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ON THE CONVERGENCE OF STEADY STATE MULTIREGION DIFFUSION CALCULATIONS

A. C. Downing, Jr.

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ON THE CONVERGENCE OF STEADY STATE MULTIREGION DIFFUSION CALCULATIONS

Arthur C. Downing, Jr.

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ABSTRACT

The basic technique for solving multiregion diffusion problems is the finite difference method. Implicit in this method is the assumption that if the grid size were allowed to shrink to zero the finite difference solutions would converge to a solution of the differential problem. This report is an investigation into the justification of this assumption. Previous work has demonstrated convergence only for the one-region Dirichlet problem.

A new formulation of the finite difference problem is described which admits an additive analog of Green's identity. With this tool it is shown that the grid solutions converge at interior points to a function satisfying the diffusion equation. The behavior at interfaces is also studied, and it appears that suitable convergence properties can be established there, although one step in the proof has not yet been justified.

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INTRODUCTION

The steady-state diffusion equation arises in the mathematical treatment of diverse physical phenomena, such as heat transfer, nuclear reactors, and chemical processes. Present-day design of devices based on these phenomena demands that proper account be taken of the fact that the diffusion takes place in several distinct media or regions. Within any one region the concentration of the diffusing substance satisfies an elliptic partial differential equation. Across each interface separating two distinct regions or media, the concentration and its gradient will not both be continuous, but must satisfy prescribed differential conditions, known as interface conditions. Such problems are known as multiregion diffusion problems.

Since the arrival of high-speed stored-program computers, enormous amounts of scientific manpower and money have been spent in obtaining approximate solutions of multiregion diffusion problems. The basic technique employed is to replace the differential problem by a finite difference problem obtained by superimposing upon the several regions a rectangular lattice or mesh and to solve for values of the unknown function at the nodes of the lattice. Implicit in this technique is the assumption that if the lattice spacing were allowed to shrink to zero the corresponding finite difference solutions would converge to the solution of the differential problem.

This report is primarily concerned with an investigation of the mathematical justification of this assumption. The classical paper of

Courant, Friedrichs, and Lewy in 1928 includes a proof for the special case of the Dirichlet problem for a single region. They assert that their method is applicable to other elliptic differential equations and other boundary conditions, and they indicate an awareness of the difficulties that will arise in demonstrating the necessary bounds for more general differential equations. Later, in 1941, Petrovskiĭ produced another convergence proof for the one-region Dirichlet problem, but his method makes strong use of the properties of superharmonic functions and hence does not appear too useful with other equations. Some additional history is given by Rosenbloom (1952). With the exception of Petrovskiĭ's work, the problem has been virtually untouched for 31 years.

The question of convergence at interfaces has never been raised in the literature.

Recently a related question has been answered for the multigroup multiregion reactor calculation. Habetler and Martino (1958) showed that if the equations for the separate groups are solved cyclically - the so-called "outer" iteration - then the process converges to a solution of the multiregion problem. But this assumes an exact solution for a partial differential problem for each group, not just a solution of the corresponding finite difference problem. The solution of the latter problem is obtained usually by a relaxation procedure which is referred to as the "inner" iteration. The study reported here was concerned with the convergence of this inner iteration.

Clearly, convergence cannot be demonstrated for every formulation of the finite difference problem. So the first effort was to find a formulation for which convergence might be demonstrated, and attention has

been fixed upon a method for treating interfaces which admits an additive analog of Green's first identity. A fundamental obstacle to the analysis of the properties of finite difference multiregion problems has been the lack of a suitable analog of this identity. Such identities are easily obtained for a single region, but they fail to be additive for regions sharing a common interface, at least with the customary approach for specifying the geometrical location of surfaces. This report introduces an alternate approach which admits a Green's identity with the desired additive property. Beyond this theoretical advantage, the finite difference formulation used here eliminates the ambiguous situations which arise in the customary formulation of multiregion problems. Moreover, the matrix of the system of finite difference equations is positive definite. Hence, it is well suited to numerical solution.

For this particular formulation it has been possible to show that the finite difference solutions will converge to a function satisfying the diffusion equation in the interior of each region and, moreover, with the usual interface conditions, to show that the solution of the differential problem is unique. The behavior at the interfaces has also been studied, and it appears that suitable convergence properties can be established there, although one step in the proof has not yet been justified. This is discussed in Chapter 4, page 74. It does not seem likely that the failure to obtain this result indicates a basic difficulty in the approach.

The general method of proof follows that of Courant, Freidrichs, and Lewy very closely. But, whereas they proved only convergence in the

mean at a boundary, it appears that actual pointwise convergence on the interfaces and boundaries can be demonstrated almost everywhere. All results obtained are valid for N-dimensions.

