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Citation for published version (APA):

Hernández, H., Massart, T. J., Peerlings, R. H. J., & Geers, M. G. D. (2018). A stabilization technique for coupled convection-diffusion-reaction equations. *International Journal for Numerical Methods in Engineering*, 116(1), 43-65. <https://doi.org/10.1002/nme.5914>

DOI:

[10.1002/nme.5914](https://doi.org/10.1002/nme.5914)

Document status and date:

Published: 05/10/2018

Document Version:

Accepted manuscript including changes made at the peer-review stage

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

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A Stabilization Technique for Coupled Convection-Diffusion-Reaction Equations

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Abstract

Partial differential equations having diffusive, convective and reactive terms appear in the modeling of a large variety of processes in several branches of science. Often, several species or components interact with each other rendering strongly coupled systems of convection-diffusion-reaction equations. Exact solutions are available in extremely few cases lacking practical interest due to the simplifications made to render such equations amenable by analytical tools. Then, numerical approximation remains the best strategy for solving these problems. The properties of these systems of equations, in particular the lack of sufficient physical diffusion, cause most traditional numerical methods to fail, with the appearance of violent and non-physical oscillations, even for the single equation case. For systems of equations, the situation is even harder due to the lack of fundamental principles guiding numerical discretization. Therefore, strategies must be developed in order to obtain physically meaningful and numerically stable approximations. Such stabilization techniques have been extensively developed for the single equation case in contrast to the multiple equations case. This paper presents a perturbation-based stabilization technique for coupled systems of 1D convection-diffusion-reaction equations. Its characteristics are discussed, providing evidence of its versatility and effectiveness through a thorough assessment.

keywords.- Finite element methods, Differential equations, Convection-diffusion equation, Stability.

1 Introduction

Partial differential equations including convection, diffusion, and reaction terms arise naturally in many branches of engineering and science. Analytical solutions of such equations are known in very few simple cases that generally lack practical interest, even if they do provide valuable mathematical, physical, or computational insights. Moreover, non-linearity, intricate boundary conditions, irregular geometries, heterogeneity in the space and time dependence of the transport coefficients complicate the situation even more, rendering the problem intractable by analytical tools. For this reason, numerical approximation methods remain the best strategy for solving such equations.

In recent decades, all well-known numerical techniques have been applied to solve such convection-diffusion-reaction equations. Finite differences, finite volumes, finite elements, spectral, or meshless methods, to name a few, are most common in the field.

These numerical techniques have been applied with different degrees of success. Some of them have excelled for some specific problems, while not obtaining satisfactory results, or even completely failing, for other problems. In this respect, a general purpose numerical methodology does not seem to be available yet. The vast majority of the above mentioned numerical methods are successful when convection, reaction, or a combination of both acting together, are largely dominated by diffusion, tending towards a *purely diffusive* process. The situation is drastically changed when either convection, reaction, or a combination of both overwhelms diffusion. In such situations, numerical instability arises when diffusion becomes less predominant for affordable meshes. The numerical approximations are usually plagued with spurious oscillations near boundary and internal layers, and can exhibit negative values even if the underlying partial differential equation only accepts non-negative solutions.

This stability problem is inherent to the numerical discretization scheme, and not to the underlying partial differential equation. When the discretization is refined the magnitude of the oscillations decreases or they even completely disappear, yielding a smooth numerical approximation.

This suggests that the lack of numerical stability and the subsequent oscillations appear because the discretization is too coarse to adequately capture all the physics of the governing transport mechanisms. This can also be interpreted as a lack of richness of the approximation space to fully capture the behavior of the function underlying the solution of the continuous model. In several cases, the refinement required to get acceptable numerical approximations is so excessive that the approximation process becomes prohibitive in computational terms.

Over the years, ad hoc discretization strategies or stabilization techniques have been developed to overcome such difficulties. Finite difference method practitioners have defined several techniques in this respect, such as upwinding schemes, the use of high order schemes, or the use of fitted meshes [1, 2, 3, 4, 5]. Flux reconstruction, total variation diminishing techniques, high order schemes, essentially non-oscillatory schemes, and their weighted version are now well established techniques in the finite volume method community [6, 7, 8]. Streamline upwind Petrov-Galerkin, Galerkin least-squares, discontinuous Galerkin schemes; bubble enrichment; algebraic sub-grid scale approaches, finite increment calculus, spurious oscillations at layers diminishing techniques, and boundary layer elements, among others, have been devised over the years in the finite element method community [9, 10, 11, 12, 13, 14, 15, 16, 17].

These techniques exhibit different degrees of success, and many of them have not been designed for general purposes. Some are focused on the convection-diffusion case, while others were developed for the diffusion-reaction case. Moreover, some techniques are able to yield exact nodal values when dealing with a *single* convection-diffusion-reaction equation in a one-dimensional configuration [13, 17]. In the finite difference and the finite element method communities, most of the approaches use the advective form of the partial differential equation [18, 21, 19, 20]. On the other hand, the divergence form is preferred by the finite volume and spectral method communities [24, 23, 25, 22]. In view of the significant number of contributions dealing with these difficulties, one may get the misleading impression that these instability problems have been fully solved.

Yet, little attention has been paid to *systems* of convection-diffusion-reaction equations, although they also arise naturally in several branches of science such as bio-mechanics [26], combustion [27], computer science [28], ecology [29], economy [30], epidemiology [31], finance [32], groundwater pollution [33], heat transfer [34], neuroscience [35], physiology [36], seepage flow [37], solid mechanics [38] or turbulence [39]. The reason for this immaturity is the lack of a maximum principle when going from a single transport equation towards systems of coupled equations in the most general form. This continuous maximum principle does not hold when the equations are strongly coupled through the convective terms [40, Chapter 3, Section 8, pp. 192].

In a contribution by Abrahamson, Keller, and Kreiss [41], a stabilization technique for systems of one dimensional convection-diffusion-reaction equations in steady state, i.e. a system of ordinary differential equations, has been proposed and successfully applied. This technique is a direct extension of a previously developed upwinding scheme for first order derivative terms [43, 44, 42, 45].

Additional progress in the approximations for systems of convection-diffusion-reaction equations until the late 1990's has been mainly made by the finite difference method community. The issue has been addressed by extending techniques previously used for discretizing a single equation. The most representative approaches consist of the use of upwind finite differences for the convective terms on layer adapted meshes according to the construction proposed by Shishkin and Bakhvalov [3, 46]. In these papers, theoretical developments have unraveled the conditions for a continuous maximum principle to be valid. In other cases compatibility conditions are derived and used instead. For finite volumes, the strategies have been similar. Discontinuous and high order approximations, upwinding and adaptive meshes were the most successful techniques to deal with coupled equations [48, 47]. In the finite element method context, streamline upwind Petrov-Galerkin, Galerkin least-squares, algebraic sub-grid scale with high order elements together with shock capturing techniques have been the most successful techniques [33, 27, 38, 49]. In general, and within all these methodologies, the case of systems of equations has been traditionally tackled using techniques previously successful in the case of a single equation. The same guiding strategy is followed in the present paper.

The main aim here is to present a stabilization technique for a system of coupled convection-diffusion-reaction equations able to resolve the main shortcomings of the above mentioned stabilization techniques such as mesh fitting or the need to adapt the mesh, the requirement of high order or discontinuous approximations and the introduction of excessive diffusive up-winded differences. This methodology extends

a recently proposed approach for a single equation, described in [50], to a general system of convection-diffusion-reaction equations. The methodology is conceptually based on perturbing the original partial differential equation, the discretized form of which on a particular discretization is on beforehand known to yield an unstable approximation, by modifying its transport coefficients to obtain a well behaved numerical approximation without altering the physics [51, 9]. The required modification or perturbation is optimally determined as the smallest possible one that still guarantees stability. These perturbations are chosen in such a way that certain compatibility conditions analogous to a maximum principle are satisfied. Once the computed perturbations are injected in the classical Bubnov-Galerkin finite element method, they deliver smooth and stable numerical approximations.

Applications to several coupled systems of partial differential equations in one dimension arising from different phenomena are presented. These results demonstrate the use of the developed technique for simulating problems modeled by systems of convection-diffusion-reaction equations with an affordable computational effort. Examples showing the reliability of the approach are presented through several thorough and detailed numerical assessments.

The one-dimensional character of the presented perturbation-based stabilization technique allows the use of simple analytical tools to study its behavior and properties, allowing to fully focus on the main difficulty this paper deals with, i.e. the strong coupling of the systems of equations at hand. At the same time it represents the first and necessary stage towards its extension to multi-dimensional configurations. Progress in the treatment of *strongly coupled* convection-diffusion-reaction equations would represent a step forward in the numerical approximation of mathematical models for which the main simplifying assumptions done in fluid dynamics community, by far the most active in the development of stabilization techniques, are not valid.

