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COMPUTING STABILIZATION PARAMETERS IN NUMERICAL MODELS FOR ADVECTIVE-DIFFUSIVE TRANSPORT PROBLEMS

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ABSTRACT

Numerical modelling in Fluid Mechanics is particularly difficult in high-advective fluid problems. The Finite Element Method, which has been succesfully applied to very challenging problems in Computational Mechanics, presents some troubles in the resolution of high velocity fluid problems due to the appearance of important oscillations of the solution in specific parts of the domain.

In this paper, we consider the advective-diffusive transport differential equation, which models a great number of problems in engineering. We briefly review the origin of the numerical oscillations and the alternative approaches proposed to overcome these phenomena, and we propose a procedure to obtain stabilization parameters in Petrov-Galerkin formulations from the eigenvalue analysis of the elemental matrices in the discretized problem. Finally, we present and discuss the results obtained for different tests problems.

1. INTRODUCTION

1.1. Mathematical model: the advective-diffusive transport equation

As it is well-known, the numerical solution of fluid problems obtained by means of Galerkin type Finite Element formulations presents some instabilities for medium and high values of the fluid velocity [1,2]. In order to understand the reasons of this anomalous behaviour, we focuse our attention to the advective-diffusive transport differential equation, which can also be interpreted as the "linear version" of the Navier-Stokes equations, and we can study the numerical oscillations in a linear problem.

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In the transport phenomena in a fluid media there are two different main processes: the "diffusion", which can be mathematically 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 $\boldsymbol{K}$ the diffusion tensor of the fluid; and the "convection" or "advection" process, which appears when the fluid moves and any substance within it will be carried along or "convected" by the mainstream velocity. For a 1D case, this process can be modelled by the hyperbolic equation:

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

being u the fluid velocity. Obviously, the dominance of one process over the other will determine the main nature of the transport in a particular case.

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

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

with the following boundary and initial conditions

$$\boldsymbol{\nabla} \phi \cdot \boldsymbol{n} = 0 \ \text{ in } \Gamma_1; \quad \boldsymbol{\nabla} \phi \cdot \boldsymbol{n} = q \ \text{ in } \Gamma_2; \quad \boldsymbol{\nabla} \phi \cdot \boldsymbol{n} = \gamma - a\phi \ \text{ in } \Gamma_3; \quad \phi(\boldsymbol{x}, 0) = f(\boldsymbol{x}), \boldsymbol{x} \in \Omega, \tag{4}$$

being Γ_1, Γ_2 and Γ_3 different parts of the boundary Γ where the above conditions are prescribed ($\Gamma_1 \cup \Gamma_2 \cup \Gamma_3 = \Gamma$). In general, γ, k, a, q and f are time and position dependants data.

1.2. Variational statement of the problem and Numerical model

A variational form of the boundary-value problem defined in (3) and (4) can be written as

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

which must hold for all members w and w_{Γ_2} of suitable classes of test functions defined in Ω and Γ_2[3]. Now, the application of Green's Identity allows to obtain the following weak variational statement:

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

The FEM numerical model of this problem requires the definition of a discrete approach to its solution and the partition of the domain Ω in e elements ($\Omega_1 \cup \Omega_2 \cup \Omega_3 \cup ... \cup \Omega_e$, so that $\Omega_i \cap \Omega_j = 0$, $i \neq j$); therefore, a finite element discretization Ω_h of domain Ω is obtained. Next, the definition of a basis of local shape functions p_j so that

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

and the selection of n test functions w_i leads to the linear system of equations:

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

being

$$\begin{aligned} B_{ij} &= \int_{\Omega_h} w_i p_j \; d\Omega_h, \quad i,j = 1,n \\ A_{ij} &= \int_{\Omega_h} (\mathbf{u}\cdot\boldsymbol{\nabla} p_j) w_i \; d\Omega_h + \int_{\Omega_h} k\boldsymbol{\nabla} p_j \cdot \boldsymbol{\nabla} w_i \; d\Omega_h + \int_{\Gamma_{2_h}} a k w_i p_j \; d\Gamma_{2_h}, \quad i,j = 1,n \\ c_i &= \int_{\Gamma_{2_h}} \gamma k w_i d\Gamma_{2_h}, \quad i = 1,n \end{aligned} \tag{9}$$

2. NUMERICAL INSTABILITIES IN GALERKIN TYPE APPROACHES

The Galerkin type weighting ($w_i = p_i$, $i = 1,n$), which has been successfully used in the finite element solution of a great number of problems in solid mechanics, produces unstable numerical schemes when it is applied to advective-diffusive transport problems with medium and high values of the velocity of the fluid. In these cases, it can be shown [3,4] that the Galerkin type numerical model 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. Next, we ilustrate the appearance of these complex eigenvalues and its influence in the problem.

