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A STABILIZED FINITE ELEMENT APPROACH FOR ADVECTIVE-DIFFUSIVE TRANSPORT PROBLEMS

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Abstract. *As it is well-known, the numerical simulation in fluid mechanics is quite difficult specially when the velocity of the fluid is important. These problems are reflected in the appearance of numerical oscillations when Finite Element approaches with Galerkin weighting are used. In last years, some alternative formulations have been proposed in order to overcome these problems: Streamline Upwind Petrov Galerkin Methods, Space-time Galerkin Least Squares Methods, Subgrid Scale Methods, Characteristic Galerkin Method, etc. In this paper, we focuse our attention in the advective-diffusive transport differential equation, and its application to engineering problems. Thus, we present a brief review of the causes of appearance of these numerical oscillations and a short revision of the numerical schemes proposed for the stabilization of advective-dominant problems. Then, a numerical formulation based on a Petrov Galerkin scheme and a procedure to obtain stabilization parameters for 1D, 2D and 3D problems are proposed. Finally, we present different numerical test problems, and we show the feasability of this formulation with its application to an engineering problem: the evolution of a water pollutant spilt in a harbour area.*

1 INTRODUCTION

Numerical simulation in Fluid Mechanics is quite difficult particularly in situations in which the velocity field of the fluid is elevated. The Finite Element Method, which has been successfully applied to a great deal of problems in Computational Mechanics, presents serious troubles in the resolution of high-advective fluid problems [1, 2]. These problems are reflected in the appearance of important oscillations of the solution in some areas of the domain.

In order to understand the key of this behaviour, we focuse our attention in the advective-diffusive transport differential equation (which can also be interpreted as the *linear version* of the Navier-Stokes equations). In this way, we can study these phenomena of the numerical oscillations in a linear problem. In this paper, we firstly revise their origin, and review alternative approaches proposed to Galerkin formulation to overcome this problem. Moreover, a new procedure to obtain stabilization parameters in Petrov-Galerkin formulations [3, 4] is proposed. We present different advective-diffusive and high-advective test problems, solved by different numerical techniques. On the other hand, we study the application of these techniques to the solution of a practical engineering problem: the evolution of a water pollutant spilt in a harbour area (in the example presented in this paper, we analyze a 2d problem, so it is assumed that the concentration of the pollutant is fixed along the water column of each point of the domain [5, 6]).

2 MATHEMATICAL MODEL OF THE PROBLEM

2.1 General statement of the physical problem

There are two different processes in transport phenomena in fluid media. The first one is the so-called *diffusion*, and it can be described by the parabolic equation

$$\frac{\partial \phi}{\partial t} = \nabla \cdot (\boldsymbol{K} \nabla \phi) \tag{1}$$

where ϕ is the transported unknown and $\boldsymbol{K}$ is the diffusion tensor of the fluid. The second process appears when the fluid moves: any substance within it will be carried along or "convected", by the mainstream velocity. This is the *convection* or *advection* process, which can be described in a 1D problem by the hyperbolic equation:

$$\frac{\partial \phi}{\partial t} + c\frac{\partial \phi}{\partial x} = 0 \tag{2}$$

being c the fluid velocity. It is obvious that the dominance of one effect over the other will determine whether the transport is mainly due to diffusion or to advection.

Taking into account both processes and considering an isotropic medium, the advective-diffusive transport problem is given by the partial differential equation

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \phi = \boldsymbol{\nabla} \cdot (k \boldsymbol{\nabla} \phi) \quad \text{in } \Omega, \quad \mathrm{t} > 0 \tag{3}$$

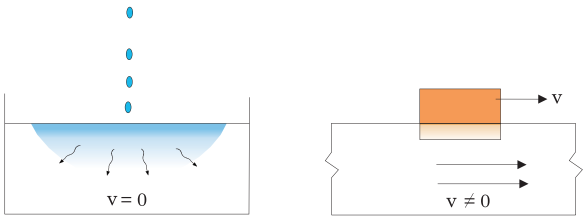

Figure 1: Diffusion and Advection processes in transport phenomena.

with the following boundary and initial conditions

$$\boldsymbol{\nabla}\phi \cdot \boldsymbol{n} = 0 \quad \text{in } \Gamma_1 \; ; \qquad \boldsymbol{\nabla}\phi \cdot \boldsymbol{n} = q \quad \text{in } \Gamma_2 \; ;$$

$$\boldsymbol{\nabla}\phi \cdot \boldsymbol{n} = \gamma - a\phi \quad \text{in } \Gamma_3 \; ;$$

$$\phi(\boldsymbol{x}, 0) = f(\boldsymbol{x}) \; , \; \boldsymbol{x} \in \Omega \; , \tag{4}$$

being Γ_1, Γ_2 and Γ_3 different portions of the boundary Γ where the conditions defined in (4) are prescribed, so that $\Gamma_1 \cup \Gamma_2 \cup \Gamma_3 = \Gamma$. In general, γ, k, a, q and $f(\boldsymbol{x})$ are time and position dependants data.

