the resulting method is nonlinear.

In the literature, many proposals for the parameter $\widetilde{\varepsilon}$ can be found and we refer to [1, 2] for a review and computational comparison. One of the most successful formulas is

$$\widetilde{\varepsilon}|_K = \eta\, \frac{\mathrm{diam}(K)\, |\mathscr{L}_h u_h - f|}{2\, |\nabla u_h|} \qquad \forall\, K \in \mathscr{T}_h\,,$$

where η is a user-chosen parameter. From now on, the notion 'SOLD method' will mean that the crosswind diffusion term $(\widetilde{\varepsilon}\, P\nabla u_h, P\nabla v_h)$ together with this choice of $\widetilde{\varepsilon}$ is used. In the framework of parameter optimization, the parameter η will be considered piecewise constant. If an optimization of η is not considered, we set $\eta = 0.7$.

4 A posteriori optimization of stabilization parameters

In this section, we describe basic ideas of our approach to a posteriori optimization of stabilization parameters. For clarity of the presentation, we shall restrict ourselves to $u_b = 0$.

Let us write a linear or nonlinear stabilized method in the abstract form:

Given a stabilization parameter $y_h \in Y_h$, find $u_h \in V_h$ such that $R_h(u_h, y_h) = 0$.

Here, Y_h is a finite-dimensional space of functions on Ω and the operator R_h maps the space $V_h \times Y_h$ into the dual space V_h'. E.g., for the SUPG method introduced in Section 2, we have

$$\langle R_h(u_h, y_h), v_h \rangle = a(u_h, v_h) + (\mathscr{L}_h u_h - f, y_h\, \mathbf{b} \cdot \nabla v_h) - (f, v_h)$$

and Y_h can be the space of piecewise constant functions on Ω. To emphasize that the approximate solution u_h depends on the choice of the stabilization parameter $y_h \in Y_h$, we shall write $u_h(y_h)$ instead of u_h in the following.

We introduce a functional $I_h : V_h \to \mathbb{R}$ such that $I_h(u_h(y_h))$ represents a measure of the error or the quality of $u_h(y_h)$. We assume that the solution $u_h(y_h)$ improves if the functional $\Phi_h(y_h) := I_h(u_h(y_h))$ decreases. Thus, our aim is to find $y_h \in Y_h$ such that $\Phi_h(y_h)$ is 'small'. This is a constrained nonlinear optimization problem since y_h has to be nonnegative and smaller than some upper bound. E.g., for the SUPG method,

$$0 \le y_h|_K \le 10\, \tau_K \qquad \forall\, K \in \mathscr{T}_h\,, \tag{3}$$

where τ_K is defined by (2). The factor 10 can be changed to another value but numerical experiments indicate that the factor should not differ too much from 10.

Common minimization algorithms require at least the knowledge of the derivative of the function which should be minimized. Thus, we have to compute the Fréchet derivative of the functional Φ_h. Using the chain rule, we obtain

$$D\Phi_h(y_h) = DI_h(u_h(y_h))Du_h(y_h)\,.$$

However, it is not efficient to compute $D\Phi_h(y_h)$ using this formula since it requires the solution of $\dim Y_h$ linear problems of the size of the original discrete problem. Therefore, we first define the adjoint problem: Find $\psi_h(y_h) \in V_h$ such that

$$(\partial_u R_h)'(u_h(y_h), y_h)\,\psi_h(y_h) = DI_h(u_h(y_h))\,,$$

where $\langle(\partial_u R_h)'(w_h, y_h)v_h, \tilde{v}_h\rangle = \langle(\partial_u R_h)(w_h, y_h)\tilde{v}_h, v_h\rangle \quad \forall\, v_h, \tilde{v}_h, w_h \in V_h, y_h \in Y_h$. Since $R_h(u_h(y_h), y_h) = 0$, we have $\partial_u R_h(u_h(y_h), y_h)Du_h(y_h) + \partial_y R_h(u_h(y_h), y_h) = 0$. Thus, combining the above relations, we deduce that

