Compact Finite Volume Methods for the Diffusion Equation

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Volume Methods for the Diffusion Equation*

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Abstract

We describe an approach to treating initial-boundary value problems by finite volume methods in which the parallel between differential and difference arguments is closely maintained. By using intrinsic geometrical properties of the volume elements, we are able to describe discrete versions of the div, curl, and grad operators which lead, using summation-by-parts techniques, to familiar energy equations as well as the div curl = 0 and curl grad = 0 identities. For the diffusion equation, these operators describe compact schemes whose convergence is assured by the energy equations and which yield both the potential and the flux vector with second order accuracy. A simplified potential form is especially useful for obtaining numerical results by multigrid and ADI methods. The treatment of general curvilinear coordinates is shown to result from a specialization of these general results.

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Compact Finite
Volume Schemes for the Diffusion Equation

Introduction:

Let V be a domain with boundary surface S on which **n** is the outward unit normal. This paper describes a finite volume scheme for solving the diffusion equation for a *potential* ϕ and *flux* **u** in the form

D.E. $$\phi_t = \text{div}\,\mathbf{u} - f, \qquad \text{in } V \qquad \backslash 1 \backslash$$
$$\text{grad}\,\phi = \mathbf{u}$$

B.C. $$\alpha\,\mathbf{u}\cdot\mathbf{n} + \beta\phi = g \qquad \text{on } S, \qquad t \geq 0 \qquad \backslash 2 \backslash$$

I.C. $$\phi = g_0 \qquad \text{in } V, \qquad t = 0 \qquad \backslash 3 \backslash$$

in both the steady and unsteady cases. We recall that the solution of this problem satisfies an 'energy' equation

$$\frac{d}{dt}\int_V \phi^2\,dV + \int_V \mathbf{u}\cdot\mathbf{u}\,dV = \int_S \phi\,\mathbf{u}\cdot d\mathbf{S} - \int_V \phi\,f\,dV \qquad \backslash 4 \backslash$$

which follows by multiplying the first equation in \1\ by ϕ and integrating by parts. We also recall that when $f = 0$ the maximum-minimum values of ϕ either lie on the boundary S or, in case $t = 0$, in V itself.

A discrete form of these results will hold for the finite volume scheme and includes results about generalized curvilinear coordinate mappings as a special case. We will identify finite volume operators div_h, grad_h, and curl_h which are consistent with their differential counterparts and from which a discrete energy expression corresponding to \4\ will follow by simple summation-by-parts identities. The important identities $\text{div}_h\,\text{curl}_h = 0$ and $\text{curl}_h\,\text{grad}_h = 0$ will also remain valid, as we will show at a later point in the paper. A potential form involving the

operator $\mathrm{div}_h\, \mathrm{grad}_h\phi$, which is obtained by eliminating **u**, leads to a symmetric, positive definite operator to which multigrid and other fast solution techniques are applicable.

The fact that the finite volume schemes described here lead to discrete energy expressions is the principal result of this paper. It insures that the schemes converge. We will also find that the approximations to both ϕ and **u** will be second order accurate. This result is similar to that obtained for mixed finite element methods ([1], [8]) and it is possible, in fact, to view the present scheme as a finite element method which involves non-conforming elements ([2],[4]).

Many of these ideas can be illustrated most simply for steady, one-dimensional problems, for which reason we first discuss the equations $\phi' = u$, $u' = f$ in detail. We will find it natural to introduce a *primary mesh*, which is formed by the endpoints of subintervals into which the basic domain is divided, and a *dual mesh*, which is formed by the centerpoints of the primary mesh. The variables ϕ and u will be associated with the primary mesh while another variable ψ will be associated with the dual mesh. An algebraic relationship between ϕ, ψ and u on each subinterval provides an approximation to the solution operator (for which reason the scheme is called *compact*) and the solution in the large is obtained by imposing continuity conditions for ϕ and u at points of the primary mesh. Both ϕ and ψ will be found to converge with second order accuracy to the solution at the points at which they are defined. Furthermore, as noted above, although u will be defined by one-sided divided differences involving ϕ and ψ, its convergence will also be second order accurate as a result of the continuity conditions imposed.

In extending these ideas to higher dimensional problems by subdividing the solution domain V into volume elements we will also find that a primary and dual grid play a natural role. Now the variables ϕ and **u** will be associated with the centerpoints of the faces of a volume element while ψ will be associated with the center of the element. However, an additional variable ζ (or a box-variable χ) which is associated with the edges (vertices) of the element will also be required. The compact scheme will describe relationships between these variables which produce second order accurate results at the points indicated. In the method discussed here, the

non-tangential components of $\mathbf{u}$ on a face of an element are obtained with the use of one-sided differences in terms of ϕ and ψ while its tangential components are determined solely by the edge values ζ, and these are obtained in terms of ψ at points of the dual grid by bilinear interpolation. In the case of (uniform or nonuniform) Cartesian or orthogonal coordinate elements, the variables ζ as well as the tangential components of $\mathbf{u}$ on faces of elements can be obtained by postprocessing, if required.

Some of these ideas are familiar from applications of finite volume methods to fluid dynamics and are described in Peyret and Taylor [5] and in a review paper by Vinokur [9]. A focus of many such methods is on the treatment of conservation laws for inviscid fluids. As noted by these authors, the primary and dual grids often play a role in many such schemes whenever gradient terms are included, as occur when viscous effects arise. Indeed, the need to accurately approximate quantities like the stress tensor at boundaries of general domains is a principal reason to resort to finite volume methods, although their use may add significantly to the cost of computations. To understand some of the problems which can arise, the diffusion equation can serve as a useful model. We will find that the relationships between grid variables differ in important respects from those described elsewhere. Many schemes place primary emphasize on the vertex (box) variables and most methods deliberately avoid the use of one-sided differencing to approximate the flux except, perhaps, at boundaries. Although compact schemes related to those described here have been used for Cartesian grids, e.g., [2], [7], the roles of the variables were not completely developed.

The paper concludes by describing the rather staightfoward modifications which are required to treat the time-dependent problem. The result is a Crank-Nicholson-type scheme and energy arguments provide convergence estimates for the finite volume method. We are also able to show that energy arguments can be adapted to a Peaceman-Rachford ADI scheme.

This paper reflects many valuable insights gained through discussions with

colleagues. I mention with particular appreciation T.B. Gatski, D. Gottlieb, H.-O. Kreiss, and G. Strang.

I. Steady One-Dimensional Problems

I.1. Notations

On an interval $[l_-, l_+]$ consider the problem :

D.E. $$u' = f \qquad \backslash I.1a \backslash$$

$$\phi' = u$$

B.C. $$\phi = g, \quad \text{for } x = l_{\pm}. \qquad \backslash I.1b \backslash$$

The associated energy equation is

$$\int \phi f \, dx + \int u^2 \, dx = (\phi u)_{l_+} - (\phi u)_{l_-} \qquad \backslash I.2 \backslash$$

Divide $[l_-, l_+]$ into M non-overlapping subintervals $I_j \equiv \{x | \, x_{j-1/2} \le x \le x_{j+1/2}\}$ with centerpoints x_j, j=1/2, 3/2,..., M-1/2. The points x_j, j=1,2,...,M−1, are endpoints of the subintervals which lie interior to $[l_-, l_+]$. We let I_e, I_c denote the sets of indices corresponding to these points:

$$I_e = \{1, 2, ..M-1\} \quad \text{(interior endpoints)}$$

$$I_c = \{1/2, 3/2,...,M - 1/2\} \quad \text{(centerpoints)}.$$

We adopt the finite-difference notations $\Delta x_i = x_{i+1/2} - x_{i-1/2}$, $h_i = \Delta x_i / 2$, $u(x_i) = u_i$. By introducing the central average and difference operators

$$\mu \phi_j \equiv (\phi_{j+1/2} + \phi_{j-1/2})/2 \, , \quad \Delta \phi_j \equiv (\phi_{j+1/2} - \phi_{j-1/2}). \qquad \backslash I.3 \backslash$$

we can verify the summation-by-parts identities

$$\Delta(\phi\psi) = (\mu\phi)(\Delta\psi) + (\Delta\phi)(\mu\psi) \qquad \backslash I.4a \backslash$$

$$\mu(\phi\psi) = (\mu\phi)(\mu\psi) + (\Delta\phi)(\Delta\psi)/4. \qquad \backslash I.4b \backslash$$

Both will play a central role in establishing energy results.

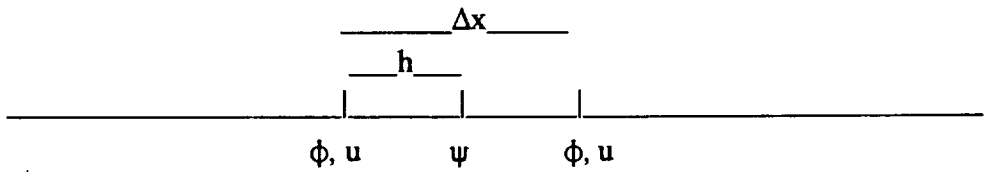

Figure 1. An interval showing the association of the variables ϕ, u with its endpoints and of ψ with its centerpoint.