In order to simplify further analysis, we will consider the problem (8) in its homogeneous form ($\boldsymbol{c} = \mathbf{0}$). Thus, by using the expansion in Taylor series, the next fully discrete forward system for the problem can be derived

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

which can be rewritten (if we denote $t^j = t$ and $t^{j+1} = t + \Delta t$) in the following form:

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

that is, the approximation to the solution in time step $j+1$ is obtained from the approximation in a time j multiplied by the factor $(\mathbf{I} - \Delta t\mathbf{B}^{-1}\mathbf{A})$. Analysis of the temporal evolution of unknown ϕ can be performed by defining a norm to this factor, which can be set in term of the eigenvalues of $\mathbf{B}^{-1}\mathbf{A}$[4]. Since the full development of this analysis is too cumbersome to be made completely explicit in this paper[3,4,5], we show their influence in an example. If we consider a 1D problem with constant physical properties and discretize the domain in a mesh of linear finite elements which size is h, the elemental matrices are given by

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

Constraining the analysis to the obtention of the steady-state response of the problem, the assembly process of the matrix $\mathbf{A}$ in (8) leads to the following linear system of equations

$$\left[\frac{u}{2}\begin{pmatrix} -1 & 1 & 0 & & & \\ -1 & 0 & 1 & & ... & \\ 0 & -1 & 0 & & & \\ & & & 0 & 1 & 0 \\ & ... & & -1 & 0 & 1 \\ & & & 0 & -1 & 1 \end{pmatrix} + \frac{k}{h}\begin{pmatrix} 1 & -1 & 0 & & & \\ -1 & 2 & -1 & & ... & \\ 0 & -1 & 2 & & & \\ & & & 2 & -1 & 0 \\ & ... & & -1 & 2 & -1 \\ & & & 0 & -1 & 1 \end{pmatrix}\right]\begin{bmatrix} \phi_1 \\ \phi_2 \\ ... \\ ... \\ ... \\ \phi_n \end{bmatrix} = \begin{bmatrix} c_1 \\ .. \\ .. \\ .. \\ \\ c_n \end{bmatrix} \quad (13)$$

In this expression, it can be seen the different contribution of diffusive and advective terms in the coefficients matrix. The advective component produces a non-symmetrical matrix, with many null elements in the main diagonal, is the origin of the apperance of the complex eigenvalues when the contribution of this matrix is dominant in the final linear system of equations, that is when advection is more important than diffussion. This effect can be shown in the following three cases corresponding to the above example for a mesh of 7 elements with different Péclet numbers ($Pe = uh/k$):

u=2, k=5, h=1, Pe=0.4 *u=12, k=5, h=1, Pe=2.4* *u=40, k=5, h=1, Pe=8*

$$\begin{bmatrix}\lambda_1\\ \lambda_2\\ \lambda_3\\ \lambda_4\\ \lambda_5\\ \lambda_6\\ \lambda_7\end{bmatrix} = \begin{bmatrix}18.828\\ 16.109\\ 12.180\\ 7.820\\ 3.891\\ 1.172\\ 0.000\end{bmatrix}; \quad \begin{bmatrix}\lambda_1\\ \lambda_2\\ \lambda_3\\ \lambda_4\\ \lambda_5\\ \lambda_6\\ \lambda_7\end{bmatrix} = \begin{bmatrix}00.0+0.00i\\ 10.0-4.14i\\ 10.0-1.48i\\ 10.0+1.48i\\ 10.0-5.98i\\ 10.0+5.98i\\ 10.0+4.14i\end{bmatrix}; \quad \begin{bmatrix}\lambda_1\\ \lambda_2\\ \lambda_3\\ \lambda_4\\ \lambda_5\\ \lambda_6\\ \lambda_7\end{bmatrix} = \begin{bmatrix}00.0+\ 0.00i\\ 10.0+34.89i\\ 10.0-34.89i\\ 10.0+24.15i\\ 10.0-24.15i\\ 10.0+\ 8.62i\\ 10.0-\ 8.62i\end{bmatrix} \quad (14)$$

According to (13), a straightforward way to stabilize the problem is to use a smaller size of element h, since then the advective component becomes less important than the diffusive one. Obviously, a remeshing procedure, which is feasible for 1D test problems, would imply an unaffordable computational cost in practice. For this reason, alternative numerical approaches have been proposed in last years to the Galerkin type weighting in order to obtain stable finite element formulations for the advective-diffusive transport equation.