The paper is organized as follows. In Section 2 the basic terminology and notations are introduced. A particular effort has been made to homogenize the different conventions used in the literature due to the variety of phenomena for which coupled convection-diffusion-reaction equations are obtained. Subsequently, the classical Bubnov-Galerkin finite element discretization is introduced in the most traditional way. Section 3 is devoted to the development of a stabilization technique for a steady state linear system of convection-diffusion-reaction equations with constant coefficients in one dimension. The particular case when the coupling coefficients vanish is discussed, for which the proposed stabilization technique simplifies to a previously proposed techniques designed for the case of a single equation. Section 4 assesses the stabilization technique through three numerical examples. The first one is of the convection-diffusion type, while the second one is of the diffusion-reaction type. Finally, the third problem is of convection-diffusion-reaction type with not only boundary layers as in the previous problems, but also internal layers. In Section 5 the performance of the presented stabilization technique is compared with those of well established stabilization techniques. This comparative study is carried out using the same numerical examples used in Section 4. Finally, Section 6 presents the main conclusions of the paper and discusses some future developments to be considered.

2 Problem definition and finite element discretization

In all generality, consider a system of m conservation equations with reaction terms of the form

$$\rho_{pq} \frac{\partial u_q}{\partial t} + \frac{\partial}{\partial x} (F_p) + \gamma_{pq} u_q = f_p, \quad (1)$$

where the use of repeated indices implies the traditional summation convention. The main variables to be approximated, u_q for $q = 1, 2, \dots, m$, are the physical quantities to be transported, F_p are their corresponding fluxes, and $f_p \in \mathbb{R}$ are the source terms, both for $p = 1, 2, \dots, m$. The reaction coefficients $\gamma_{pq} \in \mathbb{R}$, for $p, q = 1, 2, \dots, m$ will be referred to as *direct* when $p = q$ and as *coupled* when $p \neq q$. Finally, $\rho_{pq} \in \mathbb{R}^+$ are the mass coefficients, which are assumed to vanish when $p \neq q$.

The fluxes are composed of diffusive and convective contributions, i.e.

$$F_p = -\alpha_{pq} \frac{\partial u_q}{\partial x} + \beta_{pq} u_q. \quad (2)$$

Here $\alpha_{pq} \in \mathbb{R}^+$ are the diffusion coefficients and $\beta_{pq} \in \mathbb{R}$ are the convection coefficients. These diffusion and convection coefficients will also be referred to as *direct* or *coupled* using the above mentioned convention. Throughout this section all coefficients will be regarded as constants.

Substituting the flux given by Equation (2) in the general conservation Equation (1) leads to

$$\rho_{pq} \frac{\partial u_q}{\partial t} + \frac{\partial}{\partial x} \left(-\alpha_{pq} \frac{\partial u_q}{\partial x} + \beta_{pq} u_q \right) + \gamma_{pq} u_q = f_p. \quad (3)$$

which is the *divergence* form of the conservation equation due to the fact that integration over the whole domain involves, via the divergence theorem, the total flux across the boundary.

Since all the physical coefficients are regarded as constants, it is possible to expand the spatial derivative on the terms composing the flux to obtain

$$\rho_{pq} \frac{\partial u_q}{\partial t} - \alpha_{pq} \frac{\partial^2 u_q}{\partial x^2} + \beta_{pq} \frac{\partial u_q}{\partial x} + \gamma_{pq} u_q = f_p. \quad (4)$$

which is in turn the *advective* form because of the direct interpretation of the first order spatial derivative term representing convection.

With these conventions and assumptions it is possible to rewrite the system of equations (4) in matrix form as

$$\mathbf{M}\dot{\mathbf{u}} - \mathbf{A}\mathbf{u}'' + \mathbf{B}\mathbf{u}' + \mathbf{G}\mathbf{u} = \mathbf{f}, \quad (5)$$

where the superimposed dot implies differentiation in time while the prime denotes a derivative with respect to the spatial coordinate. $\mathbf{M} = \text{Diag}(\rho_{11}, \rho_{22}, \dots, \rho_{mm})$ is the *matrix of mass coefficients* and $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{G}$ are the *matrices of diffusion, convection, and reaction coefficients*, while $\mathbf{u} = [u_1, u_2, \dots, u_m]^T$ is the *vector of unknowns*. Finally, the *source vector* $\mathbf{f} = [f_1, f_2, \dots, f_m]^T$ gathers the m source terms. Care must be taken not to confuse the above matrices with the finite element matrices to be introduced afterwards.

For the sake of clarity in the notation, a single weighting function w for all the m equations is introduced and used in what follows. Notwithstanding, it is important to remark that a different weighting function can be used for each equation. Multiplying Equation (1) by such a weighting function w , and integrating over the whole spatial domain, the following weighted residuals form is obtained

$$\int_{\Omega} w \rho_{pq} \frac{\partial u_q}{\partial t} d\Omega + \int_{\Omega} w \frac{\partial}{\partial x} (F_p) d\Omega + \int_{\Omega} w \gamma_{pq} u_q d\Omega = \int_{\Omega} w f_p d\Omega, \quad (6)$$

Integrating by parts the second term in the left hand side yields

$$\int_{\Omega} w \rho_{pq} \frac{\partial u_q}{\partial t} d\Omega - \int_{\Omega} \frac{\partial w}{\partial x} F_p d\Omega + [w F_p]_{\Gamma} + \int_{\Omega} w \gamma_{pq} u_q d\Omega = \int_{\Omega} w f_p d\Omega. \quad (7)$$

It is emphasized here that this way of applying integration by parts is not standard in finite element based solutions in the fluids dynamics community. This choice, i.e. integration by part performed on the whole flux term, allows one to handle both essential and natural boundary conditions for convection-diffusion-reaction problems in a straightforward manner.

To discretize Equation (7), the weighting function w and the variable u_p are expressed as linear combinations of their corresponding nodal values using interpolation functions W_k and P_k associated with the n_e nodes within each finite element as follows

$$w = \sum_{k=1}^{n_e} W_k w_k \quad \text{and} \quad u_p = \sum_{k=1}^{n_e} P_k (u_p)_k. \quad (8)$$

Requiring the result to hold for all w_k leads to a global discretized system of the form

$$\mathbf{M}_{pq} \dot{\mathbf{u}}_q + (\mathbf{D}_{pq} + \mathbf{C}_{pq} + \mathbf{R}_{pq}) \mathbf{u}_q = \mathbf{f}_p, \quad (9)$$

where $\mathbf{M}_{pq}$ are the global mass matrices, $\mathbf{D}_{pq}$ the global diffusion matrices, $\mathbf{C}_{pq}$ are the global convection matrices and $\mathbf{R}_{pq}$ are the global reaction matrices. Again, it is emphasized that these matrices differ from those presented in Equation (5), and the same care should be taken with the unknowns and source term vectors. Nodal values of the transported quantities to be approximated are sorted in the m vectors $\mathbf{u}_q = [u_q^{(1)}, u_q^{(2)}, \dots, u_q^{(n-1)}, u_q^{(n)}]^T$ (for $q = 1, 2, \dots, m$), with n being the total number of nodes in the

finite element discretization. Furthermore, these m numerical approximations can be sorted in a single degree-of-freedom vector as

$$\mathbf{u} = \left[u_1^{(1)}, u_1^{(2)}, \dots, u_1^{(n)}, u_2^{(1)}, u_2^{(2)}, \dots, u_2^{(n)}, \dots, u_m^{(1)}, u_m^{(2)}, \dots, u_m^{(n)} \right]^T, \quad (10)$$

which will be simply referred as the numerical approximation. Finally $\mathbf{f}_p$ takes into account the m source terms f_p and boundary conditions. For simplicity, but without loss of generality, only Dirichlet boundary conditions will be considered in this work.

Instabilities in the form of node-to-node spurious oscillations appear when a problem not dominated by diffusion is approximated while using a Bubnov-Galerkin approach, i.e. with $P_k = W_k$. This phenomenon appears even in the single differential equation case, i.e. when $m = 1$. This instability problem is inherited to the multiple differential equations case, i.e. when $m > 1$.

