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(SU+C)PG: A PETROV-GALERKIN FORMULATION FOR ADVECTION-REACTION-DIFFUSION PROBLEMS

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SUMMARY

In this work we present a new method called (SU+C)PG to solve advection-reaction-diffusion (ARD) scalar equations by the Finite Element Method (FEM) [1]. Following the ideas behind SUPG [2, 3], Tezduyar and Park treated the more general ARD problem and they developed a stabilizing term for advection-reaction problems without significant diffusive boundary layers. In this work a PG extension for all situations is performed, covering the whole plane represented by the Peclet number and the dimensionless reaction number. The scheme is based in extending the super-convergence feature through the inclusion of an additional perturbation function and a corresponding proportionality constant. The proportionality constants are selected in order to verify the "super-convergence" feature. i.e. exact nodal values are obtained for a restricted class of problems (uniform mesh, no source term, constant physical properties). It is also shown that the (SU+C)PG scheme verifies the Discrete Maximum Principle (DMP), that guarantees uniform convergence of the finite element solution. Moreover, it is shown that super-convergence is closely related to the DMP, motivating the interest in developing numerical schemes that extend the super-convergence feature to a broader class of problems.

1. INTRODUCTION

In this paper we focus on the numerical solution of the ARD equation using the finite element method. Here diffusion, advection and reaction means those terms in the governing equation involving second, first and zero order derivatives of the unknown variable. This kind of equation represent a simplified model for several industrial processes, for example the simulation of electrophoresis separation phenomena and the operation of a great number of chemical reactors. In these processes both the concentration and temperature play the role of the unknown variable. Another interesting application is found in the simulation of fluid flow in a non inertial frame. This phenomenon is represented by an ARD system where the inertial forces are included in the advection term, the Coriolis forces are included in the reaction term and finally the diffusive part is due to the viscous effects. The dimensionless Reynolds and Rossby numbers quantify the relative magnitude of these forces. Both limits for high Rossby and Reynolds numbers

have a lot of numerical and physical difficulties, specially concerning with the stability of the fluid flow and the scheme used to simulate it.
Let us take the steady, linear ARD equation. As it is well known, the numerical solution of the above equation using Galerkin formulations exhibits global spurious oscillations in advection dominated problems, specially in the vicinity of discontinuities. Such drawback can be overcome by the popular SUPG method [2]. This method stabilizes the numerical scheme by adding a perturbation to the weight function producing an oscillation free solution. This perturbation is proportional to the gradient of the standard interpolation function, so that for linear constant-size elements it is an odd function with respect to the center node. The amount of perturbation to be incorporated is calculated as a function of the dimensionless Peclet number. By adding a shock capturing term one can preclude the overshoot and undershoot in the neighborhood of the discontinuities [3].
On the other hand, other kind of troubles exist in reaction dominated problems associated with the existence of local oscillations, also near discontinuities, even in the absence of advection terms. Similarly to the advection dominated problems, Tezduyar and Park [4] added a perturbation to the weight function. They choose it to be proportional to the gradient of the standard weight function, like the perturbation added for advection dominated problems, but with a different proportionality constant. The importance of the reaction term can be quantified by a dimensionless number, which we call the *reaction number* r formed by the reaction constant, the diffusivity constant and the element length. This scheme, which is called DRD, is designed to give the nodally exact solution for the homogeneous, one-dimensional analysis when the reaction number is much greater than the others and there are not diffusive boundary layers. One of the most remarkable critics to the above scheme is the impossibility to solve diffusive boundary layers. Another important critic stems from symmetry considerations under coordinate inversion $x \rightarrow -x$. In the reactive-diffusive case (null advection), the equation is invariant under this symmetry operation and it is clear that the weight function should be symmetric. Actually, this is not the case for this scheme.
In this direction this paper tries to give an answer to the above questions. We present a Petrov-Galerkin formulation proposing two different perturbations to the weight function, one of them is similar to that of SUPG scheme and the other one is symmetric. For advection-diffusion problems, the scheme reduces to the standard SUPG scheme. On the other hand, for reaction-diffusion problems only the symmetric perturbation subsists and the scheme is called CPG from *"Centered Petrov-Galerkin"*. In intermediate situations the scheme is a mixture of the two, and then the acronym (SU+C)PG. The proportionality constant for each perturbation depends on the two dimensionless numbers, Peclet number Pe and the reaction number r. We find two expressions $\alpha(\mathrm{Pe}, r)$, $\gamma(\mathrm{Pe}, r)$ similarly as with the magic function in SUPG, where α, γ are the proportionality constants for both perturbation terms. With this kind of solution, we can solve in an optimal way not only the limit cases $\mathrm{Pe} \rightarrow 0$, $r \rightarrow 0$, but also the whole Pe-r plane. Another alternative to solve the above problem, introduced by Codina[5], consists in using an SUPG formulation with shock capturing including in this last term the stabilization of the reactive effects. He demonstrated that the original equation can be transformed in a new advective-diffusive equation with a transformed velocity. Then, he applied the well known schemes for this kind of problem.