I.2. A Compact Scheme

In each subinterval I_j, construct an approximate solution using values $\phi_{j\pm1/2}$ as boundary data. Specifically,

(i) for $j \in I_c$ set

$$\Delta u_j \equiv u_{j+1/2} - u_{j-1/2} = \Delta x_j f_j \qquad \backslash I.5 \backslash$$

$$h_j u_{j+1/2} = (\phi_{j+1/2} - \psi_j) \qquad \backslash I.6a \backslash$$

$$h_j u_{j-1/2} = (\psi_j - \phi_{j-1/2}) \qquad \backslash I.6b \backslash$$

Adopting the convention that ψ_j indicates an approximation to the potential solution at the center of the interval, while $\phi_{j\pm1/2}$ indicates the approximation at its endpoints we see that \I.5\ is a central difference approximation to $u' = f$, while \I.6\ approximates $\phi' = u$ by one-sided differences. Then eqs.\I.5\, \I.6\ can be solved for $u_{j\pm1/2}$ and ψ_j in each interval in terms of $\phi_{j\pm1/2}$ considered as boundary data.

(ii) Next, require that both u and ϕ shall be continuous across every endpoint common to two intervals, i.e.,

$$[u]_i = [\phi]_i = 0 \qquad \text{for } i \in I_e \text{ (endpoints)} \qquad \backslash I.7 \backslash$$

(This is implied by our notation, since we have not distinguished between the right- and left-hand limits of u and ϕ at endpoints.) Using \I.6\ to evaluate $u_{i+1/2}$ at the right and left endpoints of the adjacent intervals $I_{i-1/2}$, $I_{i+1/2}$ we find

$$\Delta x_{i+1/2}\, u_{i+1/2} = (\psi_{i+1} - \psi_{i-1}) \qquad i \in I_e \qquad \backslash I.8\backslash$$

which indicates that the accuracy of u may be higher than that suggested by the one-sided difference expressions which originally defined u in \I.6\. Also note that \I.6\ can be used to express the continuity condition $[u]_i = 0$ in terms of ϕ, ψ with the result

$$(\phi_i - \psi_{i-1/2}) / h_{i-1/2} = (\psi_{i+1/2} - \phi_i) / h_{i+1/2} \qquad \backslash I.9a\backslash$$

and which, in the case of equal intervals, reduces to

$$\phi_i = \mu\psi_i \qquad i \in I_e \text{ (endpoints)} \qquad \backslash I.9b\backslash$$

The addition of the boundary conditions leads to a determined system of algebraic equations for the M values of ψ and the M+1 values of ϕ and u.

The special nature of this system is worth noting. By eliminating u from \I.5\ using \I.6\ we find, in the case of equal intervals,

$$(\mu\phi_i - \psi_i) = 2h^2 f \qquad i \in I_c \text{ (centerpoints)} \qquad \backslash I.10a\backslash$$

and if we also write the continuity conditions \I.9b\ in the form

$$(\mu\psi_i - \phi_i) = 0 \qquad i \in I_e \text{ (endpoints)} \qquad \backslash I.10b\backslash$$

it is evident that ϕ_i, ψ_i are the odd-even components of the solution vector of a tri-diagonal system of equations which is, thus, easily solved. In sharp contrast to \I.10\, the standard finite difference scheme for solving \I.1\ is

$$(\mu\phi_i - \psi_i) = h^2 f \qquad i \in I_c \cup I_e \qquad \backslash I.10c\backslash$$

so that some differences with standard numerical treatments of differential equations are to be expected using the schemes considered in this paper.

I.3. The Energy Equation and Convergence:

We will now show that this scheme leads to a discrete form of the energy equation \4\. For simplicity, we will assume a uniform mesh. Add and subtract the expressions

$$(\Delta x/2)\, u_{j\pm 1/2} = \pm\,(\phi_{j\pm 1/2} - \psi_j)$$

given in \I.6\ to obtain

$$\Delta x\, \mu u_j = \Delta \phi_j \qquad \text{\I.11a\}$$

$$\psi_j = \mu \phi_j - \Delta x\, \Delta u_j/4 \qquad \text{\I.11b\}$$

and we see that the approximations to ϕ and ψ are second order with respect to the center of an interval. Then, starting with

$$\Delta u_j = \Delta x\, f_j\,, \qquad \text{\I.5\}$$

multiply by ψ and use \I.11\ and \I.4\ to obtain

$$\begin{aligned} \psi\, \Delta u &= (\mu\phi - (\Delta x/4)\, \Delta u)\cdot \Delta u \qquad \text{\I.12\} \\ &= \Delta(\phi u) - (\mu u\, \Delta\phi + (\Delta x/4)(\Delta u)^2) \\ &= \Delta(\phi u) - \Delta x\, ((\mu u)^2 + (\Delta u)^2/4) \\ &= \Delta(\phi u) - \Delta x\, \mu(u^2). \end{aligned}$$

(Here and in the following we omit subscripts when no confusion is likely to arise). Summing over centerpoints of intervals

$$\sum_{I_c} (\psi_j\, \Delta u_j + \Delta x\, \mu u_j^2) = (\phi u)\Big|_{L}^{L_+} - \sum_{I_e} \left[\phi u\right]_i$$

Because of the continuity conditions, the jumps [ ] vanish and we obtain the discrete energy expression

$$\sum_{I_c} (\psi_j f_j + \mu u_j^2)\Delta x = (\phi u)\Big|_L^R \qquad \backslash I.13 \backslash$$

This result will enable us to conclude that ϕ, ψ and u converge with second order accuracy. Introduce centerpoint and endpoint norms as follows:

$$\| \psi \|_c = \left(\sum_{I_c} \psi_j^2 \Delta x \right)^{1/2} \qquad \backslash I.14a \backslash$$

$$\| u \|_e = \left((u_0^2 + u_M^2 + \sum_{I_e} u_j^2)\Delta x \right)^{1/2} \qquad \backslash I.14b \backslash$$

By summing \I.8\ and using \I.6\ we find

$$\psi_{j+1} - \phi_0 = \tfrac{1}{2} u_0 + \sum_{I_e} u_i$$

and if we also assume endpoint conditions $\phi_0 = \phi_M = 0$ we obtain the inequality

$$\| \psi \|_c \le C \| u \|_e .$$

The energy expression itself leads to the estimate

$$\| u \|_e^2 \le \| \psi \|_c \| f \|_c$$

while the continuity condition \I.9\ results in

$$\| \phi \|_e \le \| \psi \|_c .$$

Thus,

$$\| \psi \|_c \le C^2 \| f \|_c \qquad \backslash I.15 \backslash$$

$$\| u \|_e \le C \| f \|_c$$

$$\| \phi \|_e \le C^2 \| f \|_c .$$

Applying this to the homogeneous problem we conclude that $u=\phi=\psi=0$. Thus the algebraic problem has a solution which is unique. Next, interpreting f as the truncation error,

$f = O(\Delta x^2)$, and we see that ϕ, ψ, and u converge with second order accuracy.

This conclusion about the second order accuracy of u applies not only to its values at interior endpoints, as might be expected from \I.8\, but also to the values u_0 and u_M at the endpoints of $[l_-, l_+]$ itself and which, we recall, were defined in eq. \I.6\ by one-sided difference expressions.

Table 1 presents computations which verify these conclusions for the differential equation \I.1\ corresponding to the solution $\phi = x^2(1-x)^2$. Note that the errors are measured at the endpoints of intervals.

Table 1.

Error Norms

# intervals	$\|\phi_{error}\|_e$	$\|u_{error}\|_e$
6	1.234 e-2	1.851 e-2
12	3.472 e-3	9.259 e-3
24	8.680 e-4	2.893 e-3
48	2.170 e-4	7.957 e-4
96	5.425 e-5	2.080 e-4
192	1.356 e-5	5.312 e-5

Finally, we remark that more general boundary conditions involving both u and ϕ also lead to the same conclusions.

I.4. The Potential Form:

By eliminating the flux u in \I.1\ we obtain the familiar second order equation $\phi'' = f$ which we call the potential form. The difference scheme which corresponds to this may be

obtained by eliminating u in the scheme just described. To illustrate, using \I.6\, eliminate u in

$$\Delta u_j = \Delta x\, f_j \qquad \text{\I.5\}$$

to obtain

$$h^2 f_j = (\mu\phi_j - \psi_j)\,, \qquad j \in I_c \qquad \text{\I.16\}$$

$$h = \Delta x/2\,.$$

As we have seen, for uniform meshes the continuity conditions [u] = 0 result in

$$\phi_i = \mu\psi_i. \qquad i \in I_e \qquad \text{\I.9b\}$$

To these are to be added the boundary conditions

$$\phi_0 = g_-,\ \phi_M = g_+$$

When f = 0 we obtain

$$\psi = \mu\phi\,, \qquad \phi = \mu\psi \qquad \text{\I.17\}$$

and the maximum-minimum property of the solution is an immediate consequence. This can be used to develop an alternate proof of convergence.