$$D\Phi_h(y_h) = -(\partial_y R_h)'(u_h(y_h), y_h)\psi_h(y_h)\,,$$

where $\langle(\partial_y R_h)'(w_h, y_h)v_h, \tilde{y}_h\rangle = \langle(\partial_y R_h)(w_h, y_h)\tilde{y}_h, v_h\rangle \quad \forall\, v_h, w_h \in V_h, y_h, \tilde{y}_h \in Y_h$. Note that, for the SUPG method, the function $\psi_h(y_h)$ solves

$$a(v_h, \psi_h(y_h)) + (\mathscr{L}_h v_h, y_h\, \mathbf{b}\cdot\nabla\psi_h(y_h)) = \langle DI_h(u_h(y_h)), v_h\rangle \quad \forall\, v_h \in V_h$$

and the Fréchet derivative of Φ_h is given by

$$\langle D\Phi_h(y_h), \tilde{y}_h\rangle = -(\mathscr{L}_h u_h(y_h) - f, \tilde{y}_h\, \mathbf{b}\cdot\nabla\psi_h(y_h))\,.$$

5 Choice of the functional I_h

In this section, we propose various choices of the functional I_h introduced in the previous section and present numerical results illustrating the properties of these functionals.

All numerical results were computed for $\Omega = (0,1)^2$ and, in all cases, we considered a triangulation $\mathscr{T}_h$ of Ω constructed by dividing Ω into 32×32 equal squares and each square into two triangles by drawing a diagonal from bottom right to top left. The space W_h consisted of continuous piecewise linear functions. The functional Φ_h was minimized using the BFGS method [4]. The SUPG parameter was initialized by (2) and the SOLD parameter by 0. The SUPG parameter satisfied the constraints (3) and the SOLD parameter was required to be in the interval $[0,1]$.

In each iteration of the BFGS method, one has to solve once the adjoint problem and several times the discrete problem for various values of the stabilization parameter. Consequently, the cost of the computation of an optimized SUPG stabilization parameter is significantly higher than the computation of the SUPG solution for a prescribed stabilization parameter. Comparing the cost of the optimization with the cost of the solution of a nonlinear SOLD method, the difference is not so large. We believe that the higher computational cost of the parameter optimization is justified by the quality of the resulting approximate solution, cf. the examples in this section.

We denote by $\Gamma^+ = \overline{\{\mathbf{x}\in\partial\Omega\,;\,(\mathbf{b}\cdot\mathbf{n})(\mathbf{x}) > 0\}}$, $\Gamma^0 = \overline{\{\mathbf{x}\in\partial\Omega\,;\,(\mathbf{b}\cdot\mathbf{n})(\mathbf{x}) = 0\}}$ the outflow and characteristic boundaries of Ω, respectively. Furthermore, we set

