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STREAM UPWIND/PETROV GALERKIN AND GALERKIN/LEAST-SQUARES NUMERICAL APPROACHES FOR ADVECTIVE-DIFFUSIVE TRANSPORT PROBLEMS IN ENGINEERING

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Abstract. *The Finite Element method with a Galerkin type weighting is a straight-forward weighted residual method that has been successfully used in many engineering applications, specially in Solid Mechanics. However, this method yields oscillatory solutions when it is applied to high-advective problems in Fluid Mechanics. Several stabilized numerical formulations have been proposed in the last years to overcome these instabilities. The common methodology of most of these approaches is based on the addition of a term to the Galerkin formulation, in order to enhance the stability behaviour while preserving the weighting residual scheme. In this paper, we focus our attention in the Stream Upwind/Petrov Galerkin method (SUPG), and the Galerkin/least-squares method (GLS). We will review the mathematical formulation of both of them, as well as the key concept of their respective fundamentals and derivations, i.e. the exact artificial diffusion method for the SUPG and the Least Squares Finite Element method for the GLS. Finally, we will present a comparison between both methods, pointing out important coincidences and establishing their mutual relations.*

1 Introduction

On the contrary to most problems in Solid Mechanics, no unifying numerical methods are available for the wide range of problems in Fluid Mechanics. In more than three decades of development of the Finite Element Method, we can actually say that neither an universal approach for the different fluid problems has been found, nor any specific formulation has been able to offer good results for arbitrary values of the physical parameters of any given problem [1]. In the particular case of the advective-diffusive transport equation (which can also be interpreted as the linear version of the Navier-Stokes equations), it is possible to obtain good results in the case of high-diffusive problems. However, this turns out to be quite difficult in cases in which advection is the dominant phenomenon [2].

Several alternative numerical schemes have been proposed in the last years to stabilize the Galerkin weighting numerical formulation of the transport equation. In this paper, after a brief review of the Galerkin Finite Element method, we will focus our attention in two widespread stabilization methods: the Stream Upwind/Petrov Galerkin method (SUPG), and the Galerkin/least-squares method (GLS). Both attain the stability properties for high Péclet numbers in a very similar way. Thus, we will start out by studying the general formulation of the stabilized methods. As a general rule, these methods are based on the consideration of an additional term that enhances the stability behaviour of the Galerkin formulation but preserves the weighting residual scheme [2].

The study of the formulation of SUPG and GLS from two different points of view will be performed as follows. First, we will introduce the methods from the basis of the Galerkin formulation and the subsequent addition of a new term. Next, we will identify the formulation as a weighted residual scheme with modified weighting functions. Finally, a comparison of the methods, both from the theoretical point of view and by means of some 1D numerical tests, will allow us to establish the relations between them.

In order to introduce the numerical study of these methods, we consider the generic problem in terms of the unknown function u

$$\mathcal{L}(u) = f \text{ in } \Omega, \quad \mathcal{M}(u) = 0 \text{ on } \Gamma, \quad (1)$$

where $\mathcal{L}(\cdot)$ and $\mathcal{M}(\cdot)$ are the corresponding differential operators, Ω is the domain of the problem and Γ is its boundary.

We are interested in the study and in the development of efficient numerical approaches for the advective-diffusive transport equation. This differential equation governs several physical phenomena that are involved in some important application problems in civil engineering, such as the progress of the concentration distribution due to a certain pollutant spilling or dumping in a harbour or in a coastal area.

Let us consider now the steady state advective-diffusive transport problem. Our aim

is to obtain the scalar field $u = u(\mathbf{x})$ verifying

$$\begin{aligned} \mathbf{a} \cdot \nabla u - \nabla \cdot (k \nabla u) &= f \quad \text{in } \Omega, \\ u &= u_0 \quad \text{on } \Gamma_1, \quad \nabla u \cdot \mathbf{n} = \gamma - cu \quad \text{on } \Gamma_2, \end{aligned} \quad (2)$$

$$\Gamma_1 \cup \Gamma_2 = \Gamma, \quad \Gamma_1 \cap \Gamma_2 = \emptyset,$$

where $\mathbf{a}(\mathbf{x})$ is the velocity of the fluid (with $\nabla \cdot \mathbf{a} = 0$ in Ω), $k = k(\mathbf{x})$ is the diffusivity and $f(\mathbf{x})$ is a prescribed source function. Γ_1 denotes the points of the boundary where u is known, and Γ_2 denotes the points of the boundary where the flux ($\nabla u \cdot \mathbf{n}$) is prescribed.