The potential form for the discrete problem can be seen to arise as a variational problem associated with the discrete energy equation. The maximum-minimum property reflects the fact that the associated algebraic problem is symmetric and positive definite. In the general treatment, the potential form will be more suitable for numerical work, while the general form involving ϕ, ψ and u as a first order system will prove more convenient for theoretical discussions, particularly for the development of energy estimates.

II.A Compact Finite-Volume Method

We now turn to problem of treating the boundary value problem corresponding to the steady-state solution of \l\ when V is a general volume. Our objective will be to partition V into volume elements δV in such a manner that the prescribed boundary data on S can be accurately transmitted to the boundary elements and then, by solving a discrete boundary value problem in each element corresponding to a compact scheme, obtain an approximate solution in all elements which also satisfies an energy expression, thus insuring convergence. As a result, we expect to be able to treat problems posed in curvilinear coordinates as a special, but important, case.

In order to be able to generalize the arguments given earlier, a number of additional notations will have to be introduced. Before doing so, we will first present a short overview of the principal ideas which will be involved. The more detailed discussion and demonstration that the final result again leads to an energy expression and thus produces a convergent scheme may be omitted if the reader wishes to turn to the discussion of the time-dependent problem given in Part III.

II.1 An Overview:

Guided by the earlier discussion of the one-dimensional problem, we may identify the following requirements to construct a discrete approximation to div $\mathbf{u} = f$, $\mathbf{u} = \text{grad}\,\phi$ when volume elements are involved:

(i) construct consistent, discrete approximations to div $\mathbf{u}$, grad ϕ in a volume element δV in terms of variables associated with $\mathbf{u}$ and ϕ at appropriate points of δV,

(ii) further relate these variables as may be required so as to lead to a determined

and consistent system of algebraic equations from which **u** and ϕ can be determined whenever boundary conditions are prescribed on S, and

(iii) develop a difference calculus which allows summation-by-parts identities to be applied to volume elements and thereby lead to a discrete energy expression from which a convergence argument can be constructed.

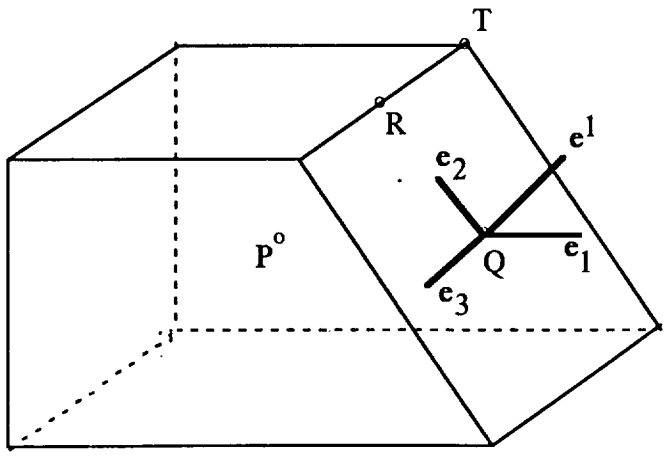

Figure 2. A normal volume element; P, Q,R, are the centers of the volume δV, a face δS, and an edge on which T is a vertex. Shown at Q is a basis [**e**] and $\mathbf{e}^1$, the unit normal to δS.

We will confine our attention to hexahedral volume elements δV, although we will allow certain of its vertices to coalesce, thereby including tetrahedra and related elements in our discussion. Figure 2 indicates the centerpoint P of δV, the center Q of an oriented face δS, and a representative centerpoint R of an edge of δS on which T is a vertex. In addition to the variables $\phi(Q)$, $\psi(P)$ introduced in our discussion of the 1-dimensional problem, we will also associate another variable $\zeta(R)$ with points R. These variables will approximate the potential solution at the

points indicated. Later, we will also associate a variable χ with the vertex points T. Section II.2 introduces notations which allow us to describe various geometrical properties of an element and from which averaging and difference operators, corresponding to \I.4\, can be introduced.

Section II.3 describes discrete approximations to the operators div and grad. The approximation to div u is based on the use of Gauss' Theorem in a volume element. Centerpoint quadrature approximations to the surface integrals involved leads to a discrete operator div_h which provides an intrinsically consistent, second order accurate, approximation to div **u** in terms of the normal components of **u** at centerpoints of faces δS. This is a familiar idea in finite volume methods. An approximation to **u** = grad ϕ will result from the integral form

$$\int_C \mathbf{u}\cdot\mathbf{dx} = \phi(B) - \phi(A)$$

in which the points A and B are identified with the points P, Q, and R in Figure 2. A midpoint evaluation of the integral will determine two tangential components of **u** lying in a surface element in terms of the variable ζ at edges of $\delta S(Q)$. The remaining non-tangential component of **u** on dS will result by using points P and Q and a one-sided evaluation of the integral at Q. This approximation will lead to second-order accuracy as a result of imposing additional continuity conditions for the variables on δS, as occurred in the 1-dimensional case. We indicate by $\text{grad}_h\phi$ the vector **u** evaluated at each face using this construction.

The compact scheme which emerges is described in II.4 and can be summarized as follows:

(a) In each element **u**, ϕ, ψ, ζ satisfy $\text{div}_h\,\mathbf{u} = f$, $\text{grad}_h\phi = \mathbf{u}$, in which the normal components of **u** arising in $\text{div}_h\,\mathbf{u}$ are to be evaluated in terms of the components given by $\text{grad}_h\phi$.

(b) Across each oriented face δS impose the continuity conditions $[\mathbf{u}\cdot\delta S] = [\phi] = [\zeta] = 0$.

(c) If δS lies on the boundary S of V, then ϕ and ζ are to be prescribed by the data.

These conditions exactly mirror the situation discussed for the 1-dimensional problem. However, we shall find that they lead to an underdetermined system of algebraic

equations and certain additional conditions will be required. These are furnished by the

(d) completeness conditions: These conditions determine ζ at vertex points in terms of the variable ψ by the use of a bilinear interpolation which we indicate as $\zeta = \Omega(\psi)$. Among other things, This will insure that is ζ bounded in norm by ψ.

This scheme will lead to an energy equation and convergence will be assured. The potential form will also show that the maximum-minimum property also holds.

When curvilinear coordinates are used, many of the geometrical constructions required for elements will be provided analytically. Furthermore, for Cartesian or more general orthogonal grids, we will find that the variable ζ can be obtained by postprocessing the results using the completeness conditions. This emphasizes the practical advantages of utilizing regular elements throughout most of the domain V and restricting the general construction to boundary elements.

II.2. Geometrical Considerations and Notations

II.2.1. Normal Volume Elements

We call $\{\delta V\}$ a *normal* covering of V by volume elements δV, themselves called normal, if: (i) each element is a hexahedron, some of whose face areas may be allowed to vanish providing its volume τ remains positive (*degeneracy*), (ii) any face of a boundary element δV which is in contact with the boundary surface S of V is tangent to S at the centerpoint of the face. The first assumption has important consequences for the geometrical constructions which will now be described.

Figure 2 indicates a normal volume δV element with center at P and surface elements δS. Since δV is a hexahedron, P may be found as the average of the verticies of δV,

while the average of the vertices on a face yields the centerpoint Q and the average of the vertex points on an edge yields the centerpoint R. We may thus construct a righthanded, local coordinate basis

$$[\mathbf{e}(P)] \equiv (\mathbf{e}_1(P), \mathbf{e}_2(P), \mathbf{e}_3(P))$$

at P which is formed by unit vectors in directions which connect the pairs of opposite centerpoints of the faces δS which we denote as $Q_{i\pm}$, i = 1, 2, 3. The face $\delta S(Q_{i-})$ is assumed oriented into δV, while $\delta S(Q_{i+})$ is outward; these are sometimes called *inflow* and *outflow* faces. We also assume that the orientation carries over to neighboring elements by requiring that an outflow face from one element be an inflow face on its adjacent neighbor.

Our primary requirement will be to evaluate the vector $\mathbf{u}(Q)$ at the centerpoints of faces. In order to do this we will construct a unit basis $[\mathbf{e}(Q)]$ at each Q as follows: assume that $\delta S(Q)$ is the outflow face of $\delta V(P)$ and the inflow face of a neighboring element $\delta V(P')$, e.g., $Q = Q_{1+}$. We take $\mathbf{e}_1(Q)$ as a unit vector in the direction of a line connecting P and P′. Also take $\mathbf{e}_2(Q)$, $\mathbf{e}_3(Q)$ as unit vectors in directions which connect Q with the centerpoints of the edges R of $\delta S(Q)$ so that $[\mathbf{e}(Q)]$forms a right-handed basis as indicated in the Figure 2. Thus, $\mathbf{e}_2(Q)$, $\mathbf{e}_3(Q)$ are tangent vectors on $\delta S(Q)$ while $\mathbf{e}_1(Q)$ is non-tangential.

