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PETROV–GALERKIN METHODS FOR THE TRANSIENT ADVECTIVE–DIFFUSIVE EQUATION WITH SHARP GRADIENTS

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SUMMARY

A Petrov–Galerkin formulation based on two different perturbations to the weighting functions is presented. These perturbations stabilize the oscilations that are normally exhibited by the numerical solution of the transient advective–diffusive equation in the vecinity of sharp gradientes produced by transient loads and boundary layers. The formulation may be written as a generalization of the Galerkin Least Square method.

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$$\frac{\partial \phi}{\partial t} - k\frac{\partial^2 \phi}{\partial x^2} + u\frac{\partial \phi}{\partial x} = 0 \tag{1.2}$$

with initial condition

$$\phi(x, t_0) = 0$$

and boundary conditions

$$\phi(0, t) = 0$$

$$\phi(2, t) = 1$$

solved using a θ-scheme for the time integration with $\theta = 1/2$ and 14 equal size linear finite elements. With $k = 1$ and $u = 10^{-3}$ the solution is dominated by diffusion and shows strong oscillations at the early stages of the calculation.

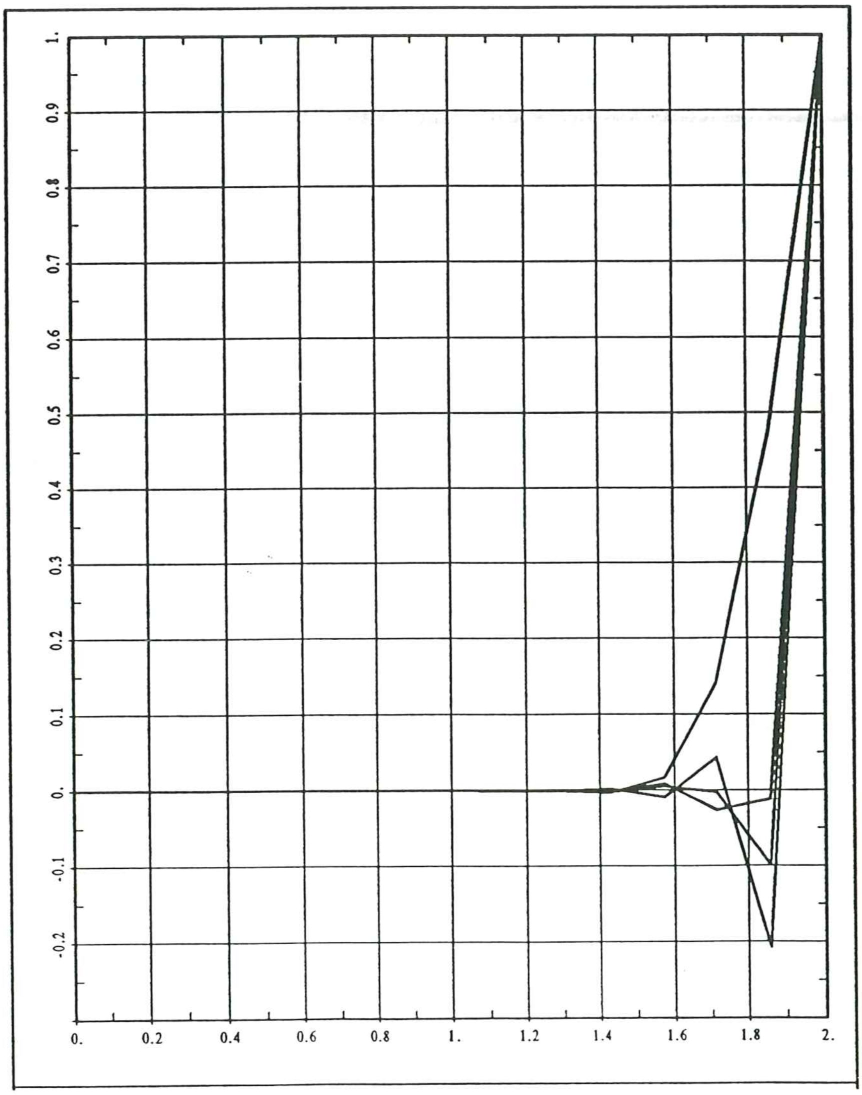


Fig. 1 First 3 time steps and 20th time step

for the diffusive dominat problem.

$u = 10^{-3}; k = 1; \Delta t = 10^{-3}.$

shock capturing term to stabilize the reactive effects. However, this approach introduces a non–linearity even in linear one–dimensional problems.

To the authors knowledge, none of the above mentioned ideas on reactive–difusion–advective problems have been used to solve the transient advective–diffusion equation. In this paper we will use the approach reported in [8], which may also be seen as a generalizaton of the Galerkin Least Square method (GLS),to approximate the solution of the time dependent equation (1.1).

It is well known that in the Petrov–Galerkin approach, a "balancing diffusion" k^* is added in order to have the exact nodal solution of the homogeneous one-dimensional linear problem. In the present formulation, both a "balancing diffusion" k^* and a "balancing advection" u^* will be added as shown below.