2. OPTIMAL NUMERICAL SCHEME FOR THE 1D PROBLEM

Let us consider the following simplified, one-dimensional form of the ARD equation:

$$
\begin{aligned}
&-k\phi'' + u\phi' + c\phi = f, \qquad 0 \le x \le 1,\\
&\phi(x=0) = \phi_0,\\
&\phi(x=1) = \phi_1,
\end{aligned}
\tag{1.1-3}
$$

where $k > 0$ represents the physical diffusivity, u the transport velocity, ϕ the scalar unknown variable, $c \ge 0$ the reaction constant and f the source term. The weak formulation is:

$$
\int_\Omega (kw_i'\phi' + uw_i\phi' + cw_i\phi)\, d\Omega + \sum_{e=1}^{N} \int_{\Omega_e} p_i(-k\phi'' + u\phi' + c\phi)\, d\Omega = \int_\Omega \tilde{w}_i f\, d\Omega, \quad i = 1, \ldots, N-1. \tag{2}
$$

Where w_i are the standard linear trial functions, $\tilde{w}_i$ the weight functions:

$$
\tilde{w}_i = w_i + p_i, \quad p_i = \alpha h w_i' + \gamma P_{2i}, \tag{3}
$$

p_i is the perturbation term and i, e are node and element indices, respectively. The first term is the well known SUPG perturbation term, whereas the second one is the new perturbation function which is intended to stabilize the reactive effects. With different expressions for the proportionality constants α and γ we obtain the (SU+C)PG method as well as those ones found in the literature:

$$
\begin{array}{lll}
\alpha = 0, & \gamma = 0, & \text{Galerkin},\\
\alpha = \coth \mathrm{Pe} - 1/Pe, & \gamma = 0, & \text{SUPG},\\
\alpha = \alpha_{\mathrm{DRD}}(r/4\mathrm{Pe}), & \gamma = 0, & \text{DRD},\\
\alpha = \alpha_{\mathrm{pr}}(\mathrm{Pe}, r), & \gamma = \gamma_{\mathrm{pr}}(\mathrm{Pe}, r), & \text{(SU+C)PG},
\end{array}
\tag{4.1-4}
$$

where α_{DRD} is given by:

$$
\alpha_{\mathrm{DRD}}(x) = \tfrac{1}{2}\{-\coth(x) + x\,[1/\sinh(x)^2 + 4/6]\}/[1 - x\,\coth(x)]. \tag{5}
$$

The dimensionless parameters Pe and r, quantifying advection and reaction, respectively, with respect to the diffusive term are defined as $\mathrm{Pe} = (uh/2k)$, $r = (ch^2/k)$. As it is usual in the SUPG context, these numerical parameters are found by requiring that the exact fundamental solutions to (1) in the homogeneous ($f \equiv 0$) case must be solutions of the discrete counterpart.