We may regard the points indicated as being related by displacement operators $E_{i\pm}$ along a direction $\mathbf{e}_i$ so that

$$Q_{i\pm} = E_{i\pm}\, P, \quad R_{i\pm,j\pm} = E_{j\pm}\, Q_{i\pm}$$

with the further understanding that (i, j, k) indicates an even permutation of (1,2,3). The averaging and difference operators defined earlier by \II.3\ may be generalized by writing

$$\mu_i\, \phi(C) \equiv (\phi(E_{i+}C) + \phi(E_{i-}C))/2\,, \quad \Delta_i\, \phi(C) \equiv (\phi(E_{i+}C) - \phi(E_{i-}C)) \qquad \text{\II.1\}$$

for a representative centerpoint C. From this it is apparent that the summation-by-parts identities \I.4\ continue to hold.

Motivated by this notation we will write also $\Delta_i x(Q)$ to indicate the distance

between the points Q_{i-} and Q_{i+} and write $h_i(Q) = \Delta_i x(Q)/2$. Also, h itself will indicate the minimum value of $h_i(P)$ for all volume elements covering V.

II.2.2. Covariant and Contravariant Bases on δV

A basis $[\mathbf{e}] \equiv (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ may be considered as a *covariant* basis from which a reciprocal *contravariant* basis $[\mathbf{e}]^{-1} \equiv (\mathbf{e}^i, \mathbf{e}^j, \mathbf{e}^k)$ can be constructed satisfying

$$\mathbf{e}^i = (\mathbf{e}_j \times \mathbf{e}_k)/\sqrt{e}, \quad \mathbf{e}_i = \sqrt{e}\cdot(\mathbf{e}^j \times \mathbf{e}^k), \quad \mathbf{e}^i\cdot\mathbf{e}_j = \delta_{ij} \qquad \backslash II.2\backslash$$

in which, if $e_{ij} \equiv \mathbf{e}_i\cdot\mathbf{e}_j$ and $e^{ij} \equiv \mathbf{e}^i\cdot\mathbf{e}^j$, then

$$e \equiv \det(e_{ij}), \qquad 1/e = \det(e^{ij}). \qquad \backslash II.3\backslash$$

Anticipating the connection to curvilinear coordinates, we call e_{ij} *element metric* coefficients at P. As a result we may write

$$\mathbf{u} = \sum u_i\mathbf{e}^i = \sum u^i\mathbf{e}_i, \qquad \backslash II.4\backslash$$

$$u^i = \sum e^{ij}u_j, \qquad u_i = \sum e_{ij}u^j$$

$$\mathbf{u}\cdot\mathbf{u} = \sum u_i u^i .$$

where $u_i = \mathbf{u}\cdot\mathbf{e}_i$ and $u^i = \mathbf{u}\cdot\mathbf{e}^i$ are the (physical) *covariant* and *contravariant* components of $\mathbf{u}$, respectively, with respect to $[\mathbf{e}]$.

Using the unit tangent vectors $\mathbf{e}_2, \mathbf{e}_3$ the oriented area of a face $\delta S(Q_{1+})$ is

$$\delta\mathbf{S} = |\delta S|\cdot\mathbf{e}_2 \times \mathbf{e}_3 = |\delta S|\sqrt{e}\cdot\mathbf{e}^i \qquad \backslash II.5\backslash$$

where

$$|\delta S| = \Delta_2 x(Q)\,\Delta_3 x(Q)$$

Thus, the covariant component δS_i of $\delta\mathbf{S}$ is $\delta S_i = |\delta S|\sqrt{e}$. Also, elementary geometrical arguments based on the fact that normal volume elements are hexahedra show that if

$$\tau_0 = \Delta_1 x\cdot\Delta_2 x\cdot\Delta_3 x$$

then the volume measure τ of δV is given by

$$\tau = \Delta_i x(Q)\,\mathbf{e}_i(P)\cdot(\delta\mathbf{S}(Q_{i-}) + \delta\mathbf{S}(Q_{i+}))/2 = \tau_0\cdot\mu_i\sqrt{e},$$

i = 1,2,3. If we also assume posiive constants c_0 and c_1 such that $c_0 h^3 \le \tau \le c_1 h^3$ and also set

$\sqrt{e_0} \equiv \mu_i \sqrt{e}$ we can summarize these geometrical results as

$$\tau = \tau_0 \cdot \sqrt{e_0}, \quad \delta S_i = \Delta_j x \Delta_k x \sqrt{e}. \qquad \backslash II.6\backslash$$

Finally, we also observe that midpoint quadrature rules result in

$$\begin{aligned} \int \mathbf{u} \cdot d\mathbf{x} &\approx \mathbf{u}(C) \cdot \Delta\, \mathbf{x}(C), \\ \int \mathbf{u} \cdot d\mathbf{S} &\approx \mathbf{u}(C) \cdot \delta \mathbf{S}(C) \qquad \backslash II.7\backslash \\ \int \mathbf{u} \cdot dV &\approx \mathbf{u}(C) \cdot \tau. \end{aligned}$$

where C is a representative centerpoint of the figure.

These facts summarize the principal properties of normal volume elements which we shall require.

II.3. The Operators $\underline{\text{div}_h}$ and $\underline{\text{grad}_h}$.

The fundamental geometrical properties of the differential operators div, curl, and grad stem from the following: div relates volume integrals with surface integrals, curl relates surface integrals with line integrals, and grad relates line integrals with endpoints. We will now describe how these properties can be systematically developed for the div and grad operators.

$\underline{\text{div}_h}$: Gauss' formula

$$\int \text{div}\, \mathbf{u}\, dV = \int \mathbf{u} \cdot \mathbf{n}\, dS$$

when applied on δV using the quadrature approximations indicated above suggests the definition

$$\tau\, \text{div}_h\, \mathbf{u} \equiv \Sigma_i\, \Delta_i\, \mathbf{u} \cdot \delta \mathbf{S} \qquad \backslash II.8\backslash$$

in which the difference operator applies to opposite face centerpoints $Q_{i\pm}$. Using the component representations for the terms on the right,

$$\text{div}_h\, \mathbf{u} = \tau^{-1}\, \Sigma_i\, \Delta_i\, u^i \cdot \delta S_i \qquad \backslash II.9\backslash$$

or, noting \II.6\,

$$\text{div}_h\, \mathbf{u} \equiv (\sqrt{e_0})^{-1}\, \Sigma_i\, \Delta_i \sqrt{e}\, u^i / \Delta_i x \qquad \backslash II.10\backslash$$

grad$_h$: The approximations to be identified with $\mathbf{u} = \text{grad}\,\phi$ will follow from the line-integral evaluation

$$\int_C \mathbf{u}\cdot\mathbf{dx} = \phi(B) - \phi(A) \qquad \text{\II.11\}$$

in which A, B are endpoints of a curve *C*. We will describe how the covariant components of **u** with respect to the bases [e(Q)] can be determined at face centerpoints.

Tangential Components:

Recalling earlier notations, suppose $\mathbf{e}_2(Q_{1+})$, $\mathbf{e}_3(Q_{1+})$ are tangent vectors to the face $\delta S(Q_{1+})$ at Q_{1+}. Evaluating \II.11\ along the line connecting the centers of opposite edges $R_{1+,2\pm}$ and $R_{1+,3\pm}$ we obtain

$$\int_C \mathbf{u}\cdot\mathbf{dx} = \zeta\,(R_{1+,j+}) - \zeta\,(R_{1+,j-}) \qquad j = 2,3$$

in which we have identified the potential variable on edges of δS by ζ. Next, use the quadrature evaluation

$$\int_C \mathbf{u}\cdot\mathbf{dx} = \Delta_j\, x\cdot(\mathbf{u}\cdot\mathbf{e}_j(Q_{1+})) = \Delta_j\, x\cdot u_j\,(Q_{1+})$$

in which u_j is the covariant component of $\mathbf{u}(Q_{1+})$. Thus,

$$\Delta_j\, x\cdot u_j\,(Q_{1+}) = \zeta\,(R_{1+,\,j+}) - \zeta\,(R_{1+,\,j-}) \qquad j = 2,3.$$
$$\equiv \Delta_j\,\zeta\,(Q_{1+}) \qquad \text{\II.12\}$$

Non-Tangential Components

We will also require evaluations of the non-tangential components of **u** at the centerpoints of faces and, as for the 1-dimensional case, want to evaluate these in terms of the value of ψ at the center P of δV and of ϕ at the centerpoints Q of its faces. Let us first introduce the one-sided difference operators

$$\Delta_i^{\pm}\,\phi(Q_{i\pm}) \equiv \pm\,[\phi(Q_{i\pm}) - \psi(P)]. \qquad \text{\II.13\}$$

Then \II.8\ leads to

$$\int \mathbf{u}\cdot\mathbf{ds} = \Delta_i^{\pm}\,\phi(Q_{i\pm})$$

in which the line integrals are to be taken between Q_{i-} and P and between P and Q_{i+}, respectively.