3 Stabilization by coefficient perturbation

The stability problems described above for the single equation case are caused by the fact that the classical Bubnov-Galerkin method applied to the considered partial differential equation does not satisfy the discrete maximum principle. This principle is the discrete counterpart of the continuous maximum principle, to be satisfied by any feasible solution of the underlying differential equation [52, 51]. However, this maximum principle has been rigorously established only for the case of a single differential equation and for weakly coupled systems of equations, i.e. not containing coupling convection terms [40, Chapter 3, Section 8, pp. 192]. When tackling systems of differential equations, barrier functions or compatibility conditions should be established and used instead [46, 4, 53, 5]. Irrespective of the problem considered, a stabilization technique is required in order to obtain physically meaningful approximations. In the present paper, the above mentioned barrier functions or compatibility conditions will not be used since their derivation is beyond the scope of the present paper. Therefore, the only guiding criterion for the stabilization technique development will be the removal of spurious oscillations. Thus, interior domain values of the approximated solutions will be allowed to be larger or smaller than the corresponding boundary values due to the fact that coupling terms between unknowns can be viewed as sources or sinks.

The key observation motivating the development of the proposed stabilization technique is that the classical Bubnov-Galerkin scheme presented in Section 2 does not generally satisfy the discrete maximum principle even for the case of a single differential equation. This renders the numerical approximation plagued with spurious unphysical oscillations for some combinations of the physical coefficients α , β , and γ and element size ℓ . One way to enforce the fulfillment of the discrete maximum principle is through mesh refinement, entailing a major increase of the computational cost. The alternative strategy is to approximate the solution of a modified, though similar, problem for which it is known in advance that its finite element approximation is free of spurious oscillations without mesh refinement. These two problems only differ in the magnitudes of the physical coefficients, leaving the differential operators, boundary conditions and source term unaltered. This has the goal of keeping the perturbed, i.e. modified, problem as similar as possible to the original physical problem. This is the working mechanism of the stabilization technique based on coefficient perturbations for the single convection-diffusion-reaction equation presented in [50]. It is therefore possible to classify the proposed perturbation-based stabilization technique as one using the *modified equation approach* [16, 13]. This technique will be heuristically extended to systems containing several coupled differential equation in Section 3.1. Then, Section 3.2 shows that this extension does indeed simplify to the single equation case when the coupling coefficients vanish. To conclude this section the consistency of the presented stabilization technique is investigated and discussed in the convection-diffusion single equation sub-case. As a result of the use of this simplified problem the analysis is substantially simplified. Dealing with the fully coupled multiple convection-diffusion-reaction equations case is algebraically rather complicated. However, one can expect that being the stabilization technique consistent for the single equation case, this desirable property will be inherited by the multiple equation case.

3.1 Stabilization of systems of coupled equations

In this section, a stabilization technique for a single convection-diffusion-reaction equation, proposed in [50], is heuristically extended to the case of multiple coupled equations. This extension is built, as for the single equation case, on the injection of the analytical solution of the linearised, homogeneous,

and steady state version of the problem at hand into the numerical stencil obtained by the finite element discretization. This injection process yields a system of algebraic equations for each differential equation composing the coupled system. The determination of the coefficient perturbations for stabilization is carried out by solving these systems of algebraic equations.

The development of the stabilization technique will make use of a simplified steady state Dirichlet boundary value problem which reads as follows

$$\frac{d}{dx} \left(-\alpha_{pq} \frac{du_q}{dx} + \beta_{pq} u_q \right) + \gamma_{pq} u_q = f_p \quad \text{in} \quad \Omega = (0, 1), \quad (11)$$

$$u_p(x=0) = u_p^L \quad \text{and} \quad u_p(x=1) = u_p^R. \quad (12)$$

The discretization of the system of differential equations by the finite element method using a uniform mesh generates $p = 1, 2, \dots, m$ numerical stencils, one for each of the p differential equations contained in system (11). These stencils take the same general form

$$-\frac{\alpha_{pq}}{\ell} \left(u_q^{(i-1)} - 2u_q^{(i)} + u_q^{(i+1)} \right) - \frac{\beta_{pq}}{2} \left(u_q^{(i-1)} - u_q^{(i+1)} \right) + \frac{\gamma_{pq}\ell}{6} \left(u_q^{(i-1)} + 4u_q^{(i)} + u_q^{(i+1)} \right) = \ell f_p^{(i)}, \quad (13)$$

which corresponds to the $[i + (p-1)m]$ -th row of the system of algebraic equations produced by the finite element method after assembly.

It is a well known fact for the single equation case, i.e. $m = 1$ that its corresponding stencil, given by Equation (13) with $p = q = 1$, should satisfy the discrete maximum principle in order to produce stable approximations. This is only achieved if the physical coefficients, together with the mesh size ℓ , satisfy the inequality

$$\frac{\alpha}{\ell^2} - \frac{|\beta|}{2\ell} - \frac{\gamma}{6} \geq 0, \quad (14)$$

where the p and q sub-indices have been omitted from because in the single equation case they are unique for each transport mechanism. Of special interest is the convection-diffusion case, i.e. when $\gamma = 0$, due to the fact that it is the most studied case in the context of finite elements for fluid dynamics. For this problem the Inequality (14) simplifies to

$$\text{Pe} \stackrel{\text{def}}{=} \frac{\beta\ell}{2\alpha} \leq 1, \quad (15)$$

where Pe is the mesh Péclet number.

The stabilization technique presented in [50] aims to enforce the fulfilment of Inequality (14) by modifying or *perturbing* the physical coefficients without reducing the mesh size ℓ in order to avoid the additional computational cost that this refinement would involve. This *perturbed* problem is therefore defined through the use of perturbed coefficients which are defined as

$$\tilde{c} = c + c^*, \quad \text{with} \quad c = \alpha_{pq}, \beta_{pq}, \gamma_{pq}, \quad \text{for} \quad p, q = 1, 2, \dots, m, \quad (16)$$

where the asterisk is used to denote the coefficients perturbations and therefore the tilde refers to the perturbed coefficients. These perturbed coefficients define the aforementioned perturbed problem, which in turn reads exactly as shown by Equation (13) but with the perturbed coefficients, with tilde, instead the physical coefficients, without tilde.

The determination of the perturbations required to get a stable numerical stencil heuristically follows the procedure developed in [50] for the single equation case, i.e. $m = 1$. This process makes use of the analytical solution of the differential equation. This analytical solution is first evaluated in the stencil points, i.e. at x_{i-1} , x_i , and x_{i+1} . These evaluations are then injected into the perturbed numerical stencil. This injection procedure gives an over-determined system of algebraic equations whose unknowns are the sought perturbations. Once the over-determination is suppressed by leaving some coefficients unperturbed, the solution of this system of algebraic equations allows determining the minimal perturbation required to obtain a stencil matching a stable approximation.

To obtain the analytical solution of the system (11), m new variables are introduced in order to convert the system of m second-order differential equations into a system of $2m$ first-order differential equations. These new variables are defined as

$$u_{j+m} = \frac{du_j}{dx} \quad \text{for } j = 1, 2, \dots, m. \quad (17)$$

After substituting Equation (17) in the system given by Equation (11) for the homogeneous case, i.e. with $f_p = 0$ for $p = 1, 2, \dots, m$, the aforementioned system of $2m$ first-order differential equations is obtained. It can be written in matrix form as

$$\frac{d\mathbf{u}}{dx} = \mathbf{K}\mathbf{u}, \quad (18)$$

with $\mathbf{u} = [u_1, u_2, \dots, u_{2m}]^T$ and the $2m \times 2m$ matrix $\mathbf{K}$ defined as

$$\mathbf{K} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{A} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{G} & \mathbf{B} \end{bmatrix}, \quad (19)$$

where $\mathbf{I}$ is the $m \times m$ identity matrix and $\mathbf{0}$ is the $m \times m$ null matrix. The $m \times m$ matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{G}$ are the diffusion, convection and reaction matrices defined in Equation (5).

With these conventions, the analytical solution of the system given by Equation (18) can be written as

$$\mathbf{u} = c_1 e^{\lambda_1 x} \mathbf{v}^{(1)} + c_2 e^{\lambda_2 x} \mathbf{v}^{(2)} + \dots + c_{2m} e^{\lambda_{2m} x} \mathbf{v}^{(2m)}, \quad (20)$$

where λ_k and $\mathbf{v}^{(k)}$ are the $2m$ eigenvalues and eigenvectors of the matrix $\mathbf{K}$, i.e. they satisfy $\mathbf{K}\mathbf{v}^{(k)} = \lambda_k \mathbf{v}^{(k)}$ for $k = 1, 2, \dots, 2m$. The constants c_k only depend on the boundary conditions given by (12). Thus, the q -th solution of the system of equations (11) can be written as

$$u_q(x) = \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x}, \quad (21)$$

where $v_q^{(k)}$ is the q -th component of the eigenvector associated to the k -th eigenvalue.

