CHAPTER

2

Convection-Dominated Problems: Finite Element Approximations to the Convection-Diffusion-Reaction Equation

2.1 Introduction

In this chapter we are concerned with steady-state and transient solutions for equations of the type

$$\frac{\partial \mathbf{\Phi}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} + \frac{\partial \mathbf{G}_i}{\partial x_i} + \mathbf{Q} = \mathbf{0} \tag{2.1}$$

where in general $\mathbf{\Phi}$ is the basic dependent, vector-valued variable, $\mathbf{Q}$ is a source or reaction term vector, and the *flux* matrices $\mathbf{F}$ and $\mathbf{G}$ are such that

$$\begin{aligned} \mathbf{F}_i &= \mathbf{F}_i(\mathbf{\Phi}) \\ \mathbf{G}_i &= \mathbf{G}_i\left(\frac{\partial \mathbf{\Phi}}{\partial x_j}\right) \end{aligned} \tag{2.2a}$$

and in general

$$\mathbf{Q} = \mathbf{Q}(x_i, \mathbf{\Phi}) \tag{2.2b}$$

In the above, x_i and i refer, in the indicial manner, to Cartesian coordinates and quantities associated with these. A linear relationship between the source and the scalar variable in Eq. (2.2b) is frequently referred to as a reaction term.

The general equation (2.1) can be termed the *transport equation* with $\mathbf{F}$ standing for the *convective* and $\mathbf{G}$ for the *diffusive* flux quantities.

Equation (2.1) is a set of *conservation laws* arising from a balance of the quantity $\mathbf{\Phi}$ with its fluxes $\mathbf{F}$ and $\mathbf{G}$ entering and leaving a control volume. Such equations are typical of fluid mechanics which we have discussed in Chapter 1. As such equations may also arise in other physical situations, this chapter is devoted to a general discussion of their approximate solution.

The simplest form of Eqs. (2.1), (2.2a), and (2.2b) is one in which the unknown is a scalar. Most of this chapter is devoted to the solution of such equations. Throughout this book we shall show that there is no need of dealing with convection of vector-type

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quantities. Thus for the scalar form we have

$$\begin{aligned} \mathbf{\Phi} &\rightarrow \phi & \mathbf{Q} &\rightarrow Q(x_i, \phi) \\ \mathbf{F}_i &\rightarrow F_i = U_i \phi & \mathbf{G}_i &\rightarrow G_i = -k \frac{\partial \phi}{\partial x_i} \end{aligned} \tag{2.3}$$

We also now have in Cartesian coordinates a scalar equation of the form

$$\frac{\partial \phi}{\partial t} + \frac{\partial (U_i \phi)}{\partial x_i} - \frac{\partial}{\partial x_i}\left(k \frac{\partial \phi}{\partial x_i}\right) + Q = 0 \tag{2.4}$$

In the above equation, U_i is a known velocity field and ϕ is a *scalar* quantity being transported by this velocity. However diffusion can also exist and here k is the diffusion coefficient.

The term Q represents any external sources of the quantity ϕ being admitted to the system and the reaction loss or gain which itself is dependent on the function ϕ.

A simple linear relation for the reaction may be written as

$$Q = c\,\phi \tag{2.5}$$

where c is a scalar parameter. The equation can be rewritten in a slightly modified form in which the convective term has been differentiated as

$$\frac{\partial \phi}{\partial t} + \underline{U_i \frac{\partial \phi}{\partial x_i}} + \phi \frac{\partial U_i}{\partial x_i} - \frac{\partial}{\partial x_i}\left(k \frac{\partial \phi}{\partial x_i}\right) + Q = 0 \tag{2.6}$$

We note that the above form of the problem is self-adjoint with the exception of a convective term which is underlined. The reader is referred to Appendix A for the definition of self-adjoint problems. The third term in Eq. (2.6) disappears if the flow itself is such that its divergence is zero, i.e., if

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{2.7}$$

In what follows we shall discuss the scalar equation in much more detail as many of the finite element remedies are only applicable to such scalar problems and are not directly transferable to the vector form. In the CBS scheme, which we shall introduce in Chapter 3, the equations of fluid dynamics will be split so that only scalar transport occurs, where the treatment considered here is sufficient.

From Eqs. (2.6) and (2.7) we have

$$\frac{\partial \phi}{\partial t} + U_i \frac{\partial \phi}{\partial x_i} - \frac{\partial}{\partial x_i}\left(k \frac{\partial \phi}{\partial x_i}\right) + Q = 0 \tag{2.8}$$

With the variable ϕ approximated in the usual way,

$$\phi \approx \widehat{\phi} = \mathbf{N}\tilde{\mathbf{\Phi}} = \sum N_a \tilde{\phi}_a \tag{2.9}$$

the problem may be presented following the usual (weighted residual) semi-discretization process as

$$\mathbf{M}\dot{\tilde{\boldsymbol{\Phi}}} + \mathbf{H}\tilde{\boldsymbol{\Phi}} + \mathbf{f} = \mathbf{0} \tag{2.10}$$

where

$$\begin{aligned} M_{ab} &= \int_\Omega W_a N_b \mathrm{d}\Omega \\ H_{ab} &= \int_\Omega \left[W_a U_i \frac{\partial N_b}{\partial x_i} + \frac{\partial W_a}{\partial x_i} k \frac{\partial N_b}{\partial x_i} \right] \mathrm{d}\Omega \\ f_a &= \int_\Omega W_a \, Q \, \mathrm{d}\Omega + \int_{\Gamma_q} W_a \bar{q}_n \, \mathrm{d}\Omega \end{aligned}$$

Now even with standard Galerkin weighting the matrix $\mathbf{H}$ will not be symmetric. However, this is a relatively minor computational problem compared with inaccuracies and instabilities in the solution which follow the arbitrary use of the weighting function.

This chapter will discuss the manner in which these difficulties can be overcome and the approximation improved.

We shall discuss in the main address the problem of solving Eq. (2.8), i.e., the scalar form, and to simplify matters further we shall start with the idealized one-dimensional equation:

$$\frac{\partial \phi}{\partial t} + U \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x}\left(k \frac{\partial \phi}{\partial x} \right) + Q = 0 \tag{2.11}$$

The term $\phi \, \partial U / \partial x$ has been removed for simplicity, which of course is true if U is constant. The above reduces in steady state to an ordinary differential equation:

$$\begin{aligned} U \frac{\mathrm{d}\phi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k \frac{\mathrm{d}\phi}{\mathrm{d}x} \right) + Q &= 0 \\ \mathcal{L}(\phi) + Q &= 0 \end{aligned} \tag{2.12}$$

in which we shall often assume U, k, and Q to be constant. The basic concepts will be evident from the above and will later be extended to multidimensional problems, still treating ϕ as a scalar variable.

Indeed the methodology of dealing with the first space derivatives occurring in differential equations governing a problem, which lead to non-self-adjointness, opens the way for many new physical situations.

The present chapter will be divided into three parts. Part I deals with *steady-state situations* starting from Eq. (2.12), Part II with *transient solutions* starting from Eq. (2.11), and Part III with treatment of boundary conditions for convective-diffusive problems where use of "weak forms" is shown to be desirable.

Although the scalar problem will mainly be dealt with here in detail, the discussion of the procedures can indicate the choice of optimal ones, which will have much bearing on the solution of the general case of Eq. (2.1). The extension of some procedures to the vector case is presented in Appendix D.

Part I: Steady-State Problems

2.2 The steady-state problem in one dimension

2.2.1 General remarks

We consider the discretization of Eq. (2.12) with

$$\phi \approx \widehat{\phi} = \sum N_a \tilde{\phi}_a = \mathbf{N}\tilde{\boldsymbol{\phi}} \tag{2.13}$$

where N_a are shape functions and $\tilde{\boldsymbol{\phi}}$ represents a set of still unknown parameters. Here we shall take these to be the nodal values of ϕ. The weighted residual form of the one-dimensional problem is written as (see Chapter 1)

$$\int_\Omega W_a \left[U \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} \right) + Q \right] \mathrm{d}\Omega = 0 \tag{2.14}$$

Integrating the second term by parts gives

$$\int_\Omega W_a \left[U \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} + Q \right] \mathrm{d}\Omega + \int_\Omega \frac{\mathrm{d}W_a}{\mathrm{d}x} k \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} \mathrm{d}\Omega = \int_{\Gamma_q} W_a \, \bar{q}_n \, \mathrm{d}\Gamma \tag{2.15}$$

where

$$\bar{q}_n = -k \frac{\partial \widehat{\phi}}{\partial n} \quad \text{on } \Gamma_q$$

and

$$\widehat{\phi} = \bar{\phi} \quad \text{on } \Gamma_\phi$$

is assumed. For a typical internal node a the approximating equation becomes

$$K_{ab}\tilde{\phi}_b + f_a = 0 \tag{2.16}$$

where

$$\begin{aligned} K_{ab} &= \int_0^L W_a U \frac{\mathrm{d}N_b}{\mathrm{d}x} \mathrm{d}x + \int_0^L \frac{\mathrm{d}W_a}{\mathrm{d}x} k \frac{\mathrm{d}N_b}{\mathrm{d}x} \mathrm{d}x \\ f_a &= \int_0^L W_a Q \mathrm{d}x + W_a \bar{q}_n \Big|_{\Gamma_q} \end{aligned} \tag{2.17}$$

and the domain of the problem is $0 \le x \le L$.

For linear shape functions (Fig. 2.1), Galerkin weighting ($W_a = N_a$), and elements of equal size h, we have for *constant* values of U, k, and Q (see Appendix E)

$$\begin{aligned} \mathbf{K}^e &= \frac{U}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{k}{h} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \\ \mathbf{f}^e &= \frac{Q}{2} \begin{Bmatrix} 1 \\ 1 \end{Bmatrix} \end{aligned}$$

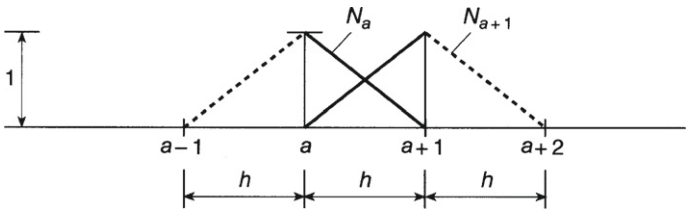

FIGURE 2.1
A linear shape function for a one-dimensional problem.

which yields a typical assembled equation (after multiplying by h/k) for an inside node "a"

$$(-Pe-1)\tilde{\phi}_{a-1}+2\tilde{\phi}_a+(Pe-1)\tilde{\phi}_{a+1}+\frac{Qh^2}{k}=0 \tag{2.18}$$

where

$$Pe=\frac{Uh}{2k} \tag{2.19}$$

is the element *Peclet* number. Incidentally, for the case of constant Q the above is identical to the usual central finite difference approximation obtained by putting

$$\frac{\mathrm{d}\phi}{\mathrm{d}x}\approx\frac{\tilde{\phi}_{a+1}-\tilde{\phi}_{a-1}}{2h} \tag{2.20a}$$

and

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\approx\frac{\tilde{\phi}_{a+1}-2\tilde{\phi}_a+\tilde{\phi}_{a-1}}{h^2} \tag{2.20b}$$

The algebraic equations (2.18) are obviously nonsymmetric and their accuracy deteriorates as the parameter Pe increases, i.e., when convective terms are of primary importance. Indeed as $Pe\to\infty$, the solution is purely oscillatory and bears no relation to the underlying problem. This may be ascertained by considering Eq. (2.18) for different element Peclet numbers and it is easy to show that with the standard Galerkin procedure oscillations in $\tilde{\phi}_a$ occur when

$$|Pe|>1 \tag{2.21}$$

To illustrate this point we consider a simple example.

Example 2.1. One-dimensional convection-diffusion ($Q=0$)

The domain of the problem considered is $0\le x\le L$ and the boundary conditions are both of Dirichlet type and given by

$$\phi(0)=1 \quad \text{and} \quad \phi(L)=0$$

We approximate the solution using nine equal size linear elements and the Galerkin form of (2.15):

$$\left[\int_0^L\left(\frac{\mathrm{d}N_a}{\mathrm{d}x}k+N_aU\right)\frac{\mathrm{d}N_b}{\mathrm{d}x}\mathrm{d}x\right]\tilde{\phi}_b=0$$

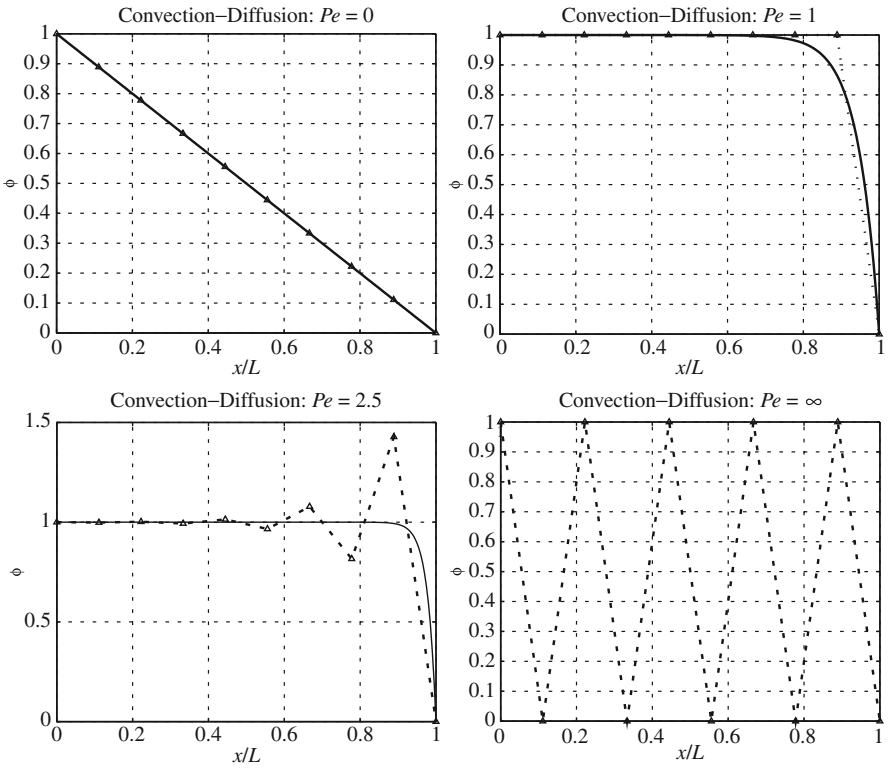

FIGURE 2.2

Approximations to $U\mathrm{d}\phi/\mathrm{d}x - k\mathrm{d}^2\phi/\mathrm{d}x^2 = 0$ for $\phi(0) = 1$ and $\phi(L) = 0$ for various Peclet numbers. Solid line: exact solution; dotted line with triangular symbol: standard Galerkin solution.

The solution shown in Fig. 2.2 with curves labeled with triangles gives results for element Peclet numbers [given by (2.19)] $Pe = 0, 1, 2.5$, and ∞ (the solution for this problem with $Pe = \infty$ is only possible for an odd number of elements). We see that as the Pe number increases above 1 the solution becomes oscillatory and progressively departs from the smooth exact solution (solid line in Fig. 2.2):

$$\phi = \frac{\mathrm{e}^{Ux/k} - \mathrm{e}^{UL/k}}{1 - \mathrm{e}^{UL/k}}$$

Of course the above is partly a problem of boundary conditions. When diffusion is omitted ($k = 0$) only a single boundary condition can be imposed and when the diffusion is small we note that the downstream boundary condition ($\phi(L) = 0$) is felt in only a very small region of a *boundary layer*.

The above example clearly demonstrates that the standard Galerkin method in which $W_a = N_a$ cannot be used to solve problems in which convective terms are large compared with those of diffusion. Of course, one can consider replacing the

weight functions N_a by other more general ones W_a (commonly called a Petrov-Galerkin weighting). Indeed for the linear one-dimensional steady-state problem we can always find weight functions which give exact solutions at the interelement nodes.

Example 2.2. Weight function for exact nodal solutions

Here we consider the problem of Example 2.1 where the weak form including Q is given by

$$\int_{x_1}^{x_2} v \left[U \frac{\mathrm{d}\phi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k \frac{\mathrm{d}\phi}{\mathrm{d}x} \right) + Q \right] \mathrm{d}x = 0$$

where $x_1 \leq x \leq x_2$ denotes the domain. After integration by parts for all derivatives on ϕ we obtain

$$\int_{x_1}^{x_2} \left[-U \frac{\mathrm{d}v}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k \frac{\mathrm{d}v}{\mathrm{d}x} \right) \right] \phi \, \mathrm{d}x + \int_{x_1}^{x_2} v \, Q \, \mathrm{d}x + v \left(U\phi - k \frac{\mathrm{d}\phi}{\mathrm{d}x} \right) \Bigg|_{x_1}^{x_2} + \frac{\mathrm{d}v}{\mathrm{d}x} k \phi \Bigg|_{x_1}^{x_2} = 0$$

in which

$$-U \frac{\mathrm{d}v}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k \frac{\mathrm{d}v}{\mathrm{d}x} \right)$$

is the *adjoint equation* for the original problem and the sign of the first derivative is opposite to that of the original operator. We note that the presence of the first derivative term makes the problem *non-self-adjoint* (see Appendix A).