We then evaluate the integrals by one-sided quadrature approximations using values of **u** at the faces to obtain

$$\int \mathbf{u}\cdot\mathbf{dx} \approx (\Delta_i x(P)/2)\cdot\mathbf{u}(Q_{i\pm})\cdot\mathbf{e}_i(Q_{i\pm})$$
$$= (\Delta_i x(P)/2)\cdot u_i(Q_{i\pm})$$

so that

$$(\Delta_i x(P)/2)\cdot u_i(Q_{i\pm}) = \Delta_i^{\pm}\phi(Q_{i\pm}) = \pm[\phi(Q_{i\pm}) - \psi(P)]. \qquad \backslash II.14\backslash$$

We can summarize this construction as follows:

grad$_h$: $\mathbf{u}(Q) = \text{grad}_h\,\phi$ expresses the set of relationships between the covariant components of u(Q) and values of ϕ, ψ, and ζ at points Q on the faces of an element given by:

Tangential components:

$$\Delta_j x\cdot u_j(Q) = \Delta_j \zeta(Q) \qquad \backslash II.12\backslash$$

Non-tangential components:

$$(\Delta_i x/2)\, u_i(Q) = \Delta_i^{\pm}\phi(Q). \qquad \backslash II.14\backslash$$

where

$$\Delta_i^{\pm}\phi(Q) \equiv \pm[\phi(Q) - \psi(P)]. \qquad \backslash II.13\backslash$$

Eqs.\II.14\ should be compared to eqs.\I.6\. By adding and subtracting these terms we obtain an equivalent form:

$$\Delta_i x(P)\,\mu_i\, u_i(P) = \Delta_i\,\phi(P), \qquad \backslash II.15\backslash$$
$$\psi(P) = \mu_i\,\phi(P) - \Delta_i x(P)\,\Delta_i\, u_i(P)/4$$

in which only centered operators at P are involved and which may be seen to be second order accurate with respect to P. These forms play an important role in establishing energy results.

II.4. A Compact Scheme

We will now return to the primary problem of solving the boundary value problem when V is a general volume with boundary S. Following our earlier discussion, we describe a compact scheme for solving the problem as follows:

(i) in each element δV solve

$$\mathrm{div}_h\, \mathbf{u} = f, \qquad \mathbf{u} = \mathrm{grad}_h\, \phi. \tag{II.16}$$

Note that $\mathrm{div}_h\, \mathbf{u} = f$ provides one equation for the six contravariant components of $\mathbf{u}$ on the faces of the element, while $\mathbf{u} = \mathrm{grad}_h\, \phi$ expresses three equations for the covariant components of $\mathbf{u}$ on each of the six sides of δV, in which the tangential components are evaluated in terms of the variable ζ at the centerpoints of edges while the nontangential components are determined by the variables ϕ and ψ.

(ii) use

$$u^i = \sum e^{ij} u_j \tag{II.17}$$

from (II.4) to relate the contravariant components to the covariant components arising in (II.16).

An important simplification will occur in this construction whenever $e^{ij} = 0$, $i \neq j$. When this situation arises we call the scheme *strongly* compact, otherwise we use the term *weakly* compact. For a strongly compact scheme the tangential components of $\mathbf{u}$ on faces will not affect the computation directly (and, thus, neither will the variable ζ) but may, if required, be determined in terms of the variable ζ by a postprocessing technique using the completeness relationships described below. This arises when Cartesian or orthogonal curvilinear grids are involved.

(iii) impose continuity conditions for $\mathbf{u}, \phi, \zeta$ on faces common to neighboring elements. In case δV is a boundary element, the data on S will be assumed to determine the data ϕ and ζ on any face tangent to S by the use of a Taylor series approximation.

We are required to calculate $\mathbf{u}$ and ϕ at the centers of the faces of elements, ψ at the centers of the elements themselves, and ζ on the edges of the faces. By examining a cube, we can verify the fact that the number of unknowns involved in the system of equations resulting from the steps just described will exceed the number of equations by just the number of interior edges of elements, i.e., those edges which are incident to four adjacent elements. This same result will also hold for a more general covering $\{\delta V\}$. In order to make the scheme determinate we will add the following

(iv) Completeness Conditions:

Let N(R) denote the centerpoints P of those volume elements which are incident to an edge having R as centerpoint. Using a bilinear interpolation, express $\zeta(R)$ in terms of the values $\psi(R)$ which are associated with the neighboring elements. The result can be written

$$\zeta(R) = \sum \omega(P)\psi(P) \qquad \backslash II.18\backslash$$

where the summation includes points P in N(R) and the weights ω are non-negative and sum to 1. As noted above, when the scheme is strongly compact \II.18\ will allow the tangential components of $\mathbf{u}$ on faces to be calculated separately.

II.5. Energy

We will now show how an energy expression can be derived. From it the existence and uniqueness of the solution of the discrete problem will follow.

Following the argument given for the one-dimensional case, use the summation rules \I.4\ and also \II.15\ to obtain

$$\begin{aligned}
\tau \, \mathrm{div}_h \, \phi \mathbf{u} &= \sum_i \Delta_i \phi u^i \delta S_i \\
&= \sum_i [\mu_i \phi \, \Delta_i u^i \delta S_i + \Delta_i \phi \, \mu_i u^i \delta S_i] \\
&= \sum_i [(\psi + 1/4 \, \Delta_i x \Delta_i u_i) \, \Delta_i u^i \delta S_i + \Delta_i x \mu_i u_i \, (\mu_i u^i \delta S_i)] \\
&= \psi \sum_i \Delta_i u^i \delta S_i + \sum_i \Delta_i x \mu_i (u_i u^i \delta S_i)
\end{aligned}$$

or, recalling that $\delta S_i = \sqrt{e}\Delta_j x \Delta_k x$,

$$\tau \, \mathrm{div}_h \, \phi \mathbf{u} = \phi \, \tau \, \mathrm{div}_h \, \mathbf{u} + \tau_0 \sum_i \mu_i (u_i \, u^i \sqrt{e})$$

so that summing over volume elements yields

$$\sum_V \mathrm{div}_h \, \phi \mathbf{u} \, \tau = \sum_V \phi \, \mathrm{div}_h \, \mathbf{u} \, \tau + \sum_V \{\sum_i \mu_i (u_i \, u^i \sqrt{e})\} \, \tau_0 \, .$$

Finally, using the telescoping property of the $\sum_V \mathrm{div}_h$ term on the left-hand side and recalling that $\tau = \tau_0 \sqrt{e_0}$, we find

$$\sum_S \phi \mathbf{u} \cdot \delta \mathbf{S} \approx \sum_V \phi \, \mathrm{div}_h \, \mathbf{u} \, \tau + \sum_V \mathbf{u} \cdot \mathbf{u} \, \tau \qquad \backslash \mathrm{II}.19 \backslash$$

which is clearly consistent with the integral form of the energy equation given by eq.\4\.

Noting that \II.18\ will insure that ζ is bounded in norm by ψ, the same arguments as were given for the one-dimensional problem will imply that this more general compact scheme converges and yields second order accuracy for ϕ, ψ, ζ and $\mathbf{u}$.

II.6. The Potential Formulation

We shall indicate how the scheme just described can be formulated solely in terms of ϕ,ψ, and ζ, corresponding to the potential form $\nabla^2\phi = f$. Again following our discussion of the one-dimensional case, we write, using \II.9\ and \II.4\,

$$\tau\, \mathrm{div}_h\, \mathbf{u} = \sum_i \Delta_i\, u^i\, \delta S_i$$
$$= \sum_i \Delta_i \left(\sum_j e^{ij} u_j\right) \delta S_i$$

or, regrouping terms:

$$\tau\, \mathrm{div}_h\, \mathbf{u} = \sum_i \Delta_i\, e^{ii} u_i\, \delta S_i + \sum_i \left(\Delta_i \sum_{j\neq i} e^{ij} u_j\right) \delta S_i \qquad \text{\II.20\}$$

Using \II.14\ in the first summation we find

$$\sum_i \Delta_i\, e^{ii}\, u_i\, \delta S_i = 2\sum_i \Delta_i\, e^{ii}\, \Delta_i^{\pm}\phi\, \delta S_i / \Delta_i x$$
$$= 4 \sum_i \mu_i\, e^{ii}\, \phi\, \delta S_i / \Delta_i x - 4\, \psi(P) \sum_i \mu_i\, e^{ii}\, \delta S_i / \Delta_i x \qquad \text{\II.21\}$$

in which the summands are evaluated at the centers of faces about the centerpoint P of the element. The second group of terms in \II.20\ involve only tangential components of $\mathbf{u}$ at face centers, and we may use \II.12\ to express these in terms of values of ζ at the edges. In this manner, all of the terms in \II.20\ may be expressed in terms of the values of ϕ, ψ, and ζ in each element. This leads to the *potential* operator $\mathrm{div}_h\, \mathrm{grad}_h\, \phi$.