The q -th component of the analytical solution can therefore be evaluated at the three nodes defining the finite element stencils (13), i.e. at x_{i-1} , x_i and x_{i+1} :

$$u_q(x_i) = u_q^{(i)} = \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i}, \quad \text{and} \quad u_q(x_{i\pm 1}) = u_q^{(i\pm 1)} = \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i} e^{\pm \lambda_k \ell}. \quad (22)$$

These expressions for $u_q^{(i-1)}$, $u_q^{(i)}$, and $u_q^{(i+1)}$ are injected in the p perturbed finite element stencils resulting from the discretization of the system of differential equations (11). Such perturbed stencils have exactly the same form as the stencils given by (13) but using the perturbed coefficients $\tilde{\alpha}_{pq}$, $\tilde{\beta}_{pq}$, and $\tilde{\gamma}_{pq}$ instead of the corresponding original coefficients α_{pq} , β_{pq} , and γ_{pq} . After taking into account the coupling through the q index, each of the p perturbed stencils can be written as

$$\begin{aligned} & \frac{\tilde{\alpha}_{pq}}{\ell} \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i} [1 - \cosh(\lambda_k \ell)] + \\ & \frac{\tilde{\beta}_{pq}}{2} \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i} \sinh(\lambda_k \ell) + \\ & \frac{\tilde{\gamma}_{pq} \ell}{6} \sum_{k=1}^{2m} c_k v_q^{(k)} e^{\lambda_k x_i} [2 + \cosh(\lambda_k \ell)] = 0. \end{aligned} \quad (23)$$

Expression (23) represents m equations (for $p = 1, 2, \dots, m$), each one corresponding to the p -th differential equation in the system (11). Expansion of the $q = 1, 2, \dots, m$ index in each of these m equations makes clear that the unknowns of the equations included in Expression (23) are the m^2 perturbed diffusion coefficients $\tilde{\alpha}_{pq}$, the m^2 perturbed convection coefficients $\tilde{\beta}_{pq}$, and the m^2 perturbed reaction coefficients $\tilde{\gamma}_{pq}$, each for $p, q = 1, 2, \dots, m$. Considering the m equations with $3m^2$ unknowns in Equation (23), attention is now focused to the summation over k . The $k = 1, 2, \dots, 2m$ index corresponds to the number

of integration constants c_k , eigenvalues λ_k , and eigenvectors $\mathbf{v}^{(k)}$. The constants c_k depend only on the boundary conditions in (12). These boundary conditions are first chosen in such a way that $c_1 \neq 0$ and $c_2 = c_3 = \dots = c_{2m} = 0$, generating m algebraic equations (for $p = 1, 2, \dots, m$), for the particular value $k = 1$. Subsequently, the boundary conditions are modified in order to get $c_1 = 0$, $c_2 \neq 0$, and $c_3 = c_4 = \dots = c_{2m} = 0$, generating this time another m algebraic equations for the value $k = 2$. This process is continued until $k = 2m$, generating m algebraic equations for each particular value of the k index. Note that after carrying out this process the product $c_k e^{\lambda_k x_i}$ can be eliminated since it appears as a common factor once a particular k has been fixed. Thus, it is possible to write the resulting $2m^2$ system of algebraic equations in a compact form as

$$\frac{\tilde{\alpha}_{pq}}{\ell} v_q^{(k)} [1 - \cosh(\lambda_k \ell)] + \frac{\tilde{\beta}_{pq}}{2} v_q^{(k)} \sinh(\lambda_k \ell) + \frac{\tilde{\gamma}_{pq} \ell}{6} v_q^{(k)} [2 + \cosh(\lambda_k \ell)] = 0, \quad (24)$$

where the eigenvalues λ_k and their corresponding eigenvectors $\mathbf{v}^{(k)}$ of the $\mathbf{K}$ matrix given by Equation (19) depend only on the transport coefficients and therefore can be easily determined through numerical computation. In order to solve this system of $2m^2$ equations with $3m^2$ unknowns, m^2 transport coefficients should be kept unperturbed, allowing to solve (24) for the remaining $2m^2$ perturbed coefficients.

Note that the expression (24) simplifies to the system of two algebraic equations obtained in [50] for the single differential equation case, i.e. when $m = 1$. The corresponding 2×2 matrix $\mathbf{K}$ is now given by

$$\mathbf{K} = \begin{bmatrix} 1 & 0 \\ 0 & \alpha \end{bmatrix}^{-1} \begin{bmatrix} 0 & 1 \\ \gamma & \beta \end{bmatrix}, \quad (25)$$

whose eigenvalues are exactly the same as the roots of the characteristic polynomial associated to the second-order convection-diffusion-reaction equation given by

$$\lambda_{1,2} = \frac{\beta}{2\alpha} \pm \sqrt{\left(\frac{\beta}{2\alpha}\right)^2 + \frac{\gamma}{\alpha}}. \quad (26)$$

This observation partially justifies the heuristic process adopted in order to extend the stabilization technique from the single equation case towards the case of systems containing m coupled equations. Additional arguments will be forwarded in the next section.

3.2 Particularization to uncoupled sets of equations

The goal of this section is to assess the validity of the extension of the presented stabilization technique to the multiple equations case. For this purpose, the special case when all coupling coefficients vanish, i.e. when $\alpha_{pq} = \beta_{pq} = \gamma_{pq} = 0$ for $p \neq q$, is considered. In this case the eigenvalues of the $\mathbf{K}$ matrix are given by

$$\lambda_{2p-1,2p} = \frac{\beta_{pp}}{2\alpha_{pp}} \pm \sqrt{\left(\frac{\beta_{pp}}{2\alpha_{pp}}\right)^2 + \frac{\gamma_{pp}}{\alpha_{pp}}}, \quad (27)$$

and their corresponding eigenvectors are in turn given by

$$\mathbf{v}^{(2p-1,2p)} = \left(\frac{\lambda_{2p-1,2p} \alpha_{pp} - \beta_{pp}}{\gamma_{pp}} \right) \hat{\mathbf{e}}^{(p)} + \hat{\mathbf{e}}^{(p+m)}, \quad (28)$$

where the vectors $\hat{\mathbf{e}}^{(i)}$ for $i = 1, 2, \dots, 2m$ have 1 in their i -th component and zeros otherwise.

Since $\alpha_{pq} = \beta_{pq} = \gamma_{pq} = 0$ for $p \neq q$, their corresponding perturbations are, for simplicity, assumed to vanish, i.e. $\alpha_{pq}^* = \beta_{pq}^* = \gamma_{pq}^* = 0$ for $p \neq q$. After substituting $q = p$ in the expression (24) and factorizing the common factor $v_p^{(k)}$, the system of equations can be compactly written as

$$v_p^{(k)} \left\{ \frac{\tilde{\alpha}_{pp}}{\ell} [1 - \cosh(\lambda_k \ell)] + \frac{\tilde{\beta}_{pp}}{2} \sinh(\lambda_k \ell) + \frac{\tilde{\gamma}_{pp} \ell}{6} [2 + \cosh(\lambda_k \ell)] \right\} = 0. \quad (29)$$

Note that only the p -th and $(p+m)$ -th entries of the $(2p-1)$ -th and the $2p$ -th eigenvectors do not vanish, i.e. $v_p^{(2p-1,2p)} \neq 0$ and $v_{p+m}^{(2p-1,2p)} \neq 0$. Thus, only the $[2(p-1)m + 2p - 1]$ -th and $[2(p-1)m + 2p]$ -th equations of the linear system are non-trivial. All the other equations generated by (29) for $k = 1, 2, \dots, 2m$ provide the trivial equality $0 = 0$. Therefore the linear system consisting originally of $2m^2$

equations is reduced to only $2m$ equations with $3m$ unknowns, i.e. the perturbed coefficients $\tilde{\alpha}_{pp}$, $\tilde{\beta}_{pp}$, and $\tilde{\gamma}_{pp}$. Furthermore, it is possible to write these equations by pairs after substituting $k = 2p - 1$ and $k = 2p$ and eliminating the common factor $v_p^{(k)}$ as

$$\frac{\tilde{\alpha}_{pp}}{\ell} [1 - \cosh(\lambda_{2p-1}\ell)] + \frac{\tilde{\beta}_{pp}}{2} \sinh(\lambda_{2p-1}\ell) + \frac{\tilde{\gamma}_{pp}\ell}{6} [2 + \cosh(\lambda_{2p-1}\ell)] = 0, \quad (30)$$

$$\frac{\tilde{\alpha}_{pp}}{\ell} [1 - \cosh(\lambda_{2p}\ell)] + \frac{\tilde{\beta}_{pp}}{2} \sinh(\lambda_{2p}\ell) + \frac{\tilde{\gamma}_{pp}\ell}{6} [2 + \cosh(\lambda_{2p}\ell)] = 0. \quad (31)$$

Note that these two equations well resemble the two algebraic equations obtained in [50] when treating the single differential equation case, i.e. when $m = 1$. This allows to conclude that when applied to an uncoupled system of convection-diffusion-reaction equations, the extended stabilization technique simplifies to m independent problems, and therefore stabilizes them independently.