Motivated by the fact that the propagation of information is in the direction of the velocity U, finite difference practitioners were the first to overcome the bad approximation problem of the central difference method. They used *one-sided* finite differences to approximate the first derivative [1–4]. Thus in place of Eq. (2.20a) and with positive U, the approximation was put as

$$\frac{\mathrm{d}\phi}{\mathrm{d}x} \approx \frac{\tilde{\phi}_a - \tilde{\phi}_{a-1}}{h} \tag{2.22}$$

changing the central finite difference form of the governing equation approximation [as given by Eq. (2.18)] to

$$(-2Pe - 1)\tilde{\phi}_{a-1} + (2 + 2Pe)\tilde{\phi}_a - \tilde{\phi}_{a+1} + \frac{Qh^2}{k} = 0 \tag{2.23}$$

With this *upwind* difference approximation, nonoscillatory solutions are obtained through the whole range of Peclet numbers as shown in Fig. 2.3 by curves labeled $\alpha = 1$. Now exact *nodal solutions* are obtained for pure diffusion ($Pe = 0$) and for pure convection ($Pe = \infty$); however, results for other values of Pe are generally not accurate.

How can such upwind differencing be introduced into a finite element scheme and generalized to more complex situations? This is the problem that we now address and indeed show that, for linear one-dimensional elements, this form of finite element solution also can result in exact nodal values for all Peclet numbers.

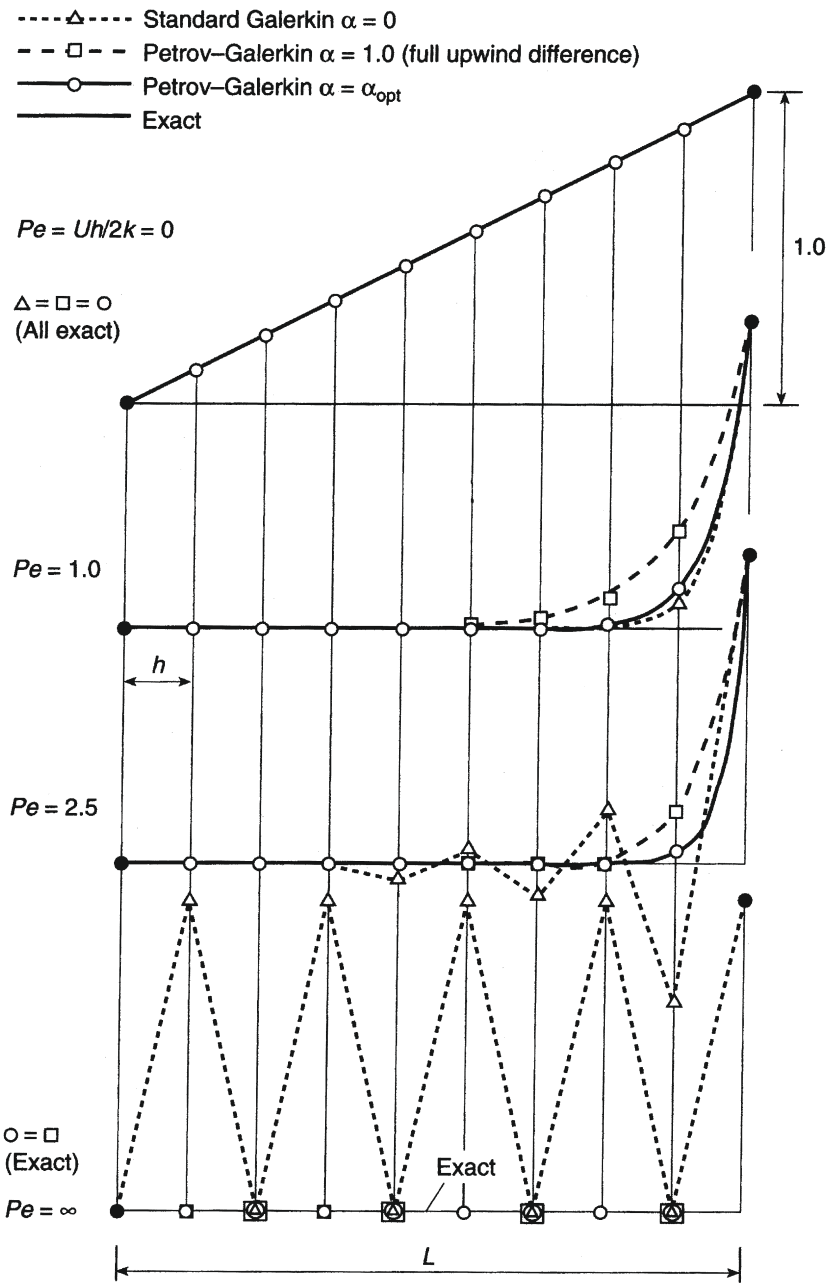

FIGURE 2.3

Approximations to $U\mathrm{d}\phi/\mathrm{d}x - k\mathrm{d}^2\phi/\mathrm{d}x^2 = 0$ for $\phi = 0$ at $x = 0$ and $\phi = 1$ at $x = L$ for various Peclet numbers.

2.2.2 Petrov-Galerkin methods for upwinding in one dimension

The first possibility is that of the use of a Petrov-Galerkin type of weighting in which $W_a \neq N_a$ [5–8]. Such weighting was first suggested by Zienkiewicz et al. [5] in 1976 and used by Christie et al. [6]. In particular, again for elements with linear shape functions N_a, shown in Fig. 2.1, we shall take weighting functions constructed as shown in Fig. 2.4 so that

$$W_a = N_a + \alpha W_a^\star \tag{2.24}$$

where $W_a^\star$ is such that (to obtain finite difference equivalent)

$$\int_{\Omega_e} W_a^\star \mathrm{d}x = \pm\frac{h}{2} \tag{2.25}$$

with the sign depending on whether U is a velocity directed toward or away from the node. With this approximation (2.15) becomes

$$\int_\Omega (N_a + \alpha W_a^\star)\left[U\frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} + Q\right]\mathrm{d}\Omega + \int_\Omega \left(\frac{\mathrm{d}N_a}{\mathrm{d}x} + \alpha\frac{\mathrm{d}W_a^\star}{\mathrm{d}x}\right)k\frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x}\,\mathrm{d}\Omega - \left(N_a + \alpha W_a^\star\right)\bar{q}_n\Big|_{\Gamma_q} = 0 \tag{2.26}$$

Various forms of $W_a^\star$ are possible, but the most convenient is the following simple definition which is, of course, a discontinuous function (continuity requirements are discussed below):

$$W_a^\star = \frac{h}{2}\frac{U}{|U|}\frac{\mathrm{d}N_a}{\mathrm{d}x} \tag{2.27}$$

where $|U|$ denotes the absolute value.

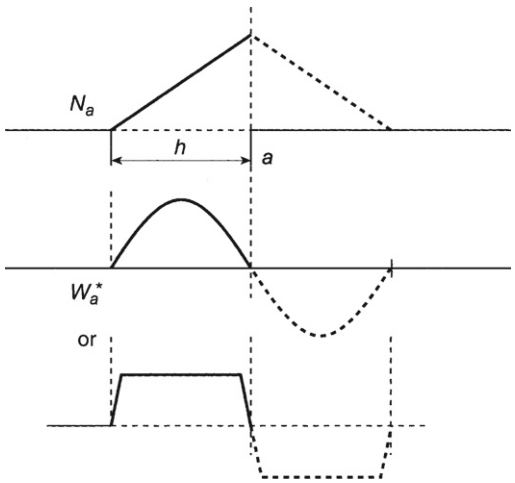

FIGURE 2.4
Petrov-Galerkin weight function $W_a = N_a + \alpha W_a^\star$. Continuous and discontinuous definitions.

With the above weighting functions the approximation from Eq. (2.15) for a typical node a becomes

$$[-Pe(\alpha+1)-1]\tilde{\phi}_{a-1}+[2+2\alpha(Pe)]\tilde{\phi}_a+[-Pe(\alpha-1)-1]\tilde{\phi}_{a+1}+\frac{Qh^2}{k}=0 \tag{2.28}$$

where Q is assumed constant for the whole domain and equal length elements are used.

Immediately we see that with $\alpha = 0$ the standard Galerkin approximation is recovered [Eq. (2.18)] and that with $\alpha = 1$ the full upwind form [Eq. (2.23)] is available, each giving exact nodal values for purely diffusive or purely convective cases respectively (Fig. 2.3).

Now if the value of α is chosen as

$$\alpha = \alpha_{\text{opt}} = \coth|Pe| - \frac{1}{|Pe|} \tag{2.29}$$

then exact nodal values will be given *for all values of Pe*. The proof of this is given in Refs. [6] and [9] for the present, one-dimensional, case where it is also shown that if

$$\alpha > \alpha_{\text{crit}} = 1 - \frac{1}{|Pe|} \tag{2.30}$$

oscillatory solutions never arise. Figure 2.5 shows the variation of α_{opt} and α_{crit} with Pe.

Although the proof of optimality for the upwinding parameter was given for the case of constant coefficients and constant size elements, nodally exact values will also be given if $\alpha = \alpha_{\text{opt}}$ is chosen for each element individually. We show some typical solutions in Fig. 2.6 for a variable source term $Q = Q(x)$ and variable element sizes.

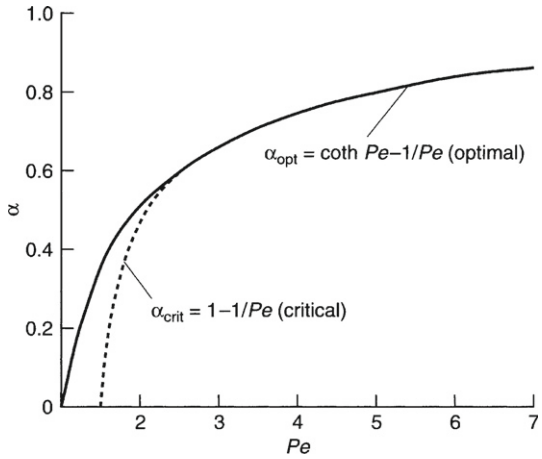

FIGURE 2.5
Critical (stable) and optimal values of the "upwind" parameter α for different values of $Pe = Uh/2k$.

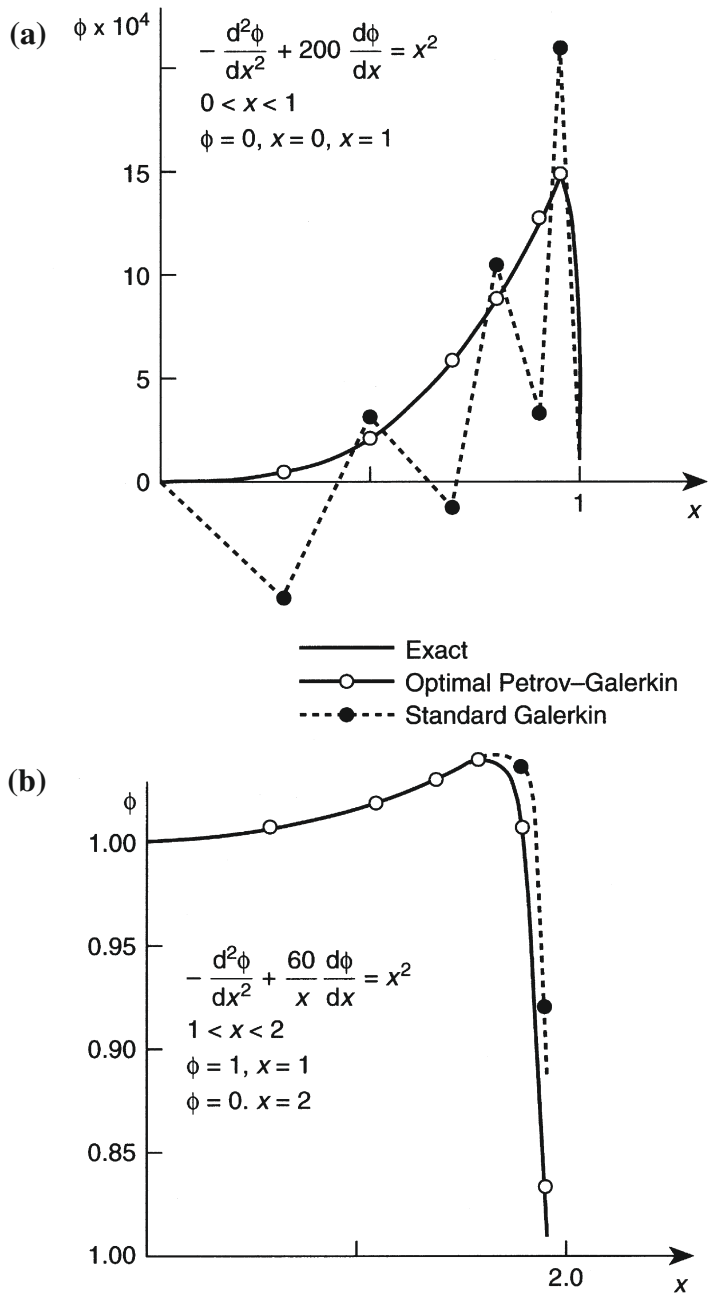

FIGURE 2.6

Application of standard Galerkin and Petrov-Galerkin (optimal) approximation: (a) variable source term equation with constants k and h; (b) variable source term with a variable U.

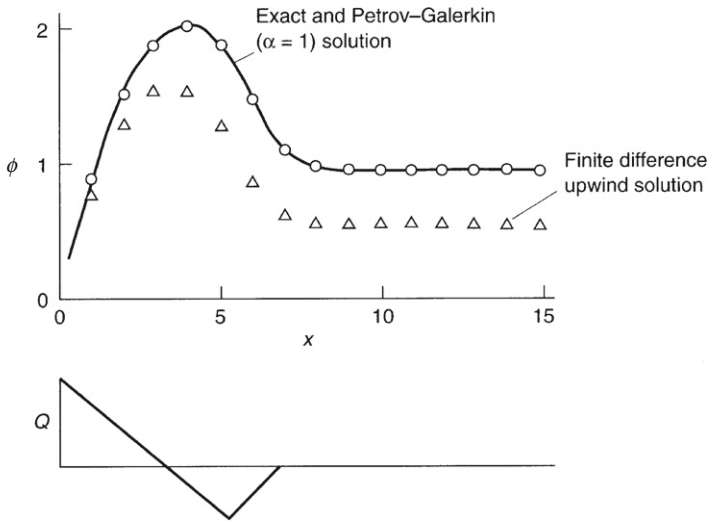

FIGURE 2.7

A one-dimensional pure convective problem ($k = 0$) with a variable source term Q and constant U. The Petrov-Galerkin procedure results in an exact solution but simple finite difference upwinding gives substantial error.

Figure 2.6(a) uses a constant convection velocity while Fig. 2.6(b) has a variable velocity [10]. Each of these is compared with a standard Galerkin solution, showing that even when the latter does not result in oscillations the accuracy is improved. Of course in the above examples the Petrov-Galerkin weighting must be applied to all terms of the equation. When this is not done (as in simple finite difference upwinding) totally wrong results will be obtained, as shown in the finite difference results of Fig. 2.7, which was used in Ref. [11] to discredit upwinding methods. The effect of α on the source term is not apparent in Eq. (2.28) where Q is constant in the whole domain, but its influence is strong when $Q = Q(x)$.

2.2.2.1 *Continuity requirements for weighting functions*

The weighting function W_a (or $W_a^\star$) introduced in Fig. 2.4 can of course be discontinuous as far as the contributions to the convective terms are concerned [see Eq. (2.17)], i.e.,

$$\int_0^L W_a \frac{\mathrm{d}(U N_b)}{\mathrm{d}x}\mathrm{d}x \quad \text{or} \quad \int_0^L W_a U \frac{\mathrm{d}N_b}{\mathrm{d}x}\mathrm{d}x$$

Clearly no difficulty arises at the discontinuity in the evaluation of the above integrals. However, when evaluating the diffusion term, we generally introduce integration by parts and evaluate such terms as

$$\int_0^L \frac{\mathrm{d}W_a}{\mathrm{d}x} k \frac{\mathrm{d}N_b}{\mathrm{d}x}\mathrm{d}x$$

in place of the form

$$-\int_0^L W_a \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}N_b}{\mathrm{d}x}\right)\mathrm{d}x$$

Here a local infinity will occur with discontinuous W_a. To avoid this difficulty we *mollify* or *smooth* the discontinuity of the $W_a^\star$ so that this occurs within the element [12] and thus avoid the discontinuity at the node in the manner shown in Fig. 2.4. Now direct integration can be used, showing in the present case zero contributions to the diffusion term.

