A nonlinear weak constraint enforcement method for advection-dominated diffusion problems

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Abstract

We devise a stabilized method to weakly enforce bound constraints in the discrete solution of advection-dominated diffusion problems. This method combines a nonlinear penalty formulation with a discontinuous Galerkin-based residual minimization method. We illustrate the efficiency of this scheme for both uniform and adaptive meshes through proper numerical examples.

Keywords: constraint enforcement, advection-diffusion-reaction, adaptive stabilized finite element method, residual minimization, discontinuous Galerkin method

1. Introduction

Standard (Galerkin) finite element methods (FEM) can yield unphysical oscillatory discrete solutions in advection-dominated regimes. A commonly used technique to overcome this weakness of the formulation is to add stabilized terms that enhance the properties of the discrete solution. Some of these techniques yield Petrov-Galerkin schemes, such as the SUPG method [7] or the streamline diffusion (SD) method [19]. Other stabilization techniques include least-squares formulations [5], variational multiscale (VMS) [18], subgrid viscosity [16], and continuous interior penalty methods (CIP) [10], among others.

Although stabilized formulations improve the robustness and accuracy of the numerical solutions, spurious undershoots and overshoots are not eliminated, especially in low-resolution meshes. These oscillations are a drawback as in many engineering applications (i.e., transport of density, concentration, or temperature) require to remain within their physical range. Violating this bounds delivers poor simulation outputs. Thus, overshoots or undershoots are controlled through proper constraint enforcement procedures. For that reason, a plethora of techniques to surmount this effect has been proposed, mostly constructed from a stabilized formulation. One of these schemes incorporates shock-capturing terms to satisfy a discrete maximum principle [8, 23]. Also, flux-corrected methods [21, 22] seek to impose the constraints by altering the system matrix. These methods are generally only first-order accurate. Higher-order schemes require terms to control and, in many times, reduce the dissipative response of the method.

More recently, an alternative constraint imposition approach –more precisely, positivity preserving– was proposed in [9]. The authors satisfy the discrete maximum principle weakly by adding a consistent penalty term to the variational formulation of a Galerkin least-squares (Ga-LS) finite element discretization. This method is flexible and can incorporate a priori lower and upper bounds on the discrete solution, by simply adding the corresponding consistent penalty term to the discrete formulation. We combine this consistent penalization with a new adaptive stabilized finite element framework that minimizes the residual in dual norms of discontinuous Galerkin (dG) methods [11]. This formulation inherits the stability and accuracy of the underlying dG approximation. The formulation seeks for a solution in a continuous trial function space which is a proper subspace of the dG function space. The resulting saddle-point problem delivers stable formulations with continuous solutions with a robust a posteriori error estimate, which can be computed on the fly to drive opti-
nal adaptive mesh refinements.

In this paper, we develop a constraint enforcement technique that combines the ideas of the nonlinear penalty method of [9], and the residual minimization technique of [11], applied to advection-dominated diffusion problems. We construct it as follows. First, we modify the corresponding bilinear dG form by adding a nonlinear penalty term to enforce constraints weakly. Next, we solve a residual minimization problem in a dG dual norm. The resulting technique minimizes weakly the violation of solution bounds and additionally delivers a robust residual estimator to guide adaptive mesh refinement. The main advantage of considering this procedure is that it results in a nonlinear saddle-point problem, with symmetric Jacobian. Therefore, an extensive procedure is that it results in a nonlinear saddle-point problem. Besides, we detail the adopted resolution refinement. The main advantage of considering this process is that it results in a nonlinear saddle-point problem, with symmetric Jacobian. Therefore, an extensive procedure is that it results in a nonlinear saddle-point problem. Henceforth, we assume that there is a real number \( \sigma_0 \geq 0 \), such that \( \sigma - \frac{\lambda}{\rho} \beta \geq \sigma_0 \) in \( \Omega \). Owing to the above assumptions, the Lax-Milgram Lemma implies that problem (2) is well posed [12]. In what follows, we assume that the exact solution \( u \) is in \( H^2(\Omega) \). If the reaction source satisfies \( \sigma \geq 0 \), problem (2) also satisfies a maximum principle, that is, under suitable assumptions on the data \( f \) and \( g \), the solution attains its maximum or minimum at the boundary. In particular, if \( f \geq 0 \) and \( g \geq 0 \), then \( u(x) \geq 0, \forall x \in \Omega \). Similarly, in pure convection-diffusion problems (i.e., if \( f = 0 \) and \( \sigma = 0 \)), then \( \min_{y \in \Omega} g(y) \leq u(x) \leq \max_{y \in \Omega} g(y), \forall x \in \Omega \). For a detailed discussion on maximum principles for elliptic second-order problems see [15].