The special case of a single convection-diffusion equation can be used to examine the effectiveness of the proposed stabilization technique through the use of affordable algebraic procedures. In this case the system eigenvalues are $\lambda_1 = \lambda = \beta/\alpha$ and $\lambda_2 = 0$ and therefore Equation (31) is satisfied trivially. Equation (30) can be re-written in this case as

$$\frac{\tilde{\alpha}}{\ell} [1 - \cosh(\lambda\ell)] + \frac{\tilde{\beta}}{2} \sinh(\lambda\ell) = 0. \quad (32)$$

Choosing the diffusion coefficient to be perturbed, i.e. $\beta^* = 0$, its corresponding perturbation is given by

$$\alpha^* = \alpha \text{Pe} [\coth(\text{Pe}) - \text{Pe}^{-1}]. \quad (33)$$

The fulfillment of the discrete maximum principle for this perturbed, i.e. modified, problem can be verified by using in the Inequality (14) the perturbed diffusion coefficient $\tilde{\alpha}$ instead of the previously used physical diffusion coefficient α . It reduces to the expression

$$\coth(\text{Pe}) \geq 1, \quad (34)$$

which irrespective of the value of the Péclet number Pe is always satisfied. Moreover, the function in Equation (33) vanishes at $\text{Pe} = 0$, i.e. when $\beta = 0$ which corresponds to the purely diffusive problem. More importantly, the perturbation given by Equation (33) tends to vanish as the mesh is refined, i.e. when $\ell \rightarrow 0$. This demonstrates that, for the simplified sub-case used here, the proposed stabilization technique is a consistent *modified equation approach* method according to the definition given in [16]. Although the analogous demonstration for strongly coupled systems of equation could become rather intricate, one could expect that the perturbations required to achieve stability will behave in the same manner, i.e. they tend to vanish as the mesh is refined, since their computation still relies on the injection of the analytical solution as in the single equation case.

4 Applications and computational assessment

This section presents three numerical examples to illustrate and assess the efficiency and consistency of the developed stabilization technique. Its main goal is to demonstrate the ability of the presented stabilization technique to successfully accommodate and handle different types of problems, independently of the underlying physics for which the system of differential equations has been established.

This goal is pursued by presenting a thorough and detailed analysis of the numerical results obtained for three examples taken from different references. In all cases the convection and reaction coefficients have been taken exactly the same as those presented in the original reference. Except in the last example, all boundary conditions have also been taken of the same type as in the original references. The modification made in the last problem is for the sake of uniformity in the assessments presented here, and more importantly because the boundary conditions chosen here more easily trigger the development of sharp boundary layers, making the problem more challenging for the stabilization technique. Thus the problems elaborated in the present assessment are all of the Dirichlet type. The domain considered always has a unit length.

Only the parameter ϵ controlling the amount of diffusion and the discretization size ℓ are modified during this study. Once these are set for a particular problem they are not varied, i.e. for a particular simulation the diffusion parameter is constant over the whole domain discretized with a uniform mesh. The parameter ϵ is always chosen as $\epsilon = 10^{-j}$ with $j = 0, 1, 2, \dots$ thus, as j increases the problem becomes less dominated by diffusion, and therefore its numerical approximation becomes more prone to numerical instabilities.

Regardless of the use of the presented stabilization technique, once the system of m differential equations has been discretized, a system of $mn \times mn$ linear algebraic equations has to be solved. For this purpose the iterative *BiCGStab* method has been used, considering future multidimensional extensions of the framework leading to large and sparse systems [54]. In all cases, the maximum number of allowed iterations is set equal to the number of nodes in the finite element mesh, although the iteration process is stopped as soon as $\|\mathbf{r}^{(k)}\|/\|\mathbf{b}\| < \epsilon_s = 10^{-6}$ is reached, with $\mathbf{r}^{(k)}$ the k -th residual vector and $\mathbf{b}$ the right hand side vector. No preconditioning is used.

4.1 Convection-diffusion system

In this section, attention is focused on a problem having no reaction terms but a full convection matrix, i.e. containing cross convection terms. It has been chosen here to perturb only the diagonal entries of the diffusion matrix in order to capture the effect of the stabilization technique in a single coefficient perturbation easy to scrutinize. Since an analytical solution is available for this problem, an error analysis can be carried out to elucidate the effectiveness of the stabilization scheme.

This problem is taken from [55], where it was treated using upwind finite differences on a Shishkin mesh. It is the simplest case among all examples solved in the present paper, where all the diffusion coefficients are equal and the convection coefficients and source terms all taken as constants.

The system consisting of $m = 3$ differential equations reads as follows

$$-\epsilon \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}_{xx} - \begin{bmatrix} 3 & -1 & -1 \\ -1 & 4 & -2 \\ -1 & -2 & 4 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}_x = \begin{bmatrix} -4 \\ 11 \\ -7 \end{bmatrix}, \quad (35)$$

with boundary condition at the left $\mathbf{u}(x=0) = [-1, 4, -1]^T$, and at the right

$$\mathbf{u}(x=1) = e^{-1/\epsilon} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + e^{-4/\epsilon} \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix} + e^{-6/\epsilon} \begin{bmatrix} 0 \\ 2 \\ -2 \end{bmatrix} + \begin{bmatrix} 1 \\ -2 \\ 0 \end{bmatrix}. \quad (36)$$

Note that the latter boundary condition depends on the diffusion parameter.

The previously mentioned analytical solution is available from [55] and reads

$$\mathbf{u}(x) = e^{-x/\epsilon} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + e^{-4x/\epsilon} \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix} + e^{-6x/\epsilon} \begin{bmatrix} 0 \\ 2 \\ -2 \end{bmatrix} + \begin{bmatrix} x \\ -2x \\ x-1 \end{bmatrix}. \quad (37)$$

Figure 1 shows the numerical approximations in terms of u_1 , u_2 , and u_3 . The results obtained with the classical Bubnov-Galerkin method are depicted in the left column, while the right column shows the results obtained with the stabilization technique. These numerical schemes are respectively referred to as *classical* and *stabilized*.

Note in the first row of Figure 1; for $\epsilon = 1$, that, having diffusion coefficients $\alpha_{pp} = 1$ for $p = 1, 2, 3$, the solutions of the classical and stabilized schemes are practically identical. Moreover, the solutions obtained using different meshes are practically indistinguishable from each other. Such smooth behavior was expected since, even for the coarsest discretization, the *direct Péclet numbers* are all smaller than one $\mathbf{Pe} = (\ell/2\epsilon) [\beta_{11}, \beta_{22}, \beta_{33}]^T = [0.15, 0.2, 0.2]^T$. This *ad hoc* Péclet numbers definition for systems of coupled convection-diffusion equations is the direct and heuristic extension of the well-known single equation case definition (15).

The situation is slightly changed when moving to the next row; for $\epsilon = 0.1$, in which oscillations start to appear in the approximation obtained by the coarsest discretization with the classical scheme. This time the Péclet numbers are $\mathbf{Pe} = [1.5, 2, 2]^T$; and therefore such an oscillatory behavior could have been expected. It disappears for the next finer mesh with corresponding Péclet numbers $\mathbf{Pe} = [0.4687, 0.625, 0.625]^T$. In the right column the effectiveness of the proposed stabilization scheme in removing the spurious oscillations, even for the coarsest mesh, is illustrated. The main features in the boundary layers are also captured, although the approximations obtained using the coarsest meshes differ from the finest meshes approximations due to the limited resolution (lack of nodes) in the boundary layer region.

Moving to the last row in the left column, it is obvious that the amplitude of the oscillations increases in the classical case as the problem gets more dominated by convection. They now even plague approximations on the finest mesh. On the other hand, the approximations obtained by the stabilized scheme, in the right column, are all free of spurious oscillations. They adequately capture the boundary layers and abrupt changes in the solutions even for the coarsest mesh for the whole range of diffusion coefficients tested.

The analytical solution of the problem can be used to assess the numerical approximation error. This analysis is done using the maximum norm, which is usually considered the most adequate for singularly perturbed problems such as convection-diffusion-reaction equations with weak diffusion [2, 56]. The analytical solution $\mathbf{u}_a$ is evaluated at the same points for which the numerical approximation on a mesh having n nodes, denoted by $\mathbf{u}_n$, is available. Thus the numerical approximation error is given by

$$E_n = \|\mathbf{u}_a - \mathbf{u}_n\|_\infty. \quad (38)$$

This numerical approximation error E_n is shown in Figure 2 as a function of the number of nodes in the finite element mesh. This is done for all values of the diffusion parameters tested for the current problem. Dashed lines are used for the results obtained with the classical scheme, while continuous lines are used for the stabilized scheme.