2.2.3 Balancing diffusion in one dimension

The comparison of the nodal equations (2.18) and (2.28) obtained on a uniform mesh and for a constant Q shows that the effect of using the Petrov-Galerkin procedure is equivalent to the use of a standard Galerkin process with the addition of a diffusion

$$k_b = \tfrac{1}{2}\alpha U h \tag{2.31}$$

to the original differential equation (2.12). The reader can easily verify that with this substituted into the original equation, thus writing now in place of Eq. (2.12)

$$U\frac{\mathrm{d}\phi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left[(k+k_b)\frac{\mathrm{d}\phi}{\mathrm{d}x}\right] + Q = 0 \tag{2.32}$$

we obtain an identical expression to that of Eq. (2.28) providing Q is constant and a standard Galerkin procedure is used.

Such *balancing diffusion* is easier to implement than Petrov-Galerkin weighting, particularly in two or three dimensions, and has some physical merit in the interpretation of the Petrov-Galerkin methods. However, it does not provide the required modification of source terms, and for instance in the example of Fig. 2.7 will give erroneous results identical with a simple finite difference, upwind, approximation.

The concept of *artificial diffusion* introduced frequently in finite difference models suffers of course from the same drawbacks and in addition cannot be logically justified.

It is of interest to observe that a central difference approximation, when applied to the original equations (or the use of the standard Galerkin process), fails by introducing a *negative diffusion* [13] into the equations. This "negative" diffusion is countered by the present, balancing, one.

2.2.4 A variational principle in one dimension

Equation (2.12), which we are considering here, is not self-adjoint and hence is not directly derivable from any variational principle. However, it was shown by Guymon et al. [14] that it is a simple matter to derive a variational principle (or ensure self-adjointness, which is equivalent) if the operator is premultiplied by a suitable function p. Thus we write a weak form of Eq. (2.12) as

$$\int_0^L vp\left[U\frac{\mathrm{d}\phi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}\phi}{\mathrm{d}x}\right) + Q\right]\mathrm{d}x = 0 \tag{2.33}$$

where $p = p(x)$ is as yet undetermined. This gives, on integration by parts,

$$\int_0^L \left[v \frac{\mathrm{d}\phi}{\mathrm{d}x} \left(pU + k \frac{\mathrm{d}p}{\mathrm{d}x} \right) + \frac{\mathrm{d}v}{\mathrm{d}x} (k\, p) \frac{\mathrm{d}\phi}{\mathrm{d}x} + v\, p\, Q \right] \mathrm{d}x + v\, k\, p \frac{\mathrm{d}\phi}{\mathrm{d}x} \Big|_0^L = 0 \tag{2.34}$$

Immediately we see that the operator can be made self-adjoint and a symmetric approximation achieved if the first term in square brackets is made zero [15]. This requires that p be chosen so that

$$pU + k \frac{\mathrm{d}p}{\mathrm{d}x} = 0 \tag{2.35a}$$

or that

$$p = C\mathrm{e}^{-Ux/k} = C\mathrm{e}^{-2\,Pe\,x/h} \tag{2.35b}$$

For such a form corresponding to the existence of a variational principle the "best" approximation is that of the Galerkin method with

$$v = \sum N_a \tilde{v}_a \qquad \text{and} \qquad \phi = \sum N_b \tilde{\phi}_b \tag{2.36}$$

where $\tilde{v}_a$ is an arbitrary parameter.

Indeed, such a formulation will, in one dimension, yield exact answers at nodes [15,16]. It must therefore be equivalent to that obtained earlier by weighting in the Petrov-Galerkin manner. Inserting the approximation of Eq. (2.36) into Eq. (2.34), with Eqs. (2.35a) and (2.35b) defining p using an origin at $x = x_a$, we have for the ath equation of the uniform mesh

$$\int_{-h}^{h} \left[\frac{\mathrm{d}N_a}{\mathrm{d}x} (k\mathrm{e}^{-2Pe\,x/h}) \frac{\mathrm{d}N_b}{\mathrm{d}x} \tilde{\phi}_b + N_a \mathrm{e}^{-2Pe\,x/h} Q \right] \mathrm{d}x = 0 \tag{2.37}$$

with $b = a - 1, a, a + 1$. This gives, after some algebra, a typical nodal equation:

$$\left(1 - \mathrm{e}^{2Pe}\right) \tilde{\phi}_{a-1} + \left(\mathrm{e}^{2Pe} - \mathrm{e}^{-2Pe}\right) \tilde{\phi}_a - \left(1 - \mathrm{e}^{-2Pe}\right) \tilde{\phi}_{a+1} + \frac{Qh^2}{2Pe\,k} \left(\mathrm{e}^{Pe} - \mathrm{e}^{-Pe}\right)^2 = 0 \tag{2.38}$$

which can be shown to be identical with the expression (2.28) *into which* $\alpha = \alpha_{\text{opt}}$ *given by Eq.* (2.29) *has been inserted.*

Here we have a somewhat more convincing proof of the optimality of the proposed Petrov-Galerkin weighting [17,18] introduced in the previous subsection. However, serious drawbacks exist. The numerical evaluation of the integrals is difficult and the equation system, though symmetric overall, is not well conditioned if p is taken as a continuous function of x through the whole domain. The second point is easily overcome by taking p to be *locally* defined, for instance taking the origin of x at point a for *all assemblies* as we did in deriving Eq. (2.38). This is permissible by arguments

given in Section 2.2.1 and is equivalent to scaling the full equation system row by row [17]. Now of course the total equation system ceases to be symmetric.

The numerical integration difficulties disappear, of course, if the simple weighting functions previously derived are used. However, the proof of equivalence is important as the problem of determining the optimal weighting is no longer necessary.

2.2.5 Galerkin least-squares approximation (GLS) in one dimension

In the preceding sections we have shown that many, apparently different, approaches have resulted in identical (or almost identical) approximations. Here another procedure is presented which again will produce similar results. In this a combination of standard Galerkin and least-squares approximation is made [19,20].

If Eq. (2.12) is rewritten as

$$\mathcal{L}(\phi) + Q = 0 \qquad \phi \approx \widehat{\phi} = \mathbf{N}\tilde{\boldsymbol{\phi}} \tag{2.39a}$$

with

$$L = U\frac{\mathrm{d}}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}}{\mathrm{d}x}\right) \tag{2.39b}$$

the standard Galerkin approximation gives for the ath equation

$$\int_\Omega N_a \left[\mathcal{L}(\widehat{\phi}) + Q\right]\mathrm{d}x = 0 \tag{2.40}$$

with boundary conditions omitted for simplicity.

Similarly, a least-squares minimization of the residual $R = \mathcal{L}(\widehat{\phi}) + Q$ results in

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\tilde{\phi}^a}\int_\Omega R^2\mathrm{d}x = \int_\Omega \frac{\mathrm{d}\mathcal{L}(\widehat{\phi})}{\mathrm{d}\tilde{\phi}^a}[\mathcal{L}(\widehat{\phi}) + Q]\mathrm{d}x \tag{2.41}$$

or

$$\int_\Omega \left[U\frac{\mathrm{d}N_a}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}N_a}{\mathrm{d}x}\right)\right](\mathcal{L}(\widehat{\phi}) + Q)\mathrm{d}x = \int_\Omega \mathcal{L}(N_a)\left[\mathcal{L}(\widehat{\phi}) + Q\right]\mathrm{d}x \tag{2.42}$$

If the final approximation is written as a linear combination of Eqs. (2.40) and (2.42), we have

$$\int_\Omega \left[N_a + \lambda\left(U\frac{\mathrm{d}N_a}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}N_a}{\mathrm{d}x}\right)\right)\right](\mathcal{L}(\widehat{\phi}) + Q)\mathrm{d}x = 0$$

or

$$\int_\Omega \left[N_a + \lambda\,\mathcal{L}(N_a)\right](\mathcal{L}(\widehat{\phi}) + Q)\mathrm{d}x = 0 \tag{2.43}$$

If the second-derivative term on N_a is omitted (as could be done assuming linear N_a and a mollification as in Fig. 2.4), Eq. (2.43) is the same as the Petrov-Galerkin

approximation with an undetermined parameter λ. Indeed, if we take

$$\lambda = \frac{\alpha h}{2|U|} \tag{2.44}$$

the approximation is identical to that of the Petrov-Galerkin method with the weighting given by Eqs. (2.24) and (2.25).

Once again we see that a Petrov-Galerkin form written as

$$\int_\Omega \left(N_a + \frac{\alpha h}{2} \frac{U}{|U|} \frac{\mathrm{d}N_a}{\mathrm{d}x} \right) \left(U \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x} \left(k \frac{\mathrm{d}\widehat{\phi}}{\mathrm{d}x} \right) + Q \right) \mathrm{d}x = 0 \tag{2.45}$$

is a result that follows from diverse approaches, though only the variational form of Section 2.2.4 and that using an exact solution of the adjoint differential equation explicitly determine the value of α that should optimally be used. In all the other derivations this value is determined by an *a posteriori* analysis.

2.2.6 Subgrid scale (SGS) approximation

The SGS method was originally introduced by Hughes [21,22] following the principles of turbulence modeling. More details on the method as applied to convection-diffusion problems are available in Ref. [23]. In this method the scalar quantity is divided into two parts $\overline{\phi}$ and ϕ', and Eq. (2.12) is written as

$$\begin{gathered} U \frac{\mathrm{d}}{\mathrm{d}x} (\overline{\phi} + \phi') - \frac{\mathrm{d}}{\mathrm{d}x} \left[k \frac{\mathrm{d}}{\mathrm{d}x} (\overline{\phi} + \phi') \right] + Q = 0 \\ \text{or} \\ \mathcal{L}(\overline{\phi}) + \mathcal{L}(\phi') + Q = 0 \end{gathered} \tag{2.46}$$

In the above split $\overline{\phi}$ is assumed to be the solution given by a finite element discretization (the so-called resolved scale) and ϕ' the unresolved, fine-scale part of the solution.

If we construct a weak form for the problem, we have

$$\int_\Omega v \left[\mathcal{L}(\overline{\phi}) + \mathcal{L}(\phi') + Q \right] \mathrm{d}x = 0 \tag{2.47}$$

where Ω is the domain considered. After integration by parts and assuming boundary conditions for ϕ' are zero at the boundaries of each element (i.e., assuming that $\overline{\phi}$ has values at element boundaries which are accurate and oscillation free) we obtain

$$\int_\Omega v \left[U \frac{\mathrm{d}\overline{\phi}}{\mathrm{d}x} + Q \right] \mathrm{d}x + \int_\Omega \frac{\mathrm{d}v}{\mathrm{d}x} k \frac{\mathrm{d}\overline{\phi}}{\mathrm{d}x} \mathrm{d}x + \int_\Omega \mathcal{L}^\star(v)\, \phi' \, \mathrm{d}x + v\, \bar{q}_n \Big|_{\Gamma_q} = 0 \tag{2.48}$$

where

$$\mathcal{L}^\star(v) = -U \frac{\mathrm{d}v}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x} \left(k \frac{\mathrm{d}v}{\mathrm{d}x} \right) \tag{2.49}$$

is the adjoint differential equation. As shown before, the solution using $\overline{\phi}$ alone with a standard Galerkin method leads to oscillatory results when convection effects are significant. Here we wish to take account of effects from the unresolved part when computing $\overline{\phi}$. From (2.46) we obtain

$$\mathcal{L}(\phi') = -(\mathcal{L}(\overline{\phi}) + Q) \tag{2.50}$$

for which the Green's function solution gives

$$\phi'(x) = -\int g(x, y)\left[\mathcal{L}\left(\overline{\phi}(y)\right) + Q\right] \mathrm{d}y \tag{2.51}$$

What we need here, however, is a simple approximation which does not require such a complex solution (and the Green's function). Using the simple approximation

$$\phi'(x) = -\beta\left[\mathcal{L}(\overline{\phi}(x)) + Q\right] \tag{2.52}$$

with *beta* appropriately defined has been shown by Codina to give accurate results [23]. Substitution of (2.52) into (2.48) gives

$$\begin{aligned}\int_\Omega v\left[U\frac{\mathrm{d}\overline{\phi}}{\mathrm{d}x} + Q\right]\mathrm{d}x + \int_\Omega \frac{\mathrm{d}v}{\mathrm{d}x}\,k\frac{\mathrm{d}\overline{\phi}}{\mathrm{d}x}\,\mathrm{d}x \\ - \int_\Omega \mathcal{L}^\star(v)\,\beta\left[\mathcal{L}(\overline{\phi}) + Q\right]\mathrm{d}x + v\,\bar{q}_n\Big|_{\Gamma_q} = 0\end{aligned} \tag{2.53}$$

If higher-order derivative terms are neglected in the above equation and $\beta = \alpha h/2|U|$, the formulation is identical to that of the Petrov-Galerkin method and the Galerkin least-squares method. However, if Q contains reaction terms such equivalence is lost and some differences occur [23].

2.2.7 The finite increment calculus (FIC) for stabilizing the convective-diffusion equation in one dimension

As mentioned in the previous sections, there are many procedures which give nearly identical results to those of the Petrov-Galerkin approximation. We shall also find a number of such procedures arising directly from the transient formulations discussed in Part II of this chapter; however, there is one further process that can be applied directly to the steady-state equation. This process was suggested by Oñate in 1998 [24] and we describe its basis below.

We start at the stage where the conservation equation of the type given by Eq. (2.6) is derived. Now instead of considering an infinitesimal control volume of length "dx," we consider a finite length δ. Expanding to one higher order by Taylor series (backwards), we obtain instead of Eq. (2.12)

$$U\frac{\mathrm{d}\phi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}\phi}{\mathrm{d}x}\right) + Q - \frac{\delta}{2}\frac{\mathrm{d}}{\mathrm{d}x}\left[U\frac{\mathrm{d}\phi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left(k\frac{\mathrm{d}\phi}{\mathrm{d}x}\right) + Q\right] = 0 \tag{2.54}$$

with δ being the finite distance which is smaller than or equal to that of the element size h. Rearranging terms and substituting $\delta = \alpha h$ we have (assuming positives U)

$$U\frac{\mathrm{d}\phi}{\mathrm{d}x} - \frac{\mathrm{d}}{\mathrm{d}x}\left[\left(k + \frac{\alpha h U}{2}\right)\frac{\mathrm{d}\phi}{\mathrm{d}x}\right] + Q - \frac{\delta}{2}\frac{\mathrm{d}Q}{\mathrm{d}x} = 0 \tag{2.55}$$

In the above equation we have omitted the higher-order expansion for the diffusion term as in the previous sections. The final equations are now obtained by applying the Galerkin method with $W_a = N_a$.

From the last equation we see immediately that a stabilizing term has been recovered and the additional term $\alpha h U/2$ is identical to that of the Petrov-Galerkin form (Eq. 2.28).

There is no need to discuss further and we see how the finite increment procedure has again yielded exactly the same result by directly modifying the conservation differential equations. In Ref. [24] it is shown further that arguments can be brought to determine α as being precisely the optimal value we have already obtained by studying the Petrov-Galerkin method.

2.2.8 Higher-order approximations

The derivation of accurate Petrov-Galerkin procedures for the convective-diffusion equation is of course possible for any order of finite element expansion. In Ref. [8] Heinrich and Zienkiewicz show how the procedure of studying exact discrete solutions can yield optimal upwind parameters for quadratic shape functions. However, here the simplest approach involves the procedures of Section 2.2.4, which are available of course for any element expansion and, as shown before, will always give an optimal approximation at nodes.

We thus recommend the reader pursue the example discussed in that section and, by extending Eq. (2.37), arrive at an appropriate equation linking the two quadratic elements of Fig. 2.8. For higher-order elements the solution gives exact values at interior nodes.

For practical purposes it is possible to extend the Petrov-Galerkin weighting of the type given in Eqs. (2.24)–(2.27) now using

$$\alpha_{\text{opt}} = \coth Pe - \frac{1}{Pe} \tag{2.56a}$$

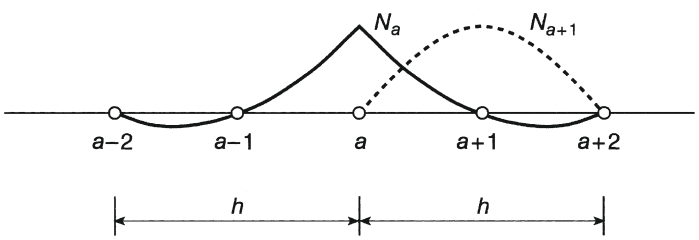

FIGURE 2.8
Assembly of one-dimensional quadratic elements.

for the midside node and

$$\alpha_{\text{opt}} = \frac{(\coth Pe - 1/Pe) - (\cosh Pe)^2(\coth 2Pe - 1/(2Pe))}{1 - (\cosh Pe)^2/2} \tag{2.56b}$$

for side nodes. A simplified procedure, though not as exact as that for linear elements, is very effective and has been used with success for solution of Navier-Stokes equations [25].