3. NUMERICAL APPROACHES FOR THE ADVECTIVE-DIFFUSIVE TRANSPORT PROBLEM

Numerical formulations proposed to stabilize the finite element equations for the transport problem are based on the selection of different types of weighting in order to enhance the diffusive contribution, that is, in the previous example the symmetrical part of the equation (13). The simplest ones directly introduce an additional diffusive term, while more recent and rigorous techniques modify the variational form in the Galerkin type weighting (SUPG[5], GLS[6], Taylor-Galerkin methods[7], Characteristic-Galerkin method[8], etc.), introducing one or more parameters which adjust the stability of the numerical approximation. Thus, the variational statement (6) of the problem is modified by the addition of a term of the general form[9]

$$\int_{\Omega_h} \mathcal{P}(w_h)\tau\mathcal{R}(p_h)d\Omega, \quad (15)$$

being $\mathcal{P}(w_h)$ an operator applied to the test functions, τ the stabilization parameters, and $\mathcal{R}(p_h)$ the residual of the differential equation:

$$\mathcal{R}(p_h) = \frac{\partial \tilde{\phi}}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \tilde{\phi} - \boldsymbol{\nabla} \cdot (k \boldsymbol{\nabla} \tilde{\phi}). \tag{16}$$

Most of the proposed stabilization methods can be included in this general framework. In the case of the Petrov-Galerkin formulations the stabilization of the numerical solution is performed upwinding the test functions against the current lines of the fluid; in the 1D case, for example, test functions $w_i(\xi)$ and trial functions $p_i(\xi)$ can be defined for linear elements as

$$p_i(\xi) = \begin{cases} p_1(\xi) = \frac{1}{2}(1-\xi) \\ \\ p_2(\xi) = \frac{1}{2}(1+\xi) \end{cases}, \quad w_i(\xi) = \begin{cases} w_1(\xi) = \frac{1}{2}(1-\xi) - \frac{\alpha}{4}(1+\xi)(1-\xi) \\ \\ w_2(\xi) = \frac{1}{2}(1+\xi) + \frac{\alpha}{4}(1+\xi)(1-\xi) \end{cases} \tag{17}$$

being α the scaling factor that controls the amount of upwind bias desired ("upwind parameter"), as it is shown in Fig. 1.