Note that the darkest line in Figure 2, corresponding to the largest diffusion parameter $\epsilon = 1$, exhibits second order convergence in the coarsest meshes range. As soon as the discretization is sufficiently refined, $n = 100$, mesh invariance is established, where round-off errors start to dominate. Note also that the error of the stabilized scheme is always lower than its classical counterpart, precisely in the second order convergence range. It can be argued that this fact is caused by the (even weak) presence of convective terms, for which the classical scheme entails instabilities. Note the increase of the approximation error for $\epsilon = 1$ when going from the penultimate to the last discretization refinement level and exclusively observed for the stabilized scheme. It is presumed that such increase of the approximation error is due to the ill-conditioning introduced in Equation (24) by the evaluation of the hyperbolic functions. For instance, in this convection-diffusion problem, with $\gamma_{pq} = 0$ and thus $\tilde{\gamma}_{pq} = 0$ for $p, q = 1, 2, 3$, Equation (24) is reduced to

$$\frac{\tilde{\alpha}_{pq}}{\ell} v_q^{(k)} [1 - \cosh(\lambda_k \ell)] + \frac{\tilde{\beta}_{pq}}{2} v_q^{(k)} \sinh(\lambda_k \ell) = 0, \quad (39)$$

which, for any $\lambda_k \neq 0$, becomes trivial in the limit when $\ell \rightarrow 0$ since $\cosh(\lambda_k \ell) \rightarrow 1$ and $\sinh(\lambda_k \ell) \rightarrow 0$, yielding an indetermination. A practical strategy to prevent such a drawback is still under development.

While decreasing the diffusion parameter, going towards brighter lines, one can notice that the second order convergence and mesh invariance ranges are shifted to the right, implying that as the problem becomes more dominated by convection coarse meshes do not have the ability to resolve the solution features any more. The stabilized scheme properly captures these features, like boundary layers, supported by the fact that the associated error is lower than the error obtained with the classical scheme.

The last case, $\epsilon = 10^{-4}$, deserves special attention. For this problem, mesh refinement does not help in reducing the error while using either the classical or the stabilized scheme, until very fine meshes are used. Further refinement is not feasible in terms of computational cost, and more importantly does not improve accuracy. In order to elucidate the latter issue, the most conservative spectral condition number estimate is evaluated, obtained for a single pure diffusive equation, i.e. $\kappa_2 = \mathcal{O}(h^{-2})$ [57]. In the present case $h^{-2} \approx 10^9$ for the finest mesh. This leads to a linear system with a huge condition number, the solution of which can be severely polluted by rounding errors [58, 59]. Obviously, this problem is of a different nature and also affects any stabilization method.

Figure 1: Numerical approximations obtained using different discretizations, darkest for the coarsest mesh consisting of $n = 10$ nodes towards brightest for the finest mesh consisting of $n = 10000$ nodes, with decreasing diffusion from top to bottom, for the classical (left) and stabilized (right) schemes.

Finally, Figure 3 shows the diffusion perturbations for the first equation, i.e. for u_1 , as a function of the discretization size for several values of the diffusion coefficient. As expected, the perturbations automatically increase as the problem becomes more dominated by convection. This is reflected by the fact that the brighter lines, which represent problems more dominated by advection, are always above the darker lines, which in turn represent diffusion dominated problems. More importantly, this plot reveals that the perturbations decrease quadratically as the mesh is refined, demonstrating the consistency of the proposed stabilization technique. The unexpected change in the slope for the line corresponding to the case with $\epsilon = 1$ when going from the penultimate to the last discretization refinement level is attributed to the same ill-conditioning introduced by the evaluation of the hyperbolic functions discussed above.

Figure 2: Numerical approximation error for various diffusion coefficients and mesh sizes. Dashed lines for the classical scheme and continuous lines for the stabilized scheme for $\epsilon = 10^{-j}$ with $j = 0, 1, 2, 3, 4$, as a function of the number of nodes in the mesh.

Figure 3: Diffusion perturbation required to achieve stability for various diffusion coefficients with $\epsilon = 10^{-j}$ with $j = 0, 1, 2, 3, 4$, as a function of the number of nodes in the mesh.

4.2 Diffusion-reaction system

Next, a diffusion-reaction type problem is considered. This problem, originally presented in [4], introduces two new characteristics: the reaction and source coefficients are dependent on the spatial coordinate and the diffusion coefficients differ. Even if the spatial variability of the coefficient is mild, it allows assessing the proposed stabilization technique in handling common difficulties faced by traditional stabilization techniques [41]. Strictly speaking, this characteristic is not a serious difficulty since, before discretization, the differential equations can be scaled in such a way that the previous case, (diffusion matrix equalling a scalar multiplied with the identity matrix) is recovered. However, this scaling may not be desired if

the original physical model is to be preserved. Again, the choice was made to compute only the direct diffusion perturbations.

The system consisting of two differential equations is given by

$$-\begin{bmatrix} \epsilon & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}_{xx} + \begin{bmatrix} 2(x+1)^2 & -(1+x^3) \\ -2\cos(\pi x/4) & 2.2e^{1-x} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 2e^x \\ 10x+1 \end{bmatrix}, \quad (40)$$

with homogeneous Dirichlet boundary conditions at both ends.

Figure 4 shows in each plot the numerical approximations obtained using different discretizations, varying the diffusion parameter row by row. The classical results are depicted in the left column and the stabilized results in the right column.

As expected, the classical and stabilized results are practically identical on the first row, corresponding to the diffusion dominated case. When reducing the diffusion parameter by two orders of magnitude, oscillations start to appear in the numerical approximations obtained with the classical scheme for the coarsest mesh. The stabilized scheme (right column) effectively removes the oscillations. Moreover it recovers the same numerical approximation irrespective of the mesh used.

By moving to the third row, more oscillations appear in the classical scheme since the problem is more dominated by reaction. Even some of the finest meshes show irregularities near the boundary layers. The corresponding numerical approximations obtained with the stabilized scheme are free of spurious oscillations and adequately capture the sharp changes at the boundary layers. It is important to emphasize that mesh invariance is confirmed despite the high reactive character of the problem at hand.

Note that, since the perturbations of the coefficients are computed in each element, the proposed stabilization scheme is able to handle spatially heterogeneous transport coefficients. This is particularly important when dealing with time dependent coefficients or even with non-linear transport equations. This same feature allows handling a variable mesh size, making the stabilization technique highly versatile and flexible.

4.3 Convection-diffusion-reaction system

In the final example, a general system involving all transport mechanisms is included. Approaching such a challenging problem involving convection, diffusion and reaction is precisely the main goal in developing the presented stabilization technique.

The problem considered was originally defined and solved using an upwind finite difference scheme in [60]. It considers a case in which the diffusion matrix is isotropic, and reads

$$\begin{aligned} -\frac{\epsilon}{2} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}_{xx} + \begin{bmatrix} r_1 & 0 & 0 \\ 0 & r_2 & 0 \\ 0 & 0 & r_3 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}_x + \dots \\ \dots + \begin{bmatrix} 2\mu_1 & -2\mu_1 & 0 \\ -\mu_2 & \mu_1 + \mu_2 & -\mu_1 \\ 0 & -2\mu_2 & 2\mu_2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}. \end{aligned} \quad (41)$$

This time, the convection coefficients are piece-wise constant and given by

$$r_k = \begin{cases} (k-1)(\lambda_1 + \lambda_2) - c & \text{if } 0 \leq x \leq b \\ (k-1)\lambda_1 - c & \text{if } b < x \leq 1 \end{cases}. \quad (42)$$

The original boundary conditions have been modified for consistency with the previous problems and to generate boundary layers challenging the stabilization scheme. They have been taken as $\mathbf{u}(x=0) = [0.25, 0, 0.1]^T$ and $\mathbf{u}(x=1) = [0, 0, 0]^T$. All diffusion and discretization parameters are the same as in the previous problem. The parameters in the convection and reaction matrices are taken $\mu_1 = 1$, $\mu_2 = 0.5$, $\lambda_1 = 1$, $\lambda_2 = 0.4$, $c = 1.2$, and $b = 0.3$. Evaluation of the convection coefficients on the two different spatial regions yields: $\mathbf{r}(0 \leq x \leq 0.3) = [-1.2, 0.3, 1.8]^T$ for the left region and $\mathbf{r}(0.3 < x \leq 1.0) = [-1.2, -0.2, 0.8]^T$ for the right region. Note that the abrupt change in the last component relates to its magnitude, while the convection direction remains unchanged. In fact, the variation is more drastic in the second component, which changes its sign. Therefore, in addition to boundary layers, internal layers are also expected.