2.2 Variational statement of the problem

In this section we present a numerical approach using the Finite Element Method with Galerkin weighting for the transport problem. First, it is necessary to define a variational formulation of (3) and (4), that can be set as follows: find ϕ so that this boundary-value problem is satisfied in the meaning of weighted-residuals

$$\int_{\Omega} \left\{ \frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}\phi - \boldsymbol{\nabla} \cdot (k\boldsymbol{\nabla}\phi) \right\} w d\Omega + \int_{\Gamma_2} \{\boldsymbol{\nabla}\phi \cdot \boldsymbol{n} - \gamma + a\phi\} \, w_{\Gamma_2} d\Gamma_2 = 0 \; , \tag{5}$$

for all tests functions w and w_{Γ_2} in Ω and Γ_2 [8]. A weak variational statement may be readily obtained by integration by parts of the diffusion term in the standard weighted-residual statement (5):

$$\int_{\Omega} \left\{ w\frac{\partial \phi}{\partial t} + w\mathbf{u} \cdot \boldsymbol{\nabla}\phi + k\boldsymbol{\nabla}\phi \cdot \boldsymbol{\nabla}w \right\} d\Omega \; + \; \int_{\Gamma_2} a\phi k w d\Gamma_2 \; = \; \int_{\Gamma_2} \gamma k w d\Gamma_2. \tag{6}$$

Next, it is necessary to introduce a discrete approach to the solution of the problem, and a partition of the domain Ω in e elements $\Omega_1 \cup \Omega_2 \cup \Omega_3 \cup ... \cup \Omega_e$ so that $\Omega_i \cap \Omega_j = 0$ $(i \neq j)$ must be performed; therefore we obtain a finite element discretization Ω_h of domain Ω. The next step is to define a basis of local shape functions p_j so that

$$\phi \approx \tilde{\phi}(\mathbf{x}, t) = \sum_{j=1}^{n} \phi_j(t) p_j(\mathbf{x}). \tag{7}$$

Finally, we must define n test functions w_i to obtain a linear system of n equations with n unknowns. This linear system is the discrete approach to the boundary-value problem defined in (3) and (4). If a Galerkin weighting scheme is applied ($p_j = w_j$, $j = 1, n$), the weak variational statement leads to the following system of linear equations:

$$\mathbf{B}\frac{d\boldsymbol{\phi}}{dt} + \mathbf{A}\boldsymbol{\phi} = \mathbf{c}, \tag{8}$$

being

$$B_{ij} = \left[\int_{\Omega_h} p_i p_j \; d\Omega_h\right],$$

$$A_{ij} = \left[\int_{\Omega_h} (\mathbf{u}\cdot\boldsymbol{\nabla} p_j) p_i \; d\Omega_h\right] + \left[k\int_{\Omega_h} \boldsymbol{\nabla} p_j \cdot \boldsymbol{\nabla} p_i \; d\Omega_h\right] + \left[ak\int_{\Gamma_{2_h}} p_i p_j \; d\Gamma_{2_h}\right],$$

$$c_i = \left[\gamma k\int_{\Gamma_{2_h}} p_i d\Gamma_{2_h}\right] \tag{9}$$

for $i, j = 1, 2...n$

Equations (8) and (9) represent the approach to the solution of a transport problem using a Finite Element formulation with Galerkin weighting. As we shall see, the choice of this weighting scheme produces high-oscillating numerical solutions in high-advective problems.

3 ORIGIN OF THE OSCILLATING BEHAVIOUR

For high-advective problems, it can be demonstrated [8, 9, 10] that the numerical scheme obtained with a Galerkin weighting is unable to propagate precisely both the *frecuency* and the *amplitude* of an eigenfunction of the analytical solution of certain problems. This frequency and this amplitude arises as a consequence of the existence of complex eigenvalues associated to a certain eigenfunction. These complex eigenvalues are the origin of the apperance of the numerical oscillations. Now, we will ilustrate the appearance of these complex eigenvalues and its influence in the problem [8].

Using Taylor series expansions we obtain the next fully discrete forward system for the problem (8)

$$\mathbf{B}\left(\frac{\boldsymbol{\phi}(t+\Delta t) - \boldsymbol{\phi}(t)}{\Delta t}\right) + \mathbf{A}\boldsymbol{\phi}(t) = \boldsymbol{c}(t) + \theta(\Delta t), \tag{10}$$

that, if we do $t^j = t$ and $t^{j+1} = t + \Delta t$, can be rewritten as

$$\boldsymbol{\phi}^{j+1} = (\mathbf{I} - \Delta t\mathbf{B}^{-1}\mathbf{A})\boldsymbol{\phi}^j + \Delta t\mathbf{B}^{-1}\boldsymbol{c}^j. \tag{11}$$

In order to simplify our analysis, we will consider the homogeneous equation ($\boldsymbol{c} = \mathbf{0}$). Thus, the solution in a time step $j+1$ can be obtained from the solution in a time j multiplied by the factor

$$(\mathbf{I} - \Delta t\mathbf{B}^{-1}\mathbf{A}). \tag{12}$$

We can analyse the temporal evolution of ϕ by defining a norm to the factor (12). This norm can be set in terms of the eigenvalues of $\mathbf{B}^{-1}\mathbf{A}$ [8]. Since the complete development of this analysis is too cumbersome to be explicited in this paper (it can be found in [8, 9, 10, 11]), we will show their influence in a particular case. In the following example it is shown that, in high-advective problems, the eigenvalues of this matrix can be complex values, and therefore the numerical solution will present spurious oscillations. If one considers a 1D case with linear finite elements (with a mesh size h), then the following expresions to the matrices defined in (9) are obtained

$$\mathbf{B} = \frac{h}{12}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}; \quad \mathbf{A} = \frac{u}{2}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{k}{h}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \tag{13}$$

If we study the steady-state response of the problem, the elemental matrices defined in (13) produce

$$\left[\frac{u}{2}\begin{pmatrix} -1 & 1 & 0 & & & \\ -1 & 0 & 1 & & \dots & \\ 0 & -1 & 0 & & & \\ & & & 0 & 1 & 0 \\ & \dots & & -1 & 0 & 1 \\ & & & 0 & -1 & 1 \end{pmatrix} + \frac{k}{h}\begin{pmatrix} 1 & -1 & 0 & & & \\ -1 & 2 & -1 & & \dots & \\ 0 & -1 & 2 & & & \\ & & & 2 & -1 & 0 \\ & \dots & & -1 & 2 & -1 \\ & & & 0 & -1 & 1 \end{pmatrix}\right]\begin{bmatrix} \phi_1 \\ \phi_2 \\ \dots \\ \dots \\ \dots \\ \phi_n \end{bmatrix} = \begin{bmatrix} c_1 \\ .. \\ .. \\ .. \\ \\ c_n \end{bmatrix}. \tag{14}$$