Let

$$\bar{k} = k + k^*$$

$$\bar{u} = u + u^*$$

be the total diffusion and advective velocity coefficients. For a uniform mesh of size h and linear finite elements the Galerkin formulation applied to Eq(2.3) gives the following difference equation at each node i :

$$\frac{(k+k^*)}{h^2}\begin{pmatrix}-\phi_{i-1}\\ 2\phi_i\\ -\phi_{i+1}\end{pmatrix} + \frac{(u+u^*)}{2h}\begin{pmatrix}-\phi_{i-1}\\ 0\phi_i\\ \phi_{i+1}\end{pmatrix} + \frac{c}{6}\begin{pmatrix}\phi_{i-1}\\ 4\phi_i\\ \phi_{i+1}\end{pmatrix} = f_i \tag{2.7}$$

The exact solution to equation (2.3) with $f_i = 0$ is of the form

$$\phi(x) = ae^{\lambda_1 x} + be^{\lambda_2 x} \tag{2.8}$$

where

$$\lambda_{1,\,2} = \frac{u}{2k} \pm \sqrt{\left(\frac{u}{2k}\right)^2 + \frac{c}{k}} \tag{2.9}$$

Replacing (2.8) in (2.7) we find:

$$k + k^* = -ch^2\frac{2 + e^{\lambda_1 h} + e^{\lambda_2 h} + 2e^{(\lambda_1+\lambda_2)h}}{6(1-e^{\lambda_1 h})(1-e^{\lambda_2 h})} \tag{2.10}$$

$$u + u^* = ch\frac{1 - e^{(\lambda_1+\lambda_2)h}}{(1-e^{\lambda_1 h})(1-e^{\lambda_2 h})} \tag{2.11}$$

When the reactive term c is small, the k^* tends to the known balancing diffusity:

$$k^* = -k + \frac{uh}{2} \coth\left(\frac{uh}{2k}\right) \tag{2.12}$$

and the numerical advection u^* goes to zero.

On the other hand, when the advective term is small, the numerical diffusion behaves like:

$$k^* = -k + \frac{ch^2}{6} + \frac{ch^2}{4 \sin h^2 \left(\sqrt{\frac{ch^2}{4k}}\right)} \tag{2.13}$$

and u^* goes to zero, which is the result obtained by Tezduyar et al. [Ref.10] for reactive dominant flows.

3. THE GENERALIZED GALERKIN LEAST SQUARE METHOD (GLS_2)

A consistent alternative to introducing the numerical coefficients k^* and u^*, as shown in the previous section, is to find weighting functions that yield the same results as Eqs. (2.7) through (2.11). In this way the physical equation is not changed, and the weighting functions are perturbated in order to obtain the desired effect. These methods are called, in general, Petrov–Galekin methods [Ref. 1–3]. The best known Petrov–Galerkin methods are the streamline–diffusion algorithms in which the weighting functions are perturbed in an unsymmetrical way in the upwind direction and the perturbation function is proportional to the gradient of the weighting function. The SUPG (streamline upwind Petrov–Galerkin) method is one of them, and it has been shown to be effective for the finite element solutions of linear advective–diffusive systems [Ref.3]. More recently, the Galerkin Least Square method [Ref. 9] has been introduced as a general methodology to obtain consistent finite element schemes that can accomodate a wider class of interpolation functions. In the GLS approach, the perturbation functions are not only proportional to the gradient of the shape functions , but to the whole operator including the Laplacian of the function. We will generalize this concept in order to include the stabilization of the reactive–diffusive–advective problem.

Let equation (1.1) be written as

$$\sum_{i=0}^{2} \mathcal{L}_i(\phi) = f \tag{3.1}$$

where

$$\mathcal{L}_2(\phi) = -\nabla \cdot k\nabla\phi \tag{3.2}$$

$$\mathcal{L}_1(\phi) = \mathbf{u}\nabla\phi \tag{3.3}$$

$$\mathcal{L}_0(\phi) = c\ \phi \tag{3.4}$$

A weighted residuals method applied to equation (3.1) consists in finding $\hat{\phi}$ such that

$$\phi \simeq \hat{\phi} = \sum_{l=1}^{n} w_l(x)\phi_l \tag{3.5}$$

by imposing that

$$\int_\Omega \tilde{w}_l(\sum_{i=0}^{2} \mathcal{L}_i(\hat{\phi}) - f)d\Omega = 0 \tag{3.6}$$

where $\tilde{w}_l$ are weighting functions.

The following approaches are recovered by an appropiate selection of the weighting functions:

a) The Galerkin approach

$$\tilde{w} = w \tag{3.7}$$

b) The SUPG technique

$$\tilde{w} = w + \tau\mathcal{L}_1(\hat{\phi}) \tag{3.8}$$

where τ is the upwind coefficient necessary to achieve stability in the proposed scheme

c) The GLS method

$$\tilde{w} = w + \tau(\sum_{i=0}^{2} \mathcal{L}_i(\hat{\phi})) \tag{3.9}$$

The name of Least–Square method was used because the perturbation to the weighting functions are the same as the operator itself.

