ON COMPUTING THE STABILIZATION PARAMETER FOR THE SOLUTION OF ADVECTIVE-DIFFUSIVE PROBLEMS OBTAINED BY FEM

Miguel Angel Moreles, Salvador Botello and Miguel Castillo

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1 Introduction

Accurate modeling of the interaction between convective and diffusive processes is a challenging task in the numerical approximation of partial differential equations. This is partly because the dimensionless parameter that measures the relative strength of the diffusion is quite small, in comparison with the advective parameter. So one often deals with situations where thin boundary and interior layers are present, and singular perturbation problems arise. See K.W. Morton [3] for a mathematical and numerical analysis of these matters.

It is widely accepted that most classical methods, finite difference, finite element, etc., require the addition of some balancing diffusion terms to obtain realistic numerical solutions of advective-diffusive problems. In particular, these additional terms smooth out local oscillation, thus stabilizing the solution in the vicinity of high gradients.

Several methods with the stabilization property have been introduced in the literature. Popular techniques are Artificial diffusion (Zienkiewicz & Taylor [7]), Streamline-Upwind Petrov-Galerkin (SUPG) (Codina [1]), Subgrid Scale (Hughes et al [2]), etc. In all cases, a proper choice of the so called stabilization parameter is of paramount importance. Unfortunately, most of the existing procedures are based on somewhat heuristic procedures.

An alternative method was introduced by Oñate [4],[5], and extended in Oñate and Manzan [6]. The method is known as the Finite Increment Calculus (FIC) method. It is based on a concept of flow balance over an infinitesimal size domain. It allows to derive most stabilized methods using physical arguments. Additionally, the FIC approach provides a general framework for computing the stabilization parameters in an objective manner.

A careful study of the FIC method shows some room for improvement. In the context of the steady state advection-diffusion equation, we present some unwanted aspects of the method, and appropriate modifications to correct them.

The first step in the FIC method is to derive stabilized versions of the classical advective-diffusive equations, as well as stabilized versions of the Neumann boundary conditions. The infinitesimal size domain to derive such boundary
conditions, does not correspond to the size of the domains in the interior. We shall show that this inconsistency is corrected when considering the weak formulation of the stabilized equation.

The stabilization parameter is computed in each domain of discretization, e.g. in each element when using FEM. The iterative scheme for computation of the stabilization parameter, say \( \alpha^{(e)} \), is roughly as follows:

1. Solve the stabilized problem by FEM with an initial guess of \( \alpha^{(e)}_0 \) and \( \alpha^{(e)}_0 \).
   
   Let \( \alpha^{(e)}_0 = \alpha^{(e)}_0 \).

2. Compute an enhanced solution of the stabilized problem with parameter \( \alpha^{(e)}_c \).

3. In terms of both solutions, compute an enhanced stabilization parameter, \( \alpha^{(e)}_+ \).

4. Repeat 2 and 3 until a satisfactory stable numerical solution is found or else \( \|\alpha^{(e)}_+ - \alpha^{(e)}_0\| \leq \varepsilon \), where \( \varepsilon \) is a prescribed tolerance.

Computing an enhanced solution in 2, can be achieved by projecting into the original mesh an improved solution obtained via global/local smoothing. Our proposal is to smooth out the solution using a technique based on distributional derivatives. This technique proves to be simple, cheap and effective.

A more delicate matter is the computation of \( \alpha^{(e)}_+ \) in 3. The expressions for this computation involve residuals that may lead to roundoff/overflow errors. Here we propose residuals by localizing the weak formulation, this device leads to a stable computation of \( \alpha^{(e)}_+ \). Moreover, a stable numerical solution is obtained.

The outline is as follows.

In Section 2, we present the classical advection-diffusion equation, as well as the stabilized equation in the interior of the domain. Next, the weak formulation is derived obtaining the stabilized Neumann boundary condition rigorously.

A proposal for the computation of the stabilization parameter, is presented in Section 3. Here we also introduce a technique to compute an enhanced solution.