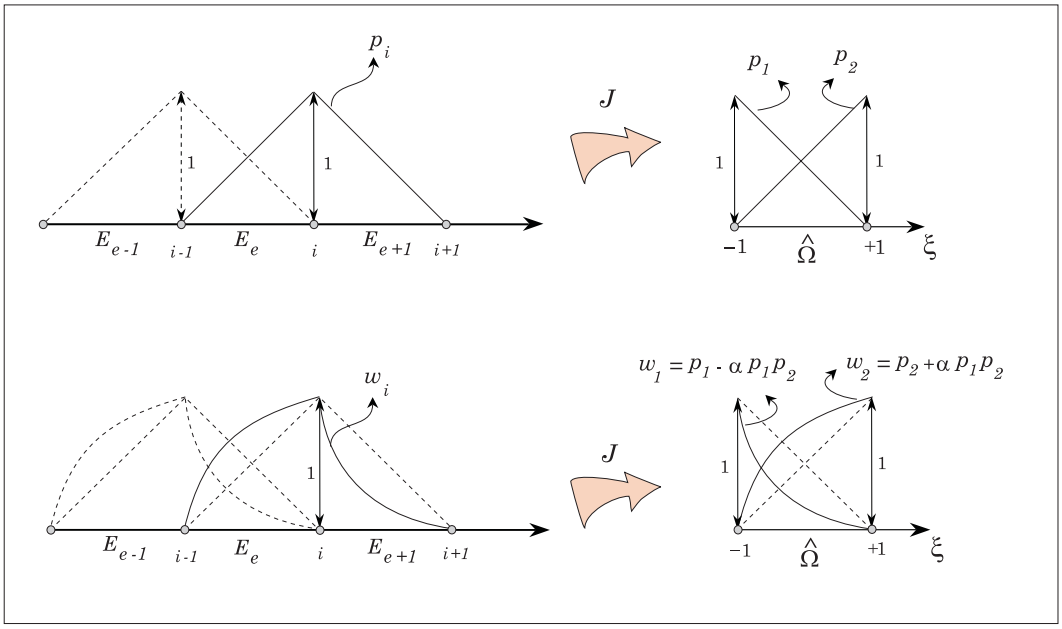

Fig. 1.-Standard piecewise-linear basis functions and quadratically based test functions for Petrov-Galerkin approaches.

If we recover the 1D example presented in (12) and introduce a bias in the test functions, we can show the stabilization mechanism of the numerical model. Thus, taking into account the trial and the test functions defined in (17), the following linear system of equations is obtained, instead of (8):

$$\left(\mathbf{B} \frac{d\boldsymbol{\phi}}{dt} + \mathbf{A}\boldsymbol{\phi} \right) + \alpha \left(\widehat{\mathbf{B}} \frac{d\boldsymbol{\phi}}{dt} + \widehat{\mathbf{A}}\boldsymbol{\phi} \right) = \mathbf{c}, \tag{18}$$

where the elemental matrices associated to the cuadratic bias $\widehat{\mathbf{B}}$, $\widehat{\mathbf{A}}$ are given by

$$\widehat{\mathbf{B}}^e = \frac{h}{12} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}; \quad \widehat{\mathbf{A}}^e = \frac{u}{6} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + k \, \mathbf{0}. \tag{19}$$

Now, in this approach it is added a new advective term (there is no new diffusive contribution), which is a symmetrical matrix and will contribute to stabilize the numerical scheme balancing the contribution of the non-symmetrical matrix $\mathbf{A}^e$ in the assembled matrix of coefficients of the final system. It is important to notice that this analysis can also be made for high-order elements and 2D and 3D problems, obtaining similar conclusions[3,4].

It is obvious that the obtention of suitable stabilization parameters for this kind of finite element approaches is now the key of the problem[10]. Nowadays, computation of stabilization parameters for finite element approaches of the advective-diffusive transport equation remains an open field of study[11]. Thus, for example, some approaches propose the computation of the "best" parameter analitically or imposing the exact solution at nodes (which is possible to obtain for simple 1D problems), by the comparison of results from a poor mesh with those obtained from an enriched mesh, or by means of smoothing procedures, and parameters for 1D problems are heuristically used for 2D and 3D cases in practice.

In previous works[3,12], we have proposed a different method for the computation of the stabilization parameter. As we have shown, the ill-conditioning character of the numerical formulation based on Galerkin type weighting is due to the assembling of non-symmetrical elemental matrices, which may have complex eigenvalues in high-advective fluid problems, that produce oscillating solutions of the problem. The stabilization approaches try to overcome this fact by modifying the variational form and so, the elemental matrices associated to advection, just like we have presented in the above examples for a Petrov-Galerkin formulation. Our proposal is to obtain the stabilization parameter from the information of the eigenvalues of the elemental matrices: the elemental matrices are computed starting with a null stabilization parameter (i.e., we use a Galerkin type weghting approach), and we obtain (or estimate) the set of eigenvalues $\{\lambda_i\}$ of each elemental matrix. If all of them are real numbers, then the stabilization parameter remains equals zero, but if it should not be so, then the value of the stabilization parameter is increased until no complex eigenvalues in the elemental matrices appear.

In this point, it is important to remark an essential characteristic of this proposal: it is absolutely general and independent of the dimension of the problem. The stabilization parameters are not computed in an heuristic way, and it is also possible to use this methodology if source and reactive terms are considered in the transport differential equation. Consequently, it is a general technique, very simple from a conceptual point of view, that stabilizes the finite element equations of the problem by analyzing only its elemental matrices.

At present, we have obtained very promising results in the cases studied until now [3,12] for 1D and 2D problems. In the next section, we present a 1D test numerical test to demonstrate the feasability of the proposed method for computing stabilization parameters and we discuss the results obtained.