Given that in this work we focus on advection-dominated cases, that is, when \( ||\sigma||_{\infty}, ||K||_{\infty} \ll ||\beta||_{\ell} \), when \( \ell \) is a length scale, we conveniently split the boundary \( \partial \Omega \equiv \Gamma \cup \Gamma_0 \cup \Gamma_+ \), with

\[
\begin{align*}
\Gamma_- &= \{ x \in \Gamma ; \beta \cdot n < 0 \} \quad \text{(inflow boundary)}, \\
\Gamma_0 &= \{ x \in \Gamma ; \beta \cdot n = 0 \} \quad \text{(characteristic boundary)}, \\
\Gamma_+ &= \{ x \in \Gamma ; \beta \cdot n > 0 \} \quad \text{(outflow boundary)},
\end{align*}
\]

where \( n \) represents the outward normal vector to \( \Gamma \).

2. Model problem: diffusion–advection–reaction

In this section, we present all the required ingredients for the constraint enforcement method in the context of advection-diffusion-reaction problems. Let \( \Omega \) be an open, bounded Lipschitz domain in \( \mathbb{R}^d, d \in \{2, 3\} \), with boundary \( \partial \Omega \); \( \beta : \Omega \to \mathbb{R}^d \) be an advective velocity field; \( K \in \mathbb{R}^{d \times d} \) be a diffusion tensor, assumed to be continuous, symmetric and positive-definite; and \( \sigma : \Omega \to \mathbb{R} \) is a reaction coefficient. We assume that \( f : \Omega \to \mathbb{R} \) is a given source term, and \( g : \Gamma \to \mathbb{R} \) is a prescribed Dirichlet boundary condition. We consider the following advection-diffusion-reaction problem:

\[
\begin{align*}
A(u) &:= -\nabla \cdot (K \nabla u) + \beta \cdot \nabla u + \sigma u = f, \quad \text{in } \Omega, \\
u &\equiv g, \quad \text{on } \Gamma,
\end{align*}
\]

where, using the standard notation, we assume that \( \beta \in [W^{\frac{1}{2},\infty}(\Omega)]^d, \sigma \in L^2(\Omega), f \in L^2(\Omega) \) and \( g \in H^{1/2}(\partial \Omega) \). Then, the weak formulation of (1) becomes:

\[
\begin{align*}
&\text{Find } u \in H^1(\Omega), \text{ such that:} \\
&(K \nabla u, \nabla v)_{\Omega} + (\beta \cdot \nabla u, v)_{\partial \Omega} + (\sigma u, v)_{\Omega} = (f, v)_{\Omega}, \\
&v \in H^1_0(\Omega)
\end{align*}
\]

\[(2)\]

where \((\cdot, \cdot)_{\Omega}\) denotes the \( L^2 \)-scalar product on \( \Omega \).

In this section, we describe the dG variational formulation that we enlarge by including the constraint enforcement penalty terms.