Chapters 6 and 7 are not part of the convergence proof. They contain some new and possibly interesting results which were obtained in an abortive attempt to extend the convergence proof to more general finite difference formulations.

This investigation began in 1954 with an idea for avoiding ambiguous points in the finite difference formulation of multiregion reactor problems. I am grateful to Dr. Ward C. Sangren for his encouragement in developing this idea. To two men I am particularly indebted. Without their patience, confidence, and skilled direction this study could not have been completed. They are Dr. Alston S. Householder of Oak Ridge National Laboratory and Professor Robert C. F. Bartels of the University of Michigan. And finally I wish to express my gratitude to Wilma Campbell and Caila Cox for their painstaking care in typing the manuscript for reproduction.

Chapter 1

PRELIMINARY REMARKS

Definitions

The regions to be considered are regular regions in N-dimensional space. Thus a region is closed, bounded, and has a surface which is a closed, bounded regular surface of dimension N - 1. A region may be triangulated and, hence, may be represented as the union of a finite number of N-dimensional (sub)regions, each with exactly N + 1 curved faces. The triangulation may be made sufficiently small that each face of any (sub)region is a regular surface element; that is, for some orientation of the axes, the face may be represented in the form

$$\xi_1 = F(\xi_2, \xi_3, \ldots, \xi_N) ,$$

where F is a continuously differentiable function. Two subregions may intersect in one or more vertices or edges, but in at most one (N-1)-dimensional face. In the latter case, the entire face is common to both subregions (by the definition of triangulation) and is known as an interface.

Explicit use will be made of the fact that for any particular choice of the coordinate axes, any interface may be further subdivided into a finite number of surface elements, each of which has the property that the angle between the normal to the surface and at least one of the coordinate directions is uniformly bounded away from 90°. Explicit use will also be made of Green's integral theorem, which is valid for a union of regular regions.

Let x denote a point in N-dimensional space whose coordinates

are $(\xi_1, \xi_2, \ldots, \xi_N)$. Let m_s be any N-tuple whose elements are integers with m_0 the zero N-tuple. If x_0 is any arbitrary vector, then the union of all points with coordinates of the form $x_0 + m_s h$, where h is any positive number, is an infinite lattice of points, usually called a grid. The constant h is referred to as the grid size or grid spacing. Each point of the lattice is known as a grid point. The neighbors of any grid point $x_s = x_0 + m_s h$ are all those points which may be represented in the form $x_s \pm e_i h$, where e_i is a unit coordinate vector; that is, e_i is the N-tuple whose ith element has the value unity and all other elements are zero. The intersection of a region and a grid is a finite collection of points which constitute a grid region. In general, the notation for a region will be R and that of the corresponding grid region G or G_h. A grid function or grid solution is defined over some grid region G.

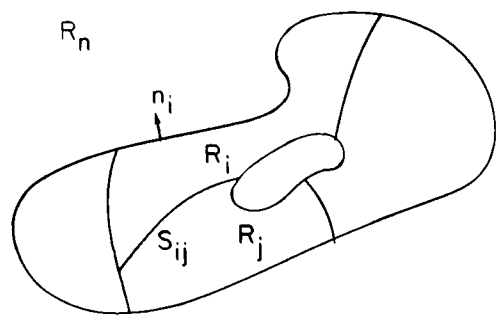
Frequent use will be made of functions which possess continuous partial derivatives over a region. The precise interpretation of this concept is the following: A partial derivative is said to be continuous over a region R provided the partial derivative exists at every interior point of R and coincides there with a function which is continuous over R. Moreover, the value of the partial derivative at a point on the boundary will be taken to be the value of the continuous function at that point. A function is said to be of class $C^{(m)}$ over a region R if it is continuous over R and all its partial derivatives of order not greater than m exist and are continuous over R.

Particular attention is called to two novel definitions. A function f will be said to be of class $M^{(r)}$ over R if f, together with

each of its partial derivatives of order not exceeding r, exists and is bounded over R. A function ρ will be said to be of class $L^2[M^{(r)}, R]$ if ρ^2, together with the square of each of its partial derivatives of order not exceeding r, has a bounded integral over R.

