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DON'T SUPPRESS THE WIGGLES - THEY'RE TELLING YOU SOMETHING!

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ABSTRACT

The subject of oscillatory solutions (wiggles), which sometimes result when the conventional Galerkin finite element method is employed to approximate the solution of certain partial differential equations, is addressed. It is argued that there is an important message behind these wiggles and that the appropriate response to it involves a combination of: reexamination of the imposed boundary conditions, judicious mesh refinement (via isoparametric elements) in critical areas, and sometimes even admitting that the problem, as posed, is just too difficult to solve adequately on an 'affordable' mesh. It is further argued that it is usually an inappropriate response to develop methods which a priori suppress these wiggles and thereby lead to claims that these unconventional FEM techniques are actually improvements and can be used to solve difficult problems on coarse meshes.

INTRODUCTION

Since the main purpose of this paper is to advocate the use of conventional Galerkin finite element methods (abbreviated GFEM), over those applications of FEM wherein one or more non-conventional or non-Galerkin modifications are invoked, we begin by defining the important features of GFEM: the conventional Galerkin weighted residual method is consistently applied to all terms in the equations and sufficiently accurate quadrature methods (e.g. Gauss-Legendre; see Leone et al. (1)) are employed, especially on the advection terms; this leads, in particular, to (a) centered-difference-like treatment of advection terms, and (b) the consistent mass matrix for coupling time derivative terms. In addition, for time-dependent problems, we extend our definition to include the requirement that the solution of the ordinary differental equations (ODE's) resulting from the spatial discretization is sufficiently accurate that time integration errors contribute in a (nearly) negligible way to the total error of the approximation. (Once the effect of spatial discretization error is sufficiently well understood, the *confounding effects of time integration errors can be reconsidered and* re-introduced for reasons of economy and cost-effectiveness.)

GFEM are prone to generate oscillatory 'solutions' (or wiggles; generally occurring in a 'node-to-node' manner) under many conditions and from many physical simulations, ranging from simple heat conduction to the Navier-Stokes (NS) equations. We believe, and will attempt to demonstrate (via rational arguments and numerical examples) that rarely, if ever, should these wiggles be artificially suppressed (damped) a priori by using an unconventional FEM 'designed' for that purpose, because these wiggles are broadcasting a strong signal regarding the accuracy of the simulation in describing the important physics of the continuum. Artificial (and usually ad hoc) damping mechanisms can be deceptive to the point of depriving the analyst from obtaining any truly useful or accurate information from the results. 'More difficult' problems require appropriately more expensive computations if the physics causing the difficulty is to be well-simulated (and not a conveniently modified, cheaper computation, of a different - and simpler - problem). The advantage of GFEM is that it usually 'announces' the nature of the difficulty (via oscillations) if the selected mesh is inappropriate for the problem at hand - and more - it provides the impetus and even the guidance for generating a more appropriate mesh (via rezoning in the region where wiggles are generated). Fortunately, the inherent flexibility of isoparametric finite elements (and good mesh generation codes) provides exactly the tools necessary to allow the analyst to intelligently remesh the domain, judiciously employing finer, graded zoning, and only in the critical areas. We believe that this aspect of FEM should be more thoroughly exploited so that good solutions can be obtained, on reasonable meshes which are well-designed, even for difficult problems. After all, FEM codes pay a high overhead (not to mention development cost) for the flexibility of isoparametric elements - they should be well-utilized. This belief is in contrast to what (too) many researchers in FEM have been pursuing of late - they seem to be mesmerized by 'smooth is beautiful' and are spending (too) much time and effort in generating FEM schemes which duplicate (with some improvements of course) the poor-but-smooth results of many finite difference simulations on coarse grids.

For example, "upwind methods" on the advection terms, which have long been resorted to in FDM (finite difference methods), especially when solving the resulting linear algebraic systems by 'relaxation' (iterative) techniques wherein diagonal dominance (which is not assured using centered differences) is often essential for guaranteeing convergent iterations, have recently been introduced into FEM formulations, mostly by ad hoc methods, and largely for a different reason; most FEM codes use direct methods on the linear systems and hence, lack of diagonal dominance causes little concern (although it's probably true that 'solutions' are always easier to obtain when upwind approximations are employed). The reason the number of FEM upwind advocates is continually increasing (besides the obvious one that all FEM research is increasing) is that many people are especially sensitive to the above-mentioned wiggles, and, believing that they should be suppressed, are vying for the honor of devising the first, or best, 'FEM wiggle suppressant' technique.

In this paper we present an alternative viewpoint regarding upwinding, via FEM or FDM; viz, "Upwinding can be dangerous to your health." We will elaborate on the various causes and effects of wiggles when using GFEM on a variety of equations, both steady and time-dependent, with the intention of vindicating the GFEM by expressing the opinion contained in the title of this paper. Our general theme and hypothesis is the following: The best way to obtain meaningful and accurate solutions is to employ the GFEM, combined with well-designed discretized domains, and appropriate boundary conditions, such that wiggles are either minimized or eliminated; when this is accomplished, the results can be relied upon as representing an actual solution to the original problem (i.e. a reasonably 'converged' solution to the partial differential equation(s), boundary conditions (BC's), and input parameters). Any technique which a priori suppresses wiggles can be deceptively inaccurate because it will too often lead to smooth solutions on coarse meshes and will not represent solutions to the <u>original</u> problem as defined above.

In addition to addressing "upwinding", we will also mention other aspects of GFEM, related to the consistent mass (CM) matrix, which, paradoxically, in one case (advection) automatically reduces wiggles and in another (transient diffusion) causes them; in both cases we will discuss why GFEM is to be preferred over its unconventional FEM counterpart (lumped mass - LM).

Specifically, we will encompass the above issues in discussing the following general flow problems, both analytically and experimentally (via numerical examples): steady-state advection-diffusion, time dependent advection-diffusion, the transient heat (diffusion) equation, and the Navier-Stokes equations, both steady and time-dependent.

STEADY-STATE ADVECTION-DIFFUSION

One-Dimensional Flow and the Classic 'Tough' Problem

Disregarding for now the appropriateness of the downstream BC, we begin with the one-dimensional version of what has recently become a 'classic' problem (as judged by the amount of attention it has received in the literature); viz,

$$u\frac{dT}{dx} = K\frac{d^2T}{dx^2} \quad ; \quad 0<x<L \quad , \tag{1}$$

$$T = T_o \text{ at } x = 0 \quad ,$$

$$T = T_L \text{ at } x = L \quad .$$

Analytical

The exact solution of Eq. (1) is

$$\frac{T(x) - T_o}{T_L - T_o} = \frac{1 - e^{Pe\frac{x}{L}}}{1 - e^{Pe}} \tag{2}$$

where $Pe \equiv uL/K$ is the Peclet number (ratio of advective – or convective – to diffusive transport), u is the velocity and K is the diffusivity.

For small to moderate Pe, T(x) displays a solution which varies rather smoothly over the entire domain. However, as Pe is increased much beyond unity, (e.g. $Pe \cong 10$ or so), the solution becomes one of a boundary layer type in that $T(x) \approx T_o$ except in the region near $x = L$ within a boundary layer of thickness

$$\delta/L \approx 1/Pe \tag{3}$$

wherein it rapidly adjusts to the outflow boundary condition (i.e., the entire variation in the solution is contained in the vicinity of the outlet and occurs in a distance $O(\delta)$). Upstream of this boundary layer region, the flow is entirely advection-dominated and the solution appropriately degenerates to the nearly trivial solution of the pure advection equation,

$$u\frac{dT}{dx} = 0 \quad ; \quad 0<x<O(L-\delta) \quad , \tag{4}$$

$$T = T_o \text{ at } x = 0$$

which is simply $T(x) = T_o$. Only within the outflow boundary layer (OBL) is the diffusive transport significant; indeed, 'equating' advection to diffusion over a small distance δ yields

$$\frac{u(\Delta T)}{\delta} = \frac{K(\Delta T)}{\delta^2} \tag{5}$$

which leads to $\delta = K/u$ or $\delta/L = 1/Pe$, in agreement with Eq. (3).

The 'tough' problem is that in which the entire physics of the flow is contained within the thin OBL; i.e., the case where $Pe \gg 1$. Also of interest in this case is the diffusive flux at $x = L$: viz,

$$q_L \equiv -K\frac{dT}{dx}\bigg|_L = \left[\frac{K(T_L - T_o)}{L} Pe\right]\frac{e^{Pe}}{1 - e^{Pe}} \quad , \tag{6}$$

which shows that the dimensionless flux is approximately equal to (-Pe) for large Pe; we will return to this point later when discussing approximate solutions to Eq. (1).

Numerical

Numerical approximations to Eq. (1) are now considered, from both the FDM and FEM points of view.

Centered FDM or Conventional (Galerkin) FEM with Linear Approximation. Either of these techniques generates the following discretized version of Eq. (1) for node m on a uniform mesh:

$$\frac{Pg}{2}(T_{m+1} - T_{m-1}) = T_{m-1} - 2T_m + T_{m+1} \quad , \tag{7}$$

where

$$Pg \equiv \frac{u\Delta x}{K} = \frac{\Delta x}{L} Pe = Pe/M \tag{8}$$

is the grid Peclet number and there are M elements. For the boundary conditions associated with Eq. (1), it is well known and has been demonstrated many times (e.g. Roache (2), Zienkiewicz and Heinrich (3), Spalding (4), Smith (5)) that the solution of Eq. (7) can exhibit significant and spurious wiggles for $Pg > 2$. Similar behavior occurs in higher dimensions as well, so it is fruitful to understand the one-dimensional results in some detail. Toward this end, the exact solution to the discretized Eq. (7) is

$$\frac{T_m - T_o}{T_L - T_o} = \frac{1 - \left(\dfrac{1 + \frac{Pg}{2}}{1 - \frac{Pg}{2}}\right)^m}{1 - \left(\dfrac{1 + \frac{Pg}{2}}{1 - \frac{Pg}{2}}\right)^M} \quad ; \quad m = 0,1,2,\ldots,M \quad . \tag{9}$$

The very form of this equation suggests some sort of 'problem' for $Pg \geq 2$ and indeed it does occur (in the matrix solution, the eigenvalues bifurcate from the real axis at $Pg = 2$). For $Pg = 2$, the limiting form of this equation gives $T_m = T_o$ for all $m \neq M$ and $T_m = T_L$ for $m = M$ and for $Pg > 2$ it is obvious that node-to-node oscillations will occur.