4. NUMERICAL EXAMPLES

The example that we present is the 1D test —Fig. 2 a)— defined by

$$u\frac{\partial \phi}{\partial x} = k\frac{\partial^2 \phi}{\partial x^2}\ , \qquad 0 < x < L; \quad \phi(0) = \phi_0\ , \qquad \frac{\partial \phi}{\partial x}(L) = \widehat{h}[\phi_L - \phi(L)] \tag{20}$$

with the following parameters: $L = 7$, $\phi_0 = 0.001$, $\phi_L = 0.005$, $k = 0.07$ and $\widehat{h} = 1.0$.

We have analyzed the numerical results for different velocities in the domain of the problem (from $u = 0.1$ to $u = 50$), and discretizations of the domain of 10 and 50 elements. In all cases, we have considered parabolic elements[3,12] (3 nodes per element). Péclet numbers ($Pe = uh/k$) vary from 1 to 500 (in the discretization of 10 elements) and from 0.2 to 100 (in the case of 50 elements).

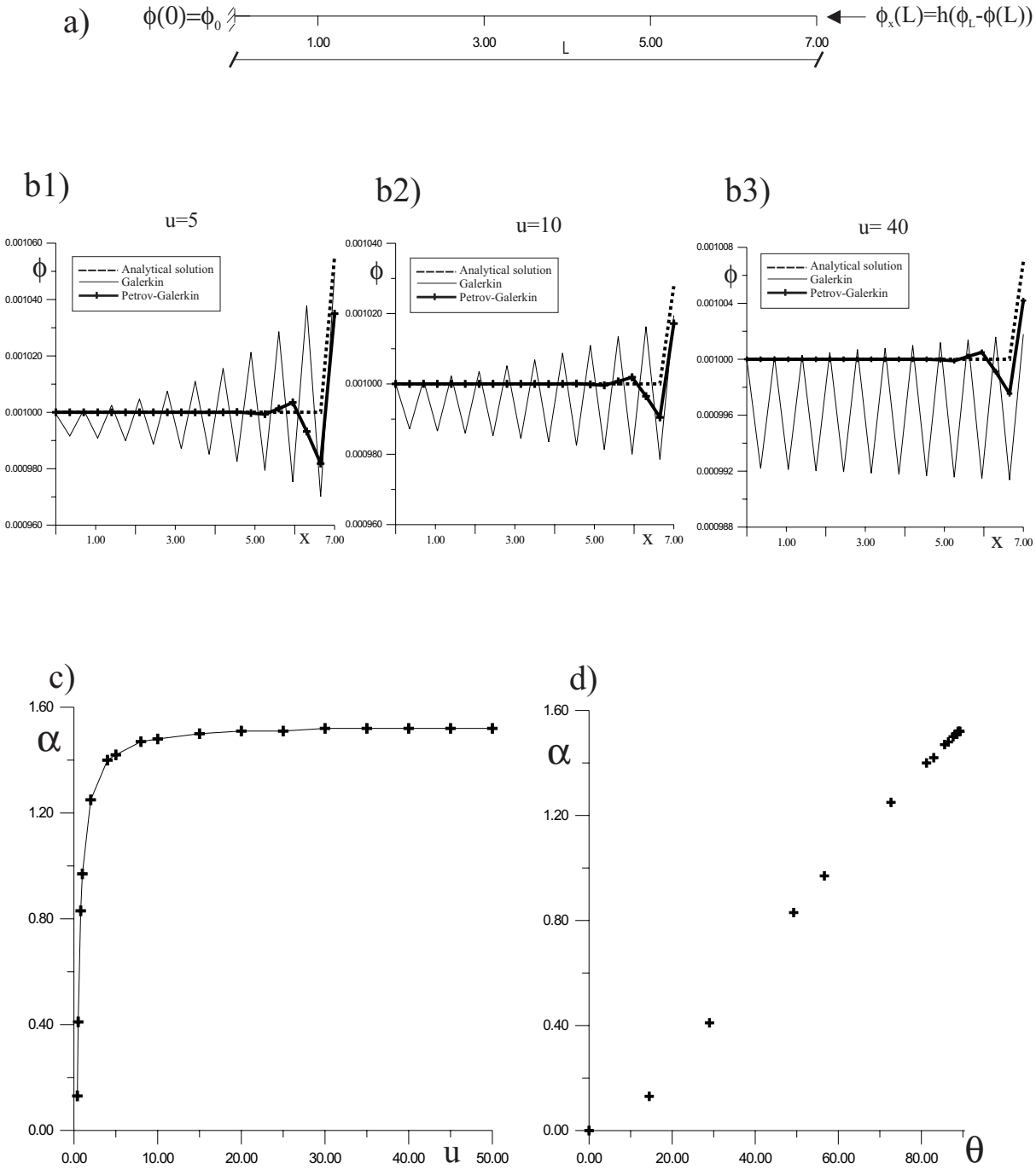

Fig. 2.- a) Domain and boundary conditions of the test problem. Results obtained with a discretization of 10 parabolic elements: **b#)** Comparison of the numerical solutions obtained with Galerkin and Petrov-Galerkin approach, and the analytical solution for different fluid velocities. **c)** Stabilization parameter α versus the fluid velocity; **d)** Stabilization parameter α versus the polar angle θ (degrees) of the eigenvalue obtained with a Galerkin approach.

Numerical results obtained with Galerkin and Petrov-Galerkin with the proposed method for computing the stabilization parameters based on the eigenvalues of the elemental matrices are presented in Fig. 2 b) and e), in comparison with the analytical solution. As it can be seen, we obtain very good numerical results and an important reduction of the oscillations (these results also agree with those obtained by using Petrov-Galerkin approaches with others methods for computing the stabilization parameters[9]). Furthermore, in Fig. 2 c) and f), we present the evolution of the stabilization parameter depending on the fluid velocity; obviously, the stabilization parameter increases when the velocity does.