The Multiregion Diffusion Problem

Consider a connected region which is the union of n regions, $R_0, \ldots, R_{n-1}$. Let the exterior be denoted by R_n. The interface between two neighboring regions R_i and R_j is denoted by S_{ij} and the exterior boundary by S_{in} or S_{nj}. In each region R_i, let $u = u_i$ be a function which satisfies an equation of the form



$$-\nabla^2 u_i + D_i u_i = \rho_i \qquad \text{in } R_i (i = 0, \ldots, n-1) \tag{1.1}$$

where $D_i \geq 0$ and of class $M^{(N+1)}$ over R_i and where ρ_i is $L^2[M^{(N+1)}, R_i]$. At each interface S_{ij}, let the functions u_i and u_j satisfy a pair of differential conditions of the type

$$\begin{aligned} u_i &= \alpha_{ij} u_j + \beta_{ij}(\nabla u_j \cdot n_j) \\ -(\nabla u_i \cdot n_i) &= \gamma_{ij} u_j + \delta_{ij}(\nabla u_j \cdot n_j) , \end{aligned} \tag{1.2}$$

where $(\nabla u_i \cdot n_i)$ is the normal derivative in the direction of the exterior normal n_i of R_i and where

$$\alpha_{ij}\,\delta_{ij} - \beta_{ij}\,\gamma_{ij} \neq 0 \qquad (i,j = 0, \ldots, n-1)\ . \tag{1.3}$$

At the outer boundary S_{ni} a single condition is imposed. It has the form

$$f_n = \alpha_{ni}u_i + \beta_{ni}(\nabla u_i \cdot n_i)\ ,$$

where $f_n \in C^{(1)}$ on each S_{ni} (but not necessarily on the union of all S_{ni}). The problem of determining a function u such that $u = u_i$ in each R_i is a multiregion diffusion problem.

The finite difference analog of this problem may be solved by a relaxation procedure. In a multicomponent problem (i.e., several diffusing substances) the problem just described is solved for each component in succession. The relaxation calculation for any one component is referred to as an inner iteration as opposed to the outer iteration, where the distinct components are treated in cyclic order. The outer iteration arises from the fact that the source ρ is a function of all the components.* This study is only concerned with the inner iteration.

Restrictions

Two types of nonhomogeneous terms are present in the multiregion diffusion problem. One type is the source function ρ_i in the diffusion equation; the other type is the function f_n in the boundary condition.

---

*The multicomponent problem for nuclear reactors is known as a multigroup problem, since the neutrons are treated in groups according to their energy ranges. For further discussion of multigroup problems see Bilodeau and Hageman (1957).

Since the problem is linear, the solution may be expressed as the sum of the solution of two problems. In one problem ρ_i is identically zero in every R_i, and in the other, f_n is identically zero on all of the surfaces S_{ni}. For convenience, the latter problem will be called the <u>nuclear reactor problem</u> to distinguish it from the former problem which is a typical <u>heat conduction problem</u>.

The initial motivation for this study was the reactor problem. However, since most of the theorems are also valid for the heat conduction problem, the theory in this report is developed, as far as possible, for the general multiregion diffusion problem. In fact, if nonhomogeneous boundary conditions are restricted to be of mixed type, then the convergence proof for the general diffusion problem is as complete as the proof for the reactor problem.

Specifically, it is assumed that the boundary conditions satisfy the following restrictions: Let $\alpha_{ni}(x) \geq 0$ and $\beta_{ni}(x) \geq 0$ and let α_{ni}, β_{ni}, and f_n be of class $C^{(1)}$ on S_{ni}. The boundary condition at any point $x \in S_{ni}$ must either have the form

$$(1.4a) \qquad 0 = \alpha_{ni} u_i + \beta_{ni}(\nabla u_i \cdot n_i) , \qquad (0 \leq i < n)$$

or have the form

$$(1.4b) \qquad f_n(x) = u_i + \beta_{ni}(\nabla u_i \cdot n_i) , \qquad (0 \leq i < n)$$

with the additional constraint that

$$(1.5) \qquad |f_n(x)/\beta_{ni}(x)| < M_0$$

is uniformly bounded. The latter restriction is used only in Theorem

4.8, a theorem which is not valid when nonhomogeneous Dirichlet conditions are admitted. Since $\alpha_{ni} = 1$ in condition (1.4b), nonhomogeneous Neumann conditions are ruled out. These restrictions permit concentration on the interface problems by avoiding digressions to handle special cases at the boundary.

To complete the proof of Theorem 4.2, it is assumed that the absorption coefficients D_i are positive and bounded away from zero. Thus the existence of a D_{min} is assumed such that $D_i \geq D_{min} > 0$ in each region R_i. This condition is always satisfied in nuclear reactor calculations. However, for the heat conduction problem, where $\rho(x)$ is identically zero in every region, this restriction on the D_i's is not required.