In this particular case, the corresponding symbolic differential operator \mathcal{L} can be expressed as the sum of two operators:

$$\mathcal{L} = \mathcal{L}_{adv} + \mathcal{L}_{dif} \quad (3)$$

being

$$\mathcal{L}_{adv} = \mathbf{a} \cdot \nabla(\cdot) \quad (4)$$

$$\mathcal{L}_{dif} = -\nabla \cdot (k \nabla(\cdot)) \quad (5)$$

2 The Galerkin Finite Element Method

The Galerkin Finite Element method is a weighted residual method. First we are required to state a variational form of the original problem. This can be set as follows: find u such that problem (1) is satisfied in the sense of weighted residuals

$$\int_{\Omega} (\mathcal{L}(u) - f)w \, d\Omega + \int_{\Gamma} (\mathcal{M}(u) - t)w_{\Gamma} \, d\Gamma = 0, \quad \forall w, w_{\Gamma} \quad (6)$$

that is: the weighted integral of the residuals of the differential equation and the boundary conditions must nullify for all members w and w_{Γ} of suitable classes of test functions defined in Ω and Γ respectively [3]. Now, for a given set of n trial functions $\{\varphi_j\}$, $j = 1, n$ defined on Ω , the unknown u can be discretized as

$$u \simeq \tilde{u} = \sum_{j=1}^n u_j \varphi_j \quad (7)$$

On a regular basis, expression (6) can not hold anymore for all test functions w and w_{Γ} , as a consequence of this approximation. However, we still can call for the verification of the variational statement (6) in a finite-dimensional context. Thus, we can impose that expression (6) nullifies at least for the collection of weighting functions

generated by a given set of n test functions $\{w_j\}, j = 1, n$ defined on Ω . In the Galerkin method, those tests functions are defined as equal to the trial functions:

$$w_j = \varphi_j \quad j = 1, n. \quad (8)$$

In Solid mechanics problems it can be demonstrated how advisable is this election from a theoretical point of view, since the Galerkin method has optimal properties of approximation for symmetric and positive-definite operators [4,5]. However, it is well-known that large scale numerical oscillations occur in Fluid mechanics problems when the Galerkin method is applied to cases with advective dominance [1]. The reason is that the advection differential operator is of first-order, and thus non-self adjoint; as a result, the Galerkin method yields a system of equations with skew-symmetric coefficients matrix, which leads to a poor numerical stability behaviour [1,6].

Thus, if we apply the Galerkin method to the advective-diffusive transport problem defined by (2), the Green's identity allows to obtain the following system of equations

$$\sum_{j=1}^n \left[\int_{\Omega} (\varphi_i \mathbf{a} \cdot \nabla \varphi_j + k \nabla \varphi_j \cdot \nabla \varphi_i) d\Omega + \int_{\Gamma_2} ck \varphi_j \varphi_i d\Gamma_2 \right] u_j = \int_{\Omega} f \varphi_i d\Omega + \int_{\Gamma_2} \gamma k \varphi_i d\Gamma_2 \quad ; \quad i = 1, \dots, n; \quad (9)$$

where the trial and test functions used in this approach must belong to suitable classes of $H^1(\Omega)$ functions. Therefore C^0 finite elements could be used [7].

3 Stabilized methods

Since the early eighties, several alternative weighted residual methods have been proposed for fluid mechanics problems in order to improve the stability, thus trying to reduce or eliminate the large scale oscillations that appear in the numerical solutions given by the Galerkin method. The common methodology of these stabilizing methods consists of adding a new term to the original Galerkin finite element method, with the general form [2,8]:

$$\int_{\tilde{\Omega}} \mathcal{R}(\tilde{u}) \boldsymbol{\tau} \mathcal{P}(\varphi_i) d\tilde{\Omega}, \quad (10)$$

where $\mathcal{R}(\tilde{u})$ is the residual of the differential equation, that is

$$\mathcal{R}(\tilde{u}) = \mathcal{L}(\tilde{u}) - f, \quad (11)$$

$\boldsymbol{\tau}$ is the stabilization parameter which tunes the contribution of the new term in the formulation (this parameter is allways positive and has dimensions of time [2]), $\mathcal{P}(\varphi_i)$ is a differential operator defined on the test functions space, and $\tilde{\Omega} = \cup \Omega_e$, being Ω_e

the interior of each element. In this way the stabilization term can be computed as a sum of integrals over the elements.