Since in the limit case of pure reaction the optimal weight function would be a Dirac's delta, it is reasonable to assume that $w + \gamma P_{2,i}$ must behave, as the reaction number is increased, in the form shown in figure 1. It is symmetric with respect to the center node i and vanishes at the neighboring nodes $i \pm 1$. For zero reaction it has to coincide with the standard "hat"linear interpolation function, whereas for increasing reaction number it has to concentrate at the center node. After some algebra, we arrive to the following system of equations defining the proportionality constants:

$$
\begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \begin{bmatrix} \alpha_{\mathrm{pr}} \\ \gamma_{\mathrm{pr}} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}, \tag{6}
$$

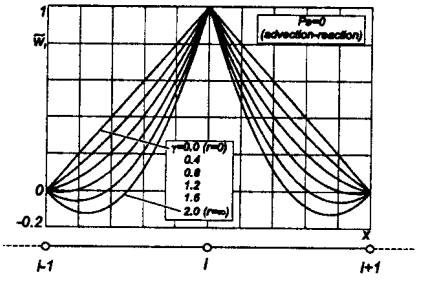


Figure 1: Weight functions for the null advection case.

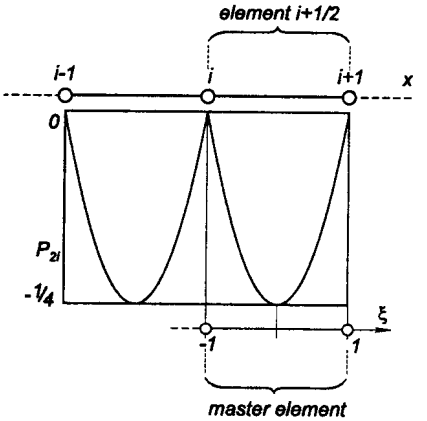


Figure 2: Proposed second perturbation function P_2.

$$
\begin{aligned}
g_{j1} &= [4\mathrm{Pe}(1-\cosh(\lambda_j h) - r\,\sinh(\lambda_j h)], \\
g_{j2} &= 2[\cosh(\lambda_j h) rm + 2\mathrm{Pe}\, a\,\sinh(\lambda_j h) + \\
&\qquad ((a-m)r)], \\
f_j &= -2[\cosh(\lambda_j h)(r/6-1) + \mathrm{Pe}\,\sinh(\lambda_j h) + (1+r/3)], \\
\lambda_j h &= \mathrm{Pe} + (-1)^{j-1}\sqrt{\mathrm{Pe}^2 + r},
\end{aligned}
\tag{7}
$$

for $j = 1, 2$, which depends only on two geometrical parameters of P_2, namely: the dimensionless semi-area a and the dimensionless first moment of one-half of the function m. We can obtain a super-convergent scheme by choosing an arbitrary function $P_2(x)$ and computing α and γ from the preceding expression. However, for an arbitrary choice we will find, in general, that the proportionality constants have singularities for certain values of Pe and r, so that a design of the P_2 function is needed to avoid singularities. A detailed analysis shows that the lowest order polynomial (inside each element) that avoids singularities is (see figure 2):

$$
P_2(\xi) = -\frac{1}{4}(1-\xi^2), \tag{8}
$$

The geometrical parameters corresponding to this function are: $a = -1/6$ and $m = -1/12$.

3. THE PROPORTIONALITY CONSTANTS

We refer to (SU+C)PG as the Petrov-Galerkin method based on the variational formulation (2), with the perturbation function defined by (3-8), and the proportionality constants defined by (6-7). In some limits the expressions are undeterminate but this singularities are removable. (This is also the case for the *"magic function"* of SUPG (see equation (4.2))). In figures 3-4 we show them, and we see that they are bounded and well-behaved: $|\alpha| \leq (1/2)$ and $0 \leq \gamma \leq 2$ for all Pe, r. Regarding consistency, it can be shown that the *"numerical additives"* vanish like $\sim h^2$ with mesh refinement. On the other hand, some desirable limits are automatically satisfied. For instance, we recover SUPG with the standard magic function in the case of null reaction:

$$
\alpha = \frac{1}{2}(\coth \mathrm{Pe} - \frac{1}{\mathrm{Pe}}), \quad \gamma = 0 \qquad \text{for } r = 0. \tag{9}
$$

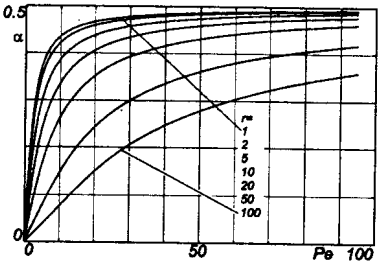


Figure 3: Proportionality constant for the standard SUPG perturbation term α as function of Pe *for constant* r.