The interface coefficients α_{ij}, β_{ij}, γ_{ij}, and δ_{ij} are assumed to be constants over the interface S_{ij}. A situation where these coefficients are only piecewise constant over S_{ij} can be reduced to the case considered here by further triangulation of the region. Furthermore, because of a conflict between sufficient conditions for uniqueness and sufficient conditions for real characteristic values, there is the added restriction that

$$\beta_{ij}\,\gamma_{ij} = 0 \qquad (0 \leq i,j < n) .$$

In any diffusion process, however, $\gamma_{ij} = 0$ unless the mathematical model assumes that some of the diffusing particles are absorbed by the interface.

Other restrictions on the interface conditions are discussed in the next section.

Interface Conditions

To carry through the convergence proof, certain natural restrictions must be placed upon the coefficients of the interface conditions. These restrictions arise from two separate considerations, one of which is deferred to the next chapter where a set of restrictions sufficient to guarantee the uniqueness of the solution of a multiregion problem is obtained. Closely related to uniqueness is the property of the homogeneous diffusion equation that an extreme value never occurs at an interior point of a region in which the equation is satisfied. To insure that maxima or minima do not occur at an interface in the multiregion problem, it will be assumed that at each interface the coefficients in equation (1.2) satisfy the restrictions

$$
\begin{aligned}
&1 \le \alpha_{ij}, \quad 0 \le \beta_{ij}, \quad 0 \le \gamma_{ij} , \\
(1.6) \qquad & \\
&0 < \alpha_{ij}\, \delta_{ij} - \beta_{ij}\, \gamma_{ij} \le \delta_{ij} .
\end{aligned}
$$

The nature of these restrictions is made clearer by noting that they imply

$$1 \le \alpha_{ij} \le 1 + \beta_{ij}\, \gamma_{ij}\, \delta_{ij}^{-1} .$$

These restrictions, and those given in the next chapter, do not constitute real qualifications on the convergence proof which follows because all of the familiar physical applications of diffusion theory have interface conditions satisfying these restrictions.

Although conditions (1.6) arise naturally in a later chapter, a brief heuristic justification will be given here. Consider the one-

dimensional behavior of the solution along the normal to the interface. For convenience here, let u denote the dependent variable to the left of the interface, let v denote it on the right, and let the independent variable in the normal direction be ξ. The interface equations may be written

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} u \\ u_\xi \end{pmatrix} = \begin{pmatrix} v \\ v_\xi \end{pmatrix} . \tag{1.7}$$

Suppose first that $\delta < 0$. If it happens that

$$u = 0 \text{ and } u_\xi < 0$$

at the interface, then $v_\xi > 0$ and no matter what value v has, there will be a minimum (see figures 1.1 and 1.2). Hence it is reasonable to require

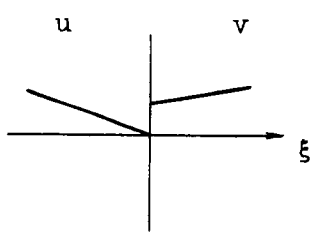


Figure 1.1

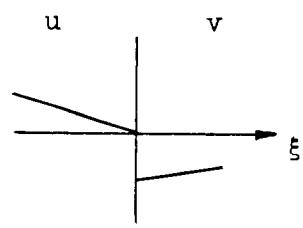


Figure 1.2

that δ be nonnegative. That it must not vanish is justified below. Assume next that $\beta < 0$. Again if $u_\xi < 0$ and $u = 0$, then $v > 0$ and there is a minimum (as in figure 1.1). Hence $\beta \geq 0$. Suppose that $\gamma < 0$. For any $u_\xi > 0$ there are sufficiently large values of $u > 0$ such that v_ξ will be negative. This implies a maximum as in figure 1.3. Finally, consider the effect of allowing $\alpha < 1$. If $u > 0$ and $u_\xi = 0$, then

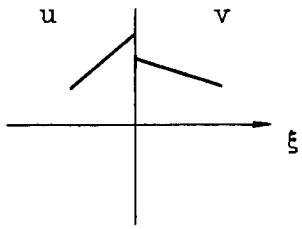


Figure 1.3

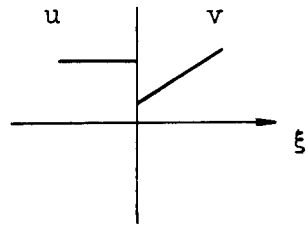


Figure 1.4

$v < u$ while $v_\xi = \gamma u > 0$, as shown in figure 1.4. (With a slight modification, the case $\gamma = 0$ can yield a similar difficulty.)