As it can be seen, the matrix of system (14) is the result of assembling the diffusive and advective terms of matrix $\boldsymbol{A}$ defined in (13). The advective component yields a non-symmetrical matrix, with many ceros in the main diagonal. This matrix is the origin of the appearance of the complex eigenvalues when advection is more important than diffusion. This circumstance is shown in the next three cases corresponding to a mesh of 7 linear elements, in which we have computed all eigenvalues for different Péclet numbers:

1. *Diffusive problem.*

u=2, k=5, h=1 , $Pe = 0.4$

$$\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \lambda_6 \\ \lambda_7 \end{bmatrix} = \begin{bmatrix} 18.828 \\ 16.109 \\ 12.180 \\ 7.820 \\ 3.891 \\ 1.172 \\ 0.000 \end{bmatrix}$$

2. *Advective problem*

u=12, k=5, h=1 , $Pe = 2.5$

$$\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \lambda_6 \\ \lambda_7 \end{bmatrix} = \begin{bmatrix} 00.0 + 0.00i \\ 10.0 - 4.14i \\ 10.0 - 1.48i \\ 10.0 + 1.48i \\ 10.0 - 5.98i \\ 10.0 + 5.98i \\ 10.0 + 4.14i \end{bmatrix} \tag{15}$$

3. *High-advective problem.*
u=40, *k=5,* *h=1* , $Pe = 40$

$$\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \lambda_6 \\ \lambda_7 \end{bmatrix} = \begin{bmatrix} 00.0 + \ 0.00i \\ 10.0 + 34.89i \\ 10.0 - 34.89i \\ 10.0 + 24.15i \\ 10.0 - 24.15i \\ 10.0 + \ 8.62i \\ 10.0 - \ 8.62i \end{bmatrix} \tag{16}$$

If we pay attention to equation (14), we can see that remeshing the domain (i.e., adopting a smaller size of element h) is a straightforward way to stabilize the problem, since the diffusive component becomes more important. Obviously, this remeshing procedure would imply a hughe increase of computational cost in practical cases, so it isn't a good solution. For this reason, some alternative formulations have been proposed to obtain stable numerical schemes. All of them establish different kinds of weighting, trying to enhance the diffusive term, i.e. the symmetrical part of the equation.

4 ALTERNATIVE FORMULATIONS TO THE PROBLEM

In last years, different alternative schemes to the Galerkin weighting have been proposed to stabilize the numerical formulation of the transport equation. Some of these are: *Streamline Upwind / Petrov-Galerkin* (*SUPG*) [12], *Space-time Galerkin/least-squares* (*ST- GLS*) [13],*Characteristic Galerkin Method* (*CG*) [14], *Subgrid Scale Method* (*SGS*) [15] and *Taylor-Galerkin Method* (*TG*) [16]. Basically, all these methods consist of the addition of a stabilizer term to the Galerkin formulation. Thus, the variational statement of problem (6)

$$\int_{\Omega_h} \left\{ w_h \frac{\partial \tilde{\phi}}{\partial t} + w_h \mathbf{u} \cdot \boldsymbol{\nabla} \tilde{\phi} + k \boldsymbol{\nabla} \tilde{\phi} \cdot \boldsymbol{\nabla} w_h \right\} d\Omega_h \ + \int_{\Gamma_{2_h}} a \tilde{\phi} k w_h d\Gamma_{2_h} \ = \int_{\Gamma_{2_h}} \gamma k w_h d\Gamma_{2_h} \ , \tag{17}$$

is modified by an additional term of the general form [17]

$$\int_{\Omega_h} \mathcal{P}(w_h) \tau \mathcal{R}(p_h) d\Omega, \tag{18}$$

where $\mathcal{P}(w_h)$ is an operator which is applied to the test functions, τ is a stabilization parameter, and $\mathcal{R}(p_h)$ is the residual of the differential equation:

$$\mathcal{R}(p_h) = \frac{\partial \tilde{\phi}}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \tilde{\phi} - \boldsymbol{\nabla} \cdot (k \boldsymbol{\nabla} \tilde{\phi}) \ . \tag{19}$$

Most classical stabilization methods for the transport equation problem fall within the previous framework. For example, Petrov-Galerkin formulations introduce this stabilization term by upwinding the test functions against the current lines; thus, in the 1D case, for a linear element, test functions $w_i(\xi)$ and trial functions $p_i(\xi)$ can be defined as

$$p_i(\xi) = \begin{cases} p_1(\xi) = \frac{1}{2}(1-\xi) \\ \\ p_2(\xi) = \frac{1}{2}(1+\xi) \end{cases}, \quad w_i(\xi) = \begin{cases} w_1(\xi) = \frac{1}{2}(1-\xi) - \frac{\alpha}{4}(1+\xi)(1-\xi) \\ \\ w_2(\xi) = \frac{1}{2}(1+\xi) + \frac{\alpha}{4}(1+\xi)(1-\xi) \end{cases} \tag{20}$$

where α is a scaling factor that specifies the amount of upwind bias desired (*upwind parameter*), as it is shown in figure 2.