In Section 4, we test the method with several examples. In all cases we show the oscillatory behavior of the FEM solution, and its stabilization after a few iterations.

We conclude our exposition with a few comments about the method and future research.

## 2 Weak formulation of stabilized advective-diffusive problems

For a transport variable \( \phi \), the classical advective-diffusive equation in a smooth domain \( \Omega \) with a distributed source \( Q \), is
\[-\nabla \cdot (D \nabla \phi) + \nu \nabla \cdot f = Q, \quad \text{in } \Omega \tag{1}\]

where \( f = \phi u \) is the advective flux vector,

\[\nabla = \begin{pmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{pmatrix}^T\]

is the gradient operator, and

\[D = \begin{bmatrix} k_x & 0 \\ 0 & k_y \end{bmatrix}\]

is the conductivity matrix. In (1) \( \nu \) is the advective flux parameter which will be assumed to be constant throughout the domain \( \Omega \).

To have a well posed problem, boundary conditions are prescribed as follows:

\[\phi - \tilde{\phi} = 0, \quad \text{on } \Gamma_\phi\]

where \( \Gamma_\phi \) is the Dirichlet boundary, where the variable is prescribed, and

\[-\nu \phi u \cdot n + (D \nabla \phi) \cdot n + \bar{q} = 0, \quad \text{on } \Gamma_q\]

where \( \bar{q} \) is the prescribed total flux across the Neumann boundary \( \Gamma_q \). As usual \( \Gamma = \partial \Omega = \Gamma_\phi \cup \Gamma_q \), and \( n \) is the outward normal vector.

When the advective term is dominant in (1) oscillating solutions are obtained by the classical methods. A remedy is to consider a stabilized version of (1), namely

\[r - \frac{1}{2} h \cdot \nabla r = 0, \quad \text{in } \Omega \tag{2}\]

where

\[r = -\nabla \cdot (D \nabla \phi) + \nu \nabla \cdot f - Q\]

The Dirichlet boundary condition remains unchanged,

\[\phi - \tilde{\phi} = 0, \quad \text{on } \Gamma_\phi \tag{3}\]

whereas, the condition on the Neumann boundary becomes

\[-\nu \phi u \cdot n + (D \nabla \phi) \cdot n + \bar{q} - \frac{1}{2} h \cdot n r = 0, \quad \text{on } \Gamma_q \tag{4}\]

Remark. It is noteworthy, that the stabilized equation (2) is equivalent, under appropriate modifications, to well known stabilization techniques, e.g., artificial diffusion, Petrov-Galerkin, etc. See Oñate & Manzan [6]. In all cases, the choice of the stabilization vector \( h \) is a nontrivial matter.
2.1 Weak formulation

Without loss of generality assume that \( \hat{\phi} = 0 \) in (3). Let \( N \) be a suitable smooth function which vanishes on \( \Gamma_\phi \). Multiply (2) by \( N \), we obtain after integration by parts

\[
(DV\phi, \nabla N) - \nu (\phi, \nabla N \cdot u) + \frac{1}{2} \left( (\nabla \cdot (DV\phi) + \nu \nabla \cdot (\phi u)), \nabla \cdot (Nh) \right) + \\
+ \int_{\Gamma_q} N \left( -DV\phi + \nu \phi u - \frac{1}{2} rNh \right) \cdot n d\Gamma = (Q, N) - \frac{1}{2} (Q, \nabla \cdot (Nh))
\]

where \((\cdot, \cdot)\) is used to denote the \( L^2 \) inner product over \( \Omega \) of either scalar or vector quantities, that is

\[
(f, g) = \int_{\Omega} f \cdot g d\Omega
\]

The first three terms in (5) define a bilinear form

\[
a_h (\phi, N) = (DV\phi, \nabla N) - \nu (\phi, \nabla N \cdot u) + \frac{1}{2} \left( (\nabla \cdot (DV\phi) + \nu \nabla \cdot (\phi u)), \nabla \cdot (Nh) \right)
\]