The subject of optimal upwinding for higher-order approximations has been studied further and Refs. [9,26,27] show the developments.

2.3 The steady-state problem in two (or three) dimensions

2.3.1 General remarks

It is clear that the application of standard Galerkin discretization to the steady-state scalar convection-diffusion equation in several space dimensions is similar to the problem discussed previously in Section 2.2.1 in one dimension and will again yield unsatisfactory answers with high oscillation for local Peclet numbers greater than unity.

The equation now considered is the steady-state version of Eq. (2.8) in multidimensions, i.e.,

$$U_i \frac{\partial \phi}{\partial x_i} - \frac{\partial}{\partial x_i}\left(k \frac{\partial \phi}{\partial x_i}\right) + Q = 0 \tag{2.57}$$

Obviously the problem is now of greater practical interest than the one-dimensional case so far discussed, and a satisfactory solution is important. Again, all of the possible numerical approaches we have discussed are applicable.

2.3.2 Streamline (upwind) Petrov-Galerkin weighting (SUPG)

The most obvious procedure is to use again some form of Petrov-Galerkin method of the type introduced in Section 2.2.2 and Eqs. (2.24)–(2.29), seeking optimality of α in some heuristic manner. Restricting attention here to two dimensions, we note immediately that the Peclet parameter

$$\mathbf{Pe} = \frac{\mathbf{U}h}{2k} \qquad \mathbf{U} = \begin{Bmatrix} U_1 \\ U_2 \end{Bmatrix} \tag{2.58}$$

is now a "vector" quantity and hence that upwinding needs to be "directional."

The first reasonably satisfactory attempt to do this consisted of determining the optimal Petrov-Galerkin formulation using $\alpha W^\star$ based on components of $\mathbf{U}$ associated to the *sides of elements* and obtaining the final weight functions by a blending procedure [7,8].

A better method was soon realized when the analogy between balancing diffusion and upwinding was established, as shown in Section 2.2.3. In two (or three) dimensions the convection is only active in the direction of the resultant element velocity $\mathbf{U}$,

and hence the corrective, or *balancing*, *diffusion* introduced by upwinding should be anisotropic with a coefficient different from zero only in the direction of the resultant velocity. This innovation introduced simultaneously by Hughes and Brooks [28,29] and Kelly et al. [10] can be readily accomplished by taking the individual weighting functions as

$$\begin{aligned} W_a &= N_a + \alpha W_a^\star \\ &\equiv N_a + \frac{\alpha h}{2}\frac{U_i}{|\mathbf{U}|}\frac{\partial N_a}{\partial x_i} \end{aligned} \tag{2.59}$$

with this last form being applicable to two and three dimensions. Here α is determined for each element by the previously found expression (2.25) written as follows:

$$\alpha = \alpha_{\text{opt}} = \coth Pe - \frac{1}{Pe} \tag{2.60}$$

where

$$Pe = \frac{|\mathbf{U}|h}{2k} \qquad \text{with} \qquad |\mathbf{U}| = \sqrt{U_i U_i} \tag{2.61}$$

The above expressions presuppose that the velocity components U_i in a particular element are substantially constant and that the element size h can be reasonably defined.

Figure 2.9 shows an assembly of a linear triangle and bilinear quadrilateral for each of which the mean resultant velocity $\mathbf{U}$ is indicated. Determination of the element size h to use in expression (2.61) is of course somewhat arbitrary. In Fig. 2.9 we show it simply as the size in the direction of the velocity vector.

The form of Eq. (2.59) is such that the "nonstandard" weighting $W^\star$ has a zero effect in the direction where the velocity is zero. Thus the balancing diffusion is only introduced in the direction of the resultant (convective) velocity vector $\mathbf{U}$.

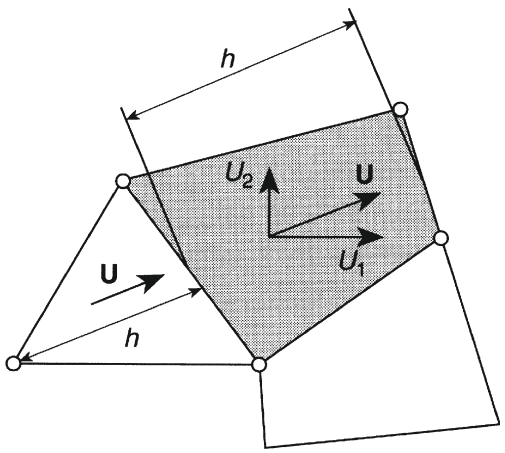

FIGURE 2.9
A two-dimensional, streamline assembly. Element size h and streamline directions.

Introducing the approximation

$$\phi \approx \widehat{\phi} = \sum_a N_a(x_i)\tilde{\phi}_a \tag{2.62}$$

and using the weights given by Eq. (2.59) the SUPG method is computed from the weighted residual form

$$\int_\Omega \left[N_a + \frac{\alpha h}{2}\frac{U_i}{|\mathbf{U}|}\frac{\partial N_a}{\partial x_i}\right]\left[\mathcal{L}(\widehat{\phi}) + Q\right] \mathrm{d}\Omega = 0 \tag{2.63}$$

or after integration by parts and introduction of the natural boundary condition on Γ_q

$$\int_\Omega \left[N_a\left(U_i\frac{\partial\widehat{\phi}}{\partial x_i} + Q\right) + \frac{\partial N_a}{\partial x_i}k\frac{\partial\widehat{\phi}}{\partial x_i} + \frac{\alpha h}{2}\frac{U_i}{|\mathbf{U}|}\frac{\partial N_a}{\partial x_i}\left(\mathcal{L}(\widehat{\phi}) + Q\right)\right]\mathrm{d}\Omega + \int_{\Gamma_q} N_a\bar{q}_n \mathrm{d}\Gamma = 0 \tag{2.64}$$

where $\bar{q}_n = -k\partial\widehat{\phi}/\partial n$. In the discretized form the "balancing diffusion" term becomes

$$\int_\Omega \frac{\partial N_a}{\partial x_i}\tilde{k}_{ij}\frac{\partial N_b}{\partial x_j}\mathrm{d}\Omega \tag{2.65}$$

with

$$\tilde{k}_{ij} = \frac{\alpha U_i U_j}{|\mathbf{U}|}\frac{h}{2} \tag{2.66}$$

This indicates a zero coefficient normal to the convective velocity vector direction. It is therefore named the *streamline balancing diffusion* [10,28,29] or streamline upwind Petrov-Galerkin process.

The streamline diffusion should allow discontinuities in the direction normal to the streamline to travel without appreciable distortion. However, with the standard finite element approximations actual discontinuities cannot be modeled and in practice some oscillations may develop. For this reason some investigators add a smoothing diffusion in the direction normal to the streamlines (crosswind diffusion) [30–33].

The mathematical validity of the procedure introduced in this section has been established by Johnson et al. [34] for $\alpha = 1$, showing convergence improvement over the standard Galerkin process. However, the proof does not include any optimality in the selection of α values as shown by Eq. (2.60).

Figure 2.10 shows a typical solution of Eq. (2.57), indicating the very small amount of "crosswind diffusion," i.e., allowing discontinuities to propagate in the direction of flow without substantial smearing [35].

A more convincing "optimality" can be achieved by applying the exponential modifying function, making the problem self-adjoint. This of course follows precisely the procedures of Section 2.2.4 and is easily accomplished if the velocities are constant

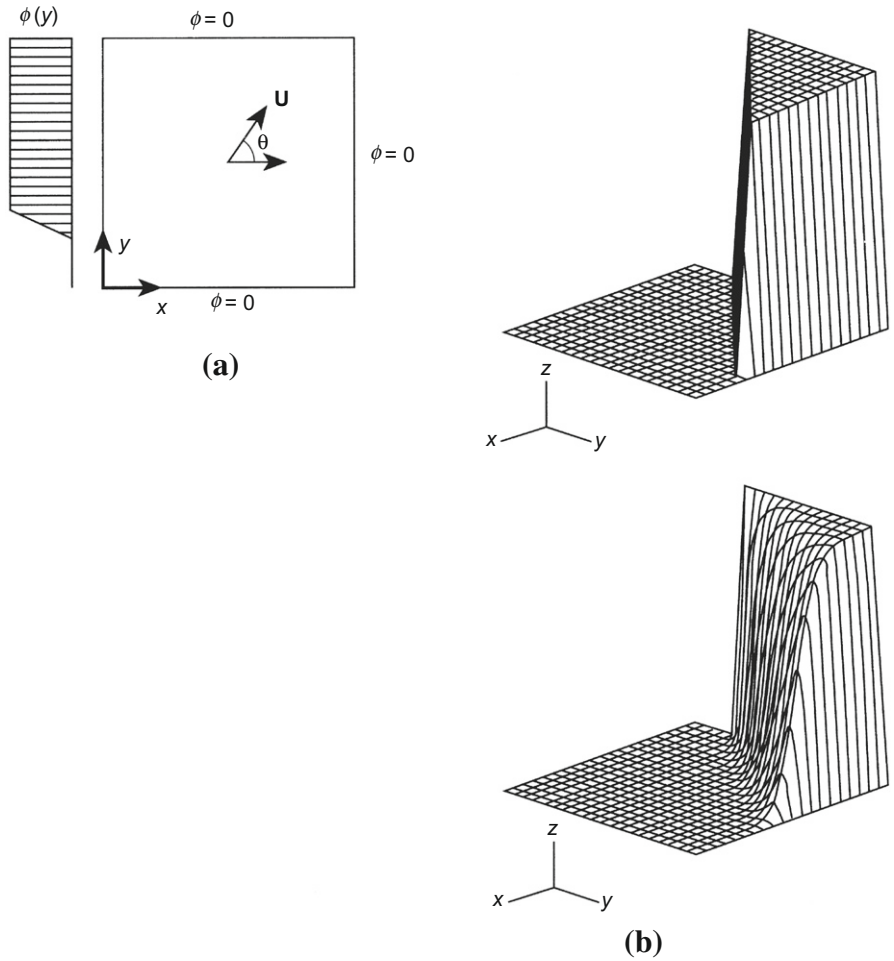

FIGURE 2.10
"Streamline" procedures in a two-dimensional problem of pure convection. Bilinear elements [35]: (a) boundary conditions for test problem; solutions for $\theta = 45°$ (top) and $\theta = 65°$.

in the element assembly domain. If velocities vary from element to element, again the exponential functions

$$p = \mathrm{e}^{-Ux'/k} \tag{2.67}$$

with x' oriented in the velocity direction in each element can be taken. This appears to have been first implemented by Sampaio [35] but problems regarding the origin of coordinates, etc., have once again to be addressed. However, the results are similar to those achieved here by the streamline upwind Petrov-Galerkin procedure.

2.3.3 Galerkin least squares (GLS) and finite increment calculus (FIC) in multidimensional problems

It is of interest to observe that the somewhat intuitive approach to the generation of the "streamline" Petrov-Galerkin weight functions of Eq. (2.59) can be avoided if the least-squares Galerkin procedure of Section 2.2.5 is extended to deal with the multidimensional equation. Simple extension of the reasoning given in Eqs. (2.39a)–(2.45) will immediately yield the weighting of Eq. (2.59).

Extension of the GLS to two or three dimensions gives (again using indicial notation)

$$\int_{\Omega} \left(N_a + \lambda \mathcal{L}(N_a)\right)\left(U_j \frac{\partial \widehat{\phi}}{\partial x_j} - \frac{\partial}{\partial x_j}\left(k \frac{\partial \widehat{\phi}}{\partial x_j}\right) + Q\right) \mathrm{d}\Omega = 0 \tag{2.68}$$

where

$$\mathcal{L}(N_a) = U_i \frac{\partial N_a}{\partial x_i} + \frac{\partial}{\partial x_i}\left(k \frac{\partial N_a}{\partial x_i}\right) \tag{2.69}$$

In the above equation after integration by parts, higher-order derivative terms of two or more are omitted for the sake of simplicity. As in one dimension [Eq. (2.43)] we have an additional weighting term. Now assuming

$$\lambda = \frac{\alpha h}{2|\mathbf{U}|} \tag{2.70}$$

we obtain an identical stabilizing term to that of the streamline Petrov-Galerkin procedure [Eq. (2.64)].

The finite increment calculus method in multidimensions can be written as [24]

$$U_j \frac{\partial \phi}{\partial x_j} - \frac{\partial}{\partial x_j}\left(k \frac{\partial \phi}{\partial x_j}\right) + Q - \frac{\delta_i}{2} \frac{\partial}{\partial x_i}\left[U_j \frac{\partial \phi}{\partial x_j} - \frac{\partial}{\partial x_j}\left(k \frac{\partial \phi}{\partial x_j}\right) + Q\right] = 0$$

or

$$\mathcal{L}(\phi) + Q - \frac{\delta_i}{2}\left[\mathcal{L}(\phi) + Q\right] = 0 \tag{2.71}$$

Note that the value of δ_i is now dependent on the coordinate direction. To obtain streamline-oriented stabilization, we simply assume that δ_i is the projection oriented along the streamlines. Now

$$\delta_i = \delta \frac{U_i}{|\mathbf{U}|} \tag{2.72}$$

With $\delta = \alpha h$ and again omitting the higher-order derivative terms in k, the streamline Petrov-Galerkin form of stabilization is obtained [Eq. (2.64)]. The reader can verify that both the GLS and FIC produce the correct weighting for the source term Q as of course is required by the Petrov-Galerkin method.

The extension of the SGS procedure to multidimensions is straightforward and follows the approach explained in Section 2.2.6.

2.4 Steady state: Concluding remarks

In Sections 2.2 and 2.3 we presented several currently used procedures for dealing with the steady-state convection-diffusion equation with a scalar variable. All of these translate essentially to the use of streamline Petrov-Galerkin discretization, though of course the modification of the basic equations to a self-adjoint form given in Section 2.2.4 provides the *full justification* of the special weighting. Which of the procedures is best used in practice is largely a matter of taste, as all can give excellent results.

The generalized representation of all the stabilization methods discussed in this part may be written as

$$\int_\Omega \left(N_a + \gamma_i \frac{\partial N_a}{\partial x_i} \right) \left[U \frac{\partial N_a}{\partial x} \widehat{\phi}^a + \frac{\partial N_1}{\partial x} k \frac{\partial N_b}{\partial x} \widehat{\phi}^b + Q \right] \mathrm{d}\Omega = 0 \tag{2.73}$$

where γ_i is a stabilizing parameter.

In the second part of this chapter dealing with transient problems it will be found that similar stabilizing forms arise directly when steady state is reached or assumed.

In this case the parameter γ_i is now replaced by another one involving the length of the time step Δt. We shall show at the end of the next section a comparison between various procedures for stabilization and will note essentially the same forms in the steady-state situation.

Part II: Transients

2.5 Transients: Introductory remarks

2.5.1 Mathematical background

The objective of this section is to develop procedures of general applicability for the solution by direct time-stepping methods of Eq. (2.1) written for scalar values of ϕ, F_i, and G_i. Starting from the scalar form Eq. (2.8)

$$\frac{\partial \phi}{\partial t} + \frac{\partial (U_i \phi)}{\partial x_i} - \frac{\partial}{\partial x_i} \left(k \frac{\partial \phi}{\partial x_i} \right) + Q = 0 \tag{2.74}$$

though consideration of the procedure for dealing with a vector-valued function is included in Appendix D. To allow a simple interpretation of the various methods and of behavior patterns the scalar equation in one dimension in nonconservation form [see Eq. (2.11)], i.e.,

$$\frac{\partial \phi}{\partial t} + U \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \left(k \frac{\partial \phi}{\partial x} \right) + Q = 0 \tag{2.75}$$

will be considered. The problem so defined is nonlinear unless U is independent of ϕ. However, the nonconservative equation (2.75) admits a spatial variation of U and is quite general.

In the general form (2.74) the main behavior patterns can be determined by a change of the independent variable x to x' such that

$$\mathrm{d}x' = \mathrm{d}x - U\,\mathrm{d}t \tag{2.76}$$

Noting that for $\phi = \phi(x', t)$ we have

$$\left.\frac{\partial \phi}{\partial t}\right|_{x \text{ const}} = \frac{\partial \phi}{\partial x'}\frac{\partial x'}{\partial t} + \left.\frac{\partial \phi}{\partial t}\right|_{x' \text{ const}} = -U\frac{\partial \phi}{\partial x'} + \left.\frac{\partial \phi}{\partial t}\right|_{x' \text{ const}} \tag{2.77}$$

The one-dimensional equation (2.75) now becomes simply

$$\frac{\partial \phi}{\partial t} - \frac{\partial}{\partial x'}\left(k\frac{\partial \phi}{\partial x'}\right) + Q(x') = 0 \tag{2.78}$$

and equations of this type can be readily discretized with self-adjoint spatial operators and solved by standard finite element Galerkin procedures [15].