While Eq. (9) approximates Eq. (2) to second order in Δx for $Pg << 1$, it is the behavior of T_m at large Pg which is of particular interest; for $Pg >> M = L/\Delta x$, Eq. (9) becomes

$$\frac{T_m - T_o}{T_L - T_o} \cong \frac{1 - (-1)^m (1 + 2m\varepsilon)}{1 - (-1)^M (1 + 2M\varepsilon)} \quad , \tag{10}$$

where $\varepsilon \equiv 2/Pg$. The behavior of Eq. (10) varies markedly depending on whether M is odd or even:

M odd:

$$\frac{T_m - T_o}{T_L - T_o} \cong \frac{\frac{1 - (-1)^m}{2} - (-1)^m \cdot m\varepsilon}{1 + M\varepsilon} \quad \text{, which yields}$$

a) m even:

$$\frac{T_m - T_o}{T_L - T_o} \cong -\frac{m\varepsilon}{1 + M\varepsilon}$$

, which (appropriately) satisfies the 'left' BC.

b) m odd:

$$\frac{T_m - T_o}{T_L - T_o} \cong 1 - (M-m)\varepsilon \quad \text{, which (appropriately) satisfies the 'right' BC.}$$

In this case the odd and even nodes 'split up' in such a way that the temperature of the even nodes remain close to T_o and that of the odd nodes is 'tied' to T_M, the result being an oscillation between odd and even nodes of approximately 'unit' amplitude (i.e., the oscillation is bounded); see also (5).

M even:

$$\frac{T_m - T_o}{T_L - T_o} \cong -\frac{1 - (-1)^m (1 + 2m\varepsilon)}{2M\varepsilon} \quad \text{, which yields}$$

a) m even:

$$\frac{T_m - T_o}{T_L - T_o} \cong \frac{m}{M} \quad \text{, which (appropriately) satisfies both BC's.}$$

b) m odd:

$$\frac{T_m - T_o}{T_L - T_o} \cong -\left(\frac{1}{M\varepsilon} + \frac{m}{M}\right) \quad \text{, which is not required to satisfy either BC.}$$

Here the odd/even separation is even more disastrous; while the even node temperatures vary linearly between the two boundary values, the odd node temperatures are essentially constant and very large, the amplitude of the resulting oscillation between even and odd nodes being proportional to Pg. For more moderate values of Pg (i.e., where the full equation - Eq. (9) - must be employed), the trend toward the above limiting cases begins for Pg > 2 and is the 'cause' of the wiggles associated with the 'tough' problem.

Pure Upwind FDM. The discretized version of Eq. (1) for this scheme is (for $u \geq 0$)

$$Pg(T_m - T_{m-1}) = T_{m-1} - 2T_m + T_{m+1} \quad , \tag{11}$$

whose solution is

$$\frac{T_m - T_o}{T_L - T_o} = \frac{1 - (1 + Pg)^m}{1 - (1 + Pg)^M} \quad . \tag{12}$$

For Pg<<1, Eq. (12) represents a first order approximation to Eq. (2); but for Pg >>1, and m > 0 it gives

$$\frac{T_m - T_o}{T_L - T_o} \cong Pg^{m-M} \tag{13}$$

which is closely approximated by $T_m = T_o$ for m=1,2,...,M-1 and $T_M = T_L$; i.e., there are no oscillations and the inlet value is properly translated across the grid - the entire change in the solution occurs between the last two nodes and is essentially independent of Pe for Pg>> 1. The upwind 'solution' to the tough problem (Pe>>1) is thus seen to be entirely different from that of the centered 'solution'; whereas the latter generates results which are spurious everywhere, the upwind solution is 'quite good' (i.e., believeable) except near the outflow wherein it displays spurious behaviour (independent of Pe). When the problem becomes tough, the upwind solution becomes constant, independent of the degree of 'toughness' (for Pg >>1; for Pg<< 1, it would retain a good description of the 'physics', albeit not as good as that from centered differences which are always more accurate for Pg < 2).

Finally, we point out that the upwind scheme can also be obtained by applying centered difference techniques to the following equation (see also Roache (2)):

$$u \frac{dT}{dx} = (K + \frac{1}{2} u\Delta x) \frac{d^2T}{dx^2} \quad ; \qquad (14)$$

from this view point, the effective diffusivity in the upwind scheme is $K + 1/2\ u\Delta x$ which leads to an effective Peclet number, $\overline{Pe}$, of

$$\overline{Pe} = \frac{Pe}{1 + \frac{1}{2} Pg} \quad . \qquad (15)$$

Hence, whenever $1/2\ u\Delta x$ is significant compared to K (or, equivalently, whenever Pg/2 is significant compared to unity), the results from the centered and upwind schemes will differ signficantly. Finally, for $Pg > \sim 5\text{-}10$, essentially all of the diffusion in the upwind scheme is numerical and the results are effectively independent of the true Peclet number.

Smart Upwind Methods. There are many upwind methods which we call 'smart' since they are based on discretized equations whose solution always agrees with Eq. (2) at the nodes. These have appeared in both the FDM and FEM literature and have the additional common property that the final result is (necessarily) independent of the means used to achieve it.

In FDM, the history of the smart upwind method appears to have begun about 25 years ago when Allen and Southwell (6) first employed it in a vorticity - stream function solution to the NS equations for viscous flow around a cylinder; i.e., Allen devised a finite difference approximation, which was later carefully analyzed by Dennis (7), based *essentially on the steady state, one-dimensional advection-diffusion* equation which is exact at the nodes. The results presented by Allen and Southwell, although undoubtedly quite impressive at that time, displayed the usual problems with upwind (or smart upwind) formulations: their downstream eddies are too short and they vary little between Re = 100 and 1000 on a too coarse mesh. This smart upwind scheme was later *'rediscovered'* by Spalding ((4); his Eqs. 26-28, *which he did not actually advocate or* test) by a more intuitive approach, and tested in two-dimensions by Raithby and Torrance (8), who found it to be useful when the flow direction was closely aligned with a coordinate axis but unacceptably diffusive otherwise. The same scheme was also employed and advocated by Briggs (9), who ostensibly generalized it to two- and three-dimensions and claims to have improved it in other ways. Finally, the scheme was again re-discovered by Fiadeiro and Veronis (10) and again 'appropriately' generalized to two- and three-dimensions, and advocated for both steady and time-dependent problems (unfortunately they too only tested the scheme for steady problems; as we discuss later, it can fail miserably for time-dependent problems). Further literature review would undoubtedly continue to reveal more and more rediscoveries of this highly touted scheme.

The first FEM result on the same subject is that by Christie et al. (11), and it was quickly adopted and generalized to two-dimensions by Huyakorn (12) and Heinrich et al. (13). These schemes were advocated as applicable to FEM formulations as they were devised by employing weighted residual methods (not Galerkin's method, however, since the asymmetric weighting functions employed are different from the basis functions). Then Heinrich and Zienkiewicz (14, see also Zienkiewicz and Heinrich (3)) extended the FEM approach to quadratic elements. Also, by a rather different approach, Hughes et al. (15 and references therein) has achieved apparently quite similar results for 4-node bilinear elements (or their one-dimensional counterpart). In contrast to the other FEM 'upwinders', who derive the final discretized equations via the method of weighted residuals, Hughes et al. obtain their upwind formulas via quadrature 'tricks' on the advection terms.

The interesting final result is that all of the above schemes (FDM and linear FEM) lead to precisely the same result for the steady-state advection-diffusion equation in one-dimension; viz, the smart upwind approximation is

$$(\tanh Pg/2)(T_{m+1} - T_{m-1}) = T_{m-1} - 2T_m + T_{m+1} \quad . \qquad (16)$$

This equation is equivalent to the central difference result except that an effective grid Peclet number,

$$\overline{Pg} \equiv 2 \tanh Pg/2 \qquad (17)$$

must be used. If Pg in Eq. (9) is replaced by $\overline{Pg}$, the resulting solution at the nodes is identical to that from the exact solution, Eq. (2). This exact formula also applies on a variable grid in the following form,

$$T_{m+1} - T_{m-1} = \coth(Pg_{m+1}/2)(T_{m+1} - T_m) + \coth(Pg_m/2)(T_{m-1} - T_m) \quad , \qquad (16a)$$

where $Pg_m \equiv u\Delta x_m/K$ is the grid Peclet number on element m. Note that $\overline{Pg} \approx Pg$ for $Pg \ll 1$ (central difference limit) and $\overline{Pg} \approx 2$ for $Pg \gg 1$ (upwind difference limit). Also note that Eq. (16) obtains from applying central differences to Eq. (1), where the diffusivity is replaced by an effective diffusivity, given by

$$\overline{K} \equiv K \cdot \frac{Pg}{2} \coth Pg/2 \quad , \qquad (18)$$

which gives $\overline{K} \to K$ as $Pg \to 0$ and $\overline{K} \to 1/2\, u\Delta x$ as $Pg \to \infty$. Thus, the smart upwind schemes look like the pure centered scheme (and are second-order accurate in Δx) for $Pg \ll 1$ and like the pure upward scheme for $Pg \gg 1$ (and accuracy is not easily estimable as a Taylor series analysis is not appropriate). But they are allegedly superior to botn in that the exact nodal values are obtained for this simple case of steady state, one-dimensional advection-diffusion. It is important to note that even these smart schemes will give results which, while still exact at the nodes, are independent of Pe if Pg is greater than about 5-10, a situation which could be quite misleading if not sufficiently well understood.