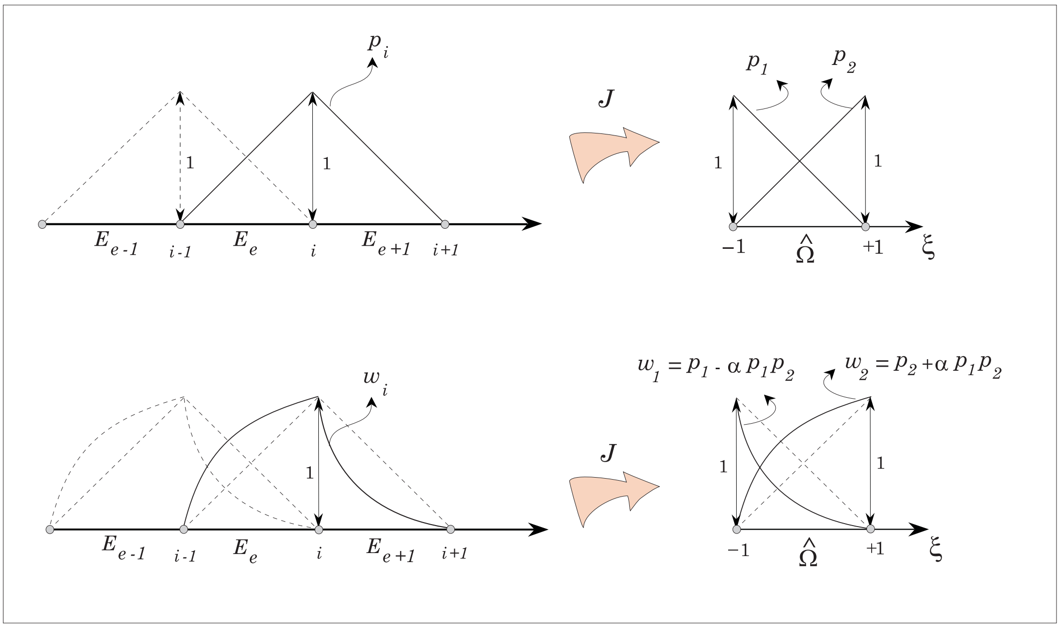

Figure 2: Standard piecewise-linear basis functions and quadratically based test functions for Petrov-Galerkin approaches.

At present, the development of a general method for computing these parameters as a function of the velocity flow is still an open field of study. Thus, some methods propose to compute this parameter by imposing exact nodal solutions [3, 4, 18], and other seek for the reduction of oscillations by the comparison of results obtained from a poor mesh with those obtained from an enriched mesh, or even by means of smoothing procedures [19].

A new method for computing these stabilization parameters will be presented below. This method is based on the analysis of the eigenvalues of elemental matrices, according to the ideas presented before. However, we will show first how the introduction of a bias in the test functions stabilizes the numerical model. Thus, if we consider a 1D case with linear elements and the test functions defined in (20), we obtain the next system of linear differential equations [8]:

$$\left(\mathbf{B}\frac{d\boldsymbol{\phi}}{dt} + u\mathbf{A}_1\boldsymbol{\phi} + k\mathbf{A}_2\boldsymbol{\phi}\right) + \alpha\left(\widehat{\mathbf{B}}\frac{d\boldsymbol{\phi}}{dt} + u\widehat{\mathbf{A}}_1\boldsymbol{\phi} + k\widehat{\mathbf{A}}_2\boldsymbol{\phi}\right) = \mathbf{c}. \tag{21}$$

It is very interesting the analysis of elemental matrices $\widehat{\mathbf{B}}$, $\widehat{\mathbf{A}}_1$ and $\widehat{\mathbf{A}}_2$ associated to the cuadratic bias, that are given by

$$\widehat{\mathbf{B}}^e \equiv \left[\widehat{b}_{ij}\right]_e = \frac{h}{12}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}, \tag{22}$$

$$\widehat{\mathbf{A}}_1^e \equiv \left[\widehat{a}_{1_{ij}}\right]_e = \frac{1}{6}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \tag{23}$$

$$\widehat{\mathbf{A}}_2^e \equiv \left[\widehat{a}_{2_{ij}}\right]_e = \mathbf{0}. \tag{24}$$

Note that elemental matrix (23) is a new advective contribution to the term appeared in (13). This is a symmetrical matrix which will contribute to stabilize the non-symmetrical matrix (13). Likewise, the new diffusive contribution given by (24) is equal to zero, so it does not perturb the symmetrical matrix (13). It is important to notice that this analysis can also be made [3, 4] for high-order elements and 2D and 3D problems, obtaining similar conclusions.

Therefore, our goal is the development of numerical formulations that produce stable schemes by the appropiate weighting of the elemental advective and diffusive matrices by means of suitable stabilization parameters.

5 BASIS OF THE PROPOSED METHOD TO COMPUTE STABILIZATION PARAMETERS

If we do not consider the terms of (9) associated to the flux prescribed in the boundary, then we obtain

$$A_{ij} = \left[\int_{\Omega_h} (\mathbf{u}\cdot\boldsymbol{\nabla} p_j) p_i \; d\Omega_h\right] + \left[\int_{\Omega_h} k\boldsymbol{\nabla} p_j \cdot \boldsymbol{\nabla} p_i \; d\Omega_h\right]. \tag{25}$$

Thus, each elemental matrix is the sum of an advective term (which yields non- symmetrical matrices) and a diffusive term (which yields symmetrical matrices). These elemental matrices may have complex eigenvalues in high-advective problems, so their assembling will produce an *ill-conditioned* problem which present an oscillating solution.

Different formulations are used to overcome this problem. For example, the Petrov-Galerkin formulation modifies the Galerkin space of weighting functions by introducing an upwinding bias in the trial functions. This modification seeks for the stabilization of the non-symmetrical matrices associated to advection, just like it was shown in (21)-(24). Now the matter is to determine the amount of this bias.

The method we propose for the calculation of these parameters is the following: Firstly, elemental matrices are computed adopting for the stabilization parameter a null value (so, we obtain a Galerkin formulation). Next, the computation (or estimation) of the set of eigenvalues $\{\lambda_i\}$ of each elemental matrix $\boldsymbol{A}_e$ is performed. If all of these eigenvalues are real numbers, then the stabilization parameter is equal to zero. However, if it should not be so, then it is necessary to increase the value of the stabilization parameter since no complex eigenvalues in the elemental matrices appear. That is, we pretend to find

$$\{\alpha_e\} \ / \ Im\{\lambda_i \ [\boldsymbol{A}_e]\} = 0, \quad i = 1, ..., n \qquad \forall e, \tag{26}$$

being $\{\alpha_e\}$ the set of stabilization parameters of each element.