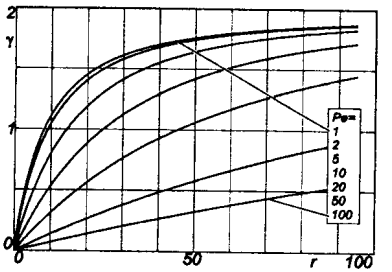


Figure 4: Proportionality constant for the second perturbation function γ as function of r for constant Pe.

On the other hand, for null advection :

$$\alpha = 0, \quad \gamma = 12\frac{\cosh(\sqrt{r})(r/6-1)+(1+r/3)}{r\,[1+\cosh(\sqrt{r})]} \qquad \text{for Pe} = 0. \tag{10}$$

The whole family of weight functions for null advection is shown in figure 1 from $\gamma = 0$ to 2. The weight function concentrates in the center node as γ increases. For $\gamma = 2$ (pure reaction) the weight function takes negative values near the neighboring nodes and it can be checked that the resulting discrete scheme reduces to collocation.
With respect to the computational cost involved in the calculation of the proportionality constants, it amounts to the evaluation of 4 exponentials, 2 square roots and 49 operations (additions, multiplications and divisions). For reference, the DRD method (expressions (4.3) and (5)) involves 3 functions and 15 operations, so that the cost of (SU+C)PG is, at most, 3 times higher than that of DRD. However, we it can be shown both theoretically (§3) and through examples (§5) that the robustness and accuracy of (SU+C)PG largely pays this extra computational cost. On the other hand, the cost for those methods that resort to non-linear feedback of the solution, like the discontinuity-capturing techniques presented in [4] or [5], depends on the precision with which the non-linear problem is solved, but we can estimate that the cost of (SU+C)PG is well below them.
Regarding the extension to multi-dimensional problems, it does not pose severe problems and the interested reader is referenced to [1].

4. THE DISCRETE MAXIMUM PRINCIPLE

It is well known that the continuum problem satisfies a maximum principle, which can be put in the following terms: if $f(x) \leq 0$ for all x, then ϕ attains its maximum at the boundaries. The question is whether the discrete scheme inherits this feature, i.e. if, for any $f(x) \leq 0$ the numerical solution satisfies: $\phi_i \leq \max\{\bar{\phi}\}$ for all i, where $\bar{\phi}$ is the value of ϕ at the boundaries.. It has been shown [10] that the satisfaction of the DMP implies uniform convergence of the finite element solution. It can be shown that the (SU+C)PG scheme verifies the *Discrete Maximum Principle* (DMP), for all Pe and r, whereas the others (Galerkin, SUPG and DRD) only satisfy the DMP in restricted regions of the Pe-r plane. We will call these regions the *stability regions* of each method. The satisfaction of the Discrete Maximum Principle can be assessed from the verification of some conditions on the coefficients of the matrix of coefficients. Furthermore, for a

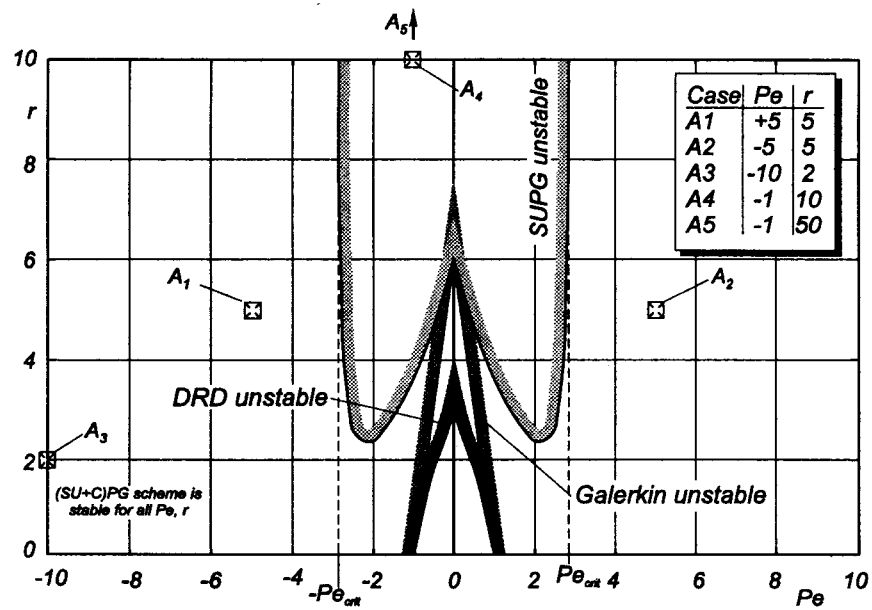


Figure 5: Stability map for Galerkin, DRD and SUPG.