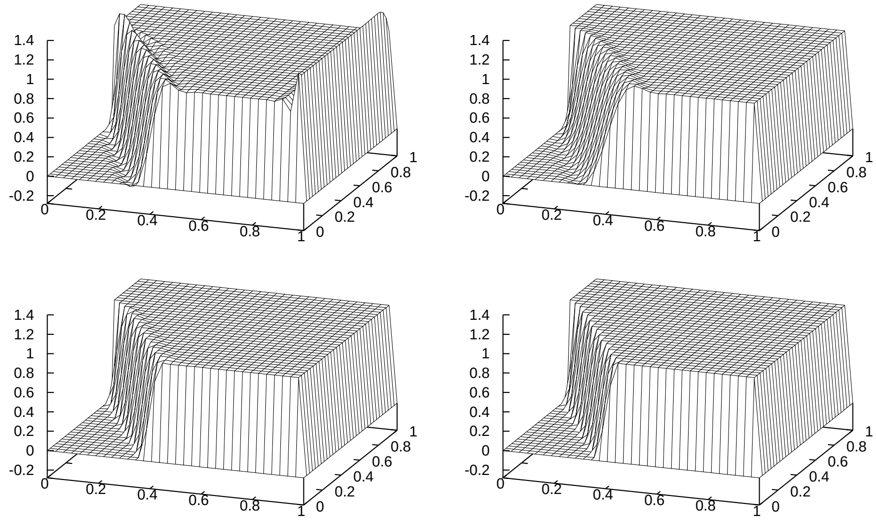

Fig. 1 Example 1: SUPG standard (top left), SUPG optimized using I_h^{res} (top right), SUPG optimized using $I_h^{\text{res}} + \alpha\, I_h^{\text{cross}}$ (bottom left), SOLD optimized using $I_h^{\text{res}} + \alpha\, I_h^{\text{cross}}$ (bottom right)

$$G_h = \bigcup_{K\in\mathscr{G}_h} \overline{K} \qquad \text{with} \qquad \mathscr{G}_h = \{K \in \mathscr{T}_h;\, \overline{K}\cap\Gamma^+ \neq \emptyset \ \text{ or } \ \overline{K}\cap\Gamma^0 \neq \emptyset\}\,.$$

Note that G_h represents a strip along Γ^+ and Γ^0 made up of elements of $\mathscr{T}_h$ having at least one vertex on these parts of the boundary. A functional characterizing the quality of an approximate solution u_h of (1) can be now defined by

$$I_h^{\text{res}}(u_h) = \|\mathscr{L}_h u_h - f\|^2_{0,\Omega\setminus G_h}\,.$$

We exclude the strip G_h since even a nodally exact solution has a large error in G_h. Let us apply the functional I_h^{res} to the numerical solution of the following example.

Example 1. (Solution with an interior layer and two exponential boundary layers) We consider the convection-diffusion equation (1) with $\Omega = (0,1)^2$, $\varepsilon = 10^{-8}$, $\mathbf{b} = (\cos(-\pi/3), \sin(-\pi/3))^T$, $c = f = 0$, $u_b(x,y) = 0$ for $x = 1$ or $y \leq 0.7$, and $u_b(x,y) = 1$ else. The function u_b could also be replaced by a function from $H^{1/2}(\partial\Omega)$ leading to the same numerical results as presented in this paper.

Fig. 1 (top left) shows the SUPG solution computed with the stabilization parameter τ_K given by (2). If we optimize the stabilization parameter using the functional I_h^{res}, the spurious oscillations along the exponential boundary layer are removed but those along the interior layer are not suppressed sufficiently. Moreover, the interior layer is smeared, see Fig. 1 (top right).

If we observe a cut through the solution in Fig. 1, top left, across the interior layer, we shall see a curve like in Fig. 2 A. We would like to compute a solution

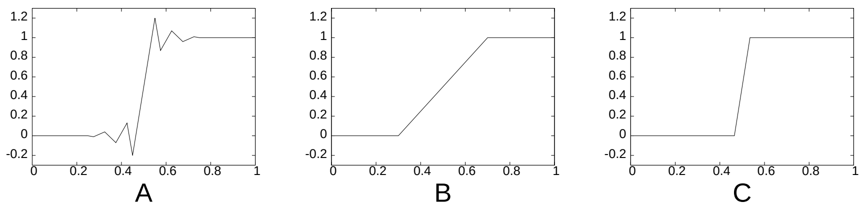

Fig. 2 Idealized cuts through approximate solutions across an interior layer

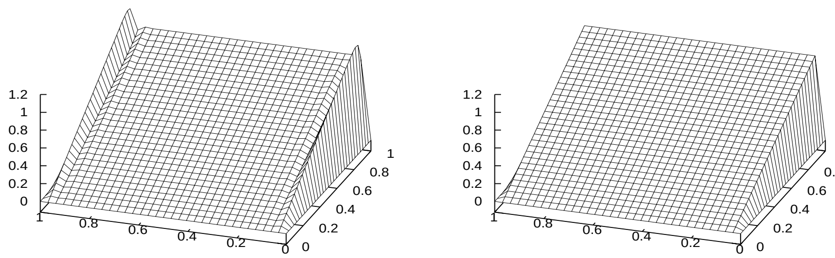

Fig. 3 Example 2: SUPG standard (left), SOLD optimized using I_h^{res} (right)