Let \( \mathcal{T}_h \) be a family of simplicial meshes of \( \Omega \). For simplicity, we assume that any mesh exactly represents \( \Omega \) in \( \mathcal{T}_h \), that is, \( \Omega \) is a polygon or a polyhedron. \( T \) denotes a generic element in \( \mathcal{T}_h \), \( h_T \) denotes the diameter of \( T \) and \( n_T \) its unit outward unit normal. We set \( h = \max_{T \in \mathcal{T}_h} h_T \). We assume, without loss of generality, that \( h \leq 1 \). We define the classical dG approximation space

\[
V_h := \{ v_h \in L^2(\Omega) \mid \forall T \in \mathcal{T}_h, v_h|_T \in \mathbb{P}^p \},
\]

where \( \mathbb{P}^p \) denotes the set of polynomials, defined over \( T \), with polynomial degree smaller or equal than \( p \).
Let \( F \) be an interior face of the mesh if there are \( T^-(F) \) and \( T^+(F) \) in \( \mathcal{T}_h \), such that \( F = T^+(F) \cap T^-(F) \), and we let \( n_F \) be the unit normal vector to \( F \) pointing from \( T^-(F) \) towards \( T^+(F) \). Similarly, \( F \) is a boundary face if there is a \( T(F) \in \mathcal{T}_h \) such that \( F = T(F) \cap \Gamma \), and we let \( n_F \) coincide with \( n \). We collect all the faces or edges into the set \( \mathcal{F}_b = \bigcup_{T \in \mathcal{T}_h} F \). We define the boundary skeleton \( \mathcal{F}_b^b \) as \( \mathcal{F}_b^b = \mathcal{F}_b \cap \Gamma \), and the internal skeleton \( \mathcal{F}_i^b = \mathcal{F}_b \setminus \mathcal{F}_b^b \). Henceforth, we deal with functions that are double-valued on \( \mathcal{F}_b^i \) and single-valued on \( \mathcal{F}_b^b \), for example, all functions in \( V_h \) have these characteristics. On interior faces, when the two branches of the function in question, \( v \), are associated with restrictions to the neighboring elements \( T^+(F) \), we denote these branches by \( v^+ \), and the jump \( \|v\|_F \) and the standard (arithmetic) average \( \|v\|_F \) as

\[
\|v\|_F := v^+ - v^-, \quad \|v\|_F := \frac{1}{2} (v^+ + v^-),
\]

On a boundary face \( F \in \mathcal{F}_b^b \), we set \( \|v\|_F = \|v\|_F \). The subscript \( F \) is omitted from the jump and average operators when there is no ambiguity. Finally, we set \( h_F \) as the diameter of the face \( F \).

Given the previous components, the dG discretized formulation for (1) reads:

\[
\begin{align*}
\text{Find } u_h & \in V_h, \text{ such that:} \\
& b_h(u_h^G, v_h) = l_h(v_h), \quad \forall v_h \in V_h, \quad \tag{3}
\end{align*}
\]

with the bilinear form

\[
b_h(u_h^G, v_h) := b_h^G(u_h^G, v_h) + b_h^{adv}(u_h^G, v_h),
\]

where

\[
b_h^G(w, v) := \sum_{T \in \mathcal{T}_h} (K \nabla w \cdot \nabla v)_{0,T} + \sum_{F \in \mathcal{F}_h} \theta (\|w\|_F, \|K \nabla v\|_F)_{0,F},
\]

\[+ \sum_{F \in \mathcal{F}_h} \eta (\|w\|_F, \|v\|_F)_{0,F},
\]

\[
b_h^{adv}(w, v) := \sum_{T \in \mathcal{T}_h} (\beta \cdot \nabla w + \sigma w, v)_{0,T} + \sum_{F \in \mathcal{F}_h} \theta (\|w\|_F, \|v\|_F)_{0,F},
\]

\[+ \sum_{F \in \mathcal{F}_h} (\beta \cdot n_F w, v)_{0,F} + \sum_{F \in \mathcal{F}_h} \eta (\|w\|_F, \|v\|_F)_{0,F},
\]

and the linear form

\[
l_h(v) := \sum_{F \in \mathcal{T}_h} (f, v)_{0,F} + \sum_{F \in \mathcal{F}_h^b} \eta (g, v)_{0,F} + \sum_{F \in \mathcal{F}_h^b} \theta (\beta, K \nabla v, n)_{0,F}.
\]