But the interface conditions can also be written with u and u_ξ as functions of v and v_ξ. Care must be exercised at this point because the interface coefficients are defined in terms of exterior normal derivatives. See equations (1.2). The form equivalent to equation (1.7) is

$$\begin{pmatrix} u \\ -u_\xi \end{pmatrix} = \frac{1}{\alpha\delta - \beta\gamma} \begin{pmatrix} \delta & \beta \\ \gamma & \alpha \end{pmatrix} \begin{pmatrix} v \\ -v_\xi \end{pmatrix}, \tag{1.8}$$

since $\partial v/\partial(-\xi)$ is $-v_\xi$. Clearly the conditions already obtained must apply to these coefficients. In particular it follows that

$$1 \le \frac{\delta}{\alpha\delta - \beta\gamma} .$$

But if $\delta \ge 0$, then $\alpha\delta - \beta\gamma$ cannot be negative, and in fact must be positive since by hypothesis the interface conditions are linearly independent (condition (1.3)). Thus

$$0 < \alpha\delta - \beta\gamma \le \delta .$$

This is the last of the inequalities in (1.6).

Chapter 2

A UNIQUENESS THEOREM

The literature on steady state, multiregion diffusion problems contains no theorems on the existence or the uniqueness of solutions. It is a corollary of the convergence proof in Chapter 4 that solutions do exist which satisfy the partial differential equation at every interior point. The extent to which such solutions satisfy the interface and boundary conditions is discussed in Chapter 5. The convergence proof, however, provides no information on the uniqueness of these solutions. Consequently, in this chapter a set of conditions upon the interface coefficients is obtained which is sufficient to guarantee the uniqueness of any solution for which Green's first integral identity is applicable. Necessary conditions are not known.

The conditions obtained are weak enough to allow the usual physical applications of diffusion theory.

Green's First Identity; and Two Lemmas

The principal analytical tool used in this chapter is one of the well-known identities due to Green. For later reference, the usual form of the identity is stated here, even though the conditions on the functions u and w may be relaxed in several respects (Kellogg, 1929; Courant and Hilbert, 1953).

Theorem. *Let u and w be two functions defined and continuous with continuous first derivatives in a (closed, regular) region R_i. Moreover, let u have continuous second derivatives in R_i. Then*

$$(2.1) \qquad \iiint_{R_i} w \nabla^2 u \, dv + \iiint_{R_i} (\nabla w \cdot \nabla u) dv = \iint_{S_i} w \, (\nabla u \cdot n_i) d\sigma \, ,$$

<u>where</u> n_i <u>is the outward normal to the surface</u> S_i <u>which bounds</u> R_i.

The surface S_i is the union of all the interfaces S_{ij} such that the region R_j is a neighbor of R_i; that is, $R_i \cap R_j = S_{ij}$ has dimension $N - 1$. The symmetric relation "R_j is a neighbor of R_i" will be written as jNi. Note that this relation is neither reflexive nor transitive. Hence, the surface integral may be expanded and Green's identity written in the form

$$(2.2) \qquad \iiint_{R_i} (w \nabla^2 u + \nabla w \cdot \nabla u) dv = \sum_{jNi} \iint_{S_{ij}} w_i \, (\nabla u_i \cdot n_i) d\sigma \, .$$

It will be necessary to sum such expressions over all R_i, and then combine terms. The following lemma is useful in carrying this out.

<u>Lemma</u> 2.1. <u>For any collection of functions</u> η_{ij} $(0 \le i,j \le n)$ <u>for which it is true that</u> $\eta_{ii} = 0$ <u>for all</u> i, <u>then</u>

$$\sum_{i=0}^{n} \sum_{j=0}^{n} \eta_{ij} = \sum_{i=0}^{n} \sum_{j=0}^{i-1} (\eta_{ij} + \eta_{ji}) \, .$$

Rewrite the sum on the left as follows:

$$\sum_{i=0}^{n} \sum_{j=0}^{i-1} \eta_{ij} + \sum_{i=0}^{n} \sum_{j=i}^{n} \eta_{ij} \, .$$

The second double sum may be transformed by interchanging the order of summation and then relabeling the indices, replacing i by j and j by i. Thus

$$\sum_{i=0}^{n} \sum_{j=i}^{n} \eta_{ij} = \sum_{j=0}^{n} \sum_{i=0}^{j} \eta_{ij} = \sum_{i=0}^{n} \sum_{j=0}^{i-1} \eta_{ji} .$$

Define

$$\eta_{ij}(f,g) \equiv \iint_{S_{ij}} f_i g_i \, d\sigma .$$

From equation (2.2) and this lemma, the following results:

<u>Lemma</u> 2.2 <u>Let</u> $k_0^2, \ldots, k_{n-1}^2$ <u>be arbitrary, positive constants and, associated with the exterior</u> R_n, <u>let</u> $k_n^2 = 0$. <u>If</u> w <u>and</u> u <u>satisfy the conditions of Green's theorem for each</u> R_i $(i = 0, \ldots, n-1)$, <u>then</u>

$$\sum_{i=0}^{n-1} k_i^2 \iiint_{R_i} (w \nabla^2 u + \nabla w \cdot \nabla u) dv$$

(2.3)

$$= \sum_{i=0}^{n} \sum_{\substack{j=0 \\ j \mathrm{N} i}}^{i-1} \left[\eta_{ij}(k^2 w, \nabla u \cdot n) + \eta_{ji}(k^2 w, \nabla u \cdot n) \right] .$$

In Chapter 4 a strictly analogous result is obtained for grid functions.

Uniqueness Conditions

If the multiregion diffusion problem does not have a unique solution, then the difference of any two distinct solutions will be a nontrivial solution of the homogeneous problem. Therefore, any set of conditions which are sufficient to guarantee that the homogeneous problem can have only the trivial solution will automatically be sufficient conditions for the uniqueness of the nonhomogeneous problem.

To obtain the homogeneous problem, replace ρ_i in equation (1.1) and f in equation (1.4b) by zero. Let w = u, and suppose that the solution

u has sufficiently strong properties that Green's identity applies to each region R_i. Then Lemma 2.2 may be applied. Solve equation (1.1) for $\nabla^2 u_i$ and substitute into identity (2.3). Similarly, replace u_i and $\nabla u_i \cdot n_i$ by their representations in terms of u_j and $\nabla u_j \cdot n_j$ as given by the interface conditions (1.2). The result, after expanding and rearranging terms, is

$$\sum_{i=0}^{n-1} k_i^2 \iiint_{R_i} (D_i u_i^2 + \nabla u_i \cdot \nabla u_i) dv$$

$$+ \sum_{i=0}^{n-1} \sum_{\substack{j=0 \\ jNi}}^{i-1} k_i^2 \left[\alpha\gamma\eta_{ji} (u,u) + \beta\delta\eta_{ji} (\nabla u \cdot n, \nabla u \cdot n) \right]$$

(2.4)

$$= \sum_{i=0}^{n} \sum_{\substack{j=0 \\ jNi}}^{i-1} \left[k_j^2 - (\alpha\delta + \beta\gamma) k_i^2 \right] \eta_{ji}(u, \nabla u \cdot n) ,$$

where the subscripts i, j have been suppressed on the coefficients α_{ij}, β_{ij}, γ_{ij}, δ_{ij}. Conditions on these coefficients which ensure that only u = 0 will satisfy equation (2.4) are easily obtained by noticing that the first summation is nonnegative and that for any u, η_{ji} (u, u) is nonnegative.

Theorem 2.1. The n-region diffusion problem — excluding the Neumann problem — has at most a unique solution if there exists an ordering of the regions R_i by index, and a set of n positive constants $k_0^2, \ldots, k_{n-1}^2$ such that coefficients of the interface conditions between neighboring regions R_i and R_j satisfy

(i) $k_j^2 = (\alpha_{ij}\,\delta_{ij} + \beta_{ij}\,\gamma_{ij})k_i^2$ <u>for</u> $0 \le j < i < n$,

(ii) α_{ij}, β_{ij}, γ_{ij}, and $\delta_{ij} \ge 0$ <u>for</u> $0 \le j < i < n$,

<u>and the coefficients of the boundary conditions satisfy</u>

(iii) $\alpha_{nj}\,\beta_{nj} \ge 0$ <u>for</u> $0 \le j < n$.

This theorem follows directly from equation (2.4), since the left-hand side must be positive whenever u is not identically zero, while the right-hand side, because of condition (i), reduces to

$$\sum_{\substack{j=0 \\ jNn}}^{n-1} k_j^2\,\eta_{jn}(u,\ \nabla u \cdot n)$$

which cannot be positive by virtue of condition (iii). Indeed, the η_{jn} are integrals over the boundary surfaces S_{nj}. But applying the boundary condition (1.4a) or (1.4b) with $f_n = 0$, it is clear that

$$\eta_{jn}(u,\nabla u \cdot n) = \begin{cases} -(\alpha_{nj}/\beta_{nj})\eta_{jn}(u,u) & , \quad \text{if } \beta_{nj} \neq 0; \\ 0 & , \quad \text{if } \beta_{nj} = 0. \end{cases}$$

<u>Remark</u> 1. The conditions imposed upon the set of constants k_i^2 in Theorem 2.1 are homogeneous in the constants. Moreover, condition (1.6) ensures that $\alpha_{ij}\delta_{ij} + \beta_{ij}\gamma_{ij} > 0$. Hence, if one set exists, then another can always be found in which no k_i^2 is less than unity. This fact will be useful in Chapter 4.