The coordinate system of Eq. (2.76) describes *characteristic directions* and the moving nature of the coordinates must be noted. A further corollary of the coordinate change is that with no conduction or source terms, i.e., when $k = 0$ and $Q = 0$, we have simply

$$\frac{\partial \phi}{\partial t} = 0 \tag{2.79a}$$

or, for the one-dimensional case,

$$\phi(x') = \phi(x - Ut) = \text{constant} \tag{2.79b}$$

along a characteristic (assuming U to be constant). This is a typical equation of a wave propagating with a velocity U in the x direction, as shown in Fig. 2.11. The wave nature is evident in the problem even if the conduction (diffusion) is not zero, and in this case we shall have solutions showing a wave that attenuates with the distance traveled.

2.5.2 Possible discretization procedures

In Part I of this chapter we have concentrated on the essential methods applicable directly to the steady-state equations. These procedures started off from somewhat heuristic considerations. The Petrov-Galerkin method was perhaps the most rational

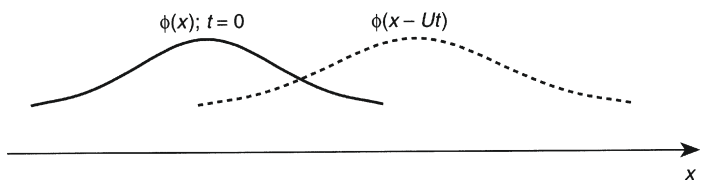

FIGURE 2.11
The wave nature of a solution with no conduction. Constant wave velocity U.

but even here the amount and the nature of the weighting functions were a matter of guesswork which was subsequently justified by consideration of the numerical error at nodal points. The Galerkin least-squares (GLS) method in the same way provided no absolute necessity for improving the answers though of course the least-squares method would tend to increase the symmetry of the equations and thus could be proved useful. It was only by results which turned out to be remarkably similar to those obtained by the Petrov-Galerkin method that we have deemed this method to be a success. The same remark could be directed at the finite increment calculus (FIC) method and indeed to other methods suggested to deal with the problems of steady-state equations.

For the transient solutions the obvious first approach would be to try again the same types of methods used in steady-state calculations and indeed much literature has been devoted to this [23,30–47]. Petrov-Galerkin methods have been used here quite extensively. However, it is obvious that the application of Petrov-Galerkin methods will lead to nonsymmetric mass matrices and these will be difficult to use for any explicit method as mass lumping is not by any means obvious.

Serious difficulty will also arise with the Galerkin least-squares (GLS) procedure even if the temporal variation is generally included by considering space-time finite elements in the whole formulation. This approach to such problems was made by Nguen and Reynen [36], Carey and Jieng [37,38], Johnson and coworkers [34,39,40], and others [41,42]. However the use of space-time elements is expensive as explicit procedures are not available.

Which way, therefore, should we proceed? Is there any other obvious approach which has not been mentioned? The answer lies in the wave nature of the equations which indeed not only permits different methods of approach but in many senses is much more direct and fully justifies the numerical procedures which we shall use later for the full fluid dynamics equations. We shall therefore concentrate on such methods and we will show that they lead to stabilizing diffusions which in form are very similar to those obtained previously by the Petrov-Galerkin method but in a much more direct manner which is consistent with the equations.

The following discussion will therefore be centered on two main directions: we will start with (1) the procedures based on the use of the *characteristics* and the wave nature directly, leading to so-called characteristic-Galerkin methods which we shall discuss in Section 2.6; and then (2) we shall proceed to approach the problem through the use of higher-order time approximations called Taylor-Galerkin methods.

Of the two approaches the first one based on the characteristics is in our view more important. However, for historical and other reasons we shall discuss both methods which for a scalar variable can be shown to give identical answers.

The solutions of convective scalar equations can be given by both approaches very simply. This will form the basis of our treatment for the solution of the full fluid mechanics equations in Chapter 3, where both explicit (time iteration) processes as well as implicit methods can be used.

Many of the methods for solving the transient scalar equations of convective diffusion have been applied to the full fluid mechanics equations, i.e., solving the full vector-valued convective-diffusive equations we presented at the beginning of the

chapter [Eq. (2.1)]. This applies in particular to the Taylor-Galerkin method which has proved to be quite successful in the treatment of high-speed compressible gas flow problems. Indeed this particular approach was the first one adopted to solve such problems. However, the simple wave concepts which are evident in the scalar form of the equations do not translate to such multivariant problems and make the procedures largely heuristic. The same can be said of the direct application of the SUPG and GLS methods to multivariant problems. The procedures such as GLS can provide a useful stabilization of difficulties encountered with incompressible behavior [15]. This does not justify their use on the full equations and we therefore recommend the alternatives to be discussed in Chapter 3.

2.6 Characteristic-based methods

2.6.1 Mesh updating and interpolation methods

We have already observed that, if the spatial coordinate is "convected" in the manner implied by Eq. (2.76), i.e., along the problem *characteristics*, then the convective, first-order, terms disappear. The remaining problem is that of simple diffusion for which discretization procedures with the standard Galerkin spatial approximation are optimal (in an energy norm sense). The most obvious use of this in the finite element context is to update the position of the mesh points in an incremental Lagrangian manner. In Fig. 2.12a we show such an update for the one-dimensional problem of Eq. (2.75) occurring in an interval Δt.

For a constant x' coordinate

$$\mathrm{d}x = U\,\mathrm{d}t \tag{2.80}$$

and for a typical nodal point a, we have

$$x_a^{n+1} = x_a^n + \int_{t_n}^{t_{n+1}} U\,\mathrm{d}t \tag{2.81}$$

where in general the "velocity" U may be dependent on x.

For a constant U we have simply

$$x_a^{n+1} = x_a^n + U\,\Delta t \tag{2.82}$$

for the updated mesh position. This is not always the case and updating generally has to be done with variable U.

On the updated mesh only the time-dependent diffusion problem needs to be solved using the Galerkin method [15].

The process of continuously updating the mesh and solving the diffusion problem on the new mesh is, of course, impractical. When applied to two- or three-dimensional configurations very distorted elements would result and difficulties will always arise near the boundaries of the domain. For these reasons it seems obvious that after completion of a single step a return to the original mesh should be made by interpolating from the updated values to the original mesh positions.

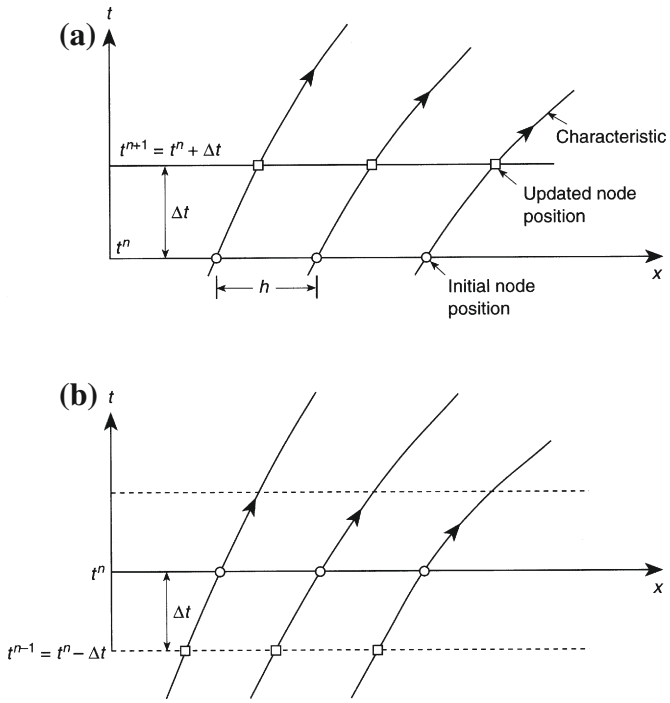

FIGURE 2.12
Mesh updating and interpolation: (a) forward and (b) backward.

This procedure can of course be reversed and characteristic origins traced backwards, as shown in Fig. 2.12b using appropriate interpolated starting values.

The method described is somewhat intuitive but has been used with success for solution of transport equations by Adey and Brebbia [48] and others as early as 1974. The procedure can be formalized and presented more generally and gives the basis of so-called characteristic-Galerkin methods [49].

The diffusion part of the computation is carried out either on the original or on the final mesh, each representing a certain approximation. Intuitively we imagine in the updating scheme that the *operator is split* with the diffusion changes occurring separately from those of convection. This idea is explained in the procedures of the next section.

2.6.2 Characteristic-Galerkin procedures

We shall consider that the equation of convective diffusion in its one-dimensional form (2.75) is split into two parts such that

$$\phi = \phi^{\star} + \phi^{\star\star} \tag{2.83}$$

and separate the differential equation into two additive parts. Accordingly,

$$\frac{\partial \phi^\star}{\partial t} + U\frac{\partial \phi}{\partial x} = 0 \tag{2.84a}$$

is a purely convective system while

$$\frac{\partial \phi^{\star\star}}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) + Q = 0 \tag{2.84b}$$

represents the self-adjoint terms [here Q contains the source, reaction, and term $(\partial U/\partial x)\phi$].

Both $\phi^\star$ and $\phi^{\star\star}$ now are approximated by expansions

$$\widehat{\phi}^\star = N_a\tilde{\phi}_a^\star \qquad \widehat{\phi}^{\star\star} = N_a\tilde{\phi}_a^{\star\star} \tag{2.85}$$

and in a single time step t^n to $t^n + \Delta t = t^{n+1}$ we shall assume that the initial conditions are

$$t = t^n \qquad \phi^\star = 0 \qquad \phi^{\star\star} = \phi^{\star n} \tag{2.86}$$

Standard Galerkin discretization of the diffusion equation allows $\tilde{\boldsymbol{\phi}}^{\star\star n+1}$ to be determined on the given fixed mesh by solving an equation of the form

$$\mathbf{M}\Delta\tilde{\boldsymbol{\phi}}^{\star\star n} = \Delta t\left[\mathbf{H}(\tilde{\boldsymbol{\phi}}^n + \theta\Delta\tilde{\boldsymbol{\phi}}^{\star\star n}) + \mathbf{f}\right] \tag{2.87}$$

with

$$\tilde{\boldsymbol{\phi}}^{\star\star n+1} = \tilde{\boldsymbol{\phi}}^{\star\star n} + \Delta\tilde{\boldsymbol{\phi}}^{\star\star n}$$

and

$$\begin{aligned} M_{ab} &= \int_\Omega N_a N_b \,\mathrm{d}\Omega \\ H_{ab} &= \int_\Omega \frac{\partial N_a}{\partial x_i}\, k\, \frac{\partial N_b}{\partial x_i}\,\mathrm{d}\Omega \\ f_a &= \int_\Omega N_a\, Q\,\mathrm{d}\Omega \end{aligned}$$

In solving the convective problem we assume that $\phi^\star$ remains unchanged along the characteristic. However, Fig. 2.13 shows how the initial value of $\phi^{\star n}$ interpolated by standard linear shape functions at time n [see Eq. (2.85)] becomes shifted and distorted. The new value is given by

$$\phi^{\star n+1} = N_a(y)\tilde{\phi}_a^{\star n} \qquad y = x + U\Delta t \tag{2.88}$$

As we require $\phi^{\star n+1}$ to be approximated by standard shape functions, we shall write a projection for smoothing of these values as

$$\int_\Omega \mathbf{N}^{\mathrm{T}}(\mathbf{N}\tilde{\boldsymbol{\phi}}^{\star n+1} - \mathbf{N}(y)\tilde{\boldsymbol{\phi}}^{\star n})\mathrm{d}x = 0 \tag{2.89}$$

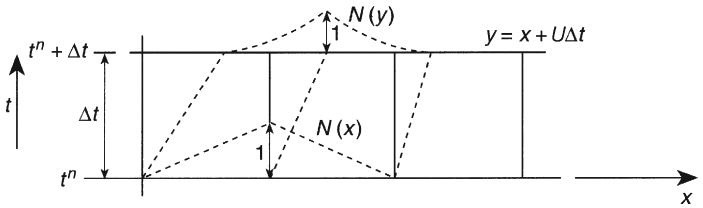

FIGURE 2.13
Distortion of convected shape function.

giving

$$\mathbf{M}\tilde{\boldsymbol{\phi}}^{\star n+1} = \int_{\Omega} [\mathbf{N}^{\mathrm{T}}\mathbf{N}(y)\mathrm{d}x]\tilde{\boldsymbol{\phi}}^{\star n} \tag{2.90}$$

The evaluation of the above integrals is of course still complex, especially if the procedure is extended to two or three dimensions. This is generally performed numerically and the stability of the formulation is dependent on the accuracy of such integration [49]. The scheme is stable and indeed exact as far as the convective terms are concerned if the integration is performed exactly (which of course is an unreachable goal). However, stability and indeed accuracy will even then be controlled by the diffusion terms where several approximations have been involved.

2.6.3 A simple explicit characteristic-Galerkin procedure

Many variants of the schemes described in the previous section are possible and were introduced quite early. References [48–59] present some successful versions. However, all methods then proposed are somewhat complex in programming and are time consuming. For this reason a simpler alternative was developed in which the difficulties are avoided at the expense of conditional stability. This method was first published in 1984 [60] and is fully described in numerous publications [61–64]. Its derivation involves a local Taylor expansion and we illustrate this in Fig. 2.14.

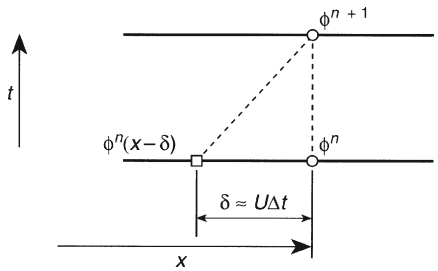

FIGURE 2.14
A simple characteristic-Galerkin procedure.

We can write Eq. (2.75) along the characteristic as

$$\frac{\partial \phi}{\partial t}(x'(t), t) - \frac{\partial}{\partial x'}\left(k\frac{\partial \phi}{\partial x'}\right) - Q(x') = 0 \tag{2.91}$$

As we can see, in the moving coordinate x', the convective acceleration term disappears and source and diffusion terms are averaged quantities along the characteristic. Now the equation is self-adjoint and the Galerkin spatial approximation is optimal. The time discretization of the above equation along the characteristic (Fig. 2.14) gives

$$\begin{aligned}\frac{1}{\Delta t}\left(\phi^{n+1} - \phi^n|_{(x-\delta)}\right) \approx\ & \theta\left[\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) - Q\right]^{n+1} \\ & + (1-\theta)\left[\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) - Q\right]^{n}|_{(x-\delta)}\end{aligned} \tag{2.92}$$

where θ is equal to zero for explicit forms and between zero and unity for semi-implicit and fully implicit forms. As we know, the solution of the above equation in moving coordinates leads to mesh updating and presents difficulties, so we will suggest alternatives. From the Taylor expansion we have

$$\phi^n|_{(x-\delta)} \approx \phi^n - \delta\frac{\partial \phi^n}{\partial x} + \frac{\delta^2}{2}\frac{\partial^2 \phi^n}{\partial x^2} + O(\Delta t^3) \tag{2.93}$$

and assuming $\theta = 0.5$

$$\begin{aligned}&\tfrac{1}{2}\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right)|_{(x-\delta)} \approx \tfrac{1}{2}\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right)^n - \frac{\delta}{2}\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right)^n\right] + O(\Delta t^2) \\ &\text{and}\quad \tfrac{1}{2}Q|_{(x-\delta)} \approx \frac{Q^n}{2} - \frac{\delta}{2}\frac{\partial Q^n}{\partial x}\end{aligned} \tag{2.94}$$

where δ is the distance traveled by a particle in the x-direction (Fig. 2.14) which is

$$\delta = \bar{U}\Delta t \tag{2.95}$$

where $\bar{U}$ is an average value of U along the characteristic. Different approximations of $\bar{U}$ lead to different stabilizing terms. The following relation is commonly used [65,66]:

$$\bar{U} = U^n - U^n\Delta t\frac{\partial U^n}{\partial x} \tag{2.96}$$

Inserting Eqs. (2.93)–(2.96) into Eq. (2.92) we have

$$\begin{aligned}\phi^{n+1} - \phi^n =\ & -\Delta t\left\{U\frac{\partial \phi^n}{\partial x} - \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right)^{n+1/2} + Q^{n+1/2}\right\} \\ & + \Delta t\left\{\frac{\Delta t}{2}\frac{\partial}{\partial x}\left[U^2\frac{\partial \phi}{\partial x}\right] - \frac{\Delta t}{2}U\frac{\partial^2}{\partial x^2}\left(k\frac{\partial \phi}{\partial x}\right) + \frac{\Delta t}{2}U\frac{\partial Q}{\partial x}\right\}^n\end{aligned} \tag{2.97a}$$

where

$$\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right)^{n+1/2} = \tfrac{1}{2}\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right)^{n+1} + \tfrac{1}{2}\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right)^{n} \tag{2.97b}$$

and

$$Q^{n+1/2} = \tfrac{1}{2}(Q^{n+1} + Q^n) \tag{2.97c}$$

In the above equation, higher-order terms are neglected. If $n+1/2$ terms in the above equations are replaced with n terms, the equations become explicit in time. This, as already mentioned, is of a similar form to those resulting from Taylor-Galerkin procedures which will be discussed fully in the next section, and the additional terms ($\Delta t^2/2$ terms) add the stabilizing diffusion in the streamline direction. For multidimensional problems, Eq. (2.97a) can be written in indicial notation and approximating $n+1/2$ terms with n terms (for the fully explicit form)

$$\begin{aligned}\phi^{n+1} - \phi^n = -\Delta t\left\{U_j\frac{\partial \phi}{\partial x_j} - \frac{\partial}{\partial x_i}\left(k\frac{\partial \phi}{\partial x_i}\right) + Q\right\}^n \\ + \Delta t\left\{\frac{\Delta t}{2}\frac{\partial}{\partial x_i}\left[U_i U_j\frac{\partial \phi}{\partial x_j}\right]\right. \\ \left. -\frac{\Delta t}{2}U_k\frac{\partial}{\partial x_k}\left[\frac{\partial}{\partial x_i}\left(k\frac{\partial \phi}{\partial x_i}\right)\right] + \frac{\Delta t}{2}U_i\frac{\partial Q}{\partial x_i}\right\}^n\end{aligned} \tag{2.98}$$