Since ϕ, ψ, and ζ are assumed continuous across faces, the continuity conditions for $\mathbf{u}$ across a face δS_i common to neighboring elements with centers at P and P′ reduce to

$$[u^i\, \delta S_i] = 0.$$

The tangential covariant components of $\mathbf{u}$ are continuous, since they are determined by ζ. Recalling \II.14\, the condition that the nontangential covariant component u_i be continuous is then

$$(\Delta_i x + \Delta_i x')\, \phi = \Delta_i x\, \psi' + \Delta_i x'\, \psi \qquad \text{\II.22\}$$

which may be compared to \I.9a\

Consider the treatment of $\nabla^2\phi = 0$ using a strongly compact scheme. In this case $e^{ij} = 0, j \neq i$ and the condition $\text{div}_h \text{ grad}_h \phi = 0$ as expressed by using \II.20\ reduces to

$$\sum_i \mu_i e^{ii} \phi \, \delta S_i / \Delta_i x = \psi(P) \sum_i \mu_i e^{ii} \delta S_i / \Delta_i x \qquad \text{\II.23\}$$

which may be written

$$\psi = \sum_i \alpha_i \phi \qquad \text{\II.24\}$$

where

$$\alpha_i = (\mu_i e^{ii} \delta S_i / \Delta_i x) / (\sum_i \mu_i e^{ii} \delta S_i / \Delta_i x), \qquad \text{\II.25\}$$

$$\sum_i \alpha_i = 1.$$

If we write the continuity condition \II.22\ as

$$\phi = \beta_i \psi + \beta_i' \psi' \qquad \beta_i + \beta_i' = 1 \qquad \text{\II.26\}$$

we can conclude that the maximum-minimum property holds. This same conclusion can be reached for a weakly compact scheme.

Referring to the energy expression, it will be seen that the potential form can also be viewed as arising from a variational problem. By using the completeness relations, the computational problem will thus reduce to determining the variables ϕ and ψ associated with a symmetric, positive definite matrix and thereby allows a variety of familiar solution techniques to be used.

II.7. Degeneracy

Recall that the definition of a normal volume element allowed for the area of one or more of its faces to vanish. Such degenerate elements play a natural role at the boundary S and are especially relevant, as will be shown shortly, in treating problems in curvilinear coodinate at the origin.

Let us suppose that a face with center Q is degenerate, i.e., $dS(Q) = 0$. Referring

to \II.8\ we see that the term involving the factor dS(Q) will not contribute to the evaluation of div_h **u** and, as a result, the contravariant component of **u**(Q) need not be computed on the face. In the potential form, this simply modifies the weight α associated with the degenerate face in \II.25\.

II.8. Curvilinear Coordinates

We will illustrate how the discussion applies when curvilinear coordinates are used. With their use the basis $(\mathbf{e}_i, \mathbf{e}_j, \mathbf{e}_k)$, which was required at each face of a volume element, can be constructed analytically, thereby considerably reducing the preliminary computational steps required. Using the potential form, we shall also illustrate the treatment of the situation at the origin which gives rise to degeneracy.

We indicate by $\mathbf{x} = \mathbf{x}(\mathbf{q})$ a mapping in general curvilinear coordinates. The vectors

$$\mathbf{g}_i = \frac{\partial \mathbf{x}}{\partial q^i} \qquad \text{\II.27\}$$

are tangent vectors on the coordinate lines formed by q^j = const. and q^k = const. so that an element of length is determined by

$$ds^2 = \sum\sum g_{ij} dq^i dq^j$$

in which g_{ij} are metric coefficients given by $g_{ij} = \mathbf{g}_i \cdot \mathbf{g}_j$. Considering $[\mathbf{g}] = (\mathbf{g}_i, \mathbf{g}_j, \mathbf{g}_k)$ as a covariant basis, a reciprocal basis $(\mathbf{g}^i, \mathbf{g}^j, \mathbf{g}^k)$ is given as

$$\mathbf{g}^i = (\mathbf{g}_j \times \mathbf{g}_k) / \sqrt{g}$$

in which $g = \det(g_{ij})$. Also, if $g^{ij} \equiv \mathbf{g}^i \cdot \mathbf{g}^j$,, then $\det(g^{ij}) = g^{-1}$.

Consider a curvilinear volume element dV which is formed as the image of a rectilinear volume element whose volume is $dq^i dq^j dq^k$. Then the edges of a face on dV given as q^i = const. are coordinate lines on which $\mathbf{g}_j$, $\mathbf{g}_k$ are tangent vectors and the oriented area of the face is

$$d\mathbf{S} = (\mathbf{g}_j \times \mathbf{g}_k)\, dq^j dq^k.$$

We may associate a normal volume element δV with dV by constructing tangent planes through the centers of the surface elements through dV. From geometrical considerations it is evident that if we make the following identifications

$$\Delta_i x\, \mathbf{e}_i = \mathbf{g}_i\, dq^i \qquad i = 1,2,3 \qquad \text{\II.28\}$$

the results of our earlier discussion will apply. If $u^i(\mathbf{g})$ indicates a contravariant component of $\mathbf{u}$ in the curvilinear system we find, in place of \II.10\,

$$\mathrm{div}_h\, \mathbf{u} \equiv (\sqrt{g_0})^{-1} \sum_i \Delta_i \sqrt{g}\, u^i(\mathbf{g}) / dq^i. \qquad \text{\II.29\}$$

Similarly, $\mathbf{u} = \mathrm{grad}_h\, \phi$, expressed earlier by \II.12\ and \II.14\, now result in

Tangential components:

$$dq^j \cdot u_j(\mathbf{g}) = \Delta_j \zeta \qquad \text{\II.30\}$$

Non-tangential components:

$$(dq^i/2)\, u_i(\mathbf{g}) = \Delta_i^{\pm} \phi. \qquad \text{\II.31\}$$

Examples

The cases of cylindrical and spherical coordinates may help illustrate these results.

Cylindrical Coordinates:

Here $\mathbf{q} = (r, \theta, z)$ and a calculation gives $\sqrt{g} = r$ and $\sqrt{g}\, g^{11} = r$, $\sqrt{g}\, g^{22} = 1/r$, $\sqrt{g}\, g^{33} = r$. The centerpoints of faces $Q_{i\pm}$ have the coordinates:

$$P_{1\pm} = (r \pm \Delta r/2, \theta, z), \quad P_{2\pm} = (r, \theta \pm \Delta\theta/2, z), \quad P_{3\pm} = (r, \theta, z \pm \Delta z/2)$$

Adopting more standard finite difference notations, let $\phi(i\Delta r, j\Delta\theta, k\Delta z) \equiv \phi_{i,j,k}$ and extend the meaning of the spatial averaging and differencing operators μ,Δ to this case by writing $(\mu_r, \mu_\theta, \mu_z)$, $(\Delta_r, \Delta_\theta, \Delta_z)$. We find that in a cell with center at $P = (i\Delta r, j\Delta\theta, k\Delta z)$

$$\mathrm{div}_h\, \mathrm{grad}_h\, \phi = \frac{4}{r}\left\{\frac{1}{2\Delta r^2}\left[(r + \Delta r/2)\, \phi_{i+1/2,j,k} + (r - \Delta r/2)\right] \phi_{i-1/2,j,k}\right. \qquad \text{\II.32\}$$
$$\left. + \frac{1}{r\Delta\theta^2}\mu_\theta\, \phi_{i,j,k} + \frac{r}{\Delta z^2}\mu_z \phi_{i,j,k} - \sigma_0\, \psi_{i,j,k}\right\}$$

in which

$$\sigma_0 = r\left(\frac{1}{\Delta r^2} + \frac{1}{\Delta z^2}\right) + \frac{1}{r\Delta\theta^2}.$$

Assuming equal spacings, the continuity conditions across faces have the form

$$\phi = \mu\psi \qquad \text{\II.33\}$$

in which $\mu = (\mu_r, \mu_\theta, \mu_z)$.

A cell with center at $(\Delta r/2, j\Delta\theta, k\Delta z)$ has the origin as a degenerate face. In this case we see that the coefficient of the value of the unknown $\phi_{0,j,k}$ vanishes, so that no assumption other than boundedness at the origin is required for the scheme.

For cells not involving boundary points, we may use the continuity condition in \II.29\ to express the result solely in terms of ψ. By adopting the notation $\delta_r \equiv \Delta_r / \Delta r$, etc. to indicate divided differences, the potential operator for such cells reduces to the form

$$\text{div}_h \, \text{grad}_h \, \phi = \left\{ \delta_r^2 + \frac{1}{r}\delta_r\mu_r + \frac{1}{r^2}\delta_\theta^2 + \delta_z^2 \right\} \psi \qquad \text{\II.34\}$$

which can be seen to be consistent with the familiar differential form in cylindrical coordinates. However, we emphasize again that the boundary conditions involving ϕ cannot be handled directly from this form but must, instead, be developed using \II.30\ directly.