The Message Behind the Wiggles

As a prelude to 'what the wiggles are saying' when using central differences (or linear GFEM), we compute the diffusive flux at x = L for comparison with the exact result - Eq. (6). These are obtained by approximating $dT/dx|_L$ by $(T_M - T_{M-1})/\Delta x$ for all discretized approximations:

a) Centered difference (Eq. 9):

$$q_L = \left[\frac{K(T_L - T_o)}{L} \cdot Pe\right] \frac{\left(\dfrac{1 + \frac{Pg}{2}}{1 - \frac{Pg}{2}}\right)^{M-1}}{\left(1 - \frac{Pg}{2}\right)\left[1 - \left(\dfrac{1 + \frac{Pg}{2}}{1 - \frac{Pg}{2}}\right)^{M}\right]} \qquad (19)$$

b) Upwind difference (Eq. 12):

$$q_L = \left[\frac{K(T_L - T_o)}{L} \cdot Pe\right] \frac{(1 + Pg)^{M-1}}{1 - (1 + Pg)^M} \quad . \qquad (20)$$

c) Smart upwind difference (Eq. 9 using $\overline{Pg}$ from Eq. 17):

$$q_L = \left[\frac{K(T_L - T_o)}{L} \cdot Pe\right] \left(\frac{2\tanh Pg/2}{1 - \tanh Pg/2} \cdot \frac{e^{-Pg}}{Pg}\right) \left(\frac{e^{Pe}}{1 - e^{Pe}}\right) \qquad (21)$$

which behaves like Eq. (19) for $Pg \ll 1$ and like Eq. (20) for $Pg \gg 1$.

Each of the above flux approximations converges to Eq. (6) as $Pg \to 0$; it is again the behavior at large Pg which is of interest. Similar to the behavior of the nodal temperatures for centered differences and M even, the flux from Eq. (19) will begin to behave erratically for $Pg > 2$ and will become total *nonsense* for large Pg (at least for M even). In contrast, both upwind and smart upwind schemes will smoothly give $q_L \cdot L/K(T_L-T_0) \to -L/\Delta x = -M$ for large Pg (say 10), which is to be compared to the exact result, -Pe; i.e., rather than increase directly with Pe, the dimensionless flux (like the temperature) approaches a constant independent of Pe (even a solution which is exact at the nodes can be deficient if the nodes are poorly located).

The behavior of the central difference scheme for Pg > 2 is a strong signal: the wiggles are saying, "The solution is becoming difficult in the region of the outflow because an important boundary layer is developing there whose thickness is small relative to the grid spacing you are using." No such signal is given by either upwinding scheme and the casual user may easily be lulled into believing his results for any Pe. The fix, of course, is to resolve (at least crudely, so that the wiggles are 'small') the OBL for large Pe; this can be easily done by grading the mesh in the outflow region - for any of the schemes. Another interpretation of the wiggles is - especially for large Pe - the solution 'resides' in the OBL and is nearly trivial outside the OBL; hence, place at least some of your nodes in the region containing the OBL.

Analogy from Ordinary Differential Equations

Another comparison between a dissipative first-order method and a non-dissipative second order method is available by considering the following ODE (or a system of ODE's if the appropriate generalizations are made):

$$\frac{dy}{dt} = -\lambda y \quad ; \quad y(0) = 1 \quad , \tag{22}$$

whose solution is

$$y = e^{-\lambda t} \tag{23}$$

The backward Euler (or fully implicit) method (BE) applied to Eq. (22) is

$$y_{n+1} = y_n - \lambda\Delta t\, y_{n+1} \tag{24}$$

whose solution (for fixed Δt) is

$$y_n = \frac{1}{(1 + \lambda\Delta t)^n} \quad . \tag{25}$$

The second order method of our analogy is the trapezoid rule (TR or "Crank-Nicolson") which approximates Eq. (22) by

$$y_{n+1} = y_n - \frac{\lambda\Delta t}{2}(y_n + y_{n+1}) \quad , \tag{26}$$

and has the solution (for fixed Δt)

$$y_n = \left(\frac{1 - \lambda\Delta t/2}{1 + \lambda\Delta t/2}\right)^n \quad . \tag{27}$$

If we liken $\lambda\Delta t$ to a grid Peclet number, then from Eqs. (9) and (12) we see that upwind advection 'looks like' BE and centered advection 'looks like' TR. The analogy goes further: Eq. 25 is first-order accurate, contains artificial (numerical) damping, and precludes oscillations regardless of step size (indeed, Δt may be chosen so that $\lambda\Delta t$ is arbitraily large and the 'exact' solution - zero - obtained in a single time step ! Like upwinding with a large grid Peclet number). On the other hand, Eq. (27) is second-order accurate, contains no artificial damping, and displays spurious oscillations for $\lambda\Delta t > 2$ (in the limit of arbitrarily large Δt, the solution is $y_n \simeq (-1)^n$ which is total nonsense - like central differencing with arbitrarily large Peclet number). The wiggles from TR are telling us that Δt is too large for the discretized approximation to be reasonable; no such warning emanates from the BE scheme and the user may be misled into believing a result which is very inaccurate. This situation could easily occur when solving systems of equations analogous to Eq. (22).

To conclude the analogy, we mention that TR will give much more accurate solutions than BE when the time step is small enough so that the discretized approximation to the continuum is 'reasonable'; ie for a fixed Δt and a desired level of accuracy, the BE scheme will require more time steps (smaller Δt). Similarly, if a 'graded mesh' (variable step size) is employed, the TR will again give the most cost-effective solution for a given required accuracy level. For example, we have solved Eq. (22) using both BE and TR in conjunction with variable Δt algorithms which control the local time truncation error. For the same error tolerance, the BE formula required typically 3-6 times as many steps as TR to reach a given time; based on maximum global errors, the results were even more dramatic: for example, for a maximum global error of 1%, the BE algorithm required 5-10 times as many steps as the TR algorithm.

We have, in fact, utilized these advantages of the TR in our time-dependent FEM code development, in which we employ both the accuracy and non-dissipative qualities of TR combined with an automatic Δt selection algorithm such that we obtain accurate, oscillation-free solutions of the Navier-Stokes and Boussinesq equations (e.g. for Karman vortex shedding of flow past a cylinder; see Gresho et al. (16,17) for further discussion of these time integration methods).

Two- and Three-Dimensions

Obviously the comparison of various schemes for solving one-dimensional problems is somewhat sterile if the schemes and the results do not generalize to two- and three-dimensions; i.e., to

$$\underline{u} \cdot \nabla T = \nabla \cdot K \nabla T \quad . \tag{28}$$

In the case of steady advection-diffusion, it appears that generalizations are usually possible, although the design of smart upwind schemes is somewhat more difficult (and perhaps less 'successful'). Also, not surprisingly, additional problems arise in higher dimensions, which we discuss below.

That the classic tough problem (high Peclet number and 'specified value' at outflow) carries over to two-dimensions has been demonstrated many times (e.g. 12, 13, 15); although mostly via the same controversial example (Gartling (18)).

We believe, however, as does Gartling (18), that there are very few cases where such an outflow BC is appropriate to the simulation . In the rare cases when this BC is appropriate, *the modeler should be cognizant of the presumably important OBL (when* advection dominates) and design an appropriately graded mesh to capture the correct solution (not the converse, as done, for example, by Heinrich et al. (13) and Huyakorn (12); they forced an OBL upon the solution yet employed a graded mesh where the largest elements were those at the outlet!).

More often than not, however, the true outflow BC is not known simply because the outflow 'boundary' is in fact fictitious, since the computational domain cannot be extended far enough in the flow direction (e.g. to infinity). Here, the best approximation available appears to be simply the natural boundary conditions of the problem (zero normal gradient) as already pointed out by Gartling (18). We will demonstrate the efficacy of this BC in simulating an infinite domain when we discuss time-dependent problems in later sections. The computational advantage of this more appropriate BC is quite signficant; there is no important OBL and therefore no need for fine zoning near the outlet.

An alternate approach to modeling infinite domains is through the use of "infinite elements" (e.g. Bettes (19)); we are not aware of any applications of these techniques to the advection-diffusion equation.

We now present a realistic example of a simulation wherein wiggles can be generated by the GFEM (and one which does not arise in one-dimension), but would probably be suppressed by any upwind scheme. In a later part of this paper, we present the velocity solution, using the GFEM, for developing flow through a channel which contains a step. These results are shown in Fig. 7 and represent what we believe is an adequate solution at Re = 200 (there are no wiggles). Using this velocity field, we solved the advection-diffusion equation (e.g. forced convection heat transfer) with the same 9-node biquadratic element as used for velocity and the following boundary conditions: $T = 0$ at the inlet, $T = 1$ on the three sides of the step, and $\partial T/\partial n = 0$ elsewhere. The problem was solved for two different Prandtl numbers (or Peclet numbers since $Pe = Pr \cdot Re$); one which is 'easy' and appropriate for the grid employed and one which is 'too difficult' for the same grid. Figure 1 shows the resulting

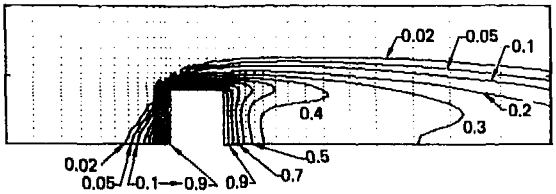


Fig. 1 Isotherms for flow over a step; Pe = Re = 200.