Therefore, if we add the new term (10) to the Galerkin formulation for a generic boundary value problem, we obtain the general formulation [2,8] of the stabilized methods

$$\int_{\Omega} (\mathcal{L}(\tilde{u}) - f) \varphi_i \, d\Omega + \int_{\tilde{\Omega}} \boldsymbol{\tau} (\mathcal{L}(\tilde{u}) - f) \mathcal{P}(\varphi_i) \, d\tilde{\Omega} = 0 \quad , \quad i = 1, \dots, n \quad (12)$$

where specific numerical formulations can be derived for different selections of the differential operator $\mathcal{P}(\varphi_i)$. As we will see in the next section, most classical stabilization methods for the steady state transport equation fall within the previous framework.

An important feature of the stabilized methods that is explicit in the general expression (12) is that the addition of this new term preserves the general weighted residual form of the Galerkin method, while stability is enhanced at the same time [4]. In fact, the general form (12) can be understood as a particular case of the weighted residual scheme (6) in which the characteristic weighting functions of the Galerkin method have been modified in the element interiors, yielding the test functions w_i :

$$\int_{\Omega} (\mathcal{L}(\tilde{u}) - f) w_i \, d\Omega = 0 \quad \forall w_i, \quad i = 1, \dots, n \quad (13)$$

$$w_i = \varphi_i + \boldsymbol{\tau} \mathcal{P}(\varphi_i) \quad (14)$$

The consequence of introducing these modified weighting functions, is that we are projecting the residual $\mathcal{R}(\tilde{u})$ of the differential equation in a different functional space [9]. Therefore, we could say that the common aim of the stabilization methods is to reduce the spurious oscillations of the numerical solution obtained by the Galerkin method, by using more adequate weighting functions.

It is important to remark that the trial functions φ_i must satisfy the continuity requirements of the Galerkin method throughout the entire domain Ω , while the term $\boldsymbol{\tau} \mathcal{P}(\varphi_i)$ is required to satisfy them in the element interiors only, but not necessarily across the element boundaries. This is due to the fact that the integration of the stabilization term (10) is only performed over the element interiors. Therefore, the evaluation of these elementwise additional terms does not upset the continuity requirements of the original variational form [10,11].

4 The Stream Upwind Petrov Galerkin Finite Element method

In the previous section we have presented the general formulation of the stabilization methods (12). Next, we will present the so-called Stream Upwind Petrov Galerkin method (SUPG) as a particular case.

For the advective-diffusive transport equation, the SUPG method consists basically in the election of the differential operator \mathcal{P} of the stabilization term (11) as equal to

the advective differential operator (4). Thus, the addition of this term to the Galerkin formulation yields [5,8]:

$$\int_{\Omega} (\mathcal{L}(\tilde{u}) - f) \varphi_i \, d\Omega + \int_{\tilde{\Omega}} \boldsymbol{\tau} (\mathcal{L}(\tilde{u}) - f) \mathcal{L}_{adv}(\varphi_i) \, d\tilde{\Omega} = 0 \quad , \quad i = 1, \dots, n \quad (15)$$