In the proposed Generalized Galerkin Least Square method (GLS2) $\tilde{w}$ is given by

$$\tilde{w} = w + \sum_{i=0}^{2} \tau_i\ \mathcal{L}_i(\hat{\phi}) \tag{3.10}$$

which requires the use of different stabilizing parameters for each of the operators involved.

In fact, we can normalize one of the coefficients τ_i in order to have 2 independent parameters as

$$\tilde{w} = w + \tau_1 \mathbf{u} \nabla w + \tau_2(-\nabla \cdot k \nabla w) \tag{3.11}$$

This formulation, includes all the previous ones as particular cases i.e.,

$$\begin{aligned}
\tau_1 = \tau_2 = 0 &\rightarrow \text{Galerkin} \\
\tau_1 \neq 0;\ \tau_2 = 0 &\rightarrow \text{SUPG} \\
\tau_1 = \tau_2 \neq 0 &\rightarrow \text{GLS} \\
\tau_1 \neq \tau_2 \neq 0 &\rightarrow \text{GLS}_2
\end{aligned}$$

In order to evaluate the stabilizing parameters τ_1 and τ_2 we will write the weighting functions (3.11) as in Ref [8]

$$\tilde{w} = w + \alpha h \mathbf{e_u} \nabla w + \gamma P_2(x) \tag{3.12}$$

where

$$\alpha = \frac{\tau_1\ |\mathbf{u}|}{h}\ ; \quad \gamma = -k\ \tau_2\ ; \quad P_2(x) = \nabla \cdot \nabla w \tag{3.13}$$

h is the size of the element and $\mathbf{e_u}$ is unit vector in the direction of $\mathbf{u}$.

The weak form of equation (3.6) is

$$\int_\Omega (\nabla \tilde{w}\ k \nabla \phi + \tilde{w}\ \mathbf{u} \nabla \phi + \tilde{w}\ c\ \phi - \tilde{w} f) d\Omega - \int_\Gamma \tilde{w}\ k \nabla \phi \cdot n\ d\Gamma = 0 \tag{3.14}$$

and using (3.12)

$$\begin{aligned}
&\int_\Omega (\nabla w\ k \nabla \phi + w\ \mathbf{u} \nabla \phi + w\ c\ \phi - w\ f) d\Omega \\
&+ \int_\Omega (P_2\ k\ \alpha\ h\ \mathbf{e_u} \nabla \phi + \nabla w\ \alpha\ h\ \mathbf{e_u} \nabla \phi + \nabla w\ \alpha\ h\ c\ \mathbf{e_u} \phi - \nabla w\ \alpha\ h\ \mathbf{e_u} f) d\Omega \\
&+ \int_\Omega (\nabla P_2\ \gamma\ k \nabla \phi + P_2\ \gamma\ \mathbf{u} \nabla \phi + P_2\ c\ \gamma\ \phi - P_2\ \gamma\ f) d\Omega \\
&- \int_\Gamma (w + \alpha\ \mathbf{e_u} \nabla w + \gamma\ P_2)\ k \nabla \phi \cdot n d\Gamma = 0
\end{aligned} \tag{3.15}$$

For linear finite elements ($\nabla \phi$ = constant) and constant f , equation (3.15) shows that the results involve specific averages of $P_2(x)$ and $\nabla P_2(x)$. For simplicity, we denote such averages as:

$$a = \frac{1}{\Omega_e} \int_{\Omega_e} P_2(x) d\Omega; \; m_i = \frac{1}{\Omega_e h} \int_{\Omega_e} x_i P_2(x); \; P_0 = \int_{\Omega_e} \nabla P_2(x) d\Omega \tag{3.16}$$

where Ω_e is the volume of each finite element.

For linear finite elements, the definition of $P_2(x)$ as (3.13) is rather arbitrary because $\nabla \cdot \nabla w$ vanishes within each element and it is a Dirac δ-function at the interfaces. On the other hand, equation (3.15) shows that the results are independent of the precise definition of $P_2(x)$, depending only on some average values over each element. Thus, any function giving the same a, m_i and P_0 values yields the same results. In Ref. [8], the authors analyzed the effect of varying the parameters a, m_i and P_0. A basic requirement is that the proportionality constants α and γ must be bounded for all combinations of the coefficients k and c . In that reference, the use of

$$a = 1/6 \quad ; \quad m_i = 1/12 \quad and \quad P_0 = 0 \tag{3.17}$$

was proposed, but different values may be used with similar results.

The stabilizing parameters α and γ (and then, τ_1 and τ_2) are computed so as to obtain the exact nodal values in the one–dimensional homogeneous problem. This situation is equivalent to the use of balancing diffusion k^* and balancing advection u^* defined in (2.10) and (2.11) respectively.

The following Peclet and reaction dimensionless numbers are defined

$$Pe = \frac{|\mathbf{u}|\, h}{2k} \quad \text{and} \quad r = \frac{c\, h^2}{k} \tag{3.18}$$

in which r , for transient problems, is a function of the time step and the time integration technique used according to eq.(2.5).