For diffusion problems, we recover well-known types of dG formulations for different choices of \( \theta \) and the penalty parameter \( \eta \) in \( b_h^{adv}(w, v) \) (e.g., see [2, 25]). Herein, for our numerical experiments we set the parameters to deliver the SIPG method, that is, \( \theta = -1 \) and, following [26], \( \eta = \eta_0 (p+1)(p+d)K/h \), being \( p \) the polynomial degree for the test functions and \( \eta_0 = 3 \). In the advective part of the bilinear form, \( b_h^{adv}(w, v) \), we use an upwinding scheme (see [6, 14]). The broken polynomial space \( V_h \) can be equipped with the following norm:

\[
\|w\|_{V_h}^{2} := \|w\|_{adv}^{2} + \|w\|_{dG}^{2},
\]

with \( \|w\|_{adv}^{2} \) representing the upwinding norm defined for advection-reaction problems and \( \|w\|_{dG}^{2} \) representing the norm defined by the interior penalty methods for diffusion problems. Thus, these norms read

\[
\|w\|_{adv}^{2} := \|w\|_{0,\Omega}^{2} + \frac{1}{2} \|\beta \cdot n\|^{2} \|w\|_{0,\Gamma}^{2},
\]

\[+ \frac{1}{2} \sum_{F \in \mathcal{F}_h^b} (|\beta \cdot n_F| \|w\|, \|w\|)_{0,F} + \sum_{F \in \mathcal{F}_h^b} h_F \|\beta \cdot \nabla w\|_{0,F}^{2},
\]

\[
\|w\|_{dG}^{2} := \|K \nabla w\|_{0,\Omega}^{2} + \sum_{F \in \mathcal{F}_h} (\eta \|w\|, \|w\|)_{0,F}.
\]

3. Weak constraint enforcement method based on residual minimization

For the sake of simplicity, in the next we assume that the aim is to enforce a positivity preserving condition, that is, \( u \geq 0 \). Other varieties of constraints, such as upper bounds or other minimal values, can also be imposed by considering a slight modification of the nonlinear term (see Remark 1).

3.1. Nonlinear consistent penalty method

Consider the following penalization term (see Remark 2):

\[
\gamma = \gamma_0 \left( \frac{|\beta|}{h} + \frac{\|K\|_{\infty}}{h^2} + \|\sigma\|_{\infty} \right)^{-1},
\]

\[
(4)
\]

3
We define \( \xi_\gamma : v_h \to \mathbb{R} \), as the function:

\[
\xi_\gamma(v_h) := [v_h - \gamma(A(v_h) - f)]_-, \quad \forall v_h \in V_h,
\]

where \( x_- = \frac{1}{2}(x - |x|) \) denotes the negative part of the real number \( x \), satisfying \( x_- = x \) if \( x < 0 \), and \( x_- = 0 \) if \( x \geq 0 \).

We define \( b_h^\gamma(u_h; v_h) \), composed by the original bilinear form \( b_h(u_h; v_h) \) and a nonlinear penalty term, as follows:

\[
b_h^\gamma(u_h; v_h) := b_h(u_h, v_h) + \langle \gamma^{-1} \xi_\gamma(u_h), v_h \rangle_h,
\]

where

\[
(\lambda_h, y_h)_h := \sum_{i,j \in T} (\lambda_h, y_h)_T.
\]

By construction, the analytical solution satisfies that \( \xi_\gamma(u) = 0 \), since \( A(u) = f \) and \( u_- = 0 \). We consider the following discrete problem:

\[
\begin{cases}
\text{Find } u_h \in V_h, \text{ such that:} \\
b_h^\gamma(u_h; v_h) = (\lambda_h(v_h), \forall v_h \in V_h.
\end{cases}
\]

Since \( \xi_\gamma(u) \) vanishes identically in \( \Omega \), exact consistency still holds for (7). Consistency still holds if we substitute the penalty parameter \( \gamma \) by a function taking uniformly positive values in \( \Omega \).