Figure 4: Numerical approximations obtained using different discretizations, darkest for the coarsest mesh consisting of $n = 16$ nodes towards brightest for the finest mesh consisting of $n = 4096$ nodes, with decreasing diffusion from top to bottom, for the classical (left) and stabilized (right) schemes.

Figure 5 shows the numerical approximations in the same format as previously. In the diffusion dominated case, in the first row, the classical and stabilized results are practically identical. Note that u_1 is convected towards the left since its corresponding convection coefficient is negative on the whole spatial domain while u_3 is convected to the opposite direction because its convection coefficient is positive on the whole domain. Thus u_1 and u_3 exhibit boundary layers at the left and right boundaries respectively. The situation is drastically different for u_2 since its boundary values are the same and its convection coefficients have opposite signs in the two different spatial regions, pointing towards the interior of the domain. Therefore, any quantity of u_2 present in the spatial domain, and generated through the reaction terms, will be transported to the point $x = b$ in which the convection coefficient changes sign. This generates a double internal layer for u_2 itself, but additionally could generate internal layers for u_1 and u_3 through the reaction coupling.

The above mentioned phenomena are more pronounced when moving to the next row, in which the diffusion has been weakened by two orders of magnitude. From these diffusion values, the approximations obtained with the classical scheme are plagued by instabilities for the coarsest meshes. The stabilized scheme solutions are free of spurious oscillations and adequately capture the boundary and internal layers. Moving to the third row, the oscillations in the classical results are so violent that at first sight all numerical approximations are useless, regardless of the mesh used. This is not the case for the stabilized scheme, since all of them still well approximate the solution of the problem at hand.

5 Comparison with other techniques

The main objective of this section is to compare the performance of the presented stabilization technique based on coefficient perturbation to other well-known stabilization techniques already available in the literature. This comparison is carried out with respect to the *Streamline Upwind Petrov-Galerkin* [9], *Galerkin Least-Squares* [61], and *Sub-Grid Scales* [62] techniques, which will be referred in what follows by their respective acronyms *SUPG*, *GLS*, and *SGS*. The restriction to only these three techniques has been made to balance conciseness in the exposition with thoroughness in the assessment. These stabilization techniques have been proposed independently, although they were all presented in a comprehensive manner in [38, 11, 18]. This generic presentation and the fact that they are the most frequently used and established methods in the finite element context, have guided the choice of including them in this comparative study.

The comparison will be carried out using the vector form of the general convection-diffusion-reaction equation (4) in steady state. The following transport operators are introduced

$$\mathcal{L}_D(\mathbf{u}) = -\frac{d}{dx} \left(\mathbf{A} \frac{d\mathbf{u}}{dx} \right), \quad \mathcal{L}_C(\mathbf{u}) = \mathbf{B} \frac{d\mathbf{u}}{dx}, \quad \text{and} \quad \mathcal{L}_R(\mathbf{u}) = \mathbf{G}\mathbf{u}, \quad (43)$$

where the sub-indices D , C , and R refer to diffusion, convection, and reaction respectively. It is possible to gather these three transport operators in a single operator $\mathcal{L}$. By doing so, Equation (4) in steady state can be expressed as

$$\mathcal{L}(\mathbf{u}) \stackrel{\text{def}}{=} \mathcal{L}_D(\mathbf{u}) + \mathcal{L}_C(\mathbf{u}) + \mathcal{L}_R(\mathbf{u}) = \mathbf{f}, \quad (44)$$

and its associated *residual* can be defined as

$$\mathcal{R}(\mathbf{u}) \stackrel{\text{def}}{=} \mathcal{L}(\mathbf{u}) - \mathbf{f}. \quad (45)$$

In order to discretize Equation (44) by finite elements via the weighted residual statement, m weighting functions, one for each of the m coupled convection-diffusion-reaction equations, are introduced and stored in a single vector as $\mathbf{w} = [w_1, w_2, \dots, w_m]^T$. After multiplying Equation (44) by $\mathbf{w}^T$ and integrating over the whole domain one obtains the classical Bubnov-Galerkin scheme, known to be unstable when either convection, reaction or a combination of both dominate over diffusion. Therefore, a stabilizing term is introduced in order to remedy such instabilities. After the introduction of this stabilizing term the weighted integral form of the system of convection-diffusion-reaction equations can be written in all generality as

$$\int_{\Omega} \mathbf{w}^T \mathcal{L}(\mathbf{u}) \, d\Omega + \sum_{e=1}^{n_e} \int_{\Omega^{(e)}} \mathcal{P}^T(\mathbf{w}) \boldsymbol{\tau} \mathcal{R}(\mathbf{u}) \, d\Omega^{(e)} = \int_{\Omega} \mathbf{w}^T \mathbf{f} \, d\Omega. \quad (46)$$

where $\mathcal{P}$ is a differential operator applied to the weighting functions, the particular definition of which depends on the stabilization technique used as discussed below. The $m \times m$ matrix $\boldsymbol{\tau}$ contains the stabilization parameters. Finally $\mathcal{R}$ is the residual already defined by Equation (45). Note that, for the sake of simplicity in the exposition, no integration by parts has been applied in Equation (46) and therefore fluxes on the boundary have not been incorporated. Moreover, the addition of the stabilization term as given here is not affected by the form (advective or divergence) of the transport equation to be discretized. Also note that such stabilization term is computed in an element-wise manner and subsequently incorporated in the global finite element system.

As mentioned above, the form of the differential operator $\mathcal{P}$ defines the stabilization technique used [38, 11, 18]. The SUPG method has been specifically designed to cope with instabilities caused by convection dominance. This fact is reflected by the form of the corresponding differential operator $\mathcal{P}_{\text{SUPG}}$, which reads

$$\mathcal{P}_{\text{SUPG}}(\mathbf{w}) = \mathcal{L}_C^T(\mathbf{w}) = \mathbf{B}^T \frac{d\mathbf{w}}{dx}. \quad (47)$$

(a) Classical, $\epsilon = 10^{-1}$.

(b) Stabilized, $\epsilon = 10^{-1}$.

(c) Classical, $\epsilon = 10^{-3}$.

(d) Stabilized, $\epsilon = 10^{-3}$.

(e) Classical, $\epsilon = 10^{-5}$.

(f) Stabilized, $\epsilon = 10^{-5}$.

Figure 5: Numerical approximations obtained using different discretizations, darkest for the coarsest mesh consisting of $n = 16$ nodes towards brightest for the finest mesh consisting of $n = 4096$ nodes, with decreasing diffusion from top to bottom, for the classical (left) and stabilized (right) schemes.

The GLS method attempts to minimize the residual associated to the differential equation via a least-squares process. Hence, the weighting functions enter in the same form of the original differential operator, i.e. $\mathcal{P}_{\text{GLS}}$ is taken as

$$\mathcal{P}_{\text{GLS}}(\mathbf{w}) = \mathcal{L}^T(\mathbf{w}) = -\frac{d}{dx} \left(\mathbf{A}^T \frac{d\mathbf{w}}{dx} \right) + \mathbf{B}^T \frac{d\mathbf{w}}{dx} + \mathbf{G}^T \mathbf{w}. \quad (48)$$

Finally, the SGS method assumes that the solution can be additively decomposed into a coarse-scale component which can be determined by the finite element method and a fine-scale component which one tries to determine analytically. Furthermore, it is assumed that these two components live in mutually orthogonal function spaces. Thus the $\mathcal{P}_{\text{SGS}}$ operator is defined as

$$\mathcal{P}_{\text{SGS}}(\mathbf{w}) = -\mathcal{L}^*(\mathbf{w}) = \frac{d}{dx} \left(\mathbf{A}^T \frac{d\mathbf{w}}{dx} \right) + \mathbf{B}^T \frac{d\mathbf{w}}{dx} - \mathbf{G}^T \mathbf{w}, \quad (49)$$

where $\mathcal{L}^*$ is the adjoint operator of $\mathcal{L}$.

Finally, the matrix containing the stabilization parameters is defined as

$$\boldsymbol{\tau} = \left[\frac{c_1}{\ell^2} \mathbf{A}_o + \frac{c_2}{\ell} \mathbf{B}_o + c_3 \mathbf{G}_o \right]^{-1}, \quad (50)$$

with

$$\mathbf{A}_o = (\mathbf{A}\mathbf{A})^{1/2}, \quad \mathbf{B}_o = (\mathbf{B}\mathbf{B})^{1/2}, \quad \text{and} \quad \mathbf{G}_o = (\mathbf{G}\mathbf{G})^{1/2}, \quad (51)$$

and $c_1 = 4$, $c_2 = 2$, and $c_3 = 1$. This definition has been proposed by Codina [38] as a straightforward extension of the single equation case in the framework of the GLS method.