The values of α and γ are obtained by solving the following 2×2 system:

$$\begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \begin{bmatrix} \alpha \\ \gamma \end{bmatrix} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} \tag{3.19}$$

where

$$\begin{aligned} g_{j1} &= 4Pe(1 - \cosh(\lambda_j)) - r \sinh(\lambda_j) \\ g_{j2} &= 2\cosh(\lambda_j)(r\, m_i - P_0) + 4Pe\, a \sinh(\lambda_j) + \\ &\quad + 2(P_0 - m_i\, r + a\, r) \\ h_j &= 2\cosh(\lambda_j)(\frac{1}{6}r - 1) + 2Pe \sinh(\lambda_j) + (2 + \frac{2}{3}r) \\ \lambda_j &= Pe + (-1)^{j-1}(Pe^2 + r)^{\frac{1}{2}} \end{aligned} \tag{3.20}$$

Figure 2 shows the curves of α and γ for different values of Pe and r when $a = 1/6$; $m_i = 1/12$ and $P_0 = 0$.

It must be noted that both parameters α and γ (and then τ_1 and τ_2) depend on both dimensionless numbers Pe and r, i.e.,

$$\tau_1 = \tau_1(Pe,\ r)$$
$$\tau_2 = \tau_2(Pe,\ r)$$

In the limit case in which one of these dimensionless numbers becomes zero, (eg: $r = 0$ for the stationary case, or $Pe = 0$ for a non–advective problem), one of the parameters becomes zero, and the other one becomes a function of the remaining dimenssionless number,

$$r = 0 \rightarrow \begin{cases} \tau_1 = \tau_1(Pe) \\ \tau_2 = 0 \end{cases}$$

$$Pe = 0 \rightarrow \begin{cases} \tau_1 = 0 \\ \tau_2 = \tau_2(r) \end{cases}$$

4.THE TRANSIENT SOLUTION

Using the GLS_2 method with the stabilizing parameters proposed in previous section, the reactive–advective–diffusive problem with constant source terms can be solved giving exact nodal values in the one–dimensional case. However, the transient advective-diffusse problem proposed in equation (2.3) has a variable generalized source term f^n which is not constant even in the case when the source term f is. In particular, in the stationary limit, the generalized source terms f^n becomes equal to the reactive term $c\phi^{n+1}$ (see equations (2.3). and (2.4)). In this limit, the equation must be solved as a non–reactive equation and the stabilizing parameter becomes the optimal parameter for the advective–diffuse case.

To overcome this difficulty a modification on the definition of the coeficient c is introduced. Equation (2.3) is now written:

$$c^*(x,t)\phi^{n+1} - \nabla \cdot k\nabla\phi^{n+1} + \mathbf{u}\nabla\phi^{n+1} = 0 \qquad (4.1)$$

with

$$c^*(x,t) = \frac{c\ \phi^{n+1} - f^n}{\phi^{n+1}} \qquad (4.2)$$

The problem is transformed into a homogeneous one but with a nonlinear reactive coefficient that varies both in space and time.