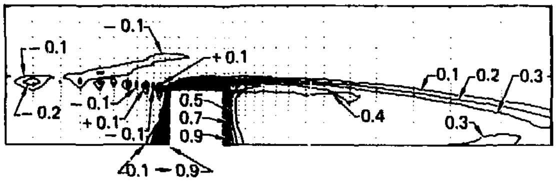
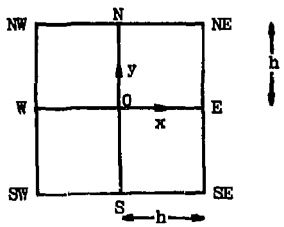


Fig. 2 Same as Fig. 1, except Pe = 2000.

temperature field for Pr = 1 (Pe = Re = 200). Here the isotherms look fairly reasonable and this is to be expected since, for Pr = 1, the thermal boundary layer thickness (δ_T, a la Eq. (3)) near the step is essentially the same as the momentum boundary layer thickness (δ_M); hence, if the velocity solution is good, so should be the temperature solution. On the other hand, Fig. 2 shows the isotherms for Pr = 10 (Pe = 2000) and the resulting wiggles upstream of the step are quite indicative of an inadequate solution (as predicted by Smith (5)). Here $\delta_T = 0.1\ \delta_M$ and is too thin to be resolved by this mesh. The problem is again caused by a solution (temperature in this case) which is advection-dominated (and thus nearly constant) upstream of the step, but which must undergo rapid change in the flow direction in the region near the step; i.e., there is a sort of boundary layer, which is especially thin near the upstream corner of the step. Note that the temperature in the lee eddy is much more reasonable; here the lower velocities cause less steep gradients and the grid can better cope with them; clearly the appropriate remedy for these wiggles is a judicious mesh refinement near the upstream portion of the step so that the important portion of the temperature solution is correctly simulated. Upwind methods would artificially thicken the thermal boundary layer (and concomitantly reduce Pe and the heat flux) so that the isotherms would 'look nice'; indeed, they would even generate smooth results for any Pe (e.g. 10^7) - but, as usual, the results would (erroneously) become independent of Pe. Finally, it appears that upwind methods can also yield poor solutions in the recirculating region, as mentioned by Raithby (20,21) who is working on smart "skew-upstream" schemes.

To conclude this section, we wish to actually display the 'central-difference nature' of the GFEM in modeling nonlinear advection in one of the simplest cases possible: the 4-node bilinear element on a regular (square) mesh. Consider the '4-patch' shown below:



The GFEM approximation to $u(\partial T/\partial x)$ at node 0 is formed as follows:

$$u \left.\frac{\partial T}{\partial x}\right|_0 = \int_{-h}^{h}\int_{-h}^{h} \phi_o \, u \frac{\partial T}{\partial x} \, dxdy \Big/ \int_{-h}^{h}\int_{-h}^{h} \phi_o \, dxdy \quad , \tag{29}$$

where

$$u = \sum_j u_j \phi_j \quad ,$$

$$T = \sum_j T_j \phi_j \quad ,$$

and ϕ_o is the basis function for the middle node. The result is

$$u \left.\frac{\partial T}{\partial x}\right|_0 = \frac{4}{9} \cdot \frac{6u_o + u_N + u_S}{8} \cdot \frac{(T_E - T_W)}{2h} + \frac{1}{9}\,\frac{u_o + u_N}{2}\,\frac{(T_{NE} - T_{NW})}{2h} + \frac{1}{9} \cdot \frac{u_o + u_S}{2}\,\frac{(T_{SE} - T_{SW})}{2h}$$

$$+ \frac{1}{9} \cdot \frac{6u_E + u_{NE} + u_{SE}}{8} \cdot \frac{(T_E - T_o)}{h} + \frac{1}{36} \cdot \frac{u_E + u_{NE}}{2}\,\frac{(T_{NE} - T_N)}{h} + \frac{1}{36} \cdot \frac{u_E + u_{SE}}{2}\,\frac{(T_{SE} - T_S)}{h}$$

$$+ \frac{1}{9} \cdot \frac{6u_W + u_{NW} + u_{SW}}{8} \cdot \frac{(T_o - T_W)}{h} + \frac{1}{36} \cdot \frac{u_W + u_{NW}}{2}\,\frac{(T_N - T_{NW})}{h} + \frac{1}{36} \cdot \frac{u_W + u_{SW}}{2}\,\frac{(T_S - T_{SW})}{h} \ . \tag{30}$$

Inspection of Eq. (30) reveals the following: (1) the GFEM treatment of advection is quite complicated and involves very intense coupling; (2) although centered difference terms clearly dominate the approximation (2/3 of the total), the remaining 1/3 is equally divided between upwind-and downwind-type differences (in such a way that the overall approximation is second-order accurate). Hence, the issue of the central difference nature of GFEM is slightly more complex than one might initially expect. Also, these nonlinear computations are obviously signficantly more costly than those from any finite difference discretization; it is generally well-accepted that FEM generates more accurate solutions than FDM on the same mesh, but clearly it must do 'much better' in order to be cost-effective - an issue which is not so well-accepted.

TIME-DEPENDENT ADVECTION-DIFFUSION

The purpose of this section is to point out the fact that while some people claim to have solved the 'wiggle problem' for steady-state advection-diffusion at large Pe, there is yet to be discovered a method for wiggle suppression which is effective and has any semblence of accuracy for time-dependent problems where the deleterious consequences of numerical diffusion are quite serious and the knowledge of the exact one-dimensional steady-state solution to the discretized equations is not very useful.

One-Dimensional Flow

The time-dependent advection diffusion equation is

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} = K \frac{\partial^2 T}{\partial x^2} \quad . \tag{31}$$

We will consider solving this equation on (0,L) subject to the following inititial and boundary conditions.

$$T(x,0) = f(x) \quad ,$$

$$T(0,t) = T_o \quad , \tag{32}$$

$$T(L,t) = T_L \quad \text{or} \quad \left.\frac{\partial T}{\partial x}\right|_L = 0 \quad .$$

In Lee et al. (22) and Gresho et al. (23) we have compared several numerical methods in the case where f(x) is a Gaussian distribution;

$$f(x) = e^{-\frac{(x-x_o)^2}{2\sigma^2}} \tag{33}$$

where σ is the standard deviation and x_o the location of the initial maximum. The results of these studies which are particularly relevant here are the following:

(1) Conventional linear finite elements are much mor accurate than central FDM - especially when Pe is large (or infinite). This is a direct consequence of the much improved phase characteristics associated with the CM matrix of the FEM.

(2) If the grid is too coarse for the attempted simulation, conventional FEM (or centered FDM for that matter) methods will advertise the fact by generating wiggles; a too-steep waveform (which contains signficant spectral content in the short wave region) and/or a too-high Peclet number and/or a fixed outflow boundary condition are all candidates for causing the wiggles. The first two are dispersion wiggles (shorter wave components are translated (advected) at the wrong speed) and can only be reduced to acceptable levels by appropriate mesh refinement. On the other hand, any upwind scheme (FEM or FDM) which we are aware of will suppress these wiggles via numerical diffusion; unfortunately, they concomitantly broaden the wave form and lower the Peclet number so that the (smooth) solution (to a different problem, in general) 'looks nice'. There is no signal or warning to indicate that the grid is too coarse for the results to be meaningful.

(3) Mass lumping is deleterious to the phase properties and thus causes more dispersion wiggles and an overall larger phase lag than the CM formulation.

(4) The FDM suggested by Briggs (9) is totally inadequate for time-dependent flows for all Peclet numbers greater than about 5 (based on σ) since the solutions then become essentially those using full upwinding and display excessive numerical diffusion (and are independent of Pe). The same conclusion was also reached by Raithby (20).

As mentioned earlier, the FDM algorithm of Briggs (et al.) is basically the same (except for the mass matrix) as that which the FEM "upwind advocates" are using for linear elements in one dimension. Hence, it is quite a simple matter to extrapolate to the conclusion that these FEM methods will also 'fail' for time-dependent flows which are advection-dominated (not even the consistent mass matrix will save them since increased phase accuracy will not reduce the numerical diffusion; in fact, as explained in Lee et al. (22), the pure upwind FDM has good phase speed properties). Furthermore, we believe that there is no 'smart' upwind scheme which could duplicate the accurate results obtained by conventional FEM methods for the pure advection (Pe = ∞) of a smooth wave form (such as a Gaussian). For nonsmooth wave forms (such as a square wave), all methods have trouble since the problem is inherently very difficult.

Recently, however, Huyakorn and Nilkuha (24) have reported some progress in the development of a time-dependent smart upwind scheme in the general context of an FEM. Unfortunately, it is not a consistent weighted residual method in the sense that different weighting functions are used for different terms (the advective and diffusive terms are weighted by the unsymmetric upstream weighting function derived from the steady-state method referred to earlier but the time derivative term is weighted in the conventional Galerkin manner, leading to the usual CM matrix). In addition to the theoretically unsound basis of the scheme, its ad hoc nature is more clearly revealed in their search for an 'optimum α' (α is the upstream weighting factor; it is 0 for central differences, 1.0 for full upwinding, and α_{opt} = coth (Pg/2) - 2/Pg for the steady state 'smart' upwinding). Whereas there is a clear reason (a la Christie et al. (11)) to use α_{opt} for steady flow (the method then is a consistent weighted residual method - a Petrov-Galerkin method - and α_{opt} is equivalent to employing Eq. (16)), there appears to be no good way to optimize the amount of upwinding (for wiggle suppressant) for time-dependent problems. Huyakorn and Nilkuha have attempted such an optimization in the context of relating it to the Courant number ($u\Delta t/\Delta x$) when using the trapezoid rule for time integration; in the limit of zero time truncation error, they suggest about 5-10% upwinding for infinite Pe. They present results which tend to justify their scheme; however, while the consistent mass matrix of FEM is shown (again) to be a definite asset in that the results are better than those employing lumped mass (with selective upwinding), even these results are, in our opinion, overly diffusive for large Pe and steep waveforms (sharp fronts). Also, it is noteworthy that they did not even refer to the equation for α_{opt} for steady flow; presumably they did test it but found it unacceptably diffusive as did we.