The SUPG method was originally developed with the aim of obtaining a new weighted residual scheme on the basis of the “exact artificial diffusion method”. In this method, one considers a modified advective-diffusive transport equation by introducing an artificial diffusion \hat{k} [5]. For the 1D case the corresponding equation is

$$a \frac{du}{dx} - (k + \hat{k}) \frac{d^2u}{dx^2} = 0 \quad ; \quad 0 \leq x \leq L \quad (16)$$

being

$$\hat{k} = \frac{|u|h}{2} \hat{\xi} \quad (17)$$

$$\hat{\xi} = \coth \alpha - \frac{1}{\alpha} \quad (18)$$

$$\alpha = \frac{|u|h}{2k}. \quad (19)$$

On the basis of these considerations, the Stream Upwind Petrov Galerkin method was formulated in order to reproduce the exact artificial diffusion method for the 1D case. Thus, in absence of the source term f , the added stabilization term yields the artificial diffusion term of the exact artificial diffusion method [5]:

$$\int_{\tilde{\Omega}} \tau \left(a \frac{d\tilde{u}}{dx} - k \frac{d^2\tilde{u}}{dx^2} \right) a \frac{d\varphi_i}{dx} \, dx = \int_{\tilde{\Omega}} \tau a^2 \frac{d\tilde{u}}{dx} \frac{d\varphi_i}{dx} \, dx = \int_{\tilde{\Omega}} \hat{k} \frac{d\tilde{u}}{dx} \frac{d\varphi_i}{dx} \, dx \quad (20)$$

where the parameter τ is given by

$$\tau = \frac{\hat{k}}{|u|^2} = \frac{h}{2|u|} \hat{\xi}. \quad (21)$$

Therefore, both methods are identical for this specific 1D problem.

As we can see, the addition of the new term in the SUPG method preserves the weighted residual numerical scheme, being the associated weighting functions

$$w_i = \varphi_i + \boldsymbol{\tau} \mathcal{L}_{adv}(\varphi_i). \quad (22)$$

On the basis of this basic idea, the SUPG method has been proposed for solving the advective-diffusive transport equation in 2D and 3D problems. In the absence of suitable theoretical results, the stabilization parameter is normally estimated in these cases by means of heuristic expressions derived from (21) and (18) for 2D/3D problems.

5 The Galerkin/Least-Squares Finite Element formulation

The Galerkin/Least-Squares method (GLS) was proposed for the first time in 1989 by Hughes et al. [4] as a methodological generalization of the SUPG method [5]. Within the general formulation of the stabilized methods (12), the Galerkin/Least-Squares method corresponds to select the differential operator \mathcal{P} as equal to the differential operator \mathcal{L} of the original problem [4,8,10]. Therefore, the stabilized term (10) in the GLS can be written as

$$\int_{\tilde{\Omega}} \boldsymbol{\tau}(\mathcal{L}(\tilde{u}) - f) \mathcal{L}(\varphi_i) d\tilde{\Omega} = 0 \quad , \quad i = 1, \dots, n. \quad (23)$$

A close look at this term shows that this election is not arbitrary at all. In order to explain it, let us consider the functional

$$\mathcal{J}(\tilde{u}) = \int_{\Omega} (\mathcal{R}(\tilde{u}))^2 W d\Omega = \int_{\Omega} (\mathcal{L}(\tilde{u}) - f)^2 W d\Omega . \quad (24)$$

For any given linear combination of the trial functions (7), and for a suitable weighting function W , this functional measures the average weighted squared error in the approximation of the solution to the generic problem (1).

Since we are interested in obtaining a suitable approximation to the exact solution of the problem, a reasonable procedure could be to minimize this functional. This yields

$$\frac{\partial}{\partial u_i} \left[\mathcal{J} \left(\sum_{j=1}^n u_j \varphi_j \right) \right] = 0 \quad , \quad i = 1, \dots, n \quad (25)$$

There is an obvious parallelism between this kind of statements and the least-squares interpolation techniques, since we finally attempt to minimize the distance between $\mathcal{L}(\tilde{u})$ and f [12]. Now, if we take into account that $\mathcal{J}(\cdot)$ is a linear differential operator and we adopt $W = 1$, the expression (25) leads to

$$\sum_{j=1}^n \left[\int_{\Omega} \mathcal{L}(\varphi_j) \mathcal{L}(\varphi_i) d\Omega \right] u_j = \int_{\Omega} f_i \mathcal{L}(\varphi_i) d\Omega \quad , \quad i = 1, \dots, n, \quad (26)$$

that, regardless of the stabilization parameter τ , is equivalent to the expression (23) evaluated in the whole domain Ω . Therefore, the new term added in the GLS method to stabilize the Galerkin method is identified as the elementwise evaluation of the least squares form of the residual of the differential equation, multiplied by the parameter τ .