Remark 2. Furthermore, condition (i) is imposed only if $j < i$ and if R_j is a neighbor of R_i. Therefore, there is one and only one condition for each interface. For the familiar problems with "slab geometry" or "spherical geometry," there are only $n - 1$ interfaces. Hence, there will always exist n constants k_i^2 which satisfy these $n - 1$ conditions.

Remark 3. When the Neumann condition, i.e., $\partial u/\partial n = 0$, is prescribed everywhere around the boundary, the n-region problem, nevertheless, has a unique solution if there is at least one interface S_{ij} at which $\gamma_{ij} > 0$ or one subregion R_i in which $D_i > 0$. Otherwise, equation (2.4) only implies that the gradient of u must be zero in each R_i.

Chapter 3

A PARTICULAR FINITE DIFFERENCE FORMULATION

The customary way for setting up a relaxation procedure is to cover the region under consideration with a rectangular net in such a way that the boundary of the region is adequately approximated by segments of the net lines. Since nodes of the net lie on the boundary, Dirichlet conditions are readily imposed upon the solution.

When this procedure is extended to multiregion problems by allowing interfaces to coincide with segments of the net, difficulties arise in the treatment of interior corner points.

Consider the Dirichlet problem depicted in figure 3.1. The simple five-point difference approximation for Laplace's equation may be used. Interface conditions such as continuity of u and a derivative condition of the type

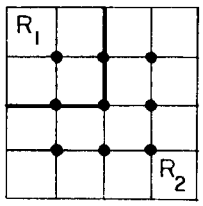


Figure 3.1

$$\delta_1 \frac{\partial u}{\partial n} \text{ (region 1)} = \delta_2 \frac{\partial u}{\partial n} \text{ (region 2)}$$

might be imposed upon the solution. The simplest and the crudest difference approximation for this condition would be to take one-sided difference quotients to approximate the derivatives. This avoids the complication of introducing fictitious points.

There are then five points in region 2 and one point in region 1

at which the partial difference equation applies. Excluding the corner point, the interface condition on the derivatives yields two more conditions, a total of eight conditions involving the nine unknown values of u. Since all other information has been used, the corner point must furnish the ninth condition. But, unfortunately, three relations are available there: the interface condition in two directions and the partial difference equation, if one pretends that the corner is an interior point of region 2. One might well question the applicability of any of these conditions at a corner. Certainly no one of them is an indisputable choice over the other two!

Very likely the difference scheme just described is the crudest possible approximation to the differential problem. By introducing fictitious points of each region which are geometrically located outside the region but adjacent to the interface, a symmetric difference scheme can be used for approximating the derivatives in the interface condition. This increases the number of unknowns, and it also yields some additional relations, since the interface points may then be treated as interior points of both regions. However, the dilemma is unchanged. The problem is still underdetermined without conditions at the corner point, and it is overdetermined if all the conditions available there are used.

The general corner point problem in two dimensions has up to four contiguous regions. Varga (1957) has shown how to obtain, at such a corner, a single integral relation which takes into account the several interface conditions and the differential equation for each region. By simple approximations for the integrals in this relation, he then obtains a single finite difference equation involving the values of u at the corner and at its four neighbors. The only restrictive feature of this method is that it

cannot be used when u is discontinuous across an interface. This is not a restriction in reactor calculations but it is a serious restriction in heat conduction problems (Carslaw and Jaeger, 1959, p. 23).

Another method for overcoming the difficulties of the corner point problem is to locate the grid points so that they are not coincident with interfaces and corners. How this may be accomplished is described in the following sections.

Description of the Center Point Grid

Consider an orthogonal lattice in Euclidean N-space which is uniform in each direction and has equal lattice spacings in each direction.* Let h be the lattice spacing. Each grid point may be thought of as being imbedded at the center of an N-cube with edges of length h. A closed N-cube is a region, which will be denoted by r_i, and the common face of two adjacent cubes r_i and r_j is an interface, s_{ij}. In this chapter attention is restricted to regions, R, which are the union of a finite number of such lattice cubes.