In this point, it is important to note an essential characteristic of this method: it is absolutely general and independent of the dimension of the problem. The stabilization parameters are not computed in an heuristic way, and it also works if internal fonts and reactive terms are considered in the transport differential equation. Consequently, it is a general methodology, very simple from a conceptual point of view, that stabilizes the numerical model of the problem by analyzing only its elemental matrices.

At present, we have obtained very promising results in the cases studied until now [8, 10, 20], and we are developing a method for the computation of these parameters using the information contained in the eigenvalues for 2D and 3D problems. Next, we present a 1D high-advective example in which is shown the feasability of the proposed method.

6 1D NUMERICAL EXAMPLE

We consider the 1D numerical test defined by (see figure 3):

$$u\frac{\partial \phi}{\partial x} = k\frac{\partial^2 \phi}{\partial x^2}\ , \qquad 0 < x < L; \quad \phi(0) = \phi_0 \ \ , \qquad \frac{\partial \phi}{\partial x}(L) = h[\phi_L - \phi(L)] \tag{27}$$

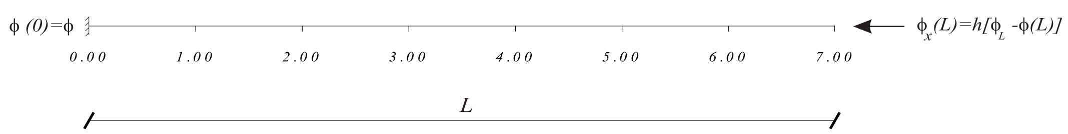

Figure 3: Domain and boundary conditions of the test problem.

The discretization parameters for this problem are as follows:

Number of elements = 10 Number of nodes per element = 3

$\phi_0 = 0.001$ $\phi_L = 0.005$ h = 1.0 Diffusion $k = 0.002$

The velocity field considered in this problem is represented in the next figure

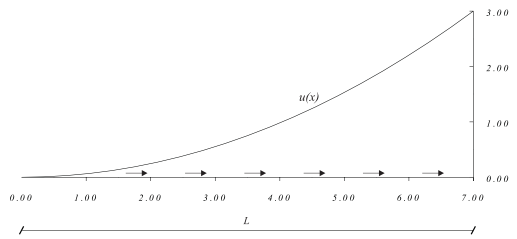

Figure 4: Velocity profile for the test problem.

This velocity profile yields the next distribution of Péclet numbers, that as it can be seen, they are very elevated at the end of the domain

Elemento	Velocidad elemental	Numero de Péclet
1	0.01250	2.18750
2	0.07250	12.68750
3	0.19250	33.68750
4	0.37250	65.18750
5	0.61250	107.18750
6	0.91250	159.68750
7	1.27250	222.68750
8	1.69250	296.18750
9	2.17250	380.18750
10	2.71250	474.68750

Figure 5: Distribution of Péclet numbers for the test problem.

Results obtained with different formulations are presented below, comparing them with the *exact* solution to the problem. This *exact* solution has been obtained by using a very dense mesh (1000 elements) and a Galerkin weighting scheme.

The formulations that have been used are:

1. *Galerkin formulation*
2. *Petrov-Galerkin formulation with "classical" determination of stabilization parameters.*
3. *Petrov-Galerkin formulation with the proposed method for computing parameters.*

In figure 6, it can be seen that oscillations in the Galerkin solution are very elevated, as it was foreseeable. This approximation is extremely poor. In the "clasical" Petrov-Galerkin approximation the computing of the stabilization parameters was made by means of the known expression [18]:

$$\alpha = \coth(\gamma) - \frac{1}{\gamma}\ , \qquad \gamma = \frac{uh}{2k} = \frac{Pe}{2}\ . \tag{28}$$

Results obtained with this formulation are much better than the previous ones. The stabilization parameter defined in (28) is obtained as a result of imposing that the nodal equations of the discrete system obtained from the finite element method have no truncation errors [18].