without spurious oscillations corresponding to Fig. 2 B or C. A candidate for a functional which prefers a solution without spurious oscillations is $\int_0^1 |u'|^p \mathrm{d}x$, where u represents the functions in Fig. 2. Denoting by d the width of the layer in Fig. 2 B or C, the integral equals d^{1-p}. Since we prefer the curve C, we have to use $p < 1$. Thus, we may consider the functional

$$I_h^{\text{cross}}(u_h) = \int_{\Omega \setminus G_h} \sqrt{|\mathbf{b}^{\perp} \cdot \nabla u_h|}\, \mathrm{d}\mathbf{x}\,,$$

where $\mathbf{b}^{\perp}$ is a unit vector orthogonal to $\mathbf{b}$. In our implementation, the square root is regularized near 0, see [3] for details. If we now optimize the SUPG stabilization parameter using a combination of I_h^{res} and I_h^{cross}, the solution improves considerably, see Fig. 1 (bottom left). Finally, if we perform the optimization with the same functional but for the SOLD method, we obtain a solution without any visible spurious oscillations and with steep layers, see Fig. 1 (bottom right).

Example 2. (Solution with one exponential and two parabolic boundary layers) We consider the convection-diffusion equation (1) with $\Omega = (0,1)^2$, $\varepsilon = 10^{-8}$, $\mathbf{b} = (1,0)^T$, $c = 0$, $f = 1$, and $u_b = 0$.

For this example, a comparison of the SUPG solution without parameter optimization and an optimized SOLD solution is given in Fig. 3. It can be observed, that the parameter optimization leads to an almost nodally exact solution.

Example 3. (Solution with two interior layers) We consider the convection-diffusion equation (1) with $\Omega = (0,1)^2$, $\varepsilon = 10^{-8}$, $\mathbf{b}(x,y) = (-y,x)^T$, and $c = f = 0$. On $\Gamma^N := \{0\} \times (0,1)$, we prescribe a homogeneous Neumann boundary condition

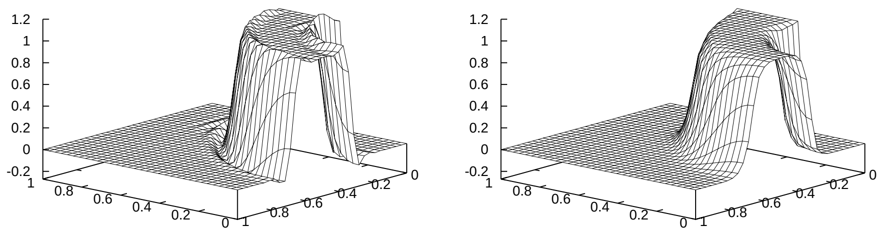

Fig. 4 Example 3: SUPG standard (left), SOLD standard (right)

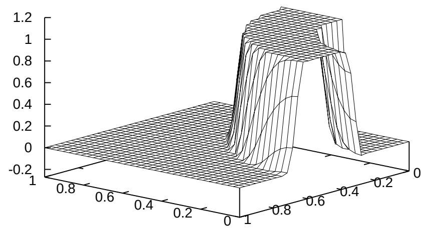

Fig. 5 Example 3: SOLD optimized using I_h^{cross}

whereas the Dirichlet boundary condition is considered only on $\Gamma^D := \partial\Omega \setminus \overline{\Gamma^N}$ with $u_b(x,y) = 1$ for $(x,y) \in (1/3, 2/3) \times \{0\}$ and $u_b(x,y) = 0$ else on Γ^D.

Fig. 4 shows results for this example obtained without parameter optimization. We see that the SOLD method suppresses the oscillations present in the SUPG solution but leads to a slight smearing of the layers. The quality of the SOLD solution obtained using parameter optimization is much better, see Fig. 5.

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