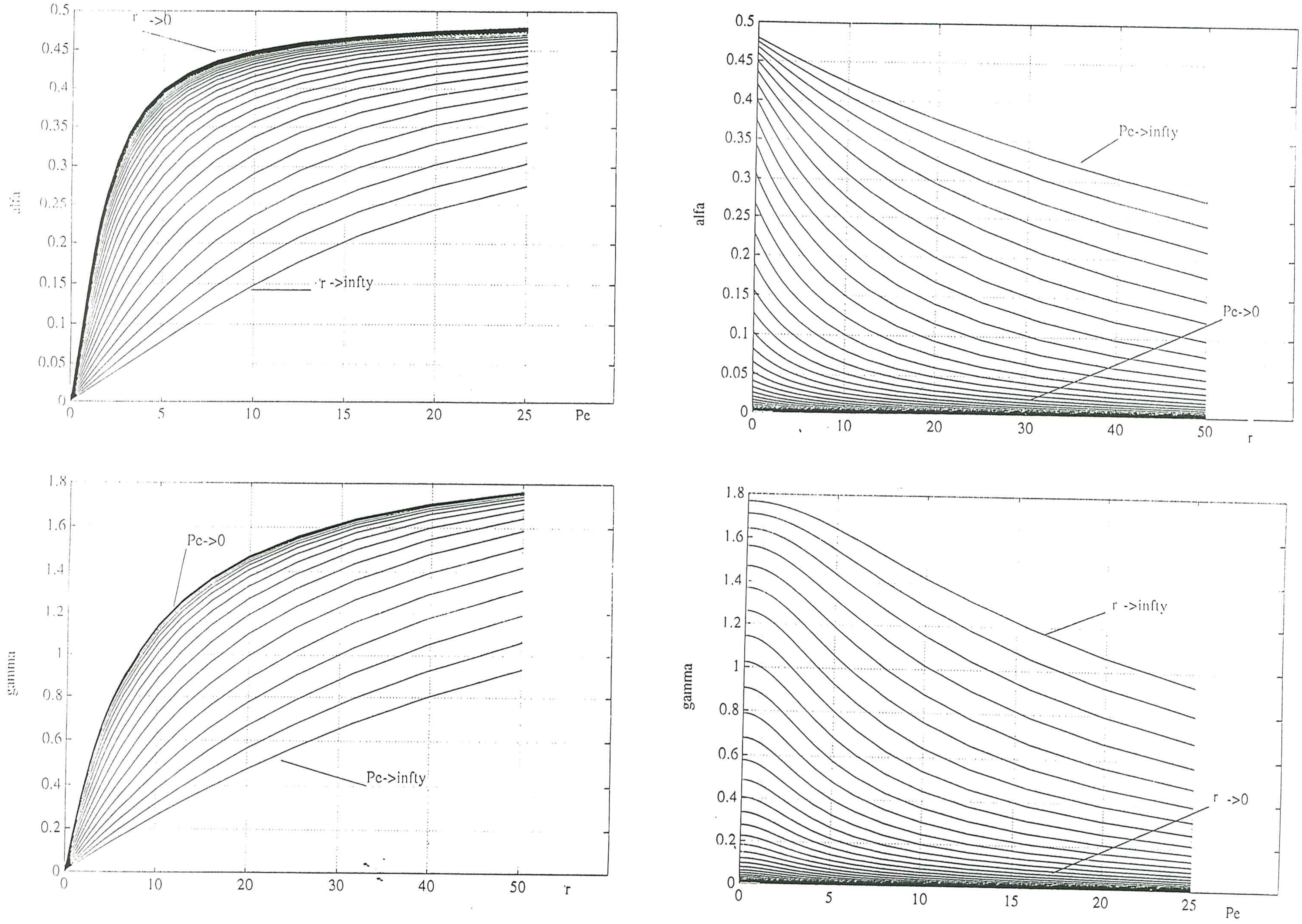


Fig. 2 Stabilization parameters as a function of Pe and r.

The problem is transformed into a homogeneous one but with a nonlinear reactive coefficient that varies both in space and time.

This coefficient may be approximated in order to retain the linearity of the problem using:

$$c^*(x,t) \simeq \frac{c\,\phi^{n+1} - c\,\phi^n}{\phi^{n+1}} \simeq c\,\frac{\phi^n - \phi^{n-1}}{\phi^n} \tag{4.3}$$

furthermore, to obtain a constant average $c^*(t)$ on all the domain:

$$c^*(t) \simeq c\,\frac{\max\left(|\phi^n - \phi^{n-1}|\right)}{\max\left(|\phi^n|\right)} \tag{4.4}$$

This last approximation has been used in the examples presented below. It must be noted that the value of c^* , given by Eq.(4.4) should be used in the evaluation of the stabilizing parameters α and γ (or τ_1 and τ_2) only. That is, the approximation (4.4) is introduced only for the evaluation of the perturbations to the weighting functions $\tilde{w}$ but not in the equation to be solved. This is important in order to retain the consistency of the solution.

Using the GLS_2 method for the transient advective–diffusive equation, with the approach (4.1)–(4.4) in the evaluation of the time dependent parameters, no spurious oscillations during the transient part and an optimally stabilized solution near the stationary state are ensured as it will be shown in the next examples.

5. NUMERICAL RESULTS

The problem of finding numerical approximations to the equation:

$$\frac{\partial \phi}{\partial t} - k\frac{\partial^2 \phi}{\partial x^2} + u\frac{\partial \phi}{\partial x} = 0 \tag{5.1}$$

with initial and boundary conditions:

$$\begin{aligned} \phi(x,\ t_0) &= 0 \\ \phi(0,\ t) &= 0 \\ \phi(2,\ t) &= 1 \end{aligned} \tag{5.2}$$

is presented for various combinations of parameters and boundary conditions.

This simple equation was chosen because it has the two types of sharp gradients under consideration. For high Peclet numbers, a boundary layer develops in the right end due to the elliptic–hyperbolic character of the equation. On the other hand, for all Peclet numbers, a sharp gradient appears at the right end during the first few time steps due to the transient solution. This sharp gradient, which is similar to a shock in a fluid mechanics problem, disappears after a few time steps if the problem is dominated by diffusion, and it will remain as the solution approaches the stationary state if the problem is dominated by advection.