uniform mesh the coefficients of the linear system of equations are constant, and, when conveniently non-dimensionalized, they depend only on the non-dimensional Pe and r numbers. Then, for each method, we can find the region of the Pe-r plane where the DMP is satisfied (see figure 5). The region of stability for Galerkin is a triangle, for pure advection the range of admissible Peclets is $|\mathrm{Pe}| < 1$, whereas for pure reaction we have $r < 6$. SUPG has a much broader range of stability. Needless to say, for pure advection all the Pe axis is in the stable zone, and for $|\mathrm{Pe}| > \mathrm{Pe}_{\mathrm{crit}}$ it is stable for all r. However, for pure reaction the range of stable reaction numbers is the same as Galerkin ($r < 6$). On the other hand the DRD method has an stable region smaller than that of Galerkin. In contrast, the (SU+C)PG scheme is uniformly stable over the whole Pe-r plane. The demonstration can be found in [1] and is based mainly on the super-convergence feature of the method. Then, it is rather independent of the particular scheme and can be extended easily to other kind of problems (system of equations, higher order schemes, for instance), *whenever the scheme is based in adjusting the numerical coefficients in order to match the solutions for the homogeneous case* (superconvergence).

5. NUMERICAL RESULTS

5.1. Experimental regions of stability. Comparison with other methods.

To experimentally confirm the stability regions deduced previously, we performed a large number of numerical experiments simulating the problem described by (1) with no source term, and $\phi_0 = 0$, $\phi_1 = 1$. The region $|\mathrm{Pe}| \leq 10$, $0 \leq r \leq 10$ was covered with a grid of 100×50 points of the form $(\pm \mathrm{Pe}_j, r_l)$ where the Pe_j and r_l, $j,l = 1,\ldots,50$ are interpolated logarithmically between 0.2 and 10. The mesh was non-uniform: the position of the inner nodes are computed as $x_j = (j + \frac{1}{2}\delta_j)\bar{h}$, where $\bar{h} = 1/N$, $N = 20$ is the number of elements and the δ_j are randomly choosed in (with a uniform density

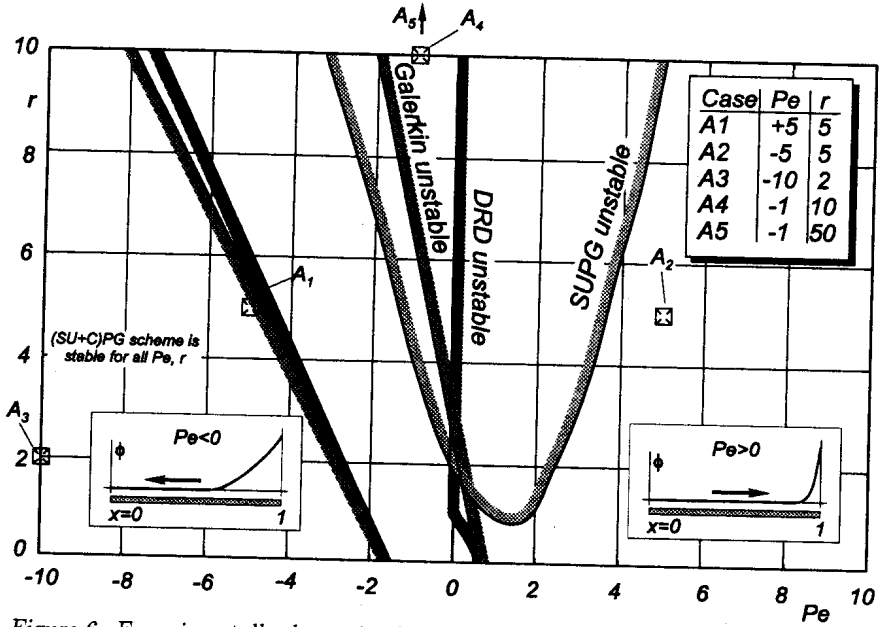
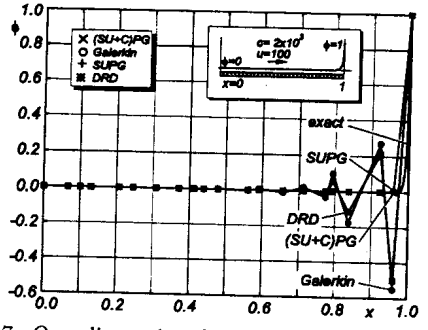
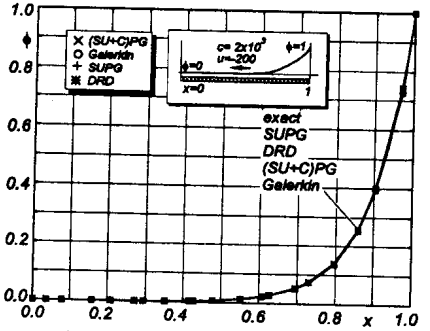