An alternative approximation for $\bar{U}$ is [65]

$$\bar{U} = \tfrac{1}{2}\left(U^{n+1} + U^n|_{(x-\delta)}\right) \tag{2.99}$$

Using the Taylor expansion

$$U^n|_{(x-\delta)} \approx U^n - \Delta t U^n\frac{\partial U^n}{\partial x} + O(\Delta t^2) \tag{2.100}$$

from Eqs. (2.92)–(2.95) and Eqs. (2.99) and (2.100) with θ equal to 0.5 we have

$$\begin{aligned}\frac{1}{\Delta t}(\phi^{n+1} - \phi^n) = -U^{n+1/2}\frac{\partial \phi^n}{\partial x} + \frac{\Delta t}{2}U^n\frac{\partial U^n}{\partial x}\frac{\partial \phi^n}{\partial x} + \frac{\Delta t}{2}U^{n+1/2}U^{n+1/2}\frac{\partial^2 \phi}{\partial x^2} \\ + \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right)^{n+1/2} - \frac{\Delta t}{2}U^{n+1/2}\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right)^n\right] \\ - Q + \frac{\Delta t}{2}U^{n+1/2}\frac{\partial Q}{\partial x}\end{aligned} \tag{2.101}$$

where

$$U^{n+1/2} = \tfrac{1}{2}(U^{n+1} + U^n) \tag{2.102}$$

As mentioned earlier, we can further approximate $n+1/2$ terms using n to get the fully explicit version of the scheme. Thus we have

$$U^{n+1/2} = U^n + O(\Delta t) \tag{2.103}$$

and similarly the diffusion term is approximated. The final form of the explicit characteristic-Galerkin method in one dimension can be written as

$$\Delta\phi = \phi^{n+1} - \phi^n = -\Delta t\left[U^n\frac{\partial\phi}{\partial x} - \frac{\partial}{\partial x}\left(k\frac{\partial\phi}{\partial x}\right) + Q\right]^n + \frac{\Delta t^2}{2}U^n\frac{\partial}{\partial x}\left[U^n\frac{\partial\phi}{\partial x} - \frac{\partial}{\partial x}\left(k\frac{\partial\phi}{\partial x}\right) + Q\right]^n \tag{2.104}$$

Generalization to multidimensions is direct and can be written in indicial notation for equations of the form Eq. (2.6):

$$\Delta\phi = -\Delta t\left[\frac{\partial(U_j\phi)}{\partial x_j} - \frac{\partial}{\partial x_i}\left(k\frac{\partial\phi}{\partial x_i}\right) + Q\right]^n + \frac{\Delta t^2}{2}U_k^n\frac{\partial}{\partial x_k}\left[\frac{\partial(U_j\phi)}{\partial x_j} - \frac{\partial}{\partial x_i}\left(k\frac{\partial\phi}{\partial x_i}\right) + Q\right]^n \tag{2.105}$$

The reader will notice the difference in the stabilizing terms obtained by two different approximations for $\bar{U}$ [Eqs. (2.98) and (2.105)]. However, as we can see the difference between them is small and when U is constant both approximations give identical stabilizing terms. In the rest of the book we shall follow the latter approximation and always use the conservative form of the equations [Eq. (2.105)].

As we proved earlier, the Galerkin spatial approximation is justified when the characteristic-Galerkin procedure is used. We can thus write the approximation

$$\phi = \mathbf{N}\tilde{\boldsymbol{\phi}} \tag{2.106}$$

and use the weighting $\mathbf{N}^{\mathrm{T}}$ in the integrated residual expression. Thus we obtain

$$\mathbf{M}(\tilde{\boldsymbol{\phi}}^{n+1} - \tilde{\boldsymbol{\phi}}^n) = -\Delta t[(\mathbf{C}\tilde{\boldsymbol{\phi}}^n + \mathbf{K}\tilde{\boldsymbol{\phi}}^n + \mathbf{f}^n) - \Delta t(\mathbf{K}_u\tilde{\boldsymbol{\phi}}^n + \mathbf{f}_s^n)] \tag{2.107}$$

In the above equation

$$\mathbf{M} = \int_\Omega \mathbf{N}^{\mathrm{T}}\mathbf{N}\mathrm{d}\Omega \qquad \mathbf{C} = \int_\Omega \mathbf{N}^{\mathrm{T}}\frac{\partial}{\partial x_i}(U_i\mathbf{N})\mathrm{d}\Omega$$
$$\mathbf{K} = \int_\Omega \frac{\partial\mathbf{N}^{\mathrm{T}}}{\partial x_i}k\frac{\partial\mathbf{N}}{\partial x_i}\mathrm{d}\Omega \qquad \mathbf{f} = \int_\Omega \mathbf{N}^{\mathrm{T}}Q\mathrm{d}\Omega + \text{b.t.} \tag{2.108}$$

and $\mathbf{K}_u$ and $\mathbf{f}_s^n$ come from the new term introduced by the discretization along the characteristics. After integration by parts, the expression of $\mathbf{K}_u$ and $\mathbf{f}_s$ is

$$\mathbf{K}_u = -\tfrac{1}{2}\int_\Omega \frac{\partial}{\partial x_i}\left(U_i\mathbf{N}^{\mathrm{T}}\right)\frac{\partial}{\partial x_i}(U_i\mathbf{N})\mathrm{d}\Omega$$
$$\mathbf{f}_s = -\tfrac{1}{2}\int_\Omega \frac{\partial}{\partial x_i}\left(U_i\mathbf{N}^{\mathrm{T}}\right)Q\mathrm{d}\Omega + \text{b.t.} \tag{2.109}$$

where b.t. stands for integrals along region boundaries. Note that the higher-order (third and above) derivatives are not included in the above equation. The boundary terms from the discretization of stabilizing terms are ignored because the original residual is zero.

The approximation is valid for any scalar convected quantity even if that is the velocity component U_i itself, as is the case with momentum-conservation equations. For this reason we have elaborated above the full details of the spatial approximation as the matrices will be repeatedly used.

It is of interest to note that the explicit form of Eq. (2.107) is only conditionally stable. For one-dimensional problems, the stability condition is given as (neglecting the effect of sources)

$$\Delta t \leq \Delta t_{\text{crit}} = \frac{h}{|U|} \tag{2.110}$$

for linear elements in the absence of diffusion. If the diffusion is present a new critical time step has to be calculated as [65,66]

$$\Delta t_{\text{crit}} = \frac{\Delta t_u \Delta t_k}{\Delta t_u + \Delta t_k} \tag{2.111}$$

where Δt_u is given by Eq. (2.110) and $\Delta t_k = h^2/2k$ is the diffusive limit for the critical one-dimensional time step. In two and three dimensions the nodal element size h is taken as the minimum of element sizes surrounding a node. In practice, however,

$$\Delta t_{\text{crit}} = min(\Delta t_u, \Delta t_k) \tag{2.112}$$

is more suitable.

Further, with $\Delta t = \Delta t_{\text{crit}}$ the steady-state solution results in an (almost) identical balancing diffusion change to that obtained by using the optimal streamline upwinding procedures discussed in Part I of this chapter. Thus if steady-state solutions are the main objective of the computation such a value of Δt should be used in connection with the $\mathbf{K}_u$ term.

A fully implicit form of solution is an expensive one involving unsymmetric matrices. However it is often convenient to apply $\theta \geq 1/2$ to the diffusive term only. We call this a *nearly* (or *quasi*) *implicit form* and if it is employed we return to the stability condition

$$\Delta t_{\text{crit}} = \frac{h}{|U|} \tag{2.113}$$

which can present an appreciable benefit.

It is of considerable interest to examine the behavior of the solution when the steady state is reached—for instance, if we use the time-stepping algorithm of Eq. (2.107) as an iterative process. Now the final solution is given by taking

$$\tilde{\boldsymbol{\phi}}^{n+1} = \tilde{\boldsymbol{\phi}}^{n} = \tilde{\boldsymbol{\phi}}$$

which gives

$$[(\mathbf{C} + \mathbf{K} - \Delta t \mathbf{K}_u]\tilde{\boldsymbol{\phi}} + \mathbf{f} - \Delta t \mathbf{f}_s = 0 \tag{2.114}$$

Inspection of Sections 2.2 and 2.3 shows that the above is identical in form with the use of the Petrov-Galerkin approximation. In the latter the matrix $\mathbf{C}$ is identical and the matrix $\mathbf{K}_u$ includes balancing diffusion of the amount given by $\frac{1}{2}\alpha U h$. However, if we take

$$\tfrac{1}{2}\alpha U h = \frac{U^2 \Delta t}{2} \tag{2.115}$$

the identity of the two schemes results. This can be written as a requirement that

$$\alpha = \frac{U \Delta t}{h} = C \tag{2.116}$$

where C is the Courant number. If $C_{critical}$ is calculated from Eq. (2.111), $C_{critical} = \sqrt{1/Pe + 1} - 1/Pe$.

In Fig. 2.15 we therefore plot the optimal value of α as given in Eq. (2.29) against Pe. *We note immediately that if the time-stepping scheme is operated at or near the critical stability limit of the lumped scheme the steady-state solution reached will be close to that resulting from the optimal Petrov-Galerkin process for the steady state*. However, if smaller time steps than the critical ones are used, the final solution, though stable, will tend toward the standard Galerkin steady-state discretization and may show oscillations if boundary conditions are such that boundary layers are created. Nevertheless, such small time steps result in very accurate transients so we can conclude that it is unlikely that optimality for transients and steady state can be reached simultaneously.

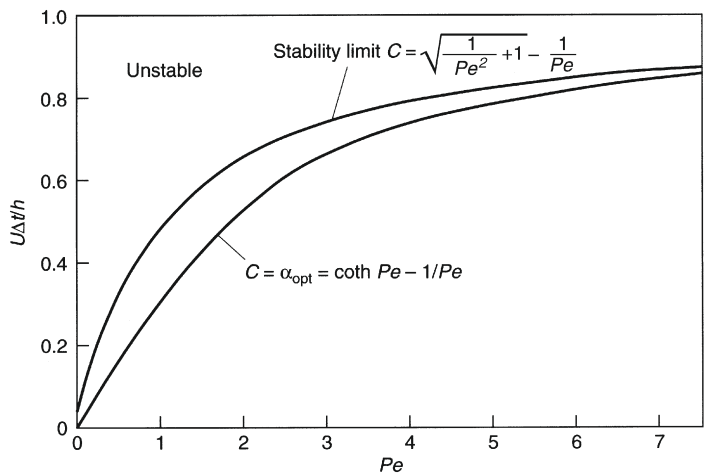

FIGURE 2.15
Stability limit for lumped mass approximation and optimal upwind parameter.

Examination of Eqs. (2.107) shows that the characteristic-Galerkin algorithm could have been obtained by applying a Petrov-Galerkin weighting

$$\left(\mathbf{N}^{\mathrm{T}} + \frac{\Delta t}{2} U_i \frac{\partial \mathbf{N}^{\mathrm{T}}}{\partial x_i}\right)$$

to the various terms of the governing Eq. (2.74) excluding the time derivative $\partial\phi/\partial t$ to which the standard Galerkin weighting of $\mathbf{N}^{\mathrm{T}}$ is attached. Comparing the above with the steady-state problem and the weighting given in Eq. (2.59) the connection is obvious.

A two-dimensional application of the characteristic-Galerkin process is illustrated in Fig. 2.16 in which we show pure convection of a disturbance in a circulating flow. It is remarkable to note that almost no dispersion occurs after a complete revolution. The present scheme is here contrasted with the solution obtained by the finite difference scheme of Lax and Wendroff [67] which for a regular one-dimensional mesh gives a scheme identical to the characteristic-Galerkin except for the mass matrix, which is always diagonal (lumped) in the finite difference scheme.

It seems that here the difference is entirely due to the proper form of the mass matrix $\mathbf{M}$ now used and we note that for transient response the importance of the consistent mass matrix is crucial. However, the numerical convenience of using the lumped form is overwhelming in an explicit scheme. It is easy to recover the performance of the consistent mass matrix by using a simple iteration. In this we write Eq. (2.107) as

$$\mathbf{M}\Delta\tilde{\boldsymbol{\phi}}^{n} = \Delta t \mathbf{S}^{n} \tag{2.117}$$

with $\mathbf{S}^{n}$ being the right-hand side of Eq. (2.107) and

$$\tilde{\boldsymbol{\phi}}^{n+1} = \tilde{\boldsymbol{\phi}}^{n} + \Delta\tilde{\boldsymbol{\phi}}^{n}$$

Substituting a lumped mass matrix $\mathbf{M}_L$ to ease the solution process we can iterate as follows:

$$\left(\Delta\tilde{\boldsymbol{\phi}}\right)_{l}^{n} = \mathbf{M}_L^{-1}[\Delta t \mathbf{S}^{n} + (\mathbf{M}_L - M)\left(\Delta\tilde{\boldsymbol{\phi}}\right)_{l-1}^{n}] \tag{2.118}$$

where l is the iteration number. The process converges very rapidly and in Fig. 2.17 we show the dramatic improvements of results in the solution of a one-dimensional wave propagation with three such iterations done at each time step. At this stage the results are identical to those obtained with the consistent mass matrix.

2.6.4 Boundary conditions: Radiation

As we have already indicated the convection-diffusion problem allows one of the conditions

$$\phi = \bar{\phi} \quad \text{on } \Gamma_u \tag{2.119a}$$

or

$$-k\left(\frac{\partial\phi}{\partial n}\right) = \bar{q} \quad \text{on } \Gamma_q \tag{2.119b}$$

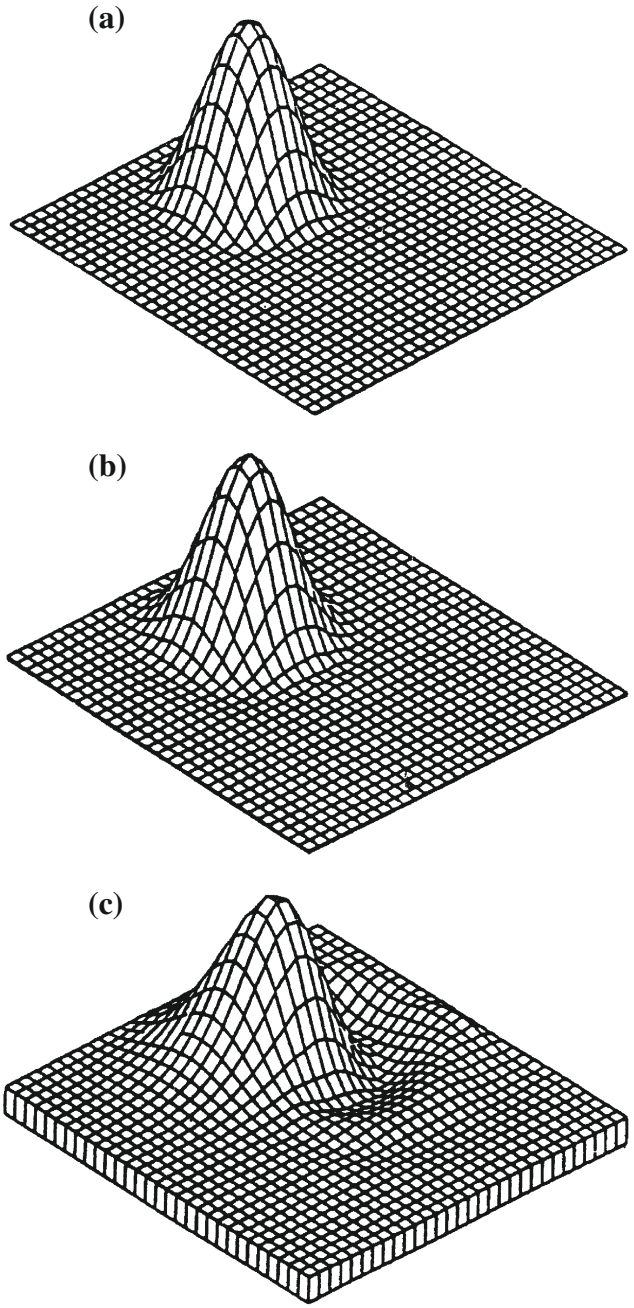

FIGURE 2.16

Advection of a Gaussian cone in a rotating fluid by characteristic-Galerkin method: (a) original form; (b) form after one revolution using consistent **M** matrix; and (c) form after one revolution using lumped mass (Lax-Wendroff).