To conclude the one-dimensional discussion, we present some numerical results which are illustrative in several ways. The exact solution to a non-dimensional form of Eq. (31) on the infinite span, with an initial condition given by Eq. (33) is

$$T = \frac{e^{-(x-x_o-t)^2/2(1+2t/Pe)}}{\sqrt{1+2t/Pe}} \quad , \tag{34}$$

where $Pe \equiv u\sigma/K$ is the Peclet number based on the 'width' of the Gaussian. Here x is in units of σ and t in units of σ/u. Eq. (31) was solved on the unit span (L = 1, u = 1, K = .004) which, for the selected value of $\sigma(.04)$, is equivalent to a dimensionless span which is 25 units long. The initial location of the Gaussian (x_o) is 3.75 and the computations were performed for Pe = 10 and stopped at t = 20, at which time almost half of the infinite-span Gaussian would have 'left the grid'. Sufficiently small time steps were employed so that errors from the time integration are negligible. Figure 3 shows the results from two grids (node locations are indicated on the abscissa) and two outflow BC's as well as the exact solution on the infinite span. For the uniform grid case, we used 40 linear elements (Δx = .625) which is a sufficiently fine grid (1.6 nodes per standard deviation) to both interpolate the initial condition adequately and to obtain fairly accurate results even for Pe = ∞ (see 22 and 23). The solid curves in Fig. 3a clearly show that the 'natural' BC ($\partial T/\partial x$ = 0 at x = L) does a very good job of simulating the infinite span result and adds further evidence (since these results also carry over to two dimensions) to the claim (18) that under most conditions, where the outflow 'boundary' is merely a model of a larger domain and hence the true outflow BC is not known, the natural (zero normal derivative) BC's are to be preferred. On the other hand, if it is known that the dependent variable must be specified at the outflow, then the problem becomes 'tough' in that an OBL will exist for large Pe. Thus, even for

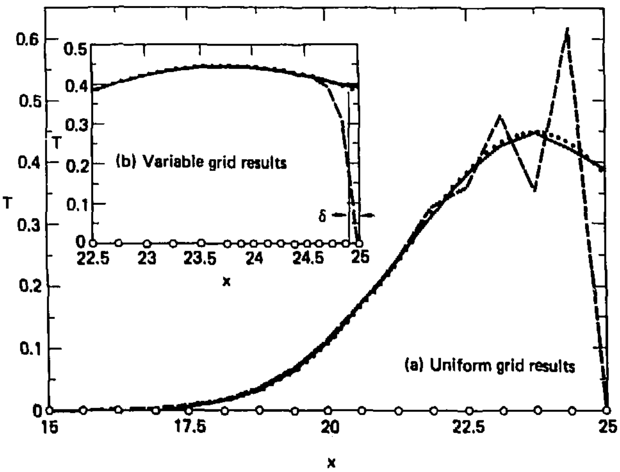


Fig. 3 Comparison of exact and FEM solutions of the time-dependent advection-diffusion equation. Dotted lines show exact solution for infinite span. Solid lines are FEM solution using $\partial T/\partial x$ = 0 at outflow. Dashed lines show FEM solution using T = 0 at outflow.

Pe = 10, $\delta \simeq .1$ and the dashed curves in Fig. 3a clearly show the inadequacy of this mesh in resolving the (presumably) important boundary layer (this mesh is more than adequate at earlier time, even for very large Pe). Rather, the wiggles which result (here the grid Peclet number is 6.25) are a signal that finer zoning is required in the region near the outlet where the solution undergoes rapid change. Note also that the wiggles are definitely caused by the specified boundary condition and that they are damped in the interior of the domain, which suggests that selective grid refinement (fine zones only near the outflow - contrary to the claim made by Huyakorn and Nilkuha (24)) is required. Fig. 3b shows the results obtained with a 'smarter' grid: this grid employs 25 elements of length 0.6 from x = 0 to x = 15 (Pg = 6), 35 elements of length .25 from 15 to 23.75 (Pg = 2.5), and 10 elements of length .125 from 23.75 to 25 (Pg = 1.25), for a total of 70 elements (This is probably an excessive grid refinement and we believe that results which would be nearly as good and more cost effective could be obtained with as few as 40-50 node points as long as a graded mesh with $\Delta x = O(\delta)$ is employed near the outlet.). In this case, the rapid variation in the solution, from the infinite-span result to zero in $O(\delta)$, is clearly shown (even at this relatively small Pe - the effect would be more pronounced at larger Pe) and, importantly, there are no wiggles - this indicates that the solution is now sufficiently accurate (i.e. believable), both within and outside the boundary layer (even with 'less than' one node located within the boundary layer). We believe that the only proper way to solve problems in which an OBL is present is to use selective mesh refinement so that the grid can 'capture' the rapid variation in the boundary layer. This conclusion applies to centered or upwind formulations and the former, being significantly more accurate, are to be preferred. Unfortunately, this leads to the requirement of employing a mesh which is adequate for the Pe in question, but this is the price to be paid for meaningful solutions.

Two-Dimensional Flow

Rather than present new results for two dimensions, we will again simply extract certain results from previous work since there are relatively few additional comments which need be made. In Gresho et al. (23), we demonstrated the efficiency of the GFEM applied to purely hyperbolic (Pe = ∞) flow in two dimensions via the 'rotating cone problem', wherein a cone of 'temperature' is placed on a square grid and advected round and round in a circular path by an imposed velocity field which describes solid body rotation. The results were basically the same as those from one dimension except for the additional demonstration that velocity vectors which are 'skew' to the mesh lines caused no problems at all (in contrast to results implied by Raithby (21) for certain upwind methods); viz, the problem was 'easy' (for the grid selected, which was 'adequate' — dispersion wiggles would appear on a 'too coarse' mesh) when CM was employed, but dispersion wiggles and phase speed error were excessive when mass lumping was invoked. Further comparisons on (essentially) the same problem were presented by Long and Pepper (25) and some additional useful results obtained: (1) Centered FDM gave similar results to LM with linear FEM, (2) full upwinding 'diffused the cone away' within one revolution and was totally useless, (3) both the temperature and the square of the temperature were very well conserved by the linear FEM using CM (this in spite of the fact that neither is guaranteed to be conserved by the conventional GFEM applied to the advective form ($\underline{u} \cdot \nabla T$) of the equation; see Lee et al (26) for further discussion of the pros and cons of conservation forms via FEM).

We believe that there is no smart FEM upwind scheme yet designed which would perform well on this totally advection-dominated problem.

THE TRANSIENT HEAT EQUATION

In this section, we will discuss the manner in which conventional GFEM can generate wiggles (which are again a signal to be regarded seriously) for 'small time' when solving the transient heat equation in one, two, or three space dimensions. We will also show how these wiggles may be suppressed by the simple and common (and ad hoc) technique of "mass lumping" and discuss the consequences of this. Finally we will generalize the results to other transient situations.

One Dimensional Heat Conduction

A simple one-dimensional example will suffice for demonstration purposes. Consider the domain ($0<x<1$) and its simplest discretization via FEM (equally spaced 'linear' elements) and the equation

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$$

$$T = 0 \quad \text{at} \quad t = 0 \quad , \tag{35}$$

$$T = 1 \quad \text{at} \quad x = 0 \quad ,$$

$$T = 0 \quad \text{at} \quad x = 1 \quad ;$$

i.e., we are considering a step change in surface temperature. Application of the GFEM to Eq. (31) yields the following system of ODE's: $M\dot{T} = -KT + f$, or

$$\frac{h}{6}\begin{bmatrix} 4 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \end{bmatrix}\begin{Bmatrix} \dot{T}_1 \\ \dot{T}_2 \\ \vdots \\ \dot{T}_N \end{Bmatrix} = \frac{1}{h}\begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \end{bmatrix}\begin{Bmatrix} T_1 \\ T_2 \\ \vdots \\ T_N \end{Bmatrix} + \frac{1}{h}\begin{Bmatrix} 1 \\ 0 \\ \downarrow \end{Bmatrix} \quad , \tag{36}$$

where there are N + 1 elements of size $h = 1/N+1$ and N degrees of freedom. The CM matrix, M, is an averaging matrix and its inverse has the property that the diagonal elements are positive and all off-diagonal elements decrease in magnitude (with a ratio of $\sim .268$) with 'distance' from the diagonal and, importantly, they oscillate in sign (in particular, the diagonals above and below the main diagonal are negative); see Oden (27). Consider now the evaluation of $\dot{T}(0)$ at which time $T = 0$; i.e.

$$\dot{T}(0) = M^{-1} \cdot f \quad . \tag{37}$$

Since f contains zeros in all but the first position, it is clear that $\dot{T}(0)$ is just 1/h times the first column of M^{-1}. Hence $\dot{T}_j(0)$ is > 0 for odd j and < 0 for even j with amplitudes which decrease with increasing j. The net result is that the temperature at all even nodes starts out in the wrong direction - the exact solution to Eq. (35) does not display any negative values of $T(x,t)$.

If the mass matrix is 'lumped' (diagonalized), by any of several ad hoc schemes (e.g. see Zienkiewicz (28) or Lee et al. (29)), the result is that $M \rightarrow hI$, where I is the identity matrix, Eq. (36) reverts to the conventional second order FDM equation, and the initital 'acceleration' is

$$\dot{T}(0) = \frac{1}{h^2}(1 \quad 0 \longrightarrow)^T \quad ; \tag{38}$$

i.e., only the first node has a non-zero derivative and none of the nodal temperatures will move 'off in the wrong direction'. At first glance, this appears to be a signficant advantage and the GFEM result looks very suspicious.

We will explore these results in more detail by solving Eq. (36) for b CM and LM and comparing these solutions with the exact solution, which is

$$T_e(x,t) = (1-x) - \frac{2}{\pi}\sum_{n=1}^{\infty} \frac{\sin n\pi x}{n} \cdot e^{-n^2\pi^2 t} \quad . \tag{39}$$

It turns out that it is fairly simple in this case to obtain a closed form solution to Eq. (36); viz

$$T_j(t) = (1 - j/N+1) - \frac{1}{N+1}\sum_{n=1}^{N} \frac{\sin n\theta}{1 - \cos n\theta} \cdot \sin jn\theta \cdot e^{-\lambda_n t} \quad , \tag{40}$$

where $\theta \equiv \pi/N+1$ and the eigenvalues (of K-M) are

$$\lambda_n^{CM} = 6(N+1)^2 \cdot \frac{1-\cos n\theta}{2+\cos n\theta} \quad \text{for CM and} \tag{41a}$$

$$\lambda_n^{LM} = 2(N+1)^2\,(1-\cos n\theta) \quad \text{for} \quad LM \quad . \tag{41b}$$

λ_n^{CM} is always greater than the exact eigenvalue ($n^2\pi^2$) since the GFEM is equivalent to the Rayleigh-Ritz variational approximation of the associated eigenvalue problem; it turns out that λ_n^{LM} is always less than $n^2\pi^2$, and by about an equal amount (the average of λ_n^{CM} and λ_n^{LM} is a much better approximation to $n^2\pi^2$).