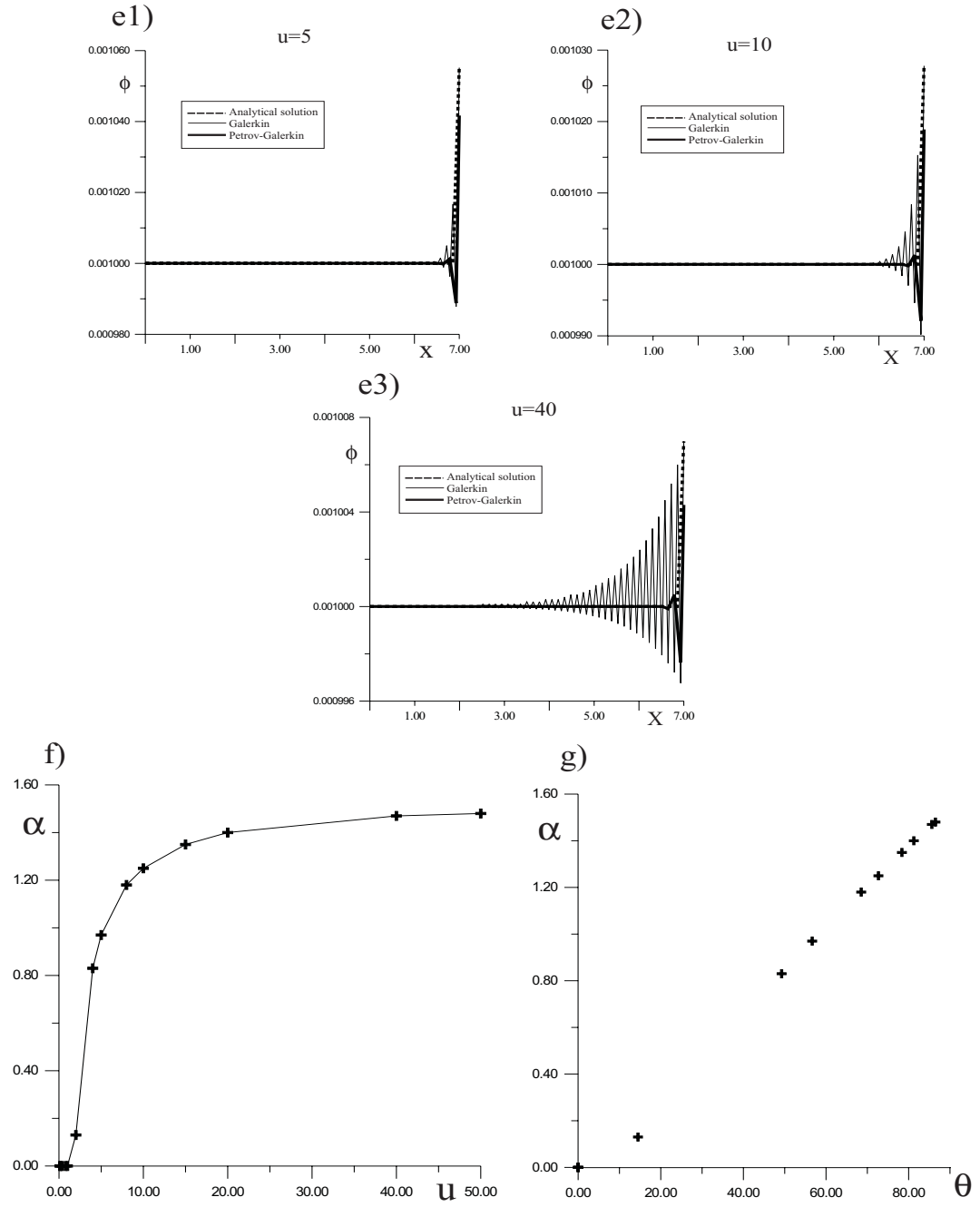

Fig. 2.-Results obtained with a discretization of 50 parabolic elements: **e#)** Comparison of the numerical solutions obtained with Galerkin and Petrov-Galerkin approach, and the analytical solution for different fluid velocities. **f)** Stabilization parameter α versus the fluid velocity; **g)** Stabilization parameter α versus the polar angle θ (degrees) of the eigenvalue obtained with a Galerkin approach.

In these examples, we remark the great advantage of the formulation that we propose since it is independent on any heuristic method for computing the stabilization parameters, which we obtain by a systematic analysis of the eigenvalues of each elemental matrix; that is, computing the stabilization parameter starting with a Galerkin type weighting approach (parameter equals zero) and increasing its value until no complex eigenvalues in the elemental matrices appears. However, we have found that there should be a faster way to obtain the stabilization parameter, since it seems to exist a clear relation between the stabilization parameter and the greater polar angle of the complex eigenvalues of an elemental matrix —Fig. 2 d) and g)— and it is independent of the fluid velocity, and the discretization level (in Fig. 3 we have represented all results together). At the