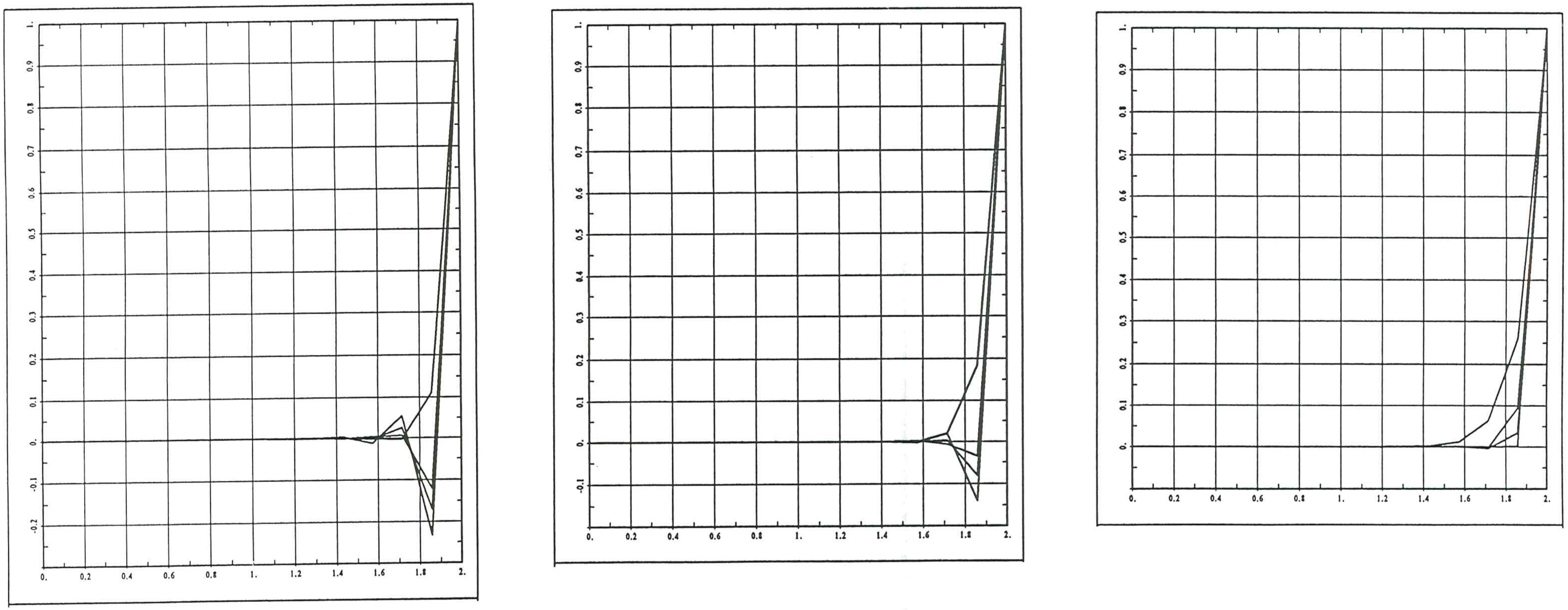
It is important to note, that the way to eliminate the spurious oscillations is different when the sharp gradients are induced by the transient evolution, than when they are produced by the advective terms.

Figure 3 shows the first three time steps and the $20th$ time step for $k = 1$ and $u = 10$. This is a case dominated by diffusion. The time step used was $\Delta t = 10^{-3}$, we use 14 equal size linear elements in space and $\theta = 1/2$ for the time integration scheme.

We can see that the Galerkin approach as well as the upwinded approach using the standard SUPG with optimal upwinding parameter both give very similar results, with spurious oscillations during the first time steps. These local oscillations dissappear before the $20th$ time step. The solutions using the new Galerkin Least Square method (GLS_2) do not present any significant oscillations.

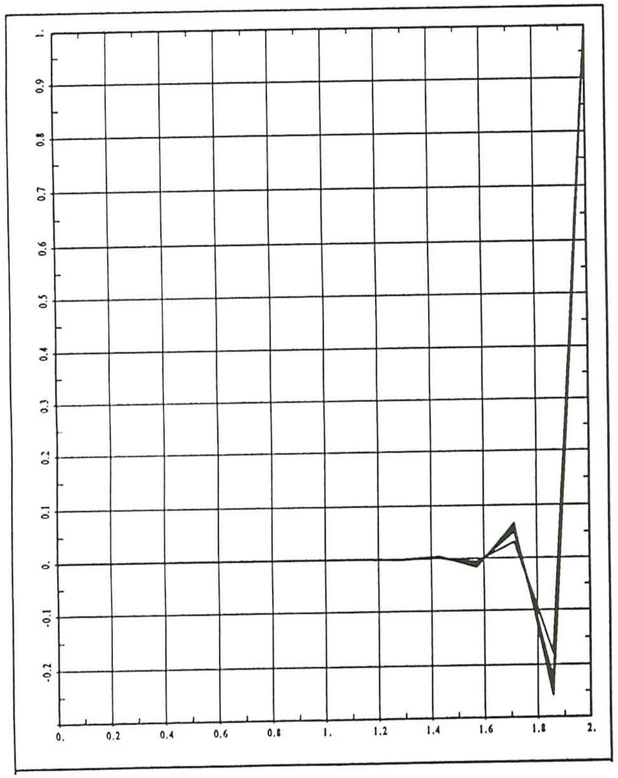
Figure 4 shows the same problem for $u = 20$. This case represents a more interesting situation because the advective terms are important enough to induce oscillations in the stationary state. The Galerkin approach (Fig. 4a) produces spurious oscillations at all time steps, including the stationary state. The optimal upwinding approach stabilizes the stationary solution but not the initial steps where large negative values of the function are present. Figura 4c shows the perfectly stabilized GLS_2 solution from $t = 0$ until the last time step.

Finally in Figure 5 the advection dominated flow with $u = 100$ is tested, for which the boundary layer is smaller than the first element, even in the stationary state. The exact solution will be $\phi = 0$ in all the interior nodes from the first time step. Figure 5a displays the oscillating behaviour obtained with the standard Galerkin approach. In Figure 5b, the optimal upwinding solution is shown. Note that no negative oscillations are obtained although the first three steps are over–diffusive. The solution approaches the correct steady–state but from above, which is not in agreement with the physics of the problem. Figure 5c shows the GLS_2 method in which the stationary solution is obtained from the first time step.