The results for N = 4 are presented in Figs. 4 and 5, along with those of the exact solution (a small N is quite sufficient for our purposes; generalization is immediate). The nodal time histories of Fig. 4 display the behavior at $t \cong 0$ predicted above; for CM, the temperatures at nodes 1 and 3 are increasing while those at nodes 2 and 4 go negative, while for LM all temperatures are positive for all time. This behavior is also seen in Fig. 5 in which temperature profiles are presented at two times; at t = .004, the CM solution displays spurious wiggles and negative temperature while the LM results are smooth and 'reasonable'. At later times ($t > \sim.02$ from Fig. 4), all temperatures from CM are positive and remain so (although the overall LM solution still appears to be slightly more accurate).

The wiggles are saying: "For this problem and this mesh (or any mesh) there is a minimum 'time of believability' ($\sim$ .02 in this case); for times less than this, the discretized solution is too inaccurate to be useful". No such message is broadcast by the wiggle-free LM results and the non-astute code user could again be fooled by methods which suppress the wiggles.

Furthermore, the heat flux at x = 0 is, for small time, $-\partial T/\partial x = 1/\sqrt{\pi t}$; i.e. it is unbounded as $t \to 0$. Conversely, the above FEM solutions give $-\partial T/\partial x \le 5$ at x = 0, which is far from accurate at small times. Equating these 'fluxes' gives $t \cong .01$, another estimate of the minimum time at which the FEM results should be used (here we have the advantage of an exact solution (the infinite span solution was used above) at our disposal; in practice this is not the case and the CM wiggles of the GFEM may be the only clue). Another estimate of the 'minimum time' is available, however, and it too is useful but not always known by the 'user'; viz, the eigenvalues of a single element: the (CM) transient heat equation for a single element is

$$\frac{h}{6}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{Bmatrix} \dot{T}_1 \\ \dot{T}_2 \end{Bmatrix} = \frac{1}{h}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \begin{Bmatrix} T_1 \\ T_2 \end{Bmatrix} \quad , \tag{42}$$

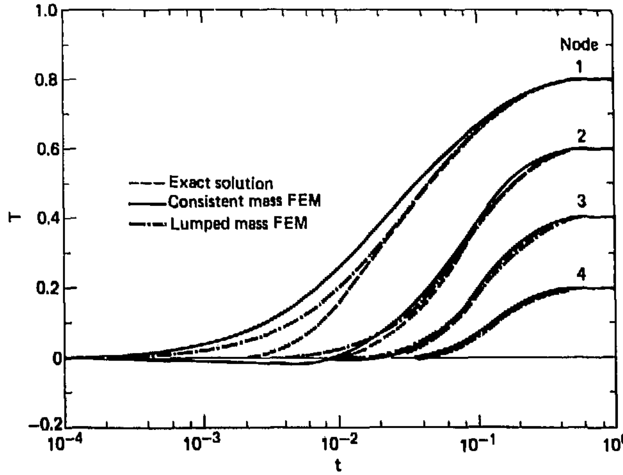


Fig. 4 Time histories of nodal temperatures for step change in surface temperature.

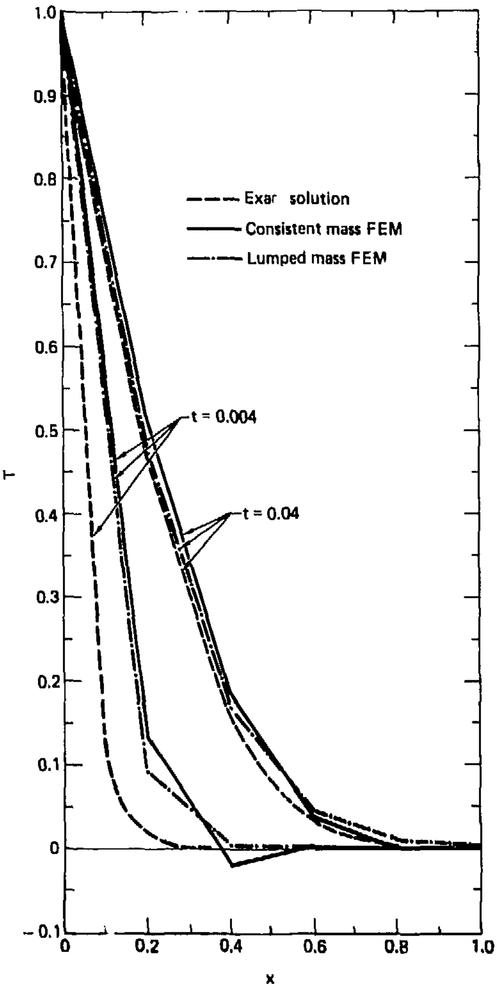


Fig. 5 Temperature profiles for a step change in surface temperature.

which gives, using $T \sim e^{-\lambda t}$ and ignoring the zero eigenvalue,

$$\lambda_e^{CM} = 12/h^2 \quad ,$$
$$\lambda_e^{LM} = 4/h^2 \quad , \qquad (43)$$

for consistent and lumped mass, respectively. These element level eigenvalues represent upper bounds (Hughes et al. (30)) to the largest eigenvalues of the assembled system, Eq. (36); hence the reciprocal of the element eigenvalue gives a lower bound to the smallest time constant of the system. For the example above, $1/\lambda_e^{CM} \cong .00333$ and $1/\lambda_e^{LM} = .01$, which can be used as lower bounds for the "minimum believable time".

The wiggles can again be reduced by judicious rezoning (small elements near $x = 0$, etc.) and better solutions obtained near $x = 0$ at 'small' time. Even here the CM formulation will cause wiggles at small time, again indicating the 'response limits' of the mesh. We should also mention that the situation becomes somewhat more complex if higher order elements are employed, since in these cases even lumped mass results can display some anomalous behavior at early time.

Generalizations

The above results are general in that they also apply in two and three dimensions and on distorted meshes of isoparametric elements. They also apply to other equations which contain time-dependence, such as the advection-diffusion equation, the Navier-Stokes equations, and the Boussinesq equations. Whenever sharp transients are present, the conventional *GFEM* may 'signal' problem areas by generating wiggles and thus providing important guidance as to the minimum believable time. In these more complicated situations, however, one must also be alert to other causes of wiggles, as discussed in other portions of this paper.

THE NAVIER-STOKES EQUATIONS

Finally, we discuss the viscous, incompressible NS equations, which are significantly more complicated owing to nonlinearities, the pressure gradient terms, and the continuity equation;

$$\rho\left(\frac{\partial \underline{u}}{\partial t} + \underline{u} \cdot \nabla \underline{u}\right) = \nabla \cdot \underline{\underline{\tau}} \qquad \nabla \cdot \underline{u} = 0 \tag{44}$$

where $\underline{u} = (u,v)$ is the velocity, ρ is the density,

$$\tau_{ij} = -P\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{45}$$

is the symmetric stress tensor, P is the pressure, and μ is the viscosity.

Steady Flows

Even with these additional complexities, however, it appears to be still true that the most basic cause of wiggles is the same as that in the simplest case (steady one-dimensional advection-diffusion); viz, the 'transported' variable must undergo a 'rapid change in a short distance' in the flow direction. For NS equations, the transported variable may be u or v and the direction may be x or y (in general of course, the flow direction is along a streamline). Rapid changes transverse to the streamlines do not seem to be serious 'wiggle generators'; even pressure singularities, which occur frequently with NS equations, and appear to generate wiggles, are generally (but perhaps not always) amenable to the above interpretation - i.e., if pressure singularities (or other difficulties in the pressure field) cause sharp velocity gradients in the flow direction, then wiggles will occur (on a mesh which is too coarse). It is also true, however, that even Stokes flow solutions (no advection) can generate wiggles; these are rapidly damped, however, away from the source, in contrast to those from NS. For examples of these wiggles, see Leone and Gresho (31).

We will attempt to demonstrate these points in the following example, which is the subject of an entire recent paper (31); this paper, in fact, may be viewed as a companion paper to the present one in that it represents a 'case study' of wiggles for a particular problem: the developing flow through a channel containing a step. The basic problem is shown in Fig. 6, in which a 'flat' inlet velocity field is forced to flow through a channel containing a step on a grid which is obviously too coarse for the Re employed

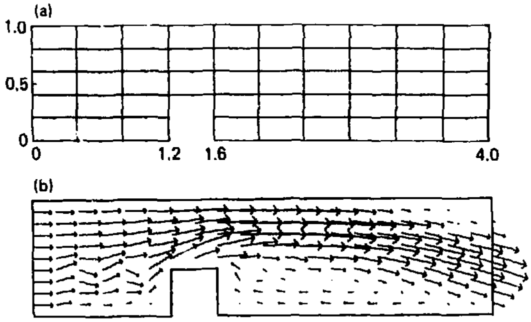


Fig. 6 Flow over a step in a channel at Re = 200; coarse grid. (a) The mesh of 48 uniform quadratic elements. (b) Velocity field.

(200). The grid (Fig. 6a) is composed of 46 equal-sized 9-node biquadratic elements (pressure is approximated bilinearly, at the 4 corner nodes of each element) and duplicates a result previously presented by Hughes et al. (15), who used these wiggles to make the claim, "We believe this problem demonstrates the inappropriateness of Gauss-Legendre integration of the convection term." - a statement with which we strongly disagree. The boundary conditions for this case are: u = 1, v = 0 at the inlet, traction-free ($f_n = f_t = 0$) at the outlet, and no slip (and no penetration; u = v = 0) along the top and bottom boundaries. The wiggles in Fig. 6b are caused by the inability of the coarse grid to resolve the rapid changes in the velocity field (principally the u-component), which should occur over a short distance as the flow approaches the step; the signal to rezone near the step is quite clear; Fig. 7 shows the solution on a refined mesh (155 elements - perhaps overly-refined if all we desire is wiggle suppression, but we were also seeking a good overall solution, including the reverse flow region) which is able to capture the gradients as the step is approached; hence, there are no wiggles and this is probably a quite good solution at Re = 200. The streamlines in Fig. 7c show separation at the trailing edge and also indicate that the flow details near the outflow are probably not as good as those closer to the step since the separation streamline leaves the grid (for further results on a longer grid, see (31)). This is also the grid and velocity solution used to solve the advection-diffusion equation discussed in an earlier section.