On the other hand, by substituting the flux boundary condition (4) on (5) we obtain a linear functional

\[
l_h (N) = (Q, N) - \frac{1}{2} (Q, \nabla \cdot (Nh)) + \int_{\Gamma_q} qNd\Gamma
\]

The bilinear form is well defined for \( \phi, N \in H^2(\Omega) \). The solution \( \phi \) must equal zero on \( \Gamma_\phi \), so we introduce the subspace \( V \) of \( H^2(\Omega) \) as follows

\[
V = \{ N \in H^2(\Omega) : N = 0, \ \text{on} \ \Gamma_q \}
\]

The weak formulation of problem (2) together with boundary conditions (3), (4) is as follows: find \( \phi \in V \) such that

\[
a_h (\phi, N) = l_h (N), \ \text{for all} \ \ N \in V \tag{6}
\]

**Remark.** If the Dirichlet data can be extended over the region \( \Omega \) to give a function \( \Phi \in H^2(\Omega) \), define

\[
\phi = \phi_0 + \Phi.
\]

The problem becomes: find \( \phi_0 \in V \) such that

\[
a_h (\phi_0, N) = l_h (N) - a_h (\Phi, N), \ \text{for all} \ \ N \in V
\]

Notice that if \( h = 0 \) the classical problem is obtained. In such a case we require functions only in \( H^1(\Omega) \).
Remark. The stabilized equation (2) is obtained by the so called FIC method introduced by Oñate [4]. Firstly, fluxes are balanced in an infinitesimal domain. Secondly, higher order Taylor polynomials are used to express all resulting function in terms of a distinctive point in the infinitesimal domain. To derive the stabilized Neumann boundary condition (4), the size of the domain is reduced to one half, and the order of expansion of the source term is also reduced. This device is rather artificial and unnecessary. Notice that to obtain the weak formulation, the stabilized Neumann boundary condition (4), arises in (5) rather naturally.

3 A proposal for computation of the stabilization parameter

For simplicity we shall illustrate the procedure to estimate the stabilization parameter when the Dirichlet data is zero.

Let us write

\[ a_h (\phi, N) = a (\phi, N) + \frac{1}{2} \left( -\nabla \cdot (D \nabla \phi) + \nu \nabla \cdot (\phi u) \right), \nabla \cdot (Nh) \]

and

\[ l_h (N) = l(N) - \frac{1}{2} (Q, \nabla \cdot (Nh)) \]

where

\[ a (\phi, N) = (D \nabla \phi, \nabla N) - \nu (\phi, \nabla N \cdot u) \]

and

\[ l(N) = (Q, N) + \int_{\Gamma} q Nd \Gamma \]

Here \( a (\phi, N) \) and \( l(N) \) correspond to the classical case.

Let us consider a finite element discretization \( \{ \Omega(e) \} \) of \( \Omega \) with index \( e \) ranging from 1 to the number of elements \( N_e \). The standard interpolation of \( \phi \) within \( \Omega(e) \) with \( n \) nodes can be written as

\[ \phi(x) \approx \hat{\phi}(x) = \sum_{j=1}^{n} \phi_j N_j(x) \]

where \( N_j \) are the FEM-basis functions and \( \phi_j \) are the nodal values.

Let us assume that the stabilization vectorial function \( h \) is constant in element \( \Omega(e) \). We write \( h \) in the form

\[ h = \alpha \left| \Omega(e) \right| p \]
where \( p \) is a constant unit vector, and \( \alpha \) is the stabilization parameter in element \( \Omega^{(e)} \). The vector \( p \) is chosen along (an approximation of) the gradient in the element \( \Omega^{(e)} \). We compute \( \alpha \) as follows.

For FEM computations, the element \( \Omega^{(e)} \) is mapped, from global to local variables, onto a canonical element, \( \Omega^{(c)} \), \( x \mapsto \xi \). From this map we may identify the shape function \( N_{j_0} \) which corresponds to the local shape function based at the origin.