present time, we are studying this possible linear (or cuasi-linear) relation and trying to explain it from a mathematically point of view, since it should represent a significant improvement in the computing of the stabilization parameter which it could be directly obtained from the eigenvalues of the elemental matrices of the Galerkin formulation with a low computational effort.

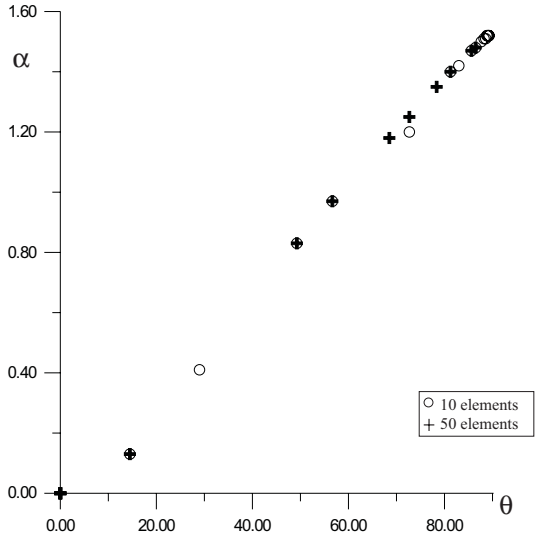

Fig. 3.-Stabilization parameter α versus the polar angle θ (degrees) of the eigenvalue obtained with a Galerkin approach (cases **d)**, and **g)** in Fig. 2).

5. CONCLUSIONS

In this paper, we have revised the origin of the numerical oscillations in the finite element solution of the advective-diffusive transport differential equation and the method that we propose for computing stabilization parameters required in Petrov-Galerkin weighting formulations. 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. The computational cost that implies the computing of the stabilization parameter from the eigenvalue analysis

of the elemental matrices of the discretization could be drastically decreased if this parameter is obtained from the polar angle of the eigenvalues of the elemental matrices in the Galerkin type weighting finite element approach.

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