Spherical Coordinates:

In this case $\mathbf{q} = (r, \varphi, \theta)$ and a calculation shows $\sqrt{g} = r^2 \sin\varphi$ while $\sqrt{g}\, g^{11} = r^2$, $\sqrt{g}\, g^{22} = \sin\varphi$, $\sqrt{g}\, g^{33} = 1$. Again assuming a uniform mesh spacing, we find in an element with center at $P = (r, \varphi, \theta)$ that

$$\text{div}_h \text{grad}_h \phi = \frac{4}{r^2 \sin\chi} \Big\{ \frac{\sin\chi}{2\Delta r^2} [(r + \Delta r/2)^2 \phi_{i+1/2,j,k} + (r - \Delta r/2)^2 \phi_{i-1/2,j,k}] + \frac{1}{2r\Delta\chi^2} [\sin(\chi + \Delta\chi/2)\phi_{i,j+1/2,k} + \sin(\chi - \Delta\chi/2)\phi_{i,j-1/2,k}] \frac{1}{\Delta\theta^2} \mu_\theta \phi_{i,j,k} - \sigma_0 \psi_{i,j,k} \Big\} \qquad \text{II.35}$$

in which

$$\sigma_0 = \Big\{ \frac{1}{\Delta r^2} (r^2 + \Delta r^2/2)\sin\chi + \frac{1}{\Delta\chi^2} \sin\chi \cos\Delta\chi/2) + \frac{1}{\Delta\theta^2} \Big\} .$$

With $\mu = (\mu_r, \mu_\chi, \mu_\theta)$ the continuity conditions again lead to $\phi = \mu\psi$. We see that the situation at the origin is exactly similar to that in the previous example; in particular, only the boundedness of the solution at the origin is required. Away from boundary cells, the continuity conditions can be used to reduce matters to the form

$$\Delta_t \psi = \frac{\Delta t}{r^2 \sin\chi} \Big\{ (r^2 + \Delta r^2/2) \sin\chi \, \delta_r^2 + 2 \sin\chi \, \delta_r \mu_r + \sin\chi \cos \Delta\chi/2) \delta_\chi^2 + \delta_\theta^2 \Big\} \psi \qquad \text{II.36}$$

which can be seen to be consistent with the potential form of the diffusion equation in spherical coordinates. We again add a precautionary note about attempting to treat the boundary conditions involving ϕ from this form.

II.9. The curl_h Operator

In our treatment of $\mathbf{u} = \text{grad}_h \phi$, emphasis was placed on evaluating the tangential components of $\mathbf{u}$ at the center Q of each face δS using a covariant basis [e(Q)]. Using II.12, these were expressed in terms of the variable ζ which was associated with the centerpoints of the

edges of the face. The completeness conditions \II.18\ were then used to relate ζ to ψ. The contravariant component of $\mathbf{u}$ which arose in the definition of $\mathrm{div}_h\mathbf{u}$ were evaluated in terms of these covariant components using \II.4\.

It is desirable, also, to also have a finite volume approximation to the curl operator which we will indicate by $\mathrm{curl}_h\mathbf{u}$. A satisfactory calculus would then yield both $\mathrm{div}_h\ \mathrm{curl}_h\mathbf{u} = 0$ as well as $\mathrm{curl}_h\ \mathrm{grad}_h\ \phi = 0$ as identities. We shall now indicate how this may be accomplished.

In Figure 2, T indicated a representative vertex of an element. Let $[\hat{\mathbf{e}}(T)]$ indicate a basis formed by the edges which intersect at T using the orientation established by $[\mathbf{e}(P)]$; also let $\hat{\mathbf{e}}(R)$ indicate the translation of $\hat{\mathbf{e}}(T)$ to the centerpoint R of an edge TT′. A suitable definition of curl_h is suggested by the following: If $\omega = \mathrm{curl}\ \mathbf{u}$, then a quadrature approximation in Stokes' formula

$$\int_{\delta S} \omega\cdot\mathbf{n}\ dS = \int_{\partial\delta S} \mathbf{u}\cdot\mathbf{ds}$$

leads to

$$\omega\cdot\delta S \approx \Delta_k\, x\cdot\Delta_j\,(\mathbf{u}\cdot\hat{\mathbf{e}}_k) - \Delta_j\, x\cdot\Delta_k\,(\mathbf{u}\cdot\hat{\mathbf{e}}_j)$$

involving the edges of a face δS. Using component representations, we are led to define curl_h in terms of the set of contravariant components ω^i associated with the faces of δV by means of

$$\omega = \mathrm{curl}_h\,\mathbf{u} \Rightarrow \quad \omega^i \equiv (\Delta_j\,\hat{u}_k/\Delta_j\,x - \Delta_k\,\hat{u}_j/\Delta_k\,x) \qquad \text{\II.32\}$$

in which the covariant components $\hat{u} = \mathbf{u}\cdot\hat{\mathbf{e}}$. With this definition the identity

$$\mathrm{div}_h\ \mathrm{curl}_h\,\mathbf{u} = 0 \qquad \text{\II.33\}$$

follows by noting the cancellation of 'line integrals' along the common edge of faces. (It is also possible to identify a vector associated with the centerpoint of dV, say $\langle \mathrm{curl}_h\mathbf{u}\rangle \equiv \sum\mu_i\omega^i\mathbf{e}_i(P)$, but this vector will not be annihilated by div_h and for which reason will not be considered further here).

As already noted, our earlier treatment of $\mathbf{u} = \mathrm{grad}_h\,\phi$ will not furnish a direct means of evaluating the covariant components $\hat{u}$ occurring above and thus we cannot interpret curl_h

$\text{grad}_h\,\phi$. In order to overcome this, introduce a new variable χ which will be defined at vertices T and is often called a *box-variable*. Recalling the intrinsic definition of grad indicated by \II.11\, we will define grad_h along edges by

$$\Delta_i x \cdot \hat{u}_i\,(R) = \Delta_i\,\chi\,(R) \qquad \text{\II.34\}$$

in which $\Delta_i x$ is the distance between vertices along an edge with direction $\hat{e}_i$ on which R is the centerpoint and $\Delta_i\,\chi\,(R)$ is the difference in values of χ at the vertex neighbors of R. Then

$$\omega^i\,(\hat{u}) \equiv (\Delta_j\,\Delta_k\,\chi\; - \Delta_k\,\Delta_j\,\chi\;) \div \Delta_j\,x \cdot \Delta_k\,x \equiv 0$$

i.e.,

$$\text{curl}_h\,\text{grad}_h\,\phi \equiv 0. \qquad \text{\II.35\}$$

This suggests a theoretical advantage in using the box-variable χ instead of ζ which was used in the earlier discussions. The most direct way to accomplish this is to define the edge variable $\zeta(R)$ as the average of χ at vertices neighboring R, i.e., $\zeta = \mu\chi$, and also re-express the consistency conditions \II.18\ so that now $\chi(T)$, rather than $\zeta(R)$, will be related to $\psi(P)$ at each interior vertex by a bilinear interpolation of the form $\chi = \Omega(\psi)$, which will now involve the six neighboring elements having T as a vertex.

III. The Time-Dependent Problem.

III.1 The Potential Form.

The potential form of the time-dependent diffusion equation \I\ is, with f = 0,

$$\phi_t = \text{div grad}\,\phi \qquad \text{\III.1\}$$

The discrete finite volume operator $\text{div}_h\,\text{grad}_h\,\phi$ corresponding to div grad ϕ has been shown to yield a discrete energy expression which corresponds to the time-independent energy terms in \4\. The principal question remaining, therefore, is how to include the term ϕ_t in the numerical scheme which will provide the approximation to the term $\frac{d}{dt}\int \phi^2 dV$ in the energy expression.

Divide [0,T] into N equal parts of width Δt, write $t_n = n\,\Delta t$, and adopt the standard finite difference notation $u(n\Delta t) = u^n$. Also, let μ_t, Δ_t indicate the central averaging and difference operators which effect the time index as indicated:

$$\mu_t u^n = (u^{n+1/2} + u^{n-1/2})/2 \qquad \text{\III.2\}$$

$$\Delta_t u^n = (u^{n+1/2} - u^{n-1/2}).$$

From \I.4\ it is evident that

$$\mu_t\psi^n\,\Delta_t\,\psi^n = \frac{1}{2}\,\Delta_t\,(\psi^n)^2. \qquad \text{\III.3\}$$

We will consider the following three-level

A. Compact Scheme.

$$\Delta_t\,\psi^n = \Delta t\,\text{div}_h\,\text{grad}_h\,\phi^n \qquad \text{\III.4a\}$$

$$\psi^n = \mu_t\psi^n \qquad \text{\III.4b\}$$

to which the appropriate continuity and completeness conditions \II.22\ and \II.18\ are understood to apply. By multiplying \III.4\ by ψ^n we obtain

$$\frac{1}{2}\,\Delta_t\,(\psi^n)^2 = \Delta t\cdot\psi^n\,\text{div}_h\,\text{grad}_h\,\phi^n \qquad \text{\III.6\}$$

in a volume element . The term on the right-hand-side has already been shown to lead to the energy expression \II.19\. Thus, by summing \III.6\ over elements in a time-strip and using the

implied continuity conditions across faces we will obtain

$$\sum_V \frac{1}{2} \Delta_t (\psi^n)^2 \tau + \Delta t \sum_V \mathbf{u}^n \cdot \mathbf{u}^n \tau = \Delta t \sum_S \phi^n \mathbf{u}^n \cdot \delta S \qquad \text{\III.7\}$$

which is the discrete energy expression which was expected.

Assuming dissipative boundary conditions in the sense of Kreiss [3], it is evident from this result that we can conclude: both ψ^n and ϕ^n are bounded in a discrete norm by the initial and boundary data. Because the scheme is consistent, this also implies that the scheme converges. (Our previous discussion of the maximum-minimum property can allow us to conclude convergence as well.)