Figure 6: Experimentally determined stability map for Galerkin, DRD and SUPG.

distribution) in the range $|\delta - j| < \delta_{\max} = 0.95$. The physical properties k, u and c were set according to the values of Peclet and reaction numbers, considered as based on the average size element $\bar{h}$. Since the exact solution is monotone we used this as the criterion for stability, i.e. the discrete solution $\{\phi_i\}$ for a given set of parameters (Pe_j, r_l) is unstable if $\phi_{i+1} < \phi_i$ for some i.

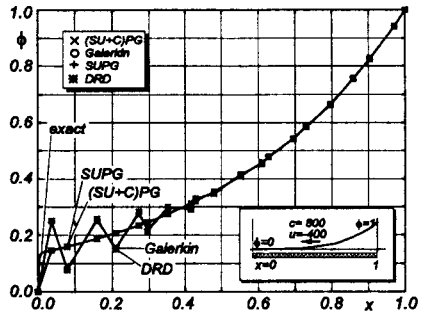


7: One-dimensional example with non-uniform mesh. Case A_1.

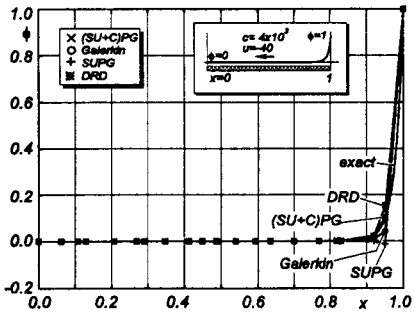


8: One-dimensional example with non-uniform mesh. Case A_2.

The resulting *stability map* is shown in figure 6. It can be seen that the right portion of the map ($\mathrm{Pe} > 0$) is similar to the stability map based on the DMP (see figure 5). The differences can be attributed to the fact that the non-dimensional mesh parameters Pe and r are based in an average element size. In contrast, the left portion is qualitatively different from the DMP version. For all methods, the stability region for $\mathrm{Pe} < 0$ is much



9: One-dimensional example with non-uniform mesh. Case A_3.



10: One-dimensional example with non-uniform mesh. Case A_4.