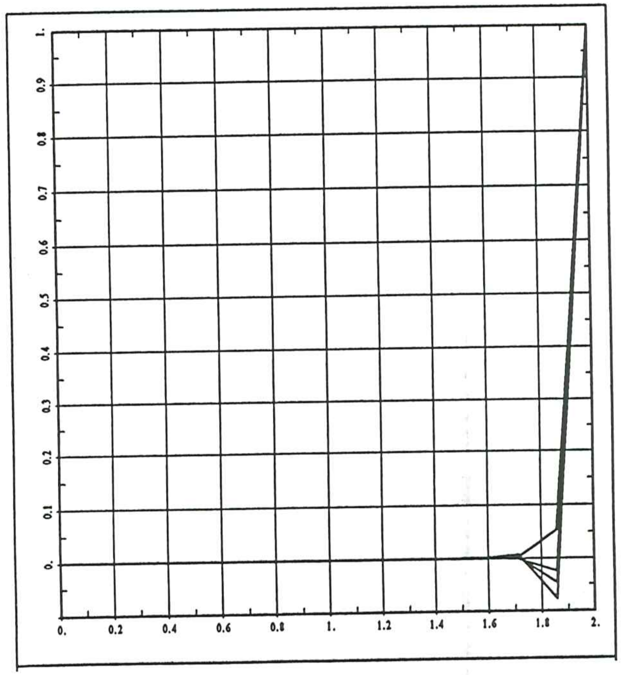


a) Galerkin b) SUPG c) GLS$_2$

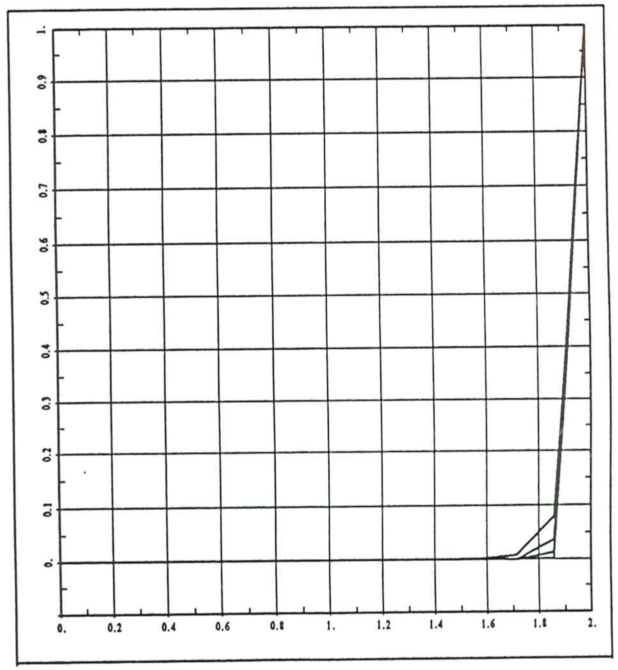
Fig. 3 Diffusive dominant problem I ($u = 10.$)



a) Galerkin

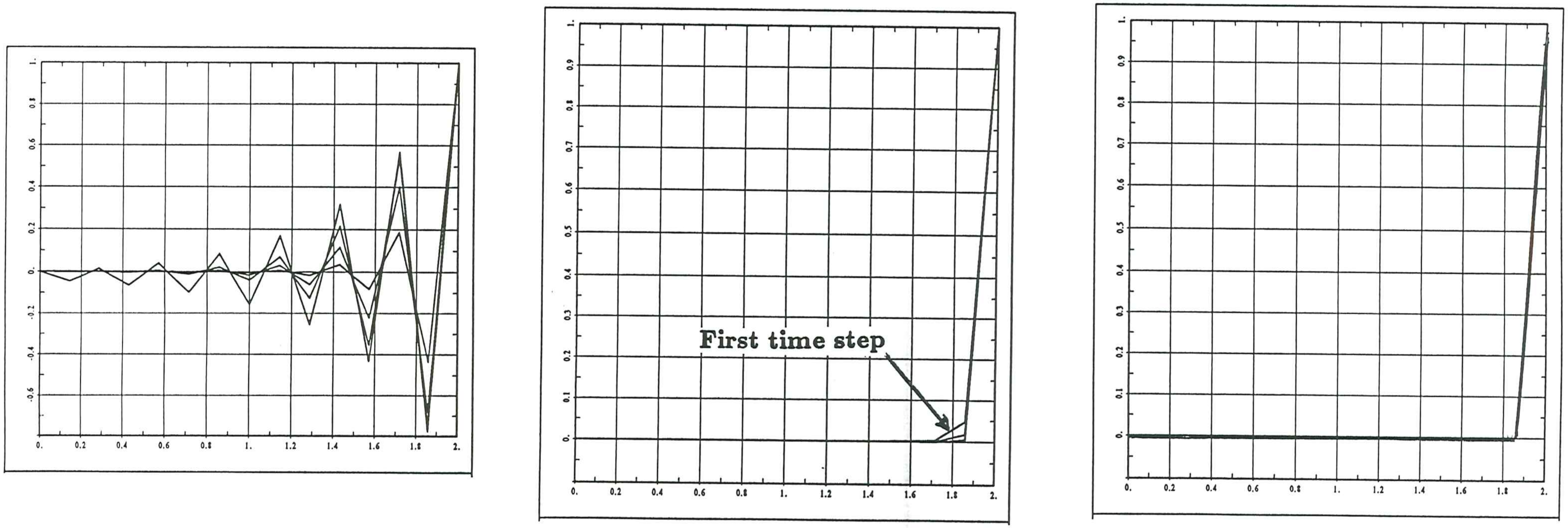


b) SUPG



c) GLS_2

Fig. 4 Advective–diffusive problem I ($u = 20.$)