In the next, related, simulation, we attempted to determine the effect of unconfined flow over a step; to do this we used a longer and higher grid (205 elements) and changed the BC's at the top to the natural boundary conditions, $f_n = f_t = 0$ (traction free), which allows flow to leave and re-enter the domain. Fig. 8 shows the results for an outflow boundary condition of f_n = v = 0 (we expected the recovery to a uni-directional flow), which is flawed by wiggles originating at the ouflow boundary. The cause of these wiggles is believed to be an outflow boundary condition which is basically incompatible with the desired interior flow; the eddy length is now quite long and the flow does not want to be unidirectional at the outlet. This incompatibility forces a rapid change in the vertical component of velocity as the outflow boundary is approached (the $u\partial v/\partial x$ term in the y-momentum equation combined with a grid Reynolds number of $\sim$60 at the outlet) and the oscillations in v are a signal to 'change something' (a signal which, if our explanation of the cause is correct, would not be given by any upwind method); e.g. the domain should be lengthened, and/or the 'tough' BC changed. We chose the simpler and cheaper route, replaced v = 0 by $f_t = 0$ at the outlet, and the results are shown in Fig. 9; clearly this natural boundary condition is more compatible as the solution is now quite smooth (and v is far from zero at the outlet, especially in the eddy region). Finally, Fig. 9b shows the corresponding streamlines which, when compared with those in Fig. 7c, show signficant changes: the eddy is much longer, stronger, and separation now occurs from the top of the step.

In addition to Hughes et al., Zienkiewicz and Heinrich (32) have been experimenting with upwind methods on the NS equations. They show results for the

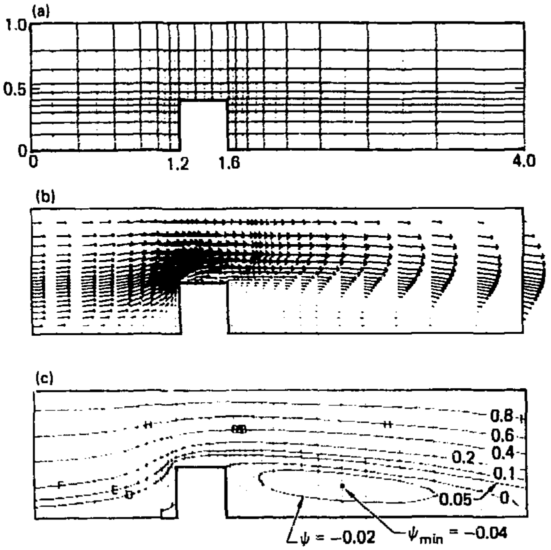


Fig. 7 Flow over a step at Re = 200; fine grid. (a) The mesh of 155 graded quadratic elements. (b) Velocity field. (c) Streamlines.

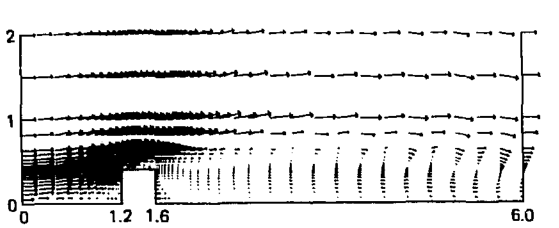


Fig. 8 Simulation of flow over a step in an unbounded domain using a too restrictive outlet boundary condition ($v = 0$).

lid-driven cavity problem on a mesh (10 x 14 bilinear elements) which is far too coarse for the Re employed (400 and 10^4) and criticize the wiggly solution from conventional GFEM. They then repeated the calculation for Re = 400 using their upwind scheme and demonstrated the smoother results attainable (they did not present results for Re = 10^4; perhaps wisely since they would probably differ little from those at Re = 400). We believe that the correct procedure for this problem is again to acknowledge the wiggles and employ judicious mesh refinement in the corner regions where rapid streamwise variations occur. Conventional GFEM should then be employed and, when the wiggles are acceptably small, the solution can be claimed to be adequate and appropriate to the actual Re employed. For further criticisms and estimates of the effective Re when upwind methods are used for the driven cavity problem, see DeVahl Davis and Mallinson (33). Finally, Tuann and Olson (34) have also recently suggested that upwind simulations on this problem are to be viewed suspiciously.

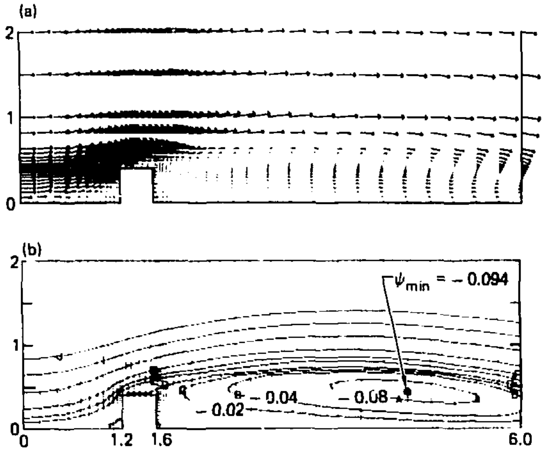


Fig. 9 Same as Fig. 8, except traction-free outflow boundary condition is employed. (a) Vector field. (b) Streamlines.

Time-Dependent Flows

We will discuss two types of time-dependent flows and the additional considerations required for their simulation. The first flow is one in which a transient flow field ultimately approaches a steady state. In these cases, the benefits accuring from the CM matrix of GFEM are the same as those discussed earlier; the wiggles at early time are defining the region of nonbelievability. For example, transient Couette flow (one-dimensional) or lid-driven cavity flow (two-dimensional) will display the awkward result that the velocities at the second row of nodes away from the driven surface and parallel to it will initially accelerate in the wrong direction. A lumped mass result will look better (all accelerations are in the right direction - at least for linear elements), yet both are inaccurate for 'small' time.

The second type of flow is one which does not display a steady-state solution, even with boundary conditions which are time-independent, such as vortex shedding behind a cylinder (see (16)) or other obstacle at a sufficiently large Re. Such flows contain 'discrete' vortices which, while definitely interacting with the external flow, are more or less transported by it. In these cases, the time-dependent NS equations will display two important characteristics of the advection-diffusion equation discussed earlier, both of which can be deleteriously affected by the use of 'smoothers' (again, if done on a 'too coarse' mesh): (1) the use of upwind methods could easily introduce sufficient "numerical viscosity" that the effective Re is significantly reduced such that the shedding phenomenon may be either misrepresented or, at worst, may not occur at all. (2) the transport of a wave-form (vortex) in the flow direction may suffer from the effects of phase speed errors (and their interaction with the surrounding flow field) if mass lumping is invoked.

SUMMARY AND FURTHER DISCUSSION

On Wiggles

In essentially all cases in which unacceptable wiggles occur, we believe that they are a strong and useful (and admittedly, often irritating) signal that some important portion of the solution (i.e. physics) is being inadequately modeled. They also indicate the 'critical' area(s) in the mesh wherein the wiggles are generated and the solution is particularly deficient. If they are pervasive or occur in 'important' regions of the mesh, judicious graded rezoning is obviously necessary. If they are not dominant at essentially all mesh locations (or at all times during a transient) and if they occur in regions of lesser importance, then the wiggle-free solution in the rest of the grid (or at larger time during a transient) is probably of acceptable accuracy. Finally, if they are small or negligible throughout the entire grid, and the overall numerical solution looks physically reasonable, then the solution of the original (continuum) equation(s) is probably adequately approximated everywhere.

Wiggles can also be a signal that there are 'problems' with the boundary conditions; either a more appropriate BC should be considered or, if the BC is appropriate, the simulation is inherently difficult and demands more attention (nodes) in the critical areas near the boundary.

Finally, wiggles tell you something about a problem with your mesh, parameter selection, and boundary conditions. Isoparametric finite elements (generally) provide the way to solve the problem in a reasonably efficient manner. The sedatives introduced by schemes which a priori eliminate wiggles induce a sense of euphoria which, while perhaps quite comfortable, can lead to bold (and usually false) claims regarding their effectiveness. These schemes can damp more than just wiggles.

On Upwinding

The upwind fallacy of 'smoother is better' is inherently dangerous and leads to a false sense of security - 'Any mesh works for any Reynolds (Peclet) number'. It is too easy to lose sight of the inherent cause of the smoothness - numerical diffusion - especially for time-dependent flow. The main premise behind upwinding is 'it works' on coarse grids (or high Re or Pe). The upwind fact is 'it works' but is only accurate if the numerical diffusion is significantly less than the physical diffusion.

We believe that upwind advocates are largely ignoring both logic and physics: logic says that less accurate methods should only be employed on meshes with more nodes and the physics of fluids says that the flow invariably becomes more complex and/or difficult at higher Re or Pe. Yet upwind methods are applied at higher Re (Pe) and on coarser meshes than is the conventional GFEM.

Upwind methods will rarely, if ever, warn the analyst that he is expecting too much from a given mesh or that he should question his results with respect to the original problem.

Upwind methods, can be fine, but generally only when used on a fine (finer) mesh. And in this case, we believe that the schemes advocated for upwinding using asymmetric weighting functions introduce sufficient additional computational complexity to make them noticeably more expensive than GFEM.