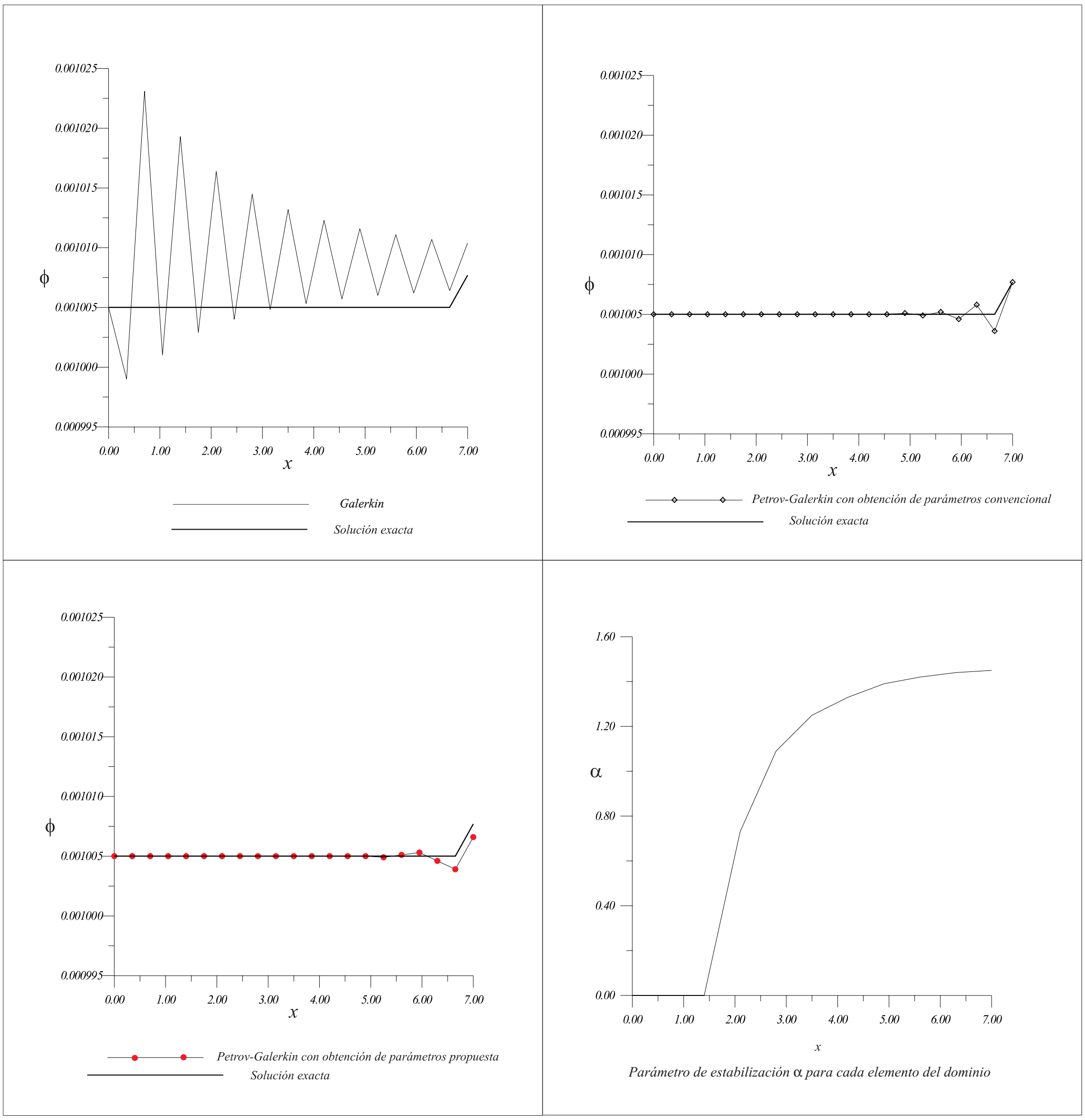

Figure 6: 1D test problem: Results obtained with different formulations.

In the case of the proposed method the computation of the stabilization parameters has been done by using 3-nodes cuadratic elements, which shape and test functions are given by:

$$p_i(\xi) = \begin{cases} p_1(\xi) = \dfrac{\xi(\xi-1)}{2} \\ p_2(\xi) = \dfrac{\xi(\xi+1)}{2} \\ p_3(\xi) = (1-\xi^2) \end{cases} \tag{29}$$

$$w_i(\xi) = \begin{cases} w_1(\xi) = \dfrac{\xi(\xi-1)}{2} - \alpha(\xi^3-\xi) \\ w_2(\xi) = \dfrac{\xi(\xi+1)}{2} - \alpha(\xi^3-\xi) \\ w_3(\xi) = (1-\xi^2) + \alpha(\xi^3-\xi) \end{cases} \tag{30}$$

Figure 6 shows the values of the stabilization parameter α and results obtained with the proposed method. As it can be seen, results are as good as ones obtained with the "classical" formulation, or even better. The reduction of the oscillations is very important and the value of the stabilization parameter is greater in those areas of the domain where the velocity is more elevated. In this example, we remark the great advantage of this formulation that it does not depend on any heuristic method for parameters computing, since a systematic analysis is performed of each elemental matrix.

7 2D APPLICATION EXAMPLE

In this section we will solve a 2D transport problem defined by equations (3) and (4) in a domain Ω defined by the harbour area of the Port of La Corunna. The problem to be solved is the evolution of a water pollutant accidentally spilt in the harbour area. First of all, it is necessary to bound somehow a semi-infinite domain. Considering this, the *open-to-sea-boundary* has been defined by an arc from the end of the dyke to the extreme of Darsena de Oza's wharf (see figure 7). As we shall see, the boundary conditions must be imposed carefully in this portion of the domain [21].

The solution to this problem will be obtained by using a finite element approach, which it is more adecquate than other numerical formulations (e.g., finite differences) [22] since it allows to deal with more complex domains and boundary conditions. The finite element mesh used and its characteristics are represented in figure 7.

7.1 Description of boundary conditions

Once it has been defined the domain and its finite element approximation, it is necessary to specify the boundary conditions (4) to be applied in each portion of the boundary. The boundary finite elements of fig. 7 are divided into three groups, according to the different boundary conditions applied. These groups are as follows:

a) Elements located in the wharves (Γ_1). In these elements, a condition of null normal flux is imposed. This assumes that there is no gain nor lost of pollutant concentration across the wharves. So,

$$\boldsymbol{\nabla}\phi \cdot \boldsymbol{n} = \frac{\partial \phi}{\partial n} = 0 \quad \text{in } \Gamma_1 \tag{31}$$

Figure 7: Domain of the problem: the harbour area of the Port of La Corunna. Finite element mesh obtained whith GEN4U system [23].

b) Elements located in the point of pollutant-spilling (Γ_2). A Neumann condition is applied in this portion of the boundary, so the flux of contaminant is prescribed as follows:

$$\boldsymbol{\nabla}\phi \cdot \boldsymbol{n} = \frac{\partial \phi}{\partial n} = q \quad \text{in } \Gamma_2 \tag{32}$$

c) Elements located in the open-to-sea-boundary (Γ_3). As it has been remarked before, this is a portion of the bondary that requires a special care. We must be able to impose a condition that simulates the effects of the rest of the ocean in the harbour area [8]. It is easy to understand that the ocean works as a spillway for the pollutant spilt in the harbour, and so it prevents from an indefinite increasing of concentration into the harbour area. This condition may be prescribed of many different ways. We have decided to impose a simple mixed boundary condition to try to reproduce this circumstance. This condition is as follows:

$$\nabla\phi \cdot \boldsymbol{n} = \frac{\partial \phi}{\partial n} = \gamma - a\phi \quad \text{in } \Gamma_3 \tag{33}$$

where γ and a are known data, which will be considered time independants.