**Remark 1.** The nonlinear form \( b_h^\gamma(u_h; v_h) \) can also impose a constraint on the upper limit of the solution. For instance, if it is known that \( u \in [u_{\min}, u_{\max}] \), \( b_h^\gamma(u_h; v_h) \) can be written as:

\[
b_h^\gamma(u_h; v_h) := b_h(u_h, v_h) + \langle \gamma^{-1} \xi_{\gamma_{\min}}(u_h), v_h \rangle_h + \langle \gamma^{-1} \xi_{\gamma_{\max}}(u_h), v_h \rangle_h,
\]

with \( \xi_{\gamma_{\min}}(u_h) := [(u_h - u_{\min}) - \gamma(A(u_h) - f)]_- \) and \( \xi_{\gamma_{\max}}(u_h) := [(u_{\max} - u_h) - \gamma(A(u_h) - f)]_- \) representing the penalty terms imposed for controlling the lower and upper limits of the solution, respectively.

**Remark 2.** The election of the stabilization term (4) is motivated by the classical stabilization parameters (SUPG, Ga-LS, VMS) for diffusive problems (see [113]), and the stabilization parameter considered in [9] for advective problems. Naïve elections of the stabilization term, such as \( \gamma \) constant, could affect the convergence of the solution.

### 3.2. Discontinuous Galerkin-based residual minimization method

We apply the adaptive stabilized method introduced in [11] to diffusion-advection-reaction problems. We seek the discrete solution in a continuous trial space (e.g., \( H^1 \)-conforming finite elements) as the minimizer of the residual measured in a suitable DG space. This procedure inherits all the desirable stability properties from the well-posed DG formulation. In practice, such a residual minimization leads to a stable saddle-point problem involving the continuous trial space and the discontinuous test space. The discrete solution delivers a residual representative that is an efficient and reliable error estimate to drive adaptive mesh refinement. Thus, we compute on the fly a discrete solution in the continuous trial space and an error representation in the discontinuous test space.

Starting from the stable dG formulation of the form (3) in \( V_h \), a trial subspace \( U_h \subset V_h \) is chosen and, rather than solving the typical square problem in \( V_h \), we state the following residual minimization:

\[
\begin{cases}
\text{Find } u_h \in U_h \subset V_h, \text{ such that:} \\
b_h(z_h, u_h) + \frac{1}{2}\|A(u_h) - B_h z_h\|_{V_h}^2 = \arg \min_{z_h \in U_h} \frac{1}{2}\|R_{V_h}^{-1}(f_h - B_h z_h)\|_{V_h}^2,
\end{cases}
\]

where the dual norm \( \| \cdot \|_{V_h^*} \) for \( v \in V_h^* \) is:

\[
\|v\|_{V_h^*} := \sup_{v_h \in V_h} \frac{\langle v, v_h \rangle_{V_h^* \times V_h}}{\|v_h\|_{V_h}},
\]

and \( b_h : U_h \to V_h^* \) is:

\[
\langle b_h(z_h, v_h) \rangle_{V_h^* \times V_h} := b_h(z_h, v_h),
\]

\[\langle \cdot, \cdot \rangle_{V_h^* \times V_h} \] denotes the duality pairing in \( V_h^* \times V_h \), and \( R_{V_h}^{-1} \) denotes the inverse of the Riesz map:

\[
R_{V_h} : V_h \to V_h^*
\]

\[
\langle R_{V_h}(y_h), v_h \rangle_{V_h^* \times V_h} := \langle y_h, v_h \rangle_{V_h}.
\]

The second equality in (9) holds, since the Riesz map is an isometric isomorphism. With all the above, it can be shown that (9) is equivalent to the following saddle-point problem (see [11]):

\[
\begin{cases}
\text{Find } (\epsilon_h, u_h) \in V_h \times U_h, \text{ such that:} \\
\langle \epsilon_h, v_h \rangle_{V_h} + b_h(u_h, v_h) = (\lambda_h(v_h), \forall v_h \in V_h, \\
b_h(z_h, \epsilon_h) = 0, \quad \forall z_h \in U_h,
\end{cases}
\]

where \( 0 < \gamma_0 < 1 \) is a user-defined constant real number.
According to [11], the well-posedness of the dG-based residual minimization method relies on the classical assumptions for well-posedness of the original dG formulation (i.e., consistency, boundedness, and stability). The residual representative is efficient and reliable under a suitable saturation assumption. The resulting linear system leads to a saddle-point problem irrespective of the symmetry properties of the dG variational formulation, opening the possibility to use efficient well-known iterative solvers for its resolution.