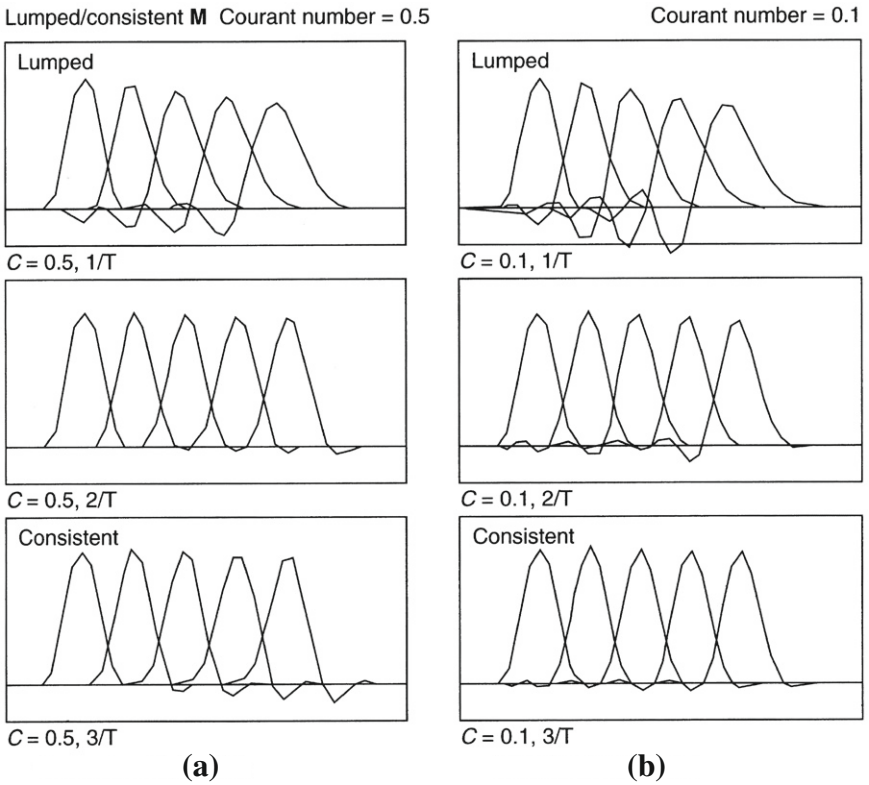

FIGURE 2.17
Characteristic-Galerkin method in the solution of a one-dimensional wave progression. Effect of using a lumped mass matrix and one of consistent iteration: (a) Courant number = 0.5; (b) Courant number = 0.1.

(where $\Gamma = \Gamma_u \bigcup \Gamma_q$) to be imposed on the boundary, providing the equation is of second order and diffusion is present.

In the case of pure convection this is no longer the case as the differential equation is of first order. Indeed this was responsible for the difficulty of obtaining a solution in the example of Fig. 2.2 when $Pe \rightarrow \infty$ and an exit boundary condition of the type given by Eq. (2.119a) was imposed. In this one-dimensional case for pure convection only the inlet boundary condition can be given; at the exit no boundary condition needs to be prescribed if U, the wave velocity, is positive.

For multidimensional problems of pure convection the same wave specification depends on the value of the normal component of U. Thus if

$$U_i n_i > 0 \tag{2.120}$$

where n_i is the outward normal vector to the boundary, the wave is leaving the problem and then no boundary condition is specified. If the problem has some diffusion, the

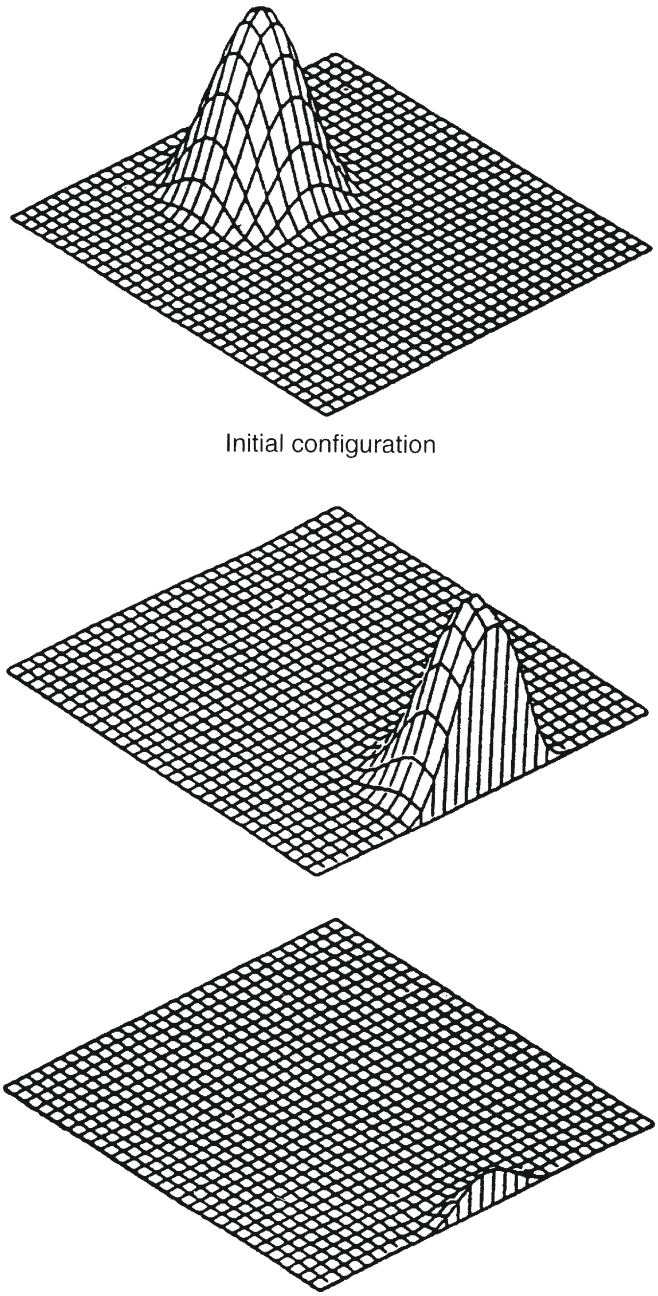

FIGURE 2.18
A Gaussian distribution advected in a constant velocity field. Boundary condition causes no reflection.

same specification of "no boundary condition" is equivalent to putting

$$-k\left(\frac{\partial \phi}{\partial n}\right) = 0 \tag{2.121}$$

at the exit boundary.

In Fig. 2.18 we illustrate, following the work of Peraire [68], how cleanly the same wave as that specified in the problem of Fig. 2.15 leaves the domain in the uniform velocity field [64,68] when the correct boundary condition is imposed.

2.7 Taylor-Galerkin procedures for scalar variables

In the Taylor-Galerkin process, the Taylor expansion in time precedes the Galerkin space discretization. Firstly, the scalar variable ϕ is expanded by the Taylor series in time [61,69]:

$$\phi^{n+1} = \phi^n + \Delta t \frac{\partial \phi^n}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 \phi^n}{\partial t^2} + O(\Delta t^3) \tag{2.122}$$

From Eq. (2.75) we have

$$\frac{\partial \phi^n}{\partial t} = \left[-U\frac{\partial \phi}{\partial x} + \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) - Q\right]^n \tag{2.123a}$$

and

$$\frac{\partial^2 \phi^n}{\partial t^2} = \frac{\partial}{\partial t}\left[-U\frac{\partial \phi}{\partial x} + \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) - Q\right]^n \tag{2.123b}$$

Substituting Eqs. (2.123a) and (2.123b) into Eq. (2.122) we have

$$\begin{aligned}\phi^{n+1} - \phi^n = &-\Delta t\left[U\frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) + Q\right]^n \\ &- \frac{\Delta t^2}{2}\frac{\partial}{\partial t}\left[U\frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) + Q\right]^n\end{aligned} \tag{2.124}$$

Assuming U and k to be constant we have

$$\begin{aligned}\phi^{n+1} - \phi^n = &-\Delta t\left[U\frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) + Q\right]^n \\ &- \frac{\Delta t^2}{2}\frac{\partial}{\partial x}\left[U\frac{\partial \phi}{\partial t} - \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial t}\right) + \frac{\partial x}{\partial t}Q\right]^n\end{aligned} \tag{2.125}$$

Inserting Eq. (2.123a) into Eq. (2.125) and neglecting higher-order terms gives

$$\begin{aligned}\phi^{n+1} - \phi^n = &-\Delta t\left[U\frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) + Q\right]^n \\ &+ \frac{\Delta t^2}{2}\frac{\partial}{\partial x}\left[U^2\frac{\partial \phi}{\partial x} - U\frac{\partial}{\partial x}\left(k\frac{\partial \phi}{\partial x}\right) + UQ\right]^n + O(\Delta t^3)\end{aligned} \tag{2.126}$$

As we can see the above equation, having assumed constants U and k, is identical to Eq. (2.104) derived from the characteristic approach. Clearly for scalar variables both characteristic- and Taylor-Galerkin procedures give identical stabilizing terms. Thus selection of a method for a scalar variable is a matter of taste. However, *the sound mathematical justification of the characteristic-Galerkin method should be emphasized here and for this reason the characteristic-Galerkin procedure forms the fundamental basis for the remainder of this text*.

The Taylor-Galerkin procedure for the convection-diffusion equation in multidimensions can be written as

$$\phi^{n+1} - \phi^n = -\Delta t \left\{ U_j \frac{\partial \phi}{\partial x_j} - \frac{\partial}{\partial x_i}\left(k \frac{\partial \phi}{\partial x_i}\right) + Q - \frac{\Delta t}{2} \frac{\partial}{\partial x_i}\left[U_i U_j \frac{\partial \phi}{\partial x_j} - U_i \frac{\partial}{\partial x_j}\left(k \frac{\partial \phi}{\partial x_j}\right) + U_i Q \right] \right\}^n \tag{2.127}$$

again showing the complete similarity with the appropriate characteristic-Galerkin form and identity when U_i and k are constant. The Taylor-Galerkin method is the finite element equivalent of the Lax-Wendroff method developed in the finite difference context [67].

The Taylor-Galerkin process has one important feature. The idea can be used directly for dealing with the vector form of the convection-diffusion equation, such as we have mentioned at the beginning of this chapter [viz. (2.1)]. This method was used with reasonable success to solve problems of high-speed gas flow. For this reason we have explained the treatment of vector valued-functions in Appendix D.

2.8 Steady-state condition

Both the Taylor-Galerkin and characteristic-Galerkin methods give an answer which compares directly with SUPG and GLS giving additional streamline diffusion (higher-order derivatives are omitted) and sources

$$\frac{\Delta t^2}{2} \frac{\partial}{\partial x_i}\left[U_i U_j \frac{\partial \phi}{\partial x_j} \right] \quad \text{and} \quad \frac{\Delta t}{2} \frac{\partial}{\partial x_i}\left[U_i Q \right] \tag{2.128}$$

with Δt replacing the coefficient αh. With the characteristic-Galerkin method being the only method that has a full mathematical justification, we feel that even for steady-state problems this should be considered as an appropriate solution technique.

2.9 Nonlinear waves and shocks

The procedures developed in the previous sections are in principle of course available for both linear and nonlinear problems (with explicit procedures of time stepping being particularly efficient for the latter). Quite generally the convective part of the

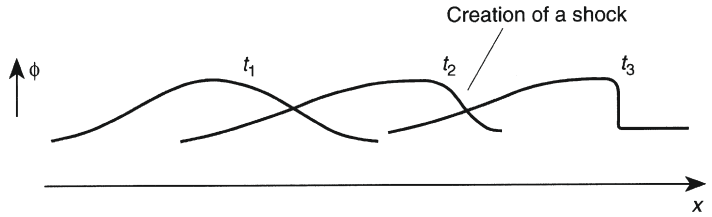

FIGURE 2.19
Progression of a wave with velocity $U = \phi$.

equation, i.e.,

$$\frac{\partial \phi}{\partial t} + \frac{\partial F_i}{\partial x_i} \equiv \frac{\partial \phi}{\partial t} + U_i \frac{\partial \phi}{\partial x_i} = 0 \tag{2.129}$$

will have the vector U_i dependent on ϕ. Thus

$$U_i \equiv \frac{\partial F_i}{\partial \phi} = U_i(\phi) \tag{2.130}$$

In the one-dimensional case with a scalar variable we shall have equations of the type

$$\frac{\partial \phi}{\partial t} + \frac{\partial F}{\partial x} \equiv \frac{\partial \phi}{\partial t} + U(\phi)\frac{\partial \phi}{\partial x} = 0 \tag{2.131}$$

corresponding to waves moving with a nonuniform velocity U. A typical problem in this category is that due to Burger, which is defined by

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x}\left(\tfrac{1}{2}\phi^2\right) = \frac{\partial \phi}{\partial t} + \phi\frac{\partial \phi}{\partial x} = 0 \tag{2.132}$$

In Fig. 2.19 we illustrate qualitatively how different parts of the wave moving with velocities proportional to their amplitude cause it to steepen and finally develop into a shock form. This behavior is typical of many nonlinear systems and in Chapter 7 we shall see how shocks develop in compressible flow at transonic and supersonic speeds.

To illustrate the necessity for the development of the shock, consider the propagation of a wave with an originally smooth profile illustrated in Fig. 2.20a. Here as we know the characteristics along which ϕ is constant are straight lines shown in Fig. 2.20b (in $x - t$ plane). These show different propagation speeds intersecting at time $t = 2$ when a discontinuous shock appears. This shock propagates at a finite speed (which here is the average of the two extreme values).