7.2 A low-advective transport problem

In this section a low advective problem is solved. This means that advective processes are less important than diffusive processes. First, we must specify the velocity field $\boldsymbol{u}(x, y, t)$ considered, which should be obtained in practice (as parameters of the boundary conditions) by means of experimental measures. However, in the example presented in this paper, we have defined it analytically (see fig. 8), only by considering the condition of incompressible flow: $\nabla \cdot \boldsymbol{u} = 0$. This field of velocity has been considered steady in time. The parameters used to solve the problem are defined below.

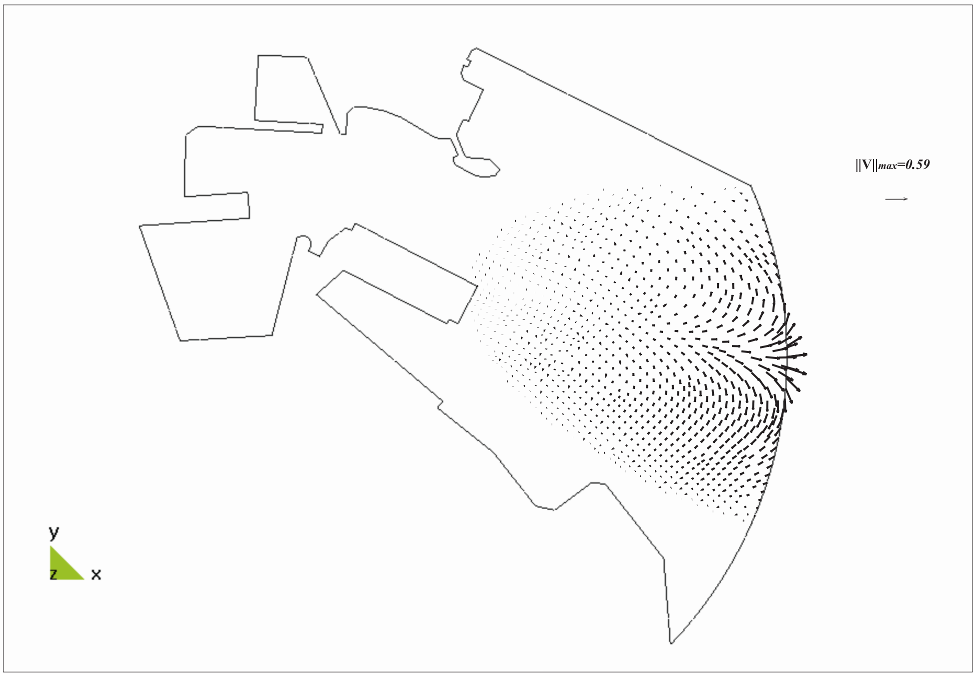

Figure 8: Velocity field analitically defined.

- Difussion $k = 10 \quad \forall\Omega$.

- Maximum Péclet number $Pe = 1.9$, taking the average length of the diagonals of the elements as the characteristic dimension.

- Γ_2 boundary conditions:

  - Oil Harbour (area of spilling)

$$\frac{\partial \phi}{\partial n} = 5 \tag{34}$$

- Γ_3 boundary conditions:

$$\nabla\phi \cdot \boldsymbol{n} = \gamma - a\phi = 5 - 0.5\phi \tag{35}$$

Results obtained for the steady-state response of this problem are shown in fig. 9. This figure presents also the results for the same problem, but considering no advection. As it can be seen, the presence of advection modifies in a very important way the distribution of water pollutant. It is also worthy to remark the increase of the pollutant concentration values all over the domain, due to the addition of the advective effects to the diffusion processes.

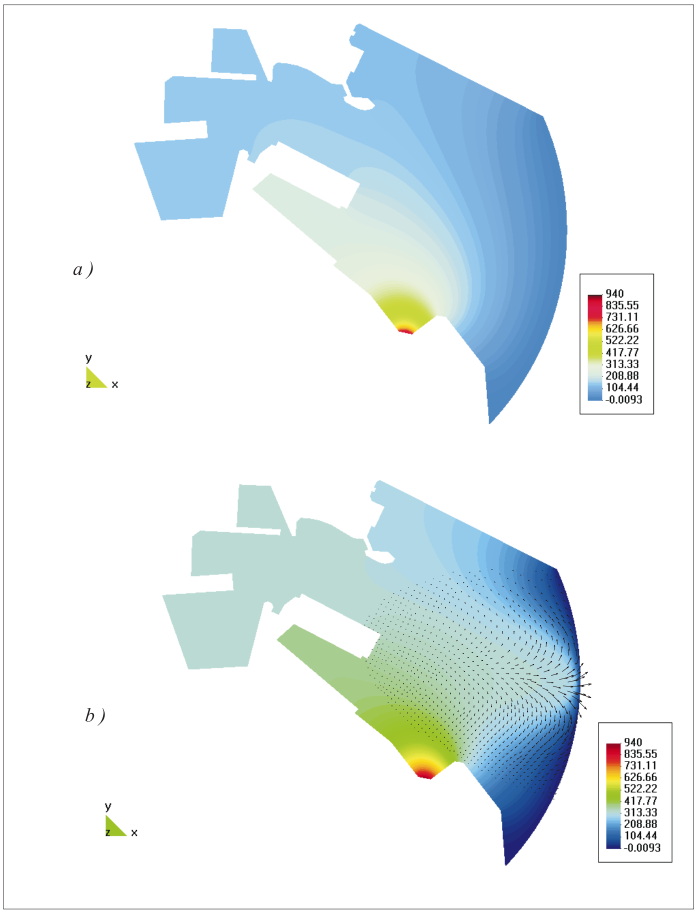

Figure 9: **a**) Solution to the pollutant spilling problem considering no advection processes. **b**) Solution to the pollutant spilling problem considering the field of velocity defined in fig. 8. (Maximum Péclet number=1.9).