3.3. Extension for the nonlinear penalty method

In this section, we extend the discrete formulation to solve a nonlinear problem of the form: \( N_h(u_h) = \ell_h \), where \( N_h : U_h \rightarrow V_h^\ast \) represents the operator that includes the nonlinear penalty term, defined as \( (N_h(z_h), v_h)_{V_h^\ast \times V_h} := b^h_1(z_h ; v_h) \). Given that \( b^h_1(z_h ; v_h) \) is built from the original bilinear form, the discrete problem (7) presents unique solution.

At the discrete level, we seek a minimizer \( u_h \in U_h \subset V_h \) for the residual \( \ell_h - N_h(z_h) \) associated to (7):

\[
\begin{align*}
\text{Find } u_h \in U_h \subset V_h, \text{ such that:} \\
\left\{ \begin{array}{ll}
1 & \| e_h - N_h(z_h) \|_{V_h^\ast}^2 \\
\text{arg min} & \| e_h - N_h(z_h) \|_{V_h^\ast}^2
\end{array} \right.
\end{align*}
\] (14)

Similar to (9), we state the nonlinear problem as a critical point of the minimizing functional, which translates into the following linear problem:

\[
\begin{align*}
\text{Find } u_h \in U_h \subset V_h, \text{ such that:} \\
\text{Find } (e_h, u_h) \in V_h \times U_h, \text{ such that:} \\
\left( R^h_1(l_h - N_h(z_h)), r \right)_{V_h^\ast \times V_h} = 0, \forall z_h \in U_h.
\end{align*}
\] (15)

\[DN_h : U_h \rightarrow V_h^\ast \text{ is defined as:}
\]

\[
\langle DN_h(u_h; z_h), v_h \rangle_{V_h^\ast \times V_h} := db^h_1(u_h; z_h, v_h).
\] (16)

where \( db^h_1(u_h; z_h, v_h) \) represents the derivative of the nonlinear form \( b^h_1(u_h; v_h) \) in the direction of an increment \( z_h \):

\[
\frac{db^h_1(u_h; z_h, v_h)}{de} := \frac{d}{de} b^h_1(u_h + \epsilon z_h; v_h)\big|_{\epsilon=0}.
\] (17)

for instance, if we can impose a positivity preserving condition through the penalty term, the derivative reads:

\[
\frac{db^h_1(u_h; z_h, v_h)}{de} := b_h(z_h, v_h) + \left( \frac{1}{\gamma} d\xi_1(u_h; z_h; v_h) \right).
\] (18)

where \( d\xi_1(u_h; z_h) = \frac{1}{\gamma} [1 - \text{sgn}(u_h - \gamma(Au_h - f))] \| z_h - \gamma A z_h \|_2 \).

The modified discrete formulation reads:

\[
\begin{align*}
\text{Find } (e_h, u_h) \in V_h \times U_h, \text{ such that:} \\
\left( (e_h, u_h), (v_h) \right)_{V_h \times U_h} + \frac{db^h_1(u_h; v_h; \gamma)}{de} = 0, \forall v_h \in V_h, \forall z_h \in U_h.
\end{align*}
\] (19)

The first line of the system (19) represents the nonlinear problem to solve, whereas the second line linearizes the constraint we seek to impose.

Remark 3. In practice, solving (19) implies that a price in the energy norm may be paid to enforce the constraints, since the residual minimization method without penalty achieves the lowest possible variational residual for the linear problem (see [11], Theorem 2).