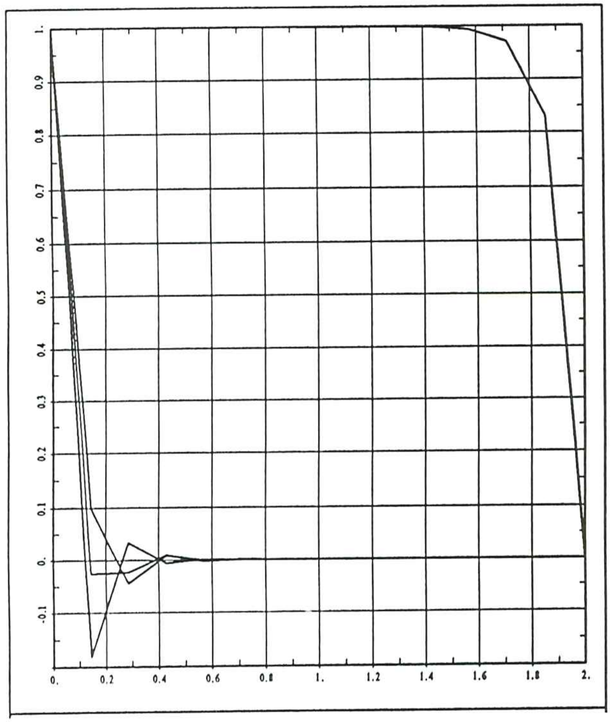


a) Galerkin

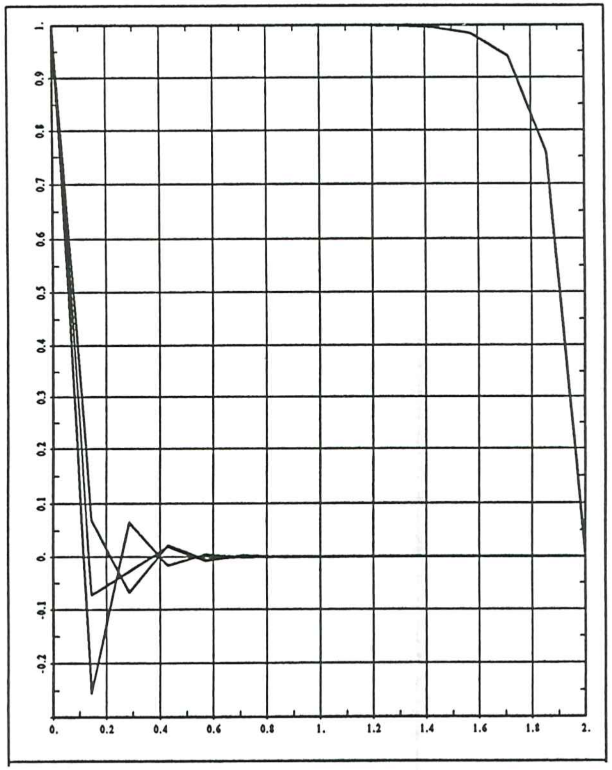
b) SUPG

c) GLS_2

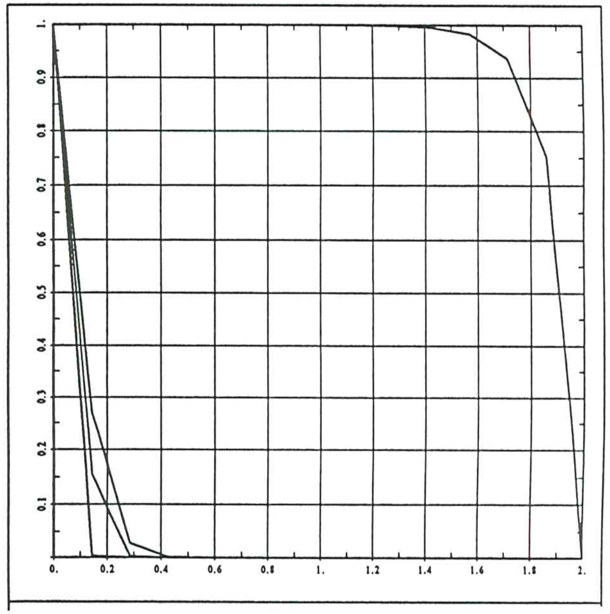
Fig. 5 Advective dominant problem I ($u = 100.$)



a) Galerkin



b) SUPG



c) GLS_2

Fig. 6 Diffusive dominant problem II ($u = 10.$)