7.3 A high-advective transport problem

In this section we will solve a very similar problem to the previous one, but adopting a bigger maximum Péclet number. Thus, we are dealing with a problem in which the importance of the advective processes is much bigger. These problems, as we have already seen

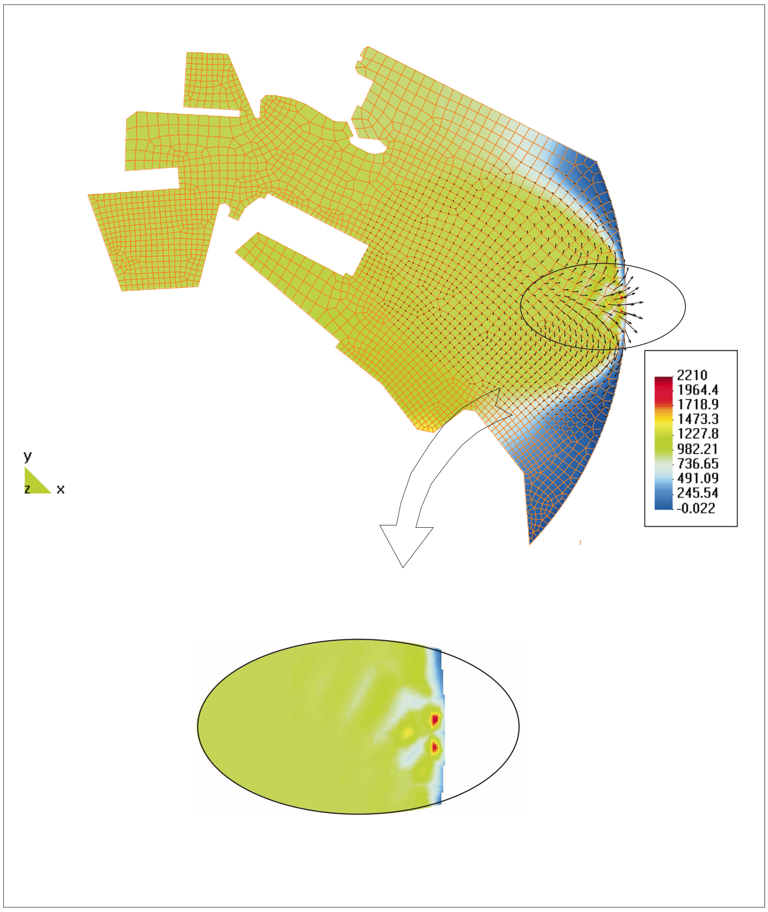

Figure 10: Solution to the pollutant spilling problem in the high-advective case (Maximum Péclet number=19). Below, detail of the zone with important oscillations in the numerical solution (it is also the zone of maximum advection).

and it is widely referenced in the bibliography [18, 9, 10], present a noticeably oscillatory behaviour, if a Galerkin weighting scheme is used. For this analysis of this example, the same field of velocity (fig. 8) will be used, and the parameters considered are the following:

- Diffusion $k = 1 \;\; \forall \Omega$.

- Maximum Péclet number $Pe = 19$.

- Γ_2 boundary conditions:

  - Oil Harbour

$$\frac{\partial \phi}{\partial n} = 5 \tag{36}$$

- Γ_3 boundary conditions:

$$\boldsymbol{\nabla} \phi \cdot \boldsymbol{n} = \gamma - a\phi = 5 - 0.5\phi \tag{37}$$

Solution to this problem (i.e. the evolution of the concetration of the pollutant) is presented in figure 10. It is important to notice the existence of important oscillations in the numerical solution in those areas of the domain where advection is more important. It can also be seen that concentrations are more elevated than in the previous problem, due to a bigger presence of advection. The appearance of these oscillations emphasizes again the poor performance of the Galerkin weighting shemes to solve high-advective transport problems. As we have already seen, there are alternative formulations [8, 17, 19, 24] which are more suitable for these problems. At present, we are developing a extension of the formulation explained in section 5, in order to compute the stabilization parameters required in Petrov-Galerkin formulations for 2D and 3D cases. This will allow us to stabilize the numerical model of problems such as those presented in this section.

8 CONCLUSIONS

In this paper, a new method for computing stabilization parameters required in Petrov-Galerkin weighting formulations has been proposed. These parameters are computed analyzing the eigenvalues of the elemental matrices of the FE discretization, by imposing that these matrices have no complex eigenvalues.

This general methodology is applicable to 1D, 2D and 3D problems and no heuristic arguments are used to obtain the stabilization parameters, what makes it more attractive. These parameters are computed during the integration and the assembly of the elemental matrices.

Results obtained in 1D problems are excellent and very promising, and they can assure a good performance of this method in 2D and 3D cases. However, the computational cost increases since the analysis of the eigenvalues of each elemental matrix of the discretization must be performed. At the present time, we are working in the development of numerical formulations that allow us to reduce the computing effort by re-using the information contained in the eigenvalues of a certain element and its adjacent ones.

Finally, it has been presented an application to an engineering problem. It has been studied the evolution of a water pollutant spilt in a harbour area. A discussion of the suitability of the boundary conditions have been made. Two different problems have been solved using a Galerkin weighting scheme. It can be seen that, as the Péclet number increases, the well-known numerical oscillations appear in those areas of the domain where the advection is more important.

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