broader than that for Pe > 0. This is because for a large part of the region Pe < 0, the solution is rather smooth, even if |Pe| and r are large. For instance, consider the cases Pe $= \pm 5$, $r = 5$ ($u = \pm 200$, $c = 2 \times 10^3$, as $\bar{h} = 1/20$), indicated as A_1 and A_2 in figure 6. The corresponding profiles can be seen in figures 7 (Pe $= +5$) and 8 (Pe $= -5$). The solution for Pe < 0 is rather smooth, since it is basically equal to the inviscid solution, which has a characteristic length of $\delta \approx |u|/c = 1/10$ and practically all methods give a qualitatively good result, even Galerkin. In contrast, the solution for $u > 0$ exhibits a thin diffusive layer, with a characteristic length $\delta \approx k/|u| = 1/200$, and only the SUPG and (SU+C)PG methods, who can cope with the strong diffusive boundary layer, give non-oscillatory results. Coming back to the Pe < 0 case, if we move deeper into the instability region of both the DRD and Galerkin methods, as for case A_3 (Pe $= -10$, $r = 2$, $u = -400$, $c = 800$, see figure 9.), then the amplitude of the mismatch at the left boundary is larger, and both DRD and Galerkin exhibit large oscillations. Up to this point, we have not found any advantage of DRD over SUPG, in fact DRD behaved very similar to Galerkin. Consider now the case A_4 (Pe $= -1$, $r = 10$; $u = -40$, $c = 4 \times 10^3$, see figure 10.). The inviscid approximation continues to be valid and the downwind boundary layer is very small, but now the characteristic length for the inviscid solution is $|u|/c = 10^{-3} \ll \bar{h}$, so that the solution is not "smooth", and SUPG exhibits oscillations whereas DRD behaves very well. If we increase r to 50 ($c = 2 \times 10^4$) case A_5, see figure 11.), the overshoot for SUPG is more pronounced, whereas DRD continues to be stable. This region, where $r \gg \|Pe|$, and Pe < 0 is the region where DRD signifies an improvement over SUPG. However, as was shown, DRD will fail whenever a diffusive boundary layer is expected. In contrast, *the (SU+C)PG method was stable uniformly over the whole* Pe-r *plane.*

5.2. Non-constant physical properties

In this example, the physical properties u and c are not constant over the domain and non-uniform meshes are used:

$$N = 20, \quad k = 1, \quad \delta_{\max} = 0.8, \quad u = \{u_1 = -1 \text{ for } x < 0.5,\ u_2 = -10 \text{ for } x < 0.5;\}$$
$$c = \{c_1 = 4 \times 10^3 \text{ for } x < 0.5; c_2 = 1 \text{ for } x < 0.5.\} \tag{12}$$

The numerical solution is shown in figure 12, along with the Galerkin solution and the exact one. While the solution in the $x \geq 1/2$ region is smooth, the solution in $x \leq 1/2$ has a transition zone with a scale length 0.015, that is smaller than the average element

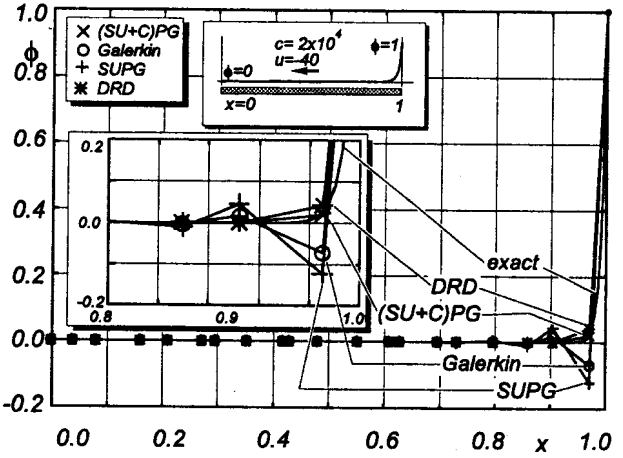
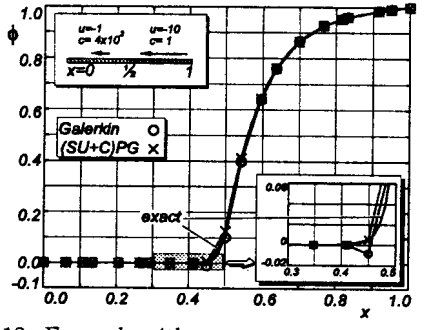
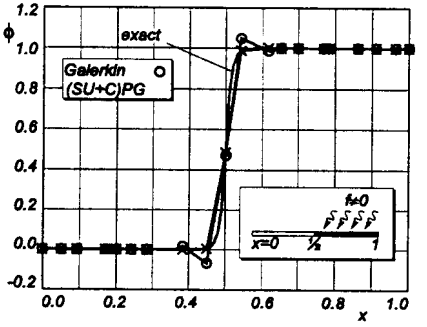


Figure 11: One-dimensional example with non-uniform mesh. Case A_5.