In such a shock the differential equation is no longer valid but the conservation integral is. We can thus write for a small length Δs around the discontinuity

$$\frac{\partial}{\partial t}\int_{\Delta s} \phi \, \mathrm{d}s + F(s + \Delta s) - F(s) = 0 \tag{2.133a}$$

or

$$C\Delta\phi + \Delta F = 0 \tag{2.133b}$$

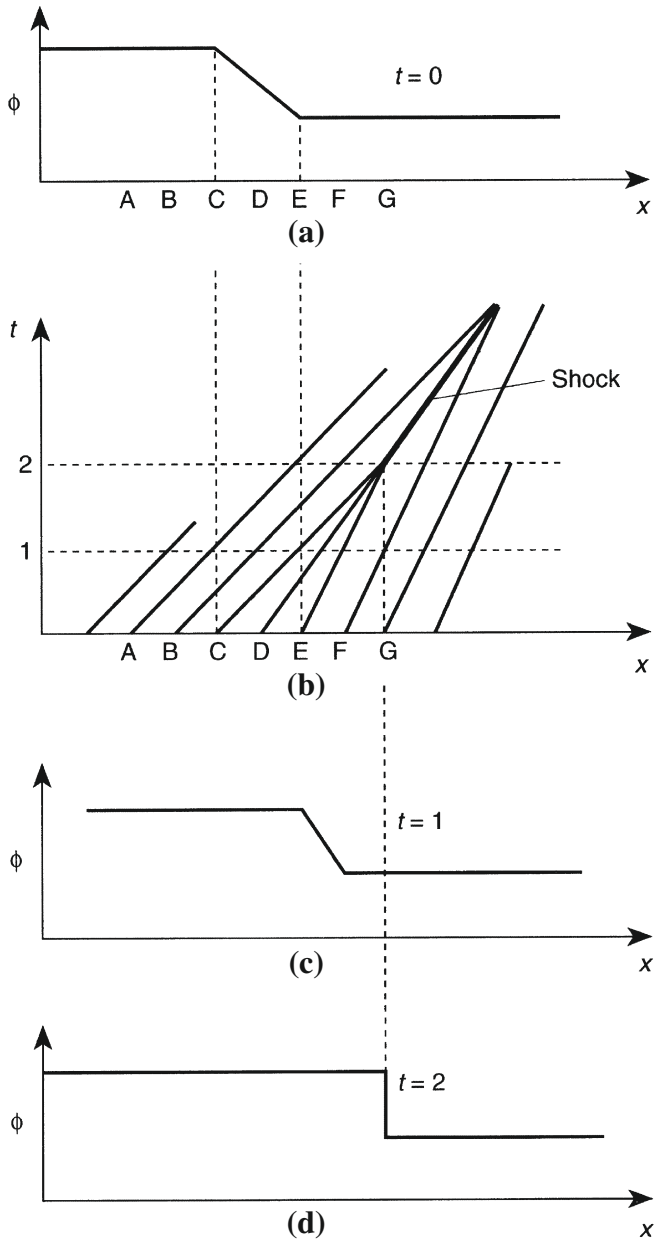

FIGURE 2.20
Development of a shock (Burger equation): (a) profile at time $t = 0$; (b) characteristics; (c) profile at time $t = 1$; (d) profile at time $t = 2$.

where $C = \lim \Delta s/\Delta t$ is the speed of shock propagation and $\Delta\phi$ and ΔF are the discontinuities in ϕ and F respectively. Eq. (2.133b) is known as the Rankine-Hugoniot condition.

We shall find that such shocks develop frequently in the context of compressible gas flow and shallow-water flow (Chapters 7 and 10) and can often exist even in the presence of diffusive terms in the equation. Indeed, such shocks are not specific to transients but can persist in the steady state. Clearly, approximation of the finite element kind in which we have postulated in general a C_0 continuity to $\widehat{\phi}$ can at best *smear* such a discontinuity over an element length, and generally oscillations near such a discontinuity arise even when the best algorithms of the preceding sections are used.

Figure 2.21 illustrates the difficulties of modeling such steep waves occurring even in linear problems in which the physical dissipation contained in the equations is incapable of smoothing the solution out reasonably, and to overcome this problem artificial diffusivity is frequently used. This artificial diffusivity must have the following characteristics:

1. It must vanish as the element size tends to zero.
2. It must not affect substantially the smooth domain of the solution.

A typical diffusivity often used is a finite element version of that introduced by Lapidus [70] for finite differences, but many other forms of local smoothing have been proposed [71,72]. The additional Lapidus-type diffusivity is of the form

$$\tilde{k} = C_{\text{Lap}} h^2 \left| \frac{\partial \phi}{\partial x} \right| \tag{2.134}$$

In the above equation C_{lap} is a coefficient and h is the element size.

In Fig. 2.22 we show a problem of discontinuous propagation in the Burger equation (2.132) and how a progressive increase of the C_{Lap} coefficient kills spurious oscillation, but at the expense of rounding of a steep wave.

For a multidimensional problem, a degree of anisotropy can be introduced and a possible expression generalizing (2.134) is

$$\tilde{k}_{ij} = C_{\text{Lap}} h^2 \frac{|V_i V_j|}{|\mathbf{V}|} \tag{2.135}$$

where

$$V_i = \frac{\partial \phi}{\partial x_i}$$

Other possibilities are open here and numerous papers have been devoted to the subject of "shock capture." We will return to this problem in Chapter 7 where its importance in the high-speed flow of gases is paramount.

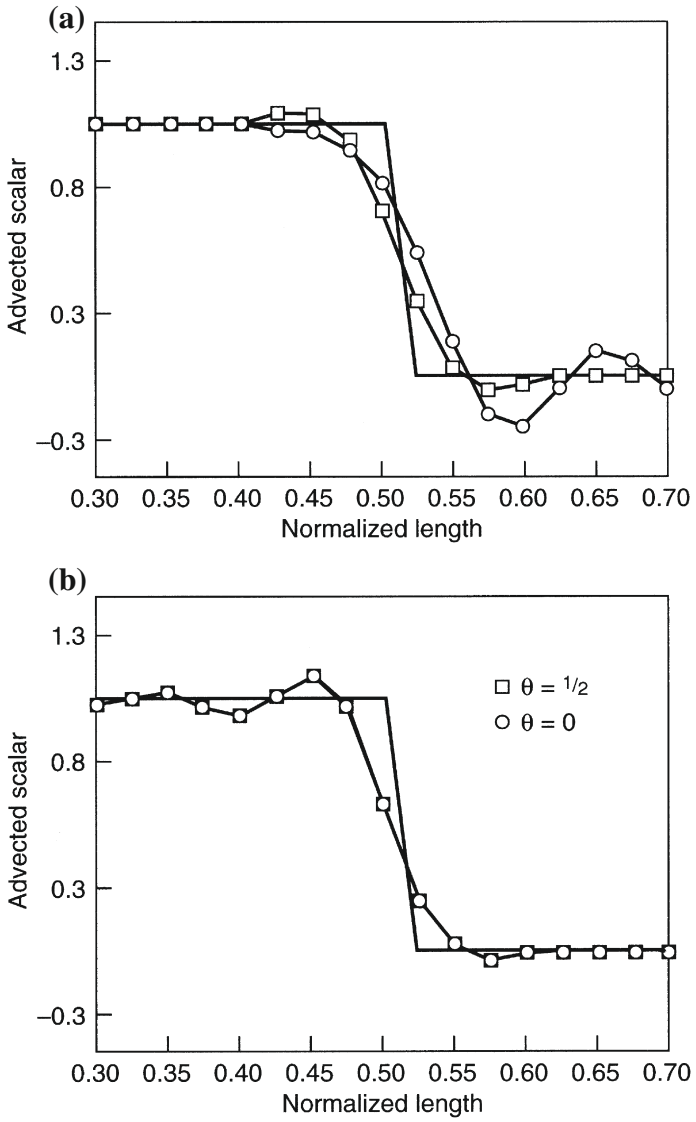

FIGURE 2.21

Propagation of a steep wave by Taylor-Galerkin process: (a) explicit methods $C = 0.5$, step wave at $Pe = 12{,}500$ and (b) explicit methods $C = 0.1$, step wave at $Pe = 12{,}500$.

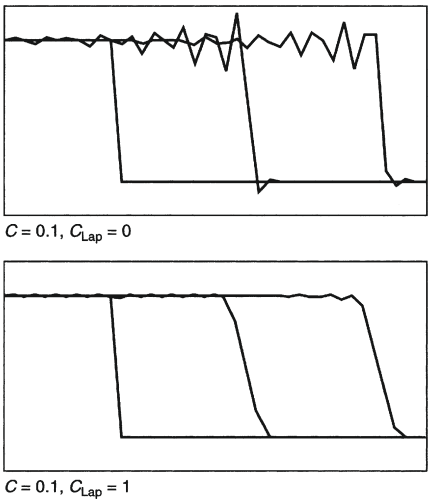

FIGURE 2.22
Propagation of a steep front in Burger's equation with solution obtained using different values of C_{Lap}.

Part III: Boundary Conditions

2.10 Treatment of pure convection

In pure convection problems the equation reduces to

$$\frac{\partial \phi}{\partial t} + U_i \frac{\partial \phi}{\partial x_i} + Q = 0 \tag{2.136}$$

It is clear that only the "inlet" values of ϕ can be set. By inlet we mean those where

$$U_i n_i < 0 \tag{2.137}$$

for n_i an outward pointing normal to the boundary.

This is particularly obvious when we consider the one-dimensional form of Eq. (2.136) in steady state:

$$U \frac{\mathrm{d}\phi}{\mathrm{d}x} + Q = 0 \tag{2.138}$$

This ordinary differential equation can only have conditions imposed on ϕ at one end of the domain. Let us consider the example where

$$U \frac{\mathrm{d}\phi}{\mathrm{d}x} + Q = 0, \quad \phi(0) = 1$$

with a constant u and Q. The Galerkin solution to Eq. (2.138) is given by

$$\int_{\Omega} N_a \left[U \frac{\mathrm{d}\phi}{\mathrm{d}x} + Q \right] \mathrm{d}x = 0 \tag{2.139}$$

As shown in Section 2.2.1 where this type of problem is solved as the limit case $Pe = \infty$ and for one-dimensional problems in which boundary conditions are imposed at both ends a purely oscillatory solution occurs. However, when properly solved with only one boundary condition imposed, i.e.,

$$\phi(0) = 1 \quad \text{for} \quad 0 < x < L$$

the correct result for the example shown in Fig. 2.2 is obtained. The same result will be obtained no matter what order finite element approximation is used.

The reader should note the solution "develops" from the inlet in an elementwise manner when Eq. (2.137) is considered. The element-by-element process eliminates the need to solve a large set of simultaneous equations (which is not a serious matter in one-dimensional problems). For two- and three-dimensional problems these savings can be quite substantial if proper boundary conditions are imposed and the process was described by Lesaint and Raviart [73].

Let us consider a one-dimensional domain as shown in Fig. 2.23a with linear elements. Since the flow direction is from the left to right, the solution at node a is influenced only by the node or element upstream. Thus the need for assembly is eliminated and the resulting discrete Galerkin finite element form of Eq. (2.139) at node a is

$$u \left(\frac{u_a - u_{a-1}}{2} \right) + \frac{Ql}{2} = 0 \tag{2.140}$$

This expression is identical to the upwind finite difference approximation discussed previously. In two-dimensional problems (Fig. 2.23b) a similar rule applies and the solution at node a is only affected by the solutions of nodes b and c as shown in

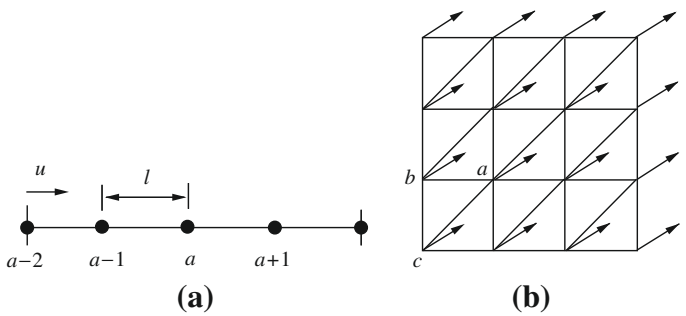

FIGURE 2.23

Solution of pure convection in element-by-element manner. Source term Q and constant u: (a) one-dimensional solution sequence; (b) tow-dimensional solution sequence.

Fig. 2.23b. The calculation can proceed using small groups of elements as illustrated in Fig. 2.23b.

The problem of pure convection is a common one in neutron transport where reaction effects are included [73,74]. We note that for compressible flow without viscosity we shall later use the so-called Euler equations [viz. Chapter 7]. Once again the values of the unknown functions will only be specified at the inlet boundaries if supersonic conditions exist.

2.11 Boundary conditions for convection-diffusion

If diffusion occurs, boundary conditions must be imposed on all boundaries. Thus, in the one-dimensional case we return to the situation discussed at the beginning of this chapter. We see immediately that the standard Galerkin process breaks down near the outlet boundary when we try to specify the value of the unknown ϕ in a "strong" (Dirichlet) manner when convection effects are important (i.e., $Pe > 1$). In such a case we shall try to impose the Dirichlet boundary condition in a "weak" manner to balance the solution between the interior and the boundary treatments. Such a weak imposition of the Dirichlet condition was presented by Nitsche in 1971 [75] and is used frequently when discontinuous Galerkin methods are discussed.

We again start with the Galerkin equation in which the diffusive term is integrated by parts yielding

$$-\int_{\Gamma} N_a n_i \left(k\,\frac{\partial \phi}{\partial x_i}\right) \mathrm{d}\Gamma = -\int_{\Gamma_\phi} N_a n_i \left(k\,\frac{\partial \phi}{\partial x_i}\right) \mathrm{d}\Gamma + \int_{\Gamma_q} N_a \bar{q}_n \mathrm{d}\Gamma \tag{2.141}$$

where the natural boundary condition has been imposed on Γ_q. When the approximate solution is used in Eq. (2.141) a contribution to the coefficient matrix arises and is given by

$$K_{ab} = -\int_{\Gamma_\phi} N_a n_i k \frac{\partial N_b}{\partial x_i} \mathrm{d}\Gamma \tag{2.142}$$

This term is clearly unsymmetric and to restore symmetry Nitsche adds two terms:

$$-\int_{\Gamma_\phi} \frac{\partial N_a}{\partial x_i} n_i k \left(\phi - \bar{\phi}\right) \mathrm{d}\Gamma + \kappa \int_{\Gamma_\phi} N_a \left(\phi - \bar{\phi}\right) \mathrm{d}\Gamma = 0$$

where κ is a parameter. In the above equation the desired value of the Dirichlet condition appears. The second term is a least-squares type term used to maintain stability of the solution. This gives the final form for the boundary integrals as

$$-\int_{\Gamma_\phi} \left[N_a n_i k \frac{\partial \phi}{\partial x_i} + \frac{\partial N_a}{\partial x_i} n_i k \left(\phi - \bar{\phi}\right)\right] \mathrm{d}\Gamma + \kappa \int_{\Gamma_\phi} N_a \left(\phi - \bar{\phi}\right) \mathrm{d}\Gamma \tag{2.143}$$

We observe as $\kappa \to \infty$ we recover the penalty method. However, Nitsche shows that choosing

$$\kappa = O(k/h)$$

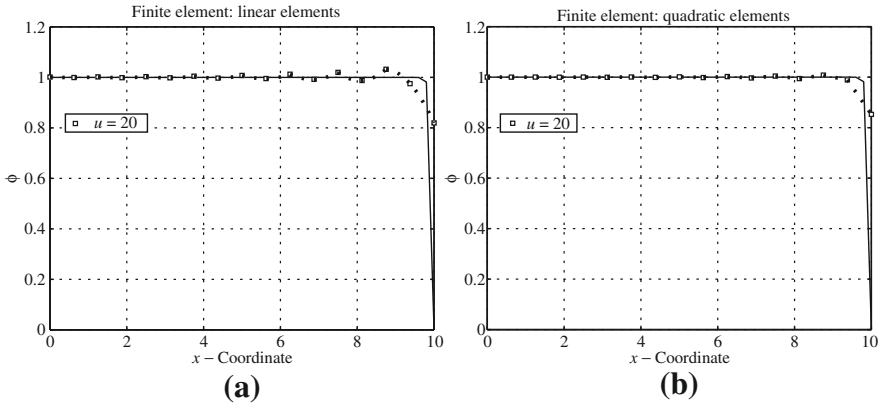

FIGURE 2.24

Solution of one-dimensional convection-diffusion problem: (a) one-dimensional linear element solution; (b) one-dimensional quadratic element solution.

where h is an element size of the mesh, an effective solution results without strong imposition of the boundary condition. In Fig. 2.24 we show results for the problem originally given in Fig. 2.2 for a large Peclet number. The overall good results are obtained *without any modification of the standard Galerkin process in the interior of the domain*.

From results shown in Fig. 2.24 using linear and quadratic elements we see immediately that the results obtained by weakening the Dirichlet condition at the outlet are quite acceptable. If we contrast these results with those obtained by using the procedures of Part I we observe that no longer are exact values obtained at nodes but the solution is accurate in the "mean." The oscillations are almost nonexistent and yet the standard Galerkin procedure is used throughout the whole domain with the special treatment confined to the outlet boundary.

2.12 Summary and concluding remarks

The reader may well be confused by the variety of apparently unrelated approaches given in this chapter. This may be excused by the fact that optimality guaranteed by the finite element approaches in elliptic, self-adjoint problems does not automatically transfer to hyperbolic non-self-adjoint ones.

The major part of this chapter is concerned with a scalar variable in the convection-diffusion reaction equation. The several procedures presented for steady-state and transient equations yield almost identical results. However the characteristic-Galerkin method is the most logical one for transient problems and gives identical stabilizing terms to that derived by the use of Petrov-Galerkin, GLS, and other procedures when the time step used is near the stability limit. For such a problem the optimality is assured simply by splitting the problem into the self-adjoint part where the direct

Galerkin approximation is optimal and an advective motion where the unknown variable remains fixed in the characteristic space.

Extension of the various procedures presented to vector variables has been made in the past and here we relegate such procedures to Appendix D as they present special problems. For this reason we recommend that when dealing with equations such as those arising in the motion of a fluid a split is made in a manner separating several scalar convection-diffusion problems for which the treatment described is used. We shall do so in the next chapter when we introduce the CBS algorithm using the *characteristic-based split*.

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