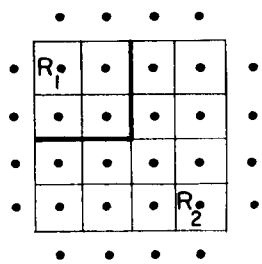
There are 2N+1 points associated with any cube r_i. They are the imbedded point and its images in the 2N faces of the cube. The latter are called <u>virtual</u> points of r_i as opposed to the imbedded or <u>real</u> point. The virtual points of r_i coincide geometrically with the real points of the cubes which are neighbors of r_i. If one or more sides of r_i coincide with the boundary of R, then the corresponding virtual points lie in the exterior of R. It should be stressed, perhaps, that each virtual point is affixed

---

*The requirements of "uniform" and "equal" are not essential for the method.

to a single cube. Thus in the interior several virtual points will possess the same geometrical location. This will also occur in the exterior whenever R is not convex.

For the two-region problem discussed in the introduction, the grid scheme based upon center points of grid cubes looks as follows:



The lattice lines remain unchanged, but the grid points are relocated and virtual ones have been added in the exterior. Each real grid point is an interior point of R_1 or R_2 at which the partial difference equation may be applied. The interface and the boundary conditions are not applied "at" grid points but on the faces of the grid cubes at points midway between two grid points. It is easily verified that the number of conditions is always exactly equal to the total number of real and virtual points.

This finite difference scheme is not entirely novel. The use of fictitious points at irregular boundaries is a commonplace technique in the relaxation methods of R. V. Southwell and his coworkers. And the possibility of centering a boundary midway between two rows of grid points was observed by Fox (1950) and, undoubtedly, by others. The proposal to formulate the entire finite difference problem by treating every grid point as an interior point of a grid cube is nevertheless new.

In addition to eliminating the ambiguity at corners where two or more regions intersect, the center point grid plan admits a finite difference

analog of Green's first integral identity which is an exact identity; that is, not just an identity to within terms which vanish as the grid size tends to zero.

Simple Properties

Let v be a grid function defined over the real and virtual points of R. The value of this function at the real point of r_i will be denoted by v_{ii}, while the value at the virtual point of r_i which lies in r_j will be denoted by v_{ij}.

Theorem 3.1. *Let v be a function with continuous first partial derivatives in R. For any $\epsilon > 0$, there exists a mesh size h sufficiently small that, if v assumes the values v_{ii} and v_{ij} at the real and virtual points of r_i, v and its exterior normal derivative evaluated at the center of the interface s_{ij} satisfy*

$$|v - 2^{-1}(v_{ij} + v_{ii})| < \epsilon ,$$

$$|\partial v/\partial n - h^{-1}(v_{ij} - v_{ii})| < \epsilon .$$

Theorem 3.2. *Let v have continuous second partial derivatives in R. For any $\epsilon > 0$ there exists an $h > 0$ such that the Laplacian evaluated at the center of any r_i in R satisfies*

$$|\nabla^2 v - h^{-2} \sum_{j \mathrm{N} i} (v_{ij} - v_{ii})| < \epsilon .$$

These theorems are consequences of Taylor's remainder theorem ar uniform continuity. Virtual points which lie outside R do not cause tro

since they may be assigned suitable values by extrapolating with the aid of the values of v and its derivatives evaluated on the boundary.

For the purpose of error analysis, however, it should be observed that when v possesses sufficiently many derivatives the expressions for v, $\partial v/\partial n$ and $\nabla^2 v$ given above are in error by at most terms of the order $O(h^2)$, at the points specified.

Theorem 3.3. *If the function v possesses bounded fourth partial derivatives in R, then for any cube r_i contained in R the value of v and its exterior normal derivative at the centroid of the interface s_{ij} satisfy*

$$v = 2^{-1}(v_{ij} + v_{ii}) + O(h^2)$$

$$\partial v/\partial n = h^{-1}(v_{ij} - v_{ii}) + O(h^2) .$$

Furthermore, the Laplacian of v at the center of r_i has the representation

$$\nabla^2 v = h^{-2} \sum_{jNi} (v_{ij} - v_{ii}) + O(h^2) .$$

Thus the partial differential equation (1.1) may be replaced by

$$-h^{-2} \sum_{jNi} (v_{ij} - v_{ii}) + D_i v_{ii} = \rho_i \tag{3.1}$$

which can be regrouped into the form

$$(2N + D_i h^2) v_{ii} - \sum_{jNi} v_{ij} = h^2 \rho_i .$$

Here, and in the following, grid functions defined only at real points are

given only a single subscript.

Interface Conditions

Corresponding to the pair of differential interface conditions given by equations (1.2), the following conditions may be imposed at the centroid of the face between r_i and r_j:

$$(3.2)\quad \begin{pmatrix} 2^{-1} & 2^{-1} \\ -h^{-1} & h^{-1} \end{pmatrix} \begin{pmatrix} v_{ij} \\