Let us form the residual
\[
 r(\hat{\phi}, \alpha) = a_h(\phi, N_{j_0}) - l_h(N_{j_0})
\]
or
\[
 r(\hat{\phi}, \alpha) = a(\phi, N_{j_0}) + \frac{1}{2} \left( \left(-\nabla \cdot (D\nabla \phi) + \nu \nabla \cdot (\phi u) \right), \nabla \cdot (N_{j_0} h) \right) - \ldots 
 l(N_{j_0}) - \frac{1}{2} (Q, \nabla \cdot (N_{j_0} h)) 
\]

By (7) we have
\[
 r(\phi, \alpha) = a(\phi, N_{j_0}) - l(N_{j_0}) + \ldots 
\]
\[
 \frac{1}{2} \alpha |\Omega^{(e)}| \left( \left(-\nabla \cdot (D\nabla \phi) + \nu \nabla \cdot (\phi u) \right), \nabla \cdot (N_{j_0} p) \right) - \ldots 
\]
\[
 \frac{1}{2} \alpha |\Omega^{(e)}| (Q, \nabla \cdot (N_{j_0} p)) 
\]

We proceed iteratively as follows. Let us assume \( \alpha_k \) is known and compute a solution \( \phi_k \) from (6) Let \( \psi_k \) be an enhanced numerical solution found by global smoothing, see below.

Solve for \( \alpha_{k+1} \) from the linear equation
\[
 r(\hat{\phi}_k, \alpha_k) - r(\hat{\psi}_k, \alpha_{k+1}) = 0 
\]
and continue with the next iteration until convergence.

**3.1 Smoothing a solution by means of distributional derivatives**

Let \( f \) be a locally integrable function defined in \( \Omega \). Then, weak derivatives of \( f \) are defined as follows
\[
 \left< \frac{\partial}{\partial x_j} f, \varphi \right> = - \left( f, \frac{\partial}{\partial x_j} \varphi \right), \quad \text{for all } \varphi \in C_c^\infty(\Omega) 
\]
we recall that if \( f \) is smooth, then its weak derivatives coincide with its classical derivatives.
Let $\hat{\phi}$ be as in (6). We approximate $\frac{\partial}{\partial x_j} \hat{\phi}$ by means of the same basis $\{N_j\}$, that is

$$\frac{\partial}{\partial x_k} \hat{\phi} = \sum_{j=1}^{n} \phi_j^k N_j$$

In light of (8) we obtain

$$\left( \sum_{j=1}^{n} \phi_j^k N_j, \varphi \right) = - \left( \hat{\phi}, \frac{\partial}{\partial x_k} \varphi \right)$$

By using $N_j$ as weighing functions, a linear systems is obtained for the unknowns $\{\phi_j^k\}$, namely

$$\sum_{j=1}^{n} (N_j, N_i) \phi_j^k = - \sum_{j=1}^{n} \phi_j^k \left( N_j, \frac{\partial}{\partial x_k} N_i \right), \quad i = 1, 2, \ldots, n$$

Notice that $\{\phi_j^k\}$ approximate the nodal values of $\frac{\partial}{\partial x_j} \hat{\phi}$.

## 4 Numerical examples

Let us test the method in some benchmark examples. Due to a large Peclet number, oscillations are exhibited when using classical numerical solutions. We illustrate this by using FEM.

**Example 1.** Consider the 1D advection-diffusion problem:

$$-0.01 \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial \phi}{\partial x} = \sin \pi x; \quad 0 \leq x \leq 1; \quad \phi_0 = \phi_1 = 0$$

In this case, the Peclet number, $\left( \frac{u L}{D} \right)$, is 2.5. The solution is attempted using a mesh of 20 linear elements. Convergence is attained only after 10 iterations of the stabilization parameter. See Figure 1.
Evolution of the solution in Example 1.

The evolution of the stabilization parameter in each element is shown in Figure 2.

Example 2. Now consider the partial differential equation:
In Figure 3, we show the evolution of the solution. Again we use a mesh of 20 linear elements. Here, the Peclet number is 5.

\[-0.005 \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial \phi}{\partial x} = 0; \quad 0 \leq x \leq 1; \quad \phi_0 = 0; \quad \phi_1 = 1\]

Notice that convergence is attained as before in 10 iterations. The stabilization parameter evolves as in Figure 4.
Evolution of the stabilization parameter in each element for Example 2.