We can summarize this in several equivalent ways, in each of which the additional continuity and completeness conditions are assumed to apply:

B: 2-step:

$$\psi^{n+1/2} - \psi^n = (\Delta t/2)\, \mathrm{div}_h\, \mathrm{grad}_h\, \phi^{n+1/2} \qquad \text{\III.8a\}$$

and

$$\psi^{n+1} - \psi^{n+1/2} = (\Delta t/2)\, \mathrm{div}_h\, \mathrm{grad}_h\, \phi^{n+1/2} \qquad \text{\III.8b\}$$

As above, this is a two-step scheme in which the first requires solving the equations in a time strip for $\phi^{n+1/2}$ and $\psi^{n+1/2}$ implicitly in terms of the boundary data for $\phi(t_{n+1/2})$ and the initial data ψ^n. With these values determined, then ψ^{n+1} can be determined explicitly from the second set of equations and furnishes initial data for the next time strip.

C: 1-step:

Eliminating ψ^n in the above scheme we find

$$\Delta_t \psi^n = \Delta t\, \mu_t\, \mathrm{div}_h\, \mathrm{grad}_h\, \phi^n \qquad \text{\III.9\}$$

This is a one-step Crank-Nicholson form.

Example:

Using our earlier 1-dimensional notations, consider the treatment of $\phi_t = \phi_{xx}$.

We find that the 1-step scheme may be written in potential form as

$$\Delta_t \psi_i^n = \kappa \mu_t (\mu\phi_i^n - \psi_i^n), \qquad i \in I_c \text{ (centerpoints)} \quad \backslash III.10a \backslash$$

where $\kappa = \Delta t / h^2$, $h = \Delta x / 2$ To this we add the continuity conditions in the form

$$\mu\psi_i^{n+1/2} - \phi_i^{n+1/2} = 0 \qquad i \in I_e \text{ (endpoints).} \quad \backslash III.10b \backslash$$

Comparing with \I.9\ we again recognize that the variables ϕ_i, ψ_i are the odd-even components of a tri-diagonal system and are therefore readily obtained at each time step.

III.2 An ADI Scheme:

Except for the one-dimensional example just considered, the basic scheme \III.4\ is implicit and effective solution methods must be considered in order to treat the general problem in higher dimensions in a practical manner. It is especially desireable that a proposed method also provide an effective means of treating the steady-state problem as well. We will now show that a Peaceman-Rachford-type ADI scheme, using a straightfoward treatment of intermediate boundary conditions, can solve the finite volume problem with second order accuracy in both space and time. Again, the existence of an energy estimate will provide the key to convergence.

We will find it convenient to make a few slight changes in some of our notations. First, we will let $\bar{v}$ indicate the time average of a variable v, i.e., let

$$\bar{v}^n \equiv \mu_t v^n \qquad \backslash III.11 \backslash$$

Also, we let

$$F_i^n \equiv \tau^{-1} \Delta_i (\mathbf{u}^n \cdot d\mathbf{S}_i) \qquad \backslash III.12 \backslash$$

so that \II.9\ leads to

$$\mathrm{div}_h\, \mathbf{u}^n \equiv F_1{}^n + F_2{}^n + F_3{}^n .$$

Then, for example, the 1-step scheme \III.10\ can be written as

$$\Delta_t \psi^n = \Delta t\, (\bar{F}_1{}^n + \bar{F}_2{}^n + \bar{F}_3{}^n) \qquad \text{\III.13\}$$

in which $\mathbf{u} = \mathrm{grad}_h\, \phi$. Finally, we indicate by g^n assumed boundary data for ϕ on S at time t^n.

Limiting our discussion to two-dimensions, consider the following 2-step scheme:

$$\psi^{n+1/2} - \psi^n = (\Delta t/2)\, (F_1{}^{n+1/2} + F_2{}^n) \qquad \text{\III.14a\}$$

$$\psi^{n+1} - \psi^{n+1/2} = (\Delta t/2)\, (F_1{}^{n+1/2} + F_2{}^{n+1}) \qquad \text{\III.14b\}$$

and note its similarity to \III.8\. Recalling our discussion of the one-dimensional example, it is evident that the first step can be solved as a one-dimensional problem using boundary conditions $\phi^{n+1/2} = g^{n+1/2}$. We solve the second step similarly, but with the boundary conditions $\phi^{n+1} = g^{n+1}$. .

Adding and subtracting \III.14a\ and \III.14a\, and relabeling the time level for purposes of later discussion, we find

$$\psi^{n+1/2} - \psi^{n-1/2} = \Delta t\, (F_1{}^n + \bar{F}_2{}^n) \qquad \text{\III.15a\}$$

$$\psi^n - \bar{\psi}^n = (\Delta t/4)\, (F_2{}^{n-1/2} - F_2{}^{n+1/2}). \qquad \text{\III.15b\}$$

The consistency of (a) with the 1-step Crank-Nicholson form \III.11\ is evident, the truncation error being $O(\Delta t^2)$. Eq.(\III.15b) is also consistent with \III.4(b)\ since the right hand term is $O(\Delta t^3)$. We may regard \III.14\ either as a scheme to approximate the solution of the compact scheme \III.4\ or as an independent scheme to solve the differential equation.

We shall show that this scheme leads to an energy estimate which is consistent with \III.7\ to within terms of $O(\Delta t^2)$. Recalling the basic energy argument in \I.11\ and the definition of F_i in \III.12\ we find

$$\psi \cdot F1 = \Delta(\phi u^1 dS_1) - \mu_1(u^1 u_1)$$

$$\bar{\psi} \cdot \bar{F}_2 = \Delta(\bar{\phi}\bar{u}^2 d\bar{S}_2) - \mu_2(\bar{u}^2 \bar{u}_2)$$

so that by multiplying \III.15a\ by $\bar{\psi}$ and then using \III.15b\ we find

$$\frac{1}{2\Delta t}\Delta_t(\psi^n)^2\,\tau + [\mu_1(u^1u_1)^n + \mu_2(\bar{u}^2\bar{u}_2)^n] = [\Delta(\phi u^1 dS_1) + \Delta(\bar{\phi}\bar{u}^2 d\bar{S}_2)] + O(\Delta t^2).$$

Summing over volume elements and noting that $\bar{\psi} = \psi + O(\Delta t^2)$, etc., we again obtain the energy expression \III.7\ to within terms $O(\Delta t^2)$. This result is sufficient to enable us to conclude that the ADI scheme converges and furnishes an approximation with the same degree of accuracy as the compact scheme \III.4\. This result is independent of any of the fixed ratios $\Delta t / (\Delta x_i)^2$ occuring in either scheme.

To treat the 3D problem, consider in place of \III.14a\, etc.,the following:

$$\begin{aligned}
\psi^{n+1/4} - \psi^n &= (\Delta t/4)\,(2F_1{}^n + F_2{}^{n+1/4}) \qquad \text{III.16}\\
\psi^{n+1/2} - \psi^{n+1/4} &= (\Delta t/4)\,(F_2{}^{n+1/4} + 2F_3{}^{n+1/2})\\
\psi^{n+3/4} - \psi^{n+1/2} &= (\Delta t/4)\,(F_2{}^{n+3/4} + 2F_3{}^{n+1/2})\\
\psi^{n+1} - \psi^{n+3/4} &= (\Delta t/4)\,(2F_1{}^{n+1} + F_2{}^{n+3/4}).
\end{aligned}$$

to which the intermediate boundary conditions $\phi^{n+k} = g^{n+k}$, k = 1/4, 1/2, 3/4, 1 apply. Then

$$\psi^{n+1} - \psi^n = \Delta t\,[(F_1{}^{n+1} + F_1{}^n)/2 + (F_2{}^{n+3/4} + F_2{}^{n+1/4})/2 + F_3{}^{n+1/2}]$$

so that the scheme is consistent with the Crank-Nicholson form. Also,

$$(\psi^{n+1} + \psi^n)/2 - \psi^{n+1/2} = (\Delta t/4)\,[(F_1{}^{n+1} - F_1{}^n) + (F_2{}^{n+3/4} - F_2{}^{n+1/4})].$$

The last pair of equations, which correspond to \III.15\ in the 2D case, can provide the basis for an energy argument, although we omit the details here.

Conclusions:

We have described a finite volume method which closely maintains the parallel between differential and difference arguments. By using intrinsic geometrical properties of the elements, we were able to describe discrete versions of the div, curl, and grad operators which led, using formal summation by parts techniques, to discrete energy equations as well as to the identities $\mathrm{div}_h\ \mathrm{curl}_h\ \mathbf{u} = 0$ and $\mathrm{curl}_h\ \mathrm{grad}_h\ \phi = 0$. The solution of the initial- boundary value problem for the diffusion equation was described directly in terms of these operators by compact schemes and the resulting energy equations insured convergence. The schemes could also be simplified to a potential form which can offer computational advantages. Finally, the treatment of general curvilinear coordinates was shown to result from a specialization of these results.

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