On Grid Peclet Number

While it is sometimes true that a grid Peclet number (or Re) cannot exceed 2 (simplistic, one-dimensional result) in order that numerical oscillations be precluded, there is another important point in this connection; viz it is the combination of large Pg (>2 or so) with large streamwise gradients in the 'advected' variable which give rise to wiggles. When this combination occurs, the GFEM results command attention. In other cases, however, the results from GFEM can be quite acceptable at very large local Reynolds numbers. For example, we have computed flow past a circular cylinder at Re = 100 and obtained very good results throughout the domain in spite of the fact that our grid Reynolds number was 100-200 in some portions of the grid (see 16); the important point is that the grid Re was sufficiently small in the critical regions where flow details were changing rapidly (of course, our outflow boundary conditions were also selected to minimize problems ($f_n = f_t = 0$) and they helped us attain good results even near the outflow boundary, similar to the step flow example discussed above, which also had a large grid Re in some portions of the grid).

On the Mass Matrix

If implicit time integration schemes are employed, we recommend that the consistent mass matrix of GFEM be retained for reasons enumerated previously; viz (1) higher phase accuracy and (2) lumped mass transients can be misleading because they tend to generate smooth results for all time. If explicit methods are chosen, then mass lumping is virtually mandatory and one sacrifices these advantages (there may be other reasons for using lumped mass matrices; for example, we believe it may be cost-effective for solving the NS equations in three dimensions - see (16)).

CONCLUDING REMARKS

Although it is frequently quite frustrating, we live with wiggles all the time in our GFEM code development and testing. However, we feel that we almost always learn something (about computational and theoretical fluid mechanics) from the wiggles and that, when they are properly reduced or eliminated (which may take several iterations) our final solutions are always much the better for it.

We do not claim to have a panacea for all wiggles (there probably is none) and have reported herein only on those with which we have dealt successfully. We are currently engaged in the analysis of other wiggles (or at least some poorly behaved velocity vectors) which, while not yet fully explained, appear to be more 'element'-related and occur frequently when simulating stratified flow via the Boussinesq equations, and occasionally with the simpler NS equations. That these current wiggles are element-related derives from studies in which one after another of our elements 'fails' in a particular simulation as the parameters are changed to make the problem more difficult (e.g. the 9-node velocity, 4-node pressure element can generate very poor solutions under certain situations). We plan to report on some these wiggles in the near future (Gresho et al., 35); further examples and discussion of these problems may also be found in the thesis of Leone (36), who has recently worked with us and our codes.

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REFERENCES

1 Leone, J., Gresho, P., Chan, S., and Lee, R., "A Note on the Accuracy of Gauss-Legendre Quadrature in the Finite Element Method," Int. J. Num. Meth. Eng., Vol. 14, 1979, pp 769-773.

2 Roache, P., Computational Fluid Dynamics, Hermosa Publishers, 1972.

3 Zienkiewicz, O. and Heinrich, J., "The Finite Element Method and Convection Problems in Fluid Mechanics", Finite Elements in Fluids - Vol. 3, John Wiley & Sons, New York, 1978, pp 1-22.

4 Spalding, D., "A Novel Finite Difference Formulation for Differential Expressions Involving Both First and Second Derivatives", Int. J. Num. Meth. Eng., Vol. 4, 1972, pp 551-559

5 Smith, R.M., "Finite Element Solutions of the Energy Equation at High Peclet Number", RD/B/N4502, April 1979, Central Electricity Generating Board, London, England.

6 Allen, D. and Southwell, R., "Relaxation Methods Applied to Determine the Motion, in Two Dimensions, of a Viscous Fluid Past a Fixed Cylinder", Quart. J. Mech. and Appl. Math., Vol VIII, pt 2, 1955, pp 129-145.

7 Dennis, S., "Finite Differences Associated with Second Order Differential Equations", Quart. J. Mech. & Appl. Math., Vol XIII, pt 4, 1960, pp 487-507.

8 Raithby, G. and Torrance, K., "Upstream-Weighted Differencing Schemes and Their Application to Elliptic Problems Involving Fluid Flow", Comp. & Fluids, Vol. 2, 1974, pp 191-206.

9 Briggs, D., "A Finite Difference Scheme for the Incompressible Advection-Diffusion Equation", Comp. Meth. Appl. Mech. & Eng., Vol. 6, 1975, pp 233-241.

10 Fiadeiro, M., and Veronis, G., "On weighted-mean schemes for the finite difference approximation to the advection-diffusion equation", Tellus, Vol. 29, 1977, pp 512-522.

11 Christie, I., Griffiths, D., Mitchell, A., and Zienkiewicz, O., "Finite Element Methods for Second Order Differential Equations with Significant First Derivatives", Int. J. Num. Meth. Eng., Vol. 10, 1976, pp 1389-1396.

12 Huyakorn, P., "Solution of steady-state, convective transport equation using an upwind finite element scheme", Appl. Math. Modeling, Vol. 1, March 1977, pp 187-195.

13 Heinrich, J., Huyakorn, P., Zienkiewicz, O., and Mitchell, A., "An 'Upwind' Finite Element Scheme for Two-Dimentional Convective Transport Equation", Int. J. Num. Meth. Eng., Vol. 11, 1977, pp 131-143.

14 Heinrich, J. and Zienkiewicz, O., "Quadratic Finite Element Schemes for Two-Dimensional Convective-Transport Problems", Int. J. Num. Meth. Eng., Vol. 11, 1977, pp 1831-1844.

15 Hughes, J., Liu, W., and Brooks, A., "Finite Element Analysis of Incompressible Viscous Flows by the Penalty Function Formulation", J. Comp. Phys., Vo. 30, Jan. 1979, pp 1-60.

16 Gresho, P., Lee, R., Sani R., and Stullich, T., "On the Time-Dependent FEM Solution of the Incompressible Navier-Stokes Equations in Two- and Three-Dimensions", Lawrence Livermore Laboratory, UCRL 81323, July 7, 1978; see also, Recent Advances in Numerical Methods in Fluids, Pineridge Press, Ltd., Swansea, U.K. (to appear, late 1979).

17 Gresho, P., Lee, R., Stullich, T., and Sani, R., "Solution of the Time-Dependent Equations via FEM", in Finite Elements in Water Resources, Proc. of 2nd International Conference, Imperial College, London, England; July, 1978, Edited by C. Brebbia, W. Gray, & G. Pinder: pp 3.45-3.64.

18 Gartling, D., "Some Comments on the Paper by Heinrich, Huyakorn, Zienkiewicz, and Mitchell", Int. J. Num. Meth. Eng., Vol. 12, 1978, pp 187-190.

19 Bettes, P., "Infinite Elements", Int. J. Num. Meth. Eng., Vol. 11, 1977, pp 53-64.

20 Raithby, G., "A Critical Evaluation of Upstream Differencing Applied to Problems Involving Fluid Flow", Comp. Meth. Appl. Mech. & Eng., Vol. 9, 1976, pp 75-103.

21 Raithby, G., "Skew Upstream Differencing Schemes for Problems Involving Fluid Flow", Comp. Meth. Appl. Mech. & Eng., Vol. 9, 1976 pp 153-164.

22 Lee, R., Gresho, P., and Sani, R., "A Comparative Study of Certain Finite-Element and Finite-Difference Methods in Advection-Diffusion Simulations", in 1976 Summer Computer Simulation Conference; July, 1976, pp 37-42.

23 Gresho, P., Lee, R., & Sani, R., "Advection-Dominated Flows, with Emphasis on the Consequences of Mass Lumping", Finite Elements in Fluids Vol. 3, John Wiley and Sons, New York, 1978, pp 335-350.

24 Huyakorn, P. and Nilkuha, K., "Solution of Transient Transport Equation Using an Upstream Finite Element Scheme", Appl. Math. Modeling, Vol. 3, Feb. 1979, pp 7-17.

25 Long, P., and Pepper, D., "A Comparison of Six Numerical Schemes for Calculating the Advection of Atmospheric Pollution", in Third Symposium on Atmospheric Turbulence, Diffusion, and Air Quality, American Meteorological Society, Oct., 1976, pp 181-187.

26 Lee, R., Gresho, P., Chan, S., and Sani, R., "A Comparison of Several Conservative Forms for Finite Element Formulations of the Incompressible Navier-Stokes or Boussinesq Equations", submitted to Third International Conference on Finite Elements in Flow Problems, to be held in Banff, Canada, June 10-13, 1980.

27 Oden, J., Finite Elements of Nonlinear Continua, McGraw-Hill, New York, 1972, p 89.

28 Zienkiewicz, O., The Finite Element Method, McGraw-Hill, London, 1977.

29 Lee, R., Gresho, P., and Sani, R., "Smoothing Techniques for Certain Primitive Variable Solutions of the Navier-Stokes Equtions", Int. J. Num. Meth. Eng., to appear (1979).

30 Hughes, T., Pister, K., and Taylor, R., "Implicit-explicit finite elements in nonlinear transient analysis", Comp. Meth. Appl. Mech. Eng., Vol. 17/18, 1979, pp 159-182.

31 Leone, J., and Gresho, P., "Finite Element Simulations of Steady, Two-Dimensional Viscous Incompressible Flow Over a Step", Submitted to J. Comp. Phys., 1979.

32 Zienkiewicz, O. and Heinrich, J., "A Unified Treatment of Steady-State Shallow Water and Two-Dimensional Navier-Stokes Equations - Finite Element Penalty Function Approach", Comp. Meth. Appl. Mech. & Eng., Vol. 17/18, 1979, pp 673-698.

33 DeVahl Davis, G., and Mallinson, G., "An Evaluation of Upwind and Central Difference Approximations by a Study of Recirculating Flow", Comp. & Fl., Vol. 4, 1976, pp 29-43.

34 Tuann, S., and Olson, M., "Review of Computing Methods for Recirculating Flows", J. Comp. Phys., Vol. 29, Oct. 1978, pp 1-19.

35 Gresho, P., Lee, R., Chan, S., and Sani, R., "A New Finite Element for Incompressible or Boussinesq Fluids", submitted to Third International Conference on Finite Elements in Flow Problems, to be held at Banff, Canada, June 10-13, 1980.

36 Leone, J.M., "Finite Element Simulations of Stratified Flow Over Simple Geometrical Obstructions and Arbitrarily Complex Terrain", Ph. D. Thesis, Iowa State University, Ames, Iowa, 1979.