Problems in two dimensions pose additional difficulties. We show the performance of our method in four troublesome examples.

Example 3. Let us consider a problem with non uniform Dirichlet boundary conditions. The data is as follows:

\[
\Omega = \left[ -\frac{1}{2}, \frac{1}{2} \right] \times \left[ -\frac{1}{2}, \frac{1}{2} \right],
\]

\[
u = [1, -2]^T,
\]

\[
k_x = k_y = 10^{-6},
\]

\[
Q(x, y) = 0,
\]

\[
\phi = \begin{cases} 
100 & (x, y) \in \Gamma_{\phi_1} \\
0 & (x, y) \in \Gamma_{\phi_2}
\end{cases}
\]

Where \( \Gamma_{\phi_1} = \{ -1/2 \} \times [1/4, 1/2] \cup \{ -1/2 \} \times [1/2, \infty \}, \Gamma_{\phi_2} = \Gamma_{\phi} \setminus \Gamma_{\phi_1} \) and \( \Gamma_{\phi} = \emptyset \).

A structured mesh of 576 linear quadrangular has been chosen (24X24 regular divisions). The initial value of \( \alpha \) is \([0, 0]^T\). Figure 5 shows the oscillatory distribution of \( \phi \) in the initial solution.
We run 10 iterations. Results are shown in Figures 7 and 8.

Final distribution of $\phi(x,y)$ in the 10th iteration of Example 3.
3D view of the Final distribution of $\phi(x, y)$ in the $10^{th}$ iteration of Example 3.

The value and distribution of the stabilization parameter are in Figures 9 and 10.

Contour of the magnitude of stabilization parameter in the $10^{th}$ iteration of Example 3.
Direction of stabilization parameter in the 10th iteration of Example 3.

**Example 4.** We have a 2D advection-diusion with Neumann and Dirchlet conditions.

\[ \Omega = [0, 1] \times [0, 1], \]
\[ u = [1, 1]^T, \]
\[ k_x = k_y = 10^{-10}, \]
\[ Q(x, y) = 0, \]
\[ \phi = \begin{cases} 
100 & (x, y) \in \Gamma_{\phi_1} \\
0 & (x, y) \in \Gamma_{\phi_2}
\end{cases} \]
\[ q_n = 0. \]

Where \( \Gamma_{\phi_1} = \{1\} \times [0, 1], \Gamma_{\phi_2} = \Gamma_\phi - \Gamma_{\phi_1}, \) and \( \Gamma_q = [0, 1] \times \{1\}. \)

A structured mesh of 400 linear quadrangular has been chosen (20x20 regular divisions). In this case, the solution is \( \phi = 0 \) in the domain, except in a neighborhood of \( \Gamma_{\phi_1}. \) In Figures 11 and 12 we can see the solution in the initial iteration with \( \alpha = [0, 0]^T. \) In Figures 13 and 14 we show the values of the principal variable in the 10th iteration. In Figures 15 and 16, we show the magnitude of the nodal parameter and corresponding direction.
Oscillatory distribution of the initial solution $\phi(x, y)$ in Example 4.

3D view of oscillatory distribution of the initial solution $\phi(x, y)$ in Example 4.

We run again ten iterations. Results in Figure 13 and 14.
Final distribution $\phi(x, y)$ in the $10^{th}$ iteration of Example 4.

3D view of the final distribution $\phi(x, y)$ in the $10^{th}$ iteration of Example 4.
Contour of the magnitude of stabilization parameter in the 10\textsuperscript{th} iteration of Example 4.

Direction of stabilization parameter in the 10\textsuperscript{th} iteration of Example 4.

**Example 5.** The following example is a non constant velocity vector in a convection diffusion problem with non uniform Dirchlet conditions.
\[\Omega = ]0, 1[ \times ]0, 1[, \]
\[u = [2y(1 - (2x - 1)^2), -2(2x - 1)(1 - y^2)]^T, \]
\[k_x = k_y = 1/200, \]
\[Q(x, y) = 0, \]
\[\bar{\phi} = \begin{cases} 
1 + \text{tanh}(10 + 20(2x - 1)) & (x, y) \in \Gamma_{\phi_1} \\
2 & (x, y) \in \Gamma_{\phi_2} \\
0 & (x, y) \in \Gamma_{\phi_3} 
\end{cases} \]

Where \(\Gamma_{\phi_1} = [1/2, 1] \times \{1\}, \Gamma_{\phi_2} = [0, 1/2] \times \{1\}, \Gamma_{\phi_3} = \Gamma_{\phi} - \Gamma_{\phi_1} - \Gamma_{\phi_2} \) and \(\Gamma_{\phi} = \emptyset\).

A structured mesh of 256 linear quadrangular has been chosen (16X16 regular divisions). In Figures 17 and 18 we can see the solution in the initial iteration with \(\alpha = [0, 0]^T\). Figures 19 and 20 shows the values of principal variable in the 10th iteration. In Figure 21 and 22, we show the magnitude of the nodal parameter and the correspondent direction.

Oscillatory distribution of \(\phi(x, y)\) in Example 5.
Figure 1: Contour of the final distribution of $\phi(x, y)$ in the $10^{th}$ iteration of Example 5.

3D view of oscillatory distribution of $\phi(x, y)$ in Example 5.
3D view of the final distribution of $\phi(x,y)$ in the 10\textsuperscript{th} iteration of Example 5.

Contour of the magnitude of stabilization parameter in the 10\textsuperscript{th} iteration of Example 5.
Direction of stabilization parameter in the 10th iteration of Example 5.

Example 6. Convection diffusion problem with Dirchlet no uniform conditions and not constant velocity. The conditions of the partial differential equation are:

\[ \Omega = ] - 1/2, 1/2[ \times ] - 1/2, 1/2[ , \]
\[ u = [0, 1]^T, \]
\[ k_x = k_y = 10^{-6}, \]
\[ Q(x, y) = 0, \]
\[ \phi = \begin{cases} 1 & (x, y) \in \Gamma_{\phi_1} \\ 0 & (x, y) \in \Gamma_{\phi_2} \end{cases} \]

where \( \Gamma_{\phi_1} = [0, 1/2] \times \{0\} \cup \{1\} \times [-1/2, 1/2], \Gamma_{\phi_2} = \Gamma_{\phi} - \Gamma_{\phi_1} \) and \( \Gamma_q = \emptyset \). A structured mesh of 625 linear quadrangular has been chosen (25X25 regular divisions). In Figures 23 and 24 the solution in the initial iteration with \( \alpha = [0, 0]^T \). Figures 25 and 26 shows the values of principal variable in the 10th iteration. Finally, in Figures 27 and 28, it is shown the magnitude of the nodal parameter and the corresponding direction.
Contour of the oscillatory distribution of $\phi(x, y)$ in the initial solution of Example 6.

3d view of the oscillatory distribution of $\phi(x, y)$ in the initial solution of Example 6.
Contour of final distribution of $\phi(x, y)$ in the 10th iteration of Example 6.

3D view of final distribution of $\phi(x, y)$ in the 10th iteration of Example 6.
Contour of the magnitude of stabilization parameter in the 10th iteration of Example 6.

Direction of stabilization parameter in the 10th iteration of Example 6.
5 Final comments

We have introduced an alternative method to compute the stabilization parameter in the FIC method. It has the following features:

- It does not require any analysis to derive an initial guess for the stabilization parameter, it starts at zero.
- Convergence is attained in a few iterations.
- It works satisfactorily with coarse meshes.

We have also presented an analysis of the weak formulation of the stabilized equation. Consequently, the stabilized Neumann boundary condition is obtained rigorously.

An important step in stabilization methods, is the computation of enhanced solutions. Based on distributional derivatives, we have introduced a simple and efficient technique.

Currently, we are testing our method on transient, as well as 3d problems. Our results are promising.

References