5.1 Convection-diffusion system

The comparison of stabilization techniques is first carried out using the convection-diffusion system (35) with boundary conditions (36). Figure 6 presents the numerical results obtained by the proposed stabilization technique, SUPG, GLS, and SGS using three different discretizations. The coarsest discretization consists of $n = 16$ nodes, the medium of $n = 64$ nodes and the finest of $n = 256$ nodes. The mesh density is reflected in the figures by the colour brightness, i.e. the darkest lines correspond to the coarsest discretization while the brightest lines correspond to the finest discretization. All results shown in Figure 6 have been obtained using a diffusion parameter $\epsilon = 10^{-2}$. Thus, the results presented here are comparable with those depicted in the last row of Figure 1 which shows the classical approximation and the perturbation-stabilized solution.

It can be observed in Figure 6 that all numerical approximations are free of spurious oscillations. The results obtained with the SUPG, GLS and SGS methods are practically indistinguishable. The numerical approximations obtained with the perturbation-based stabilization technique differ from the other approximations. The SUPG, GLS and SGS methods are obtaining approximately the same nodal values irrespective of the discretization used. The perturbation-based stabilization technique shifts the boundary layers to the right, as can be seen most clearly for u_1 and u_3 respectively in Figure 6. This effect is at the cost of accuracy, i.e. the numerical approximations rendered by the proposed stabilization scheme are notably influenced by the discretization used.

5.2 Diffusion-reaction system

Now the comparison is carried out on the diffusion-reaction problem given by Equation (40) with homogeneous Dirichlet boundary conditions at both ends for the two equations.

The numerical results obtained are depicted in Figure 7 in the same manner as in the previous subsection. The diffusion parameter has been taken as $\epsilon = 10^{-3}$. The results presented here correspond to those presented in the middle row of Figure 4; in fact, Figure 7(a) reproduces Figure 4(d).

For this diffusion-reaction problem not all results are free of spurious oscillations. Indeed, the failure of the SUPG method to obtain stable solutions in the present case is expected since this technique was not designed to cope with reaction problems. From Equation (47) it is easy to see that $\mathcal{P}_{\text{SUPG}}$ vanishes identically, providing no stabilization at all. This is not the case for the GLS method since $\mathcal{P}_{\text{GLS}}$ does not vanish, although the scheme is unable to remove the spurious oscillations close to the boundary layers.

Figure 6: Numerical approximations obtained using three different discretizations consisting of $n = 16$ nodes (darkest), of $n = 64$ nodes (medium), and of $n = 256$ nodes (brightest), for $\epsilon = 10^{-2}$, for the proposed stabilized scheme (top-left), the Streamline Upwind Petrov-Galerkin (top-right), Galerkin Least-Squares (bottom-left), and Sub-Grid Scale (bottom-right) methods. The corresponding classical results are depicted in Figure 1(e) and the perturbation approach results are repeated from Figure 1(f).

For reaction dominated problems, this limitation has been reported for both one and two-dimensional domains even for the single equation case by Donea and Huerta [18]. It has also been reported by these authors that only the SGS method is able to render numerical approximations free of spurious oscillations. However, in this case it does not provide the same nodal values when different discretizations are used, while the proposed perturbation-based stabilization technique does so.

The presented stabilization technique is thus able, for the diffusion-reaction problem at hand, to render numerical approximations free of spurious oscillations with approximately the same nodal values when using different discretizations

5.3 Convection-diffusion-reaction system

Finally, the comparison is made for the general convection-diffusion-reaction problem defined by Equation (41). The results presented in Figure 8 have been obtained using a diffusion parameter $\epsilon = 10^{-3}$ and correspond to those presented in the middle row of Figure 5.

It is worth noting that the SGS method in this case fails in rendering acceptable numerical approximations. For the present problem, it is the SUPG method that performs better, in the sense that it is capable of rendering solutions which are free of spurious oscillations and with the coarse approximation that best resembles its corresponding fine approximation. The perturbation-based stabilization technique seems to over-diffuse the first solution, i.e. u_1 , for the coarsest discretization. A similar but milder effect can be observed for the GLS method.

Figure 7: Numerical approximations obtained using three different discretizations consisting of $n = 16$ nodes (darkest), of $n = 64$ nodes (medium), and of $n = 256$ nodes (brightest), for $\epsilon = 10^{-3}$, for the proposed stabilized scheme (top-left), the Streamline Upwind Petrov-Galerkin (top-right), Galerkin Least-Squares (bottom-left), and Sub-Grid Scale (bottom-right) methods. The corresponding classical results are depicted in Figure 4(c) and the perturbation approach results are repeated from Figure 4(d).

6 Conclusions and outlook

In this paper a stabilization technique for general systems of one-dimensional coupled convection-diffusion-reaction equations with constant coefficients was developed. It is an heuristic extension, from the single equation case towards the multiple equations case, of the methodology presented in [50]. Thus, for uncoupled systems of equations the proposed stabilization technique recovers the single equation case approach. The stabilization is achieved by effectively perturbing the transport coefficients of the system of differential equations to be discretized. It can be proven that, when dealing with a system of uncoupled equations of either convection-diffusion or diffusion-reaction type, such perturbations are optimally determined to be the minimum ones required to obtain smooth and stable approximations. Additionally, it was shown through a scrupulous numerical assessment dealing with coupled systems of differential equations that the numerical approximations obtained with the stabilized scheme converge to the classical Bubnov-Galerkin solution when the mesh is sufficiently refined. The stabilization technique is applicable regardless whether the advective or the divergence form of the partial differential equation is used for the spatial discretization, making it highly flexible and general, and allowing it to deal with different types of complex boundary conditions.

Although originally developed for coupled equations with constant coefficients, the stabilization technique has also been successfully applied to equations having spatially variable convection and reaction coefficients. This renders the method particularly versatile for problems with time dependent or even non-linear transport coefficients, including also the diffusion coefficients. Furthermore, since the perturbations required to render smooth numerical approximations are computed element by element this stabilization technique is locally adaptive, properly handling variable element sizes. Finally, there is no need to compute in advance, adapt, or change the mesh at any stage of the computation. This flexibility

Figure 8: Numerical approximations obtained using three different discretizations consisting of $n = 16$ nodes (darkest), of $n = 64$ nodes (medium), and of $n = 256$ nodes (brightest), for $\epsilon = 10^{-3}$, for the proposed stabilized scheme (top-left), the Streamline Upwind Petrov-Galerkin (top-right), Galerkin Least-Squares (bottom-left), and Sub-Grid Scale (bottom-right) methods. The corresponding classical results are depicted in Figure 5(c) and the perturbation approach results are repeated from Figure 5(d).

also removes the need for ordering or scaling of the system of differential equations prior to discretization.

The comparative study carried out highlighted both the strengths and weaknesses of the presented stabilization technique with respect to well established stabilization methods. It is worth mentioning that its ability to deal satisfactorily with all three different types of problems presented here is not shared by any of the other stabilization techniques. This shows the generality of the methodology when dealing with systems of coupled convection-diffusion-reaction equations, as well as the convection-diffusion and diffusion-reaction sub-cases.

For future work, the analytical solution injected into the numerical stencil could take into account non-vanishing source terms. Moreover, the proposed stabilization technique can be extended to multidimensional configurations. The problem then arises of how to choose the direction in which the stabilizing effect has to be applied, i.e. in addition to the streamline artificial diffusion, how to determine the optimal cross-wind artificial diffusion needed to suppress persistent oscillations close to sharp gradients in the solution. Endowing the proposed stabilization technique with a shock capturing mechanism able to deal with this difficulty could be pursued as well. Although the present paper mainly focused on constant diffusion and space dependent convection and reaction coefficients in steady state with Dirichlet boundary conditions, variable diffusion coefficients, time dependency of the transport coefficients, non-linearity and other types of boundary conditions will be investigated in steady and transient states.

In this paper, the effect the stabilization technique on the general properties of the system of algebraic equations after discretization has not been addressed. In particular, the spectral properties of this system may guide one to more effective strategies to solve it, especially when using iterative methods combined with preconditioning techniques. This will be the subject of forthcoming work.

Acknowledgments

The first author would like to thank the financial support granted by the European Commission EACEA Agency, Framework Partnership Agreement 2013-0043 Erasmus Mundus Action 1b, as a part of the EM Joint Doctorate Simulation in Engineering and Entrepreneurship Development (SEED).

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