3.4. Solution scheme

Given the discrete solution pair \( (e_h^k, u_h^k) \) in a iterative step \( k \), we seek for the increment \( (\delta e_h, \delta u_h) \) in the next iteration step, such that \( u_h^{k+1} = u_h^k + \delta u_h \), and \( e_h^{k+1} = e_h^k + \delta e_h \), being \( \delta \) a relaxation parameter. The method looks for a solution pair \( (e_h^{k+1}, u_h^{k+1}) \) that accomplishes (19) to first order. We propose a solution strategy that applies Newton’s method to the nonlinear problem.

Considering this, (19) we solve the following linearized problem at the iteration \( k + 1 \):

\[
\begin{align*}
\text{Given the pair } (e_h^k, u_h^k), \text{ find } (\delta e_h, \delta u_h) \in V_h \times U_h, \text{ such that:} \\
(\delta e_h, \delta u_h) + \frac{db^h_1(u_h^k; \delta u_h, v_h)}{de} = 0, \forall v_h \in V_h, \forall z_h \in U_h.
\end{align*}
\] (20)

The matrix formulation of (20) reads

\[
\begin{pmatrix}
G & B_u \\
B_u^\top & 0
\end{pmatrix}
\begin{pmatrix}
\delta e_h \\
\delta u_h
\end{pmatrix}
=
\begin{pmatrix}
L \\
0
\end{pmatrix}
-
\begin{pmatrix}
G e_h^k + N(u_h^k) \\
B_u e_h^k
\end{pmatrix}
\] (21)

where \( G \) represents the inner product induced by the norm in the discrete space \( V_h \), \( N(u_h^k) \) is related to the nonlinear form \( b^h_1(u_h^k; v_h) \) and \( B_u \) represents the matrix associated with its linearization \( db^h_1(u_h^k; \delta u_h, v_h) \). The residual representative \( e_h \) is a function of \( u_h \). We define \( x_h = (e_h, u_h) \), comprising both the solution and the residual representative, being valid also for the increments, which allows us to rewrite (21) as:

\[
J^k \delta x_h = R^k,
\]

where

\[
J^k = \begin{pmatrix}
G & B_u \\
B_u^\top & 0
\end{pmatrix}
\text{ and } R^k = \begin{pmatrix}
L \\
0
\end{pmatrix}
-
\begin{pmatrix}
G e_h^k + N(u_h^k) \\
B_u e_h^k
\end{pmatrix}
\]
The convergence of the method depends on the step size. Thus, we use a damped Newton algorithm to control convergence [3]. Presently, we cannot provide a bound on the number of iterations the proposed algorithm needs to achieve convergence. Nevertheless, in our experience, the algorithm is efficient and has a reasonable cost compared to the original linear problem, as the next Section shows.

**Algorithm 1** Damped Newton method

1. input $\omega \in (0, 1)$, $\zeta = 0$, $k = 0$, TOL
2. compute $x_h^0 = (x_h^0, u_h^0)$
3. compute $||R_h^0||$
4. $t^k = \frac{1 + \zeta ||R_h^0||}{||R_h^0||}$
5. compute $x_h^{k+1} = x_h^k + t^k \delta x_h^k$, $||R_h^{k+1}||$
6. If $\frac{1}{t^k} \left(1 - \frac{||R_h^{k+1}||}{||R_h^k||}\right) < \omega$
7. then if $\zeta = 0$ then $\zeta = 1$ else $\zeta = 10\zeta$; go to (4)\)
8. else $\zeta = \zeta/10$; $k = k + 1$
9. If $||u^{k+1} - u^k|| < $ TOL then return else go to (3)

4. Numerical experiments

In this section, we implement the nonlinear constraint enforcement method to solve several numerical tests using FEniCS [1].

4.1. Advection problem over a quasi-uniform mesh

We simulate a pure advection problem over a quasi-uniform mesh of size $h = 0.126$. We set $\Omega := (0, 1) \times (0, 1)$ and $\beta = (3/\sqrt{10}, 1/\sqrt{10})^T$, $K = 0$, $f = 0$. The unit advection field defines that $\Gamma_-$ corresponds to the part where $xy = 0$. The exact solution is $u = \frac{1}{2}(\tanh((y - \frac{1}{4} - \frac{3}{4})/\epsilon) + 1.0)$, defining an inner layer in the solution of width $\epsilon$. We compute solutions for a sharp layer ($\epsilon = 0.01$) using both the stabilized method based on residual minimization with the addition of the nonlinear penalty term. We consider affine ($p = 1$) finite elements. Given that the source $f = 0$ and the boundary condition $0 \leq g \leq 1$ in this experiment, the solution $0 \leq u \leq 1$. Thus, we use the penalty to impose both the lower and upper bounds. Using (4), we set $\gamma_0 = 10^{-5}$. We converge after 18 iterations using $TOL = 10^{-5}$. As seen in Figures 1(a) & 1(b), penalties consistently reduce the violation of the solution bounds up to the order of $10^{-3}\%$. Figure 1(c) shows a cross-section, normal to the advective field. The formulation with penalty significantly improves the bound preservation of the solution, removing the over- and under-shoots that appear in the stabilized formulation. Finally, in Figures 2(a) and 2(b), we show the $L^2$ and $V_h$-error norm convergence, respectively, considering a sequence of uniform meshes. We note that the constraint enforcement asymptotically produces a worsen convergence in the $V_h$-norm, being in line with Remark 3, while surprisingly producing an improvement in the $L^2$-norm.

4.2. Rotating flow over an adaptive mesh

We now solve a pure-advection test problem proposed in [20]. Let $\Omega := (0, 1) \times (-1, 1)$ with $b = (-y, x)^T$, $K = 0$, $f = 0$. The convection field rotates counterclockwise, and defines $\Gamma_- = (0, 1) \times (0, 1)$, $\Gamma_+ = (0, 1) \times (1, 0)$. Boundary condition
\( g \) is:

\[
g = \begin{cases} 
0.5[1 + \tanh(\varepsilon(y - 0.35))] & \text{on } (0, 0.5) \times [0], \\
0.5[1 + \tanh(\varepsilon(0.65 - y))] & \text{on } (0.5, 1) \times [0], \\
0 & \text{elsewhere on } \Gamma_-, 
\end{cases}
\]

which produces an inner layer in the solution of width \( \varepsilon \) between 0.35 and 0.65. Similar to the previous test case, we set \( \varepsilon = 0.01 \). Figure 3(a) shows a cross-section with and without the inclusion of the penalty term. The bound penalty improves the constraint satisfaction and the inner layer slope. Besides, Figure 3(b) shows the convergence in \( L^2 \) and reflects a similar behavior than the uniform mesh case, with the error norm for the penalty formulation solution higher than the one without penalty.

4.3. Advection-dominated diffusion problem over an adaptive mesh

We use the nonlinear penalty method to solve a version of the previous test with diffusion. That is, all parameters as above except \( K = 10^{-3} \). This modification induces a boundary layer at \( x = 0 \) in the solution due to the contribution of the diffusion part. Our initial mesh is structured and has \( 4 \times 4 \) triangular elements. We set \( \gamma_0 = 10^{-4} \). Both trial and test functions are of degree \( p = 1 \). The penalty constraints both the lower and upper bounds. Figure 4 shows that the adaptive scheme with the nonlinear penalty method captures the boundary layer through a proper error estimate, minimizing the bound violation on each refinement level and thus, delivering physically meaningful solutions at each level.

5. Conclusions

We describe a nonlinear weak constraint enforcement for a new adaptive stabilized finite element method. We impose solution bounds on pure-advection and on advection-dominated diffusion problems through the addition of a nonlinear penalty term that weakly enforces the solution range in the variational formulation. The final formulation reduces the bounds violation by several orders of magnitude. Given the stability provided by the formulation, the method moderately increases the computational cost of lower-order schemes. Finally, this method performs well with adaptive formulations taking advantage of the \textit{a posteriori} error estimate obtained on the fly in the computations. Future work will look for extending the formulation to more complex constraint conditions along with a consistent formulation for transient problems.
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