For this reason, the GLS method can also be considered as a combination of the Galerkin method and the Least-squares method, where the last one provides the stabilizing properties to the GLS [13]. Thus, for a generic problem, the GLS method [10] leads to the variational form

$$\int_{\Omega} (\mathcal{L}(\tilde{u}) - f) \varphi_i d\Omega + \int_{\tilde{\Omega}} \boldsymbol{\tau}(\mathcal{L}(\tilde{u}) - f) \mathcal{L}(\varphi_i) d\tilde{\Omega} = 0 \quad , \quad i = 1, \dots, n. \quad (27)$$

The addition of the Least-Squares term to the Galerkin formulation in the GLS method implies an upwind mechanism that will improve the stability properties [13]. This is due to the *over-diffusive* behaviour of the Least-Squares Finite Element method. Considered as an additional term, this balances the *under-diffusive* behaviour of the Galerkin method. The parameter τ must tune the contribution of this LS term. Thus, it should be high enough to accomplish a stabilized method without provide over-dissipative results (as it occurs in the Least Squares finite Element Method), what precludes the obtaining of the solution in the case of sharp fronts [1].

Due to the different contributions of the advective and diffusive matrices of the Galerkin term in problems with high and low Péclet numbers, the stabilization parameter has a different dependence on the physical parameters of the problem through the entire rank of Péclet numbers. A detailed analysis on the computation of stabilization parameters can be found in references [2,4,8,10,11].

The GLS formulation can also be interpreted as a residual formulation type (13), being the corresponding modified test functions

$$w_i = \varphi_i + \tau \mathcal{L}(\varphi_i), \quad (28)$$

that is a linear combination of the specific test functions corresponding to both, the Galerkin method and the Least Squares method [9,14].

6 Theoretical comparison of SUPG and GLS methods

In the previous sections we have presented the SUPG and GLS finite element methods. Now, we can establish the relations that exist between them.

As we have seen, both methods can be considered as particular cases within the general framework presented in section 3 for the stabilized methods. Thus, both methods can be understood as weighted residual approaches, like the Galerkin method, with modified test functions. On the contrary to the Galerkin method, in which the functional spaces of the test functions and the trial functions are the same for all cases, the SUPG and GLS functional spaces corresponding to the test functions —expressions (22) and (28)— depend on the differential operator of the problem. Thus, for a given set of trial functions, differential equations corresponding to different problems will have different weighting functions, depending on the nature of the problem that is being solved [9].

However, the general methodology of both methods is the same. In fact, they become identical for certain cases. Actually, in the hyperbolic case $\mathcal{L} = \mathcal{L}_{adv}$. Therefore, substituting this operators in (15) and (23), the stabilization terms of both methods become

$$\int_{\tilde{\Omega}} \tau \mathcal{L}_{adv}(\tilde{u}) \mathcal{L}_{adv}(\phi_i) d\tilde{\Omega} \quad (29)$$

On the other hand, the trial functions being used in the resolution of the advective-diffusive problem by both methods must satisfy the same continuity and derivability

requirements of the Galerkin method. Thus, since the trial functions must belong to $H^1(\Omega)$, C^0 elements could be used [7]. Therefore, the added stabilization term plays no role in these considerations, because it is evaluated elementwise and not across the element boundaries.

If we use C^0 -linear elements, both methods become identical too [4]. In this case, the second derivative of the shape functions vanishes and thus $\mathcal{L}_{dif}(\tilde{u}) = 0$. Therefore, the stabilization term will also be given by expression (29) for both methods.

Finally, the rank of applicability of the GLS method for solving boundary value problems in Fluid Mechanics is wider than the rank of applicability of the SUPG method. The reason is that the election of the differential operator \mathcal{P} in (10) as the total operator \mathcal{L} of the original equation is just straightforward, while the splitting $\mathcal{L} = \mathcal{L}_{adv} + \mathcal{L}_{dif}$ could be questionable or pointless for a certain problem. The formulation of the GLS method overcomes this shortcoming [8,10]. As a conclusion, we could interpret the GLS method as a methodological generalization of the SUPG formulation [5,8].

7 Numerical tests

In this section we compare the performance of the Galerkin method, the Stream Upwind Petrov Galerkin method and the Galerkin Least Squares method for solving the advective-diffusive transport problem. The presented 1D tests were designed to assess the accuracy of these techniques when dealing with high-advective terms.

Accordingly to the concepts outlined before, we study the numerical solution of the following test problem: find $u = u(x)$ verifying

$$a \frac{du}{dx} - k \frac{d^2u}{dx^2} = 0 \quad , \quad 0 \leq x \leq L; \quad u(x=0) = u_0; \quad u(x=L) = u_L \quad (30)$$

with the following parameters: $a = 10$, $k = 0.09$, $L = 6$, $u_0 = 12$ and $u_L = 16$.

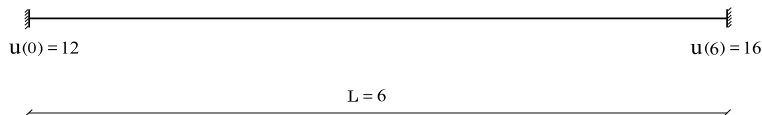


Fig. 1. Domain and boundary conditions of the 1D test problem.

Figures 2a, 2b, 2c and 2d show the approximated numerical solutions obtained by means of the Galerkin method, the SUPG method and the GLS method, for different mesh refinements, in comparison with the exact analytical solution. The presented results were computed for several increasing levels of discretization (namely, using 15, 50, 100 and 500 C^0 -quadratic elements). This produces a series of cases with decreasing Péclet numbers (22.22, 6.66, 3.33 and 0.66, respectively), and increasing accuracy and stability. Notice that the horizontal scale has been adjusted in order to depict the rightmost side of the domain, where the instabilities occur.

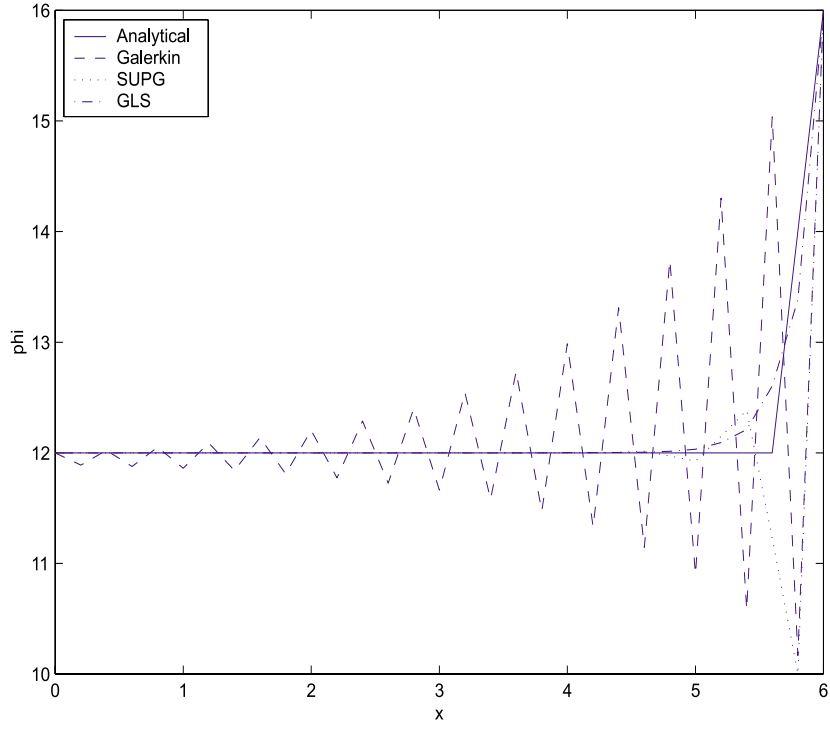


Fig. 2. Numerical solutions to (30), by using 15 C^0 -quadratic elements ($Pe=22.22$).

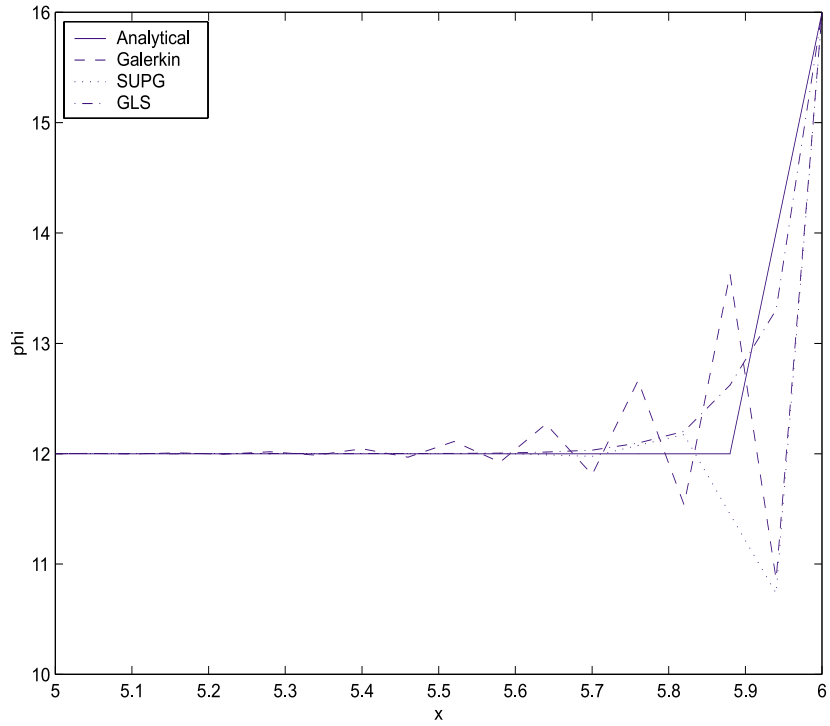


Fig. 3. Numerical solutions to (30), by using 50 C^0 -quadratic elements ($Pe=6.66$).

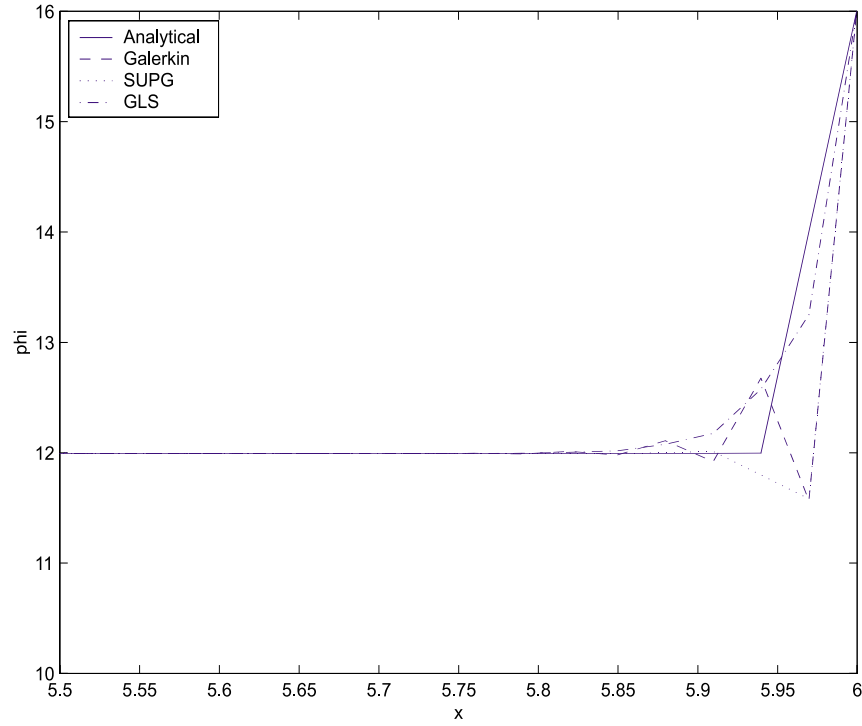


Fig. 4. Numerical solutions to (30), by using 100 C^0 -quadratic elements ($Pe=3.33$).

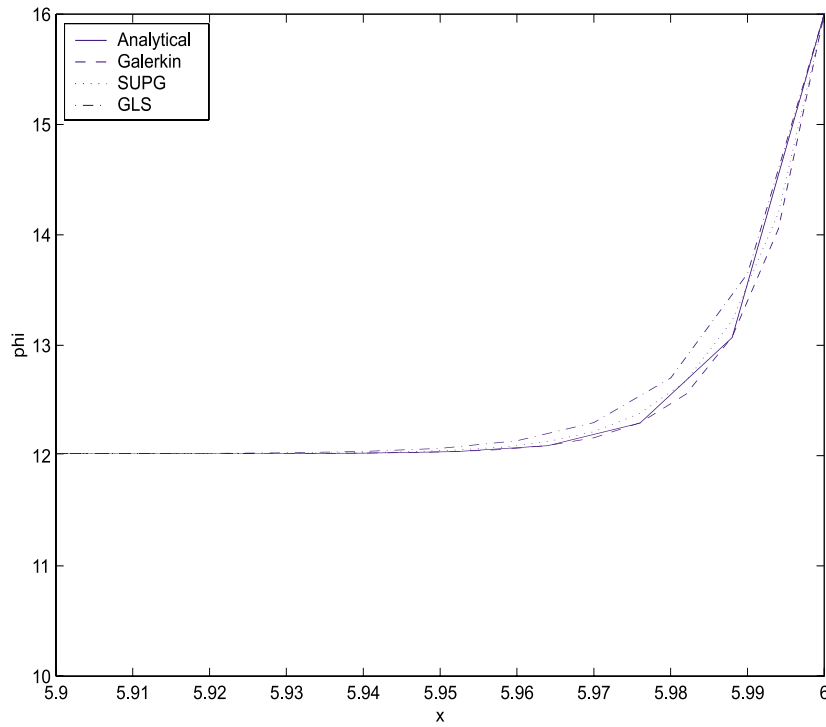


Fig. 5. Numerical solutions to (30), by using 500 C^0 -quadratic elements ($Pe=0.66$).

The Figures show that the Galerkin method yields oscillatory numerical solutions to this kind of problems, except for significantly low Péclet numbers. Therefore, obtaining acceptable results by means of the Galerkin method should normally involve an extremely high computing effort. On the other hand, the SUPG method stabilizes (markedly well) the approximated solution in most of the domain. However, the instabilities in the proximity of the sharp advective front are not fully removed by the SUPG method, except for low Péclet numbers. On the contrary, the GLS method yields a totally stable solution, even for the coarsest mesh.

It must be clear that indefinite mesh refinement can not be a proper solution to the stability problem of the Galerkin method, even though numerical oscillations diminish as discretization level increases. In fact, mesh refinement should become extremely expensive for high-advective problems, specially in the case of 2D and 3D problems. On the other hand, the Galerkin Least Squares method requires more computing effort than the SUPG method, since the complete differential operator is used in the stabilization term. However, it is worthwhile using the GLS method due to the marked improvement in the numerical solution, even for low discretization levels.

8 Conclusions

In this paper, we have reviewed the application of three widespread numerical Finite Element formulations to the advective-diffusive transport problem: the Galerkin method, the Stream Upwind/Petrov Galerkin method (SUPG) and the Galerkin/Least-Squares method (GLS).

The Galerkin method is a well-known weighted residual formulation that exhibits a very good performance in many Computational Mechanics applications, specially in the Solid Mechanics field. However, its application to Fluid Mechanics problems is precluded in practice, due to the spurious oscillations that corrupt the numerical solution in high-advective cases. Several stabilization methods have been proposed in order to overcome this obstacle.

We have analyzed the basic concepts of the stabilization methods from two different points of view: first, we consider these methods as resulting from the addition of a certain stabilization term to the Galerkin formulation; and second, we identify them as specific weighting residual formulations with modified weighting functions. This study is essential to understand their mathematical foundations and their respective performances.

We have studied two widespread stabilized methods, the SUPG method and the GLS method, paying special attention to their background. The SUPG method was originally based in the exact artificial diffusion finite difference method. On the other hand, the GLS method takes advantage of the over-dissipative effect of the Least-Squares Finite Element method to upwind the Galerkin formulation. However, both methods produce an identical formulation in specific cases, namely for the hyperbolic case or when piecewise linear elements are used. We point out that the GLS method can

be considered as a generalization of the SUPG method. Therefore, we conclude that the GLS method can be a shrewd starting point to develop more accurate numerical formulations, well supported from a mathematical point of view, for solving 2D and 3D linear and non-linear problems in fluid mechanics.

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