12: Example with non-constant physical properties. Comparison between the different methods.



13: Example with internal source and null advection. Comparison between the different methods.

size $\bar{h} = 0.05$. Consequently, Galerkin's method suffers from oscillations whereas the (SU+C)PG one remains stable.

5.3. Example with internal source and null advection

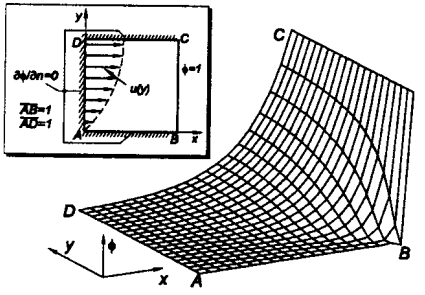
Here a source term along with non-uniform meshes are used. The physical constants, source term and boundary conditions are:

$$\begin{aligned} &N = 20, \quad k = 1, \quad u = 0, \quad c = 8 \times 10^3, \quad \delta_{\max} = 0.8, \\ &f(x) = \{0 \text{ for } x < 1/2; c \text{ for } x > 1/2;\}, \quad \phi(0) = \phi_0 = 0, \quad \phi(1) = \phi_1 = 1. \end{aligned} \tag{13}$$

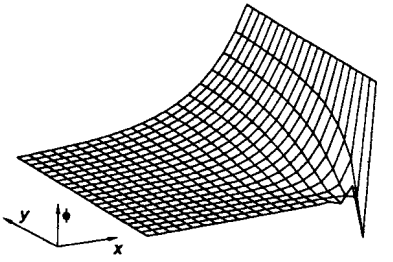
The solution ϕ is S-shaped and for $c \to \infty$ it approaches a step function about $x = 1/2$. The scale of the transition zone from $\phi = 0$ to $\phi = 1$ is $O(\sqrt{k/c})$. For large c, this discontinuity induces oscillations for the non-stabilized algorithms, so that it is a good test in order to show the benefits of the (SU+C)PG scheme. The numerical results are shown in figure 13, comparing the solution with the present method and Galerkin. For the given physical data, the scale of the transition zone from $\phi = 0$ to $\phi = 1$ is

$\sim \sqrt{k/c} = 0.011$, being smaller than the average element size $\bar{h} = 0.05$. In consequence, Galerkin method produces spurious oscillations, whereas the (SU+C)PG method does not.

5.4. *Multi-dimensional results*



14: Two-dimensional example with advection (parabolic profile). Problem description and numerical results with the (SU+C)PG scheme.



15: Two-dimensional example with advection (parabolic profile). SUPG scheme.

Finally we performed a two-dimensional example that consists in a linear convection reaction without source term but, now, the velocity is not constant [5]. The domain is the unit square $0 \leq x, y \leq 1$. The velocity $\mathbf{u} = (u, v)$ is assumed to have a parabolic profile: $u(y) = u_{\max} y^2$, $v \equiv 0$. The reaction coefficient is equal to $c = 5$, diffusivity $k = 10^{-8}$ and $u_{\max} = 1$. The mesh is uniform and consists of 20×20 elements. The boundary conditions are natural (null flux) in three of the four sides of the domain and in the fourth side we have imposed a Dirichlet condition fixing the solution value equal to 1, as shown in figure 14. Figures 14, 15 show the stabilized scheme results and the standard SUPG ones. We can observe that the oscillations obtained with the standard SUPG near the zone where a very high reaction number exists have disappeared with the stabilized scheme whereas, in the rest of the domain, both solutions are equivalent because the problem is advection dominated there.

CONCLUSIONS

This paper presents a stabilized multidimensional scheme for ARD problems that extends the SUPG method to overcome the numerical oscillations that appear from the reaction term. This numerical improvement allows to treat in an optimal way a lot of industrial interesting situations where reaction effects are important in some regions of the domain, advection effects dominates in other zones, specially if the location of these zones is *a priori* unknown. It has been shown that (SU+C)PG scheme satisfies the DMP criterion uniformly over all the Pe-r plane and it has been proved to be stable also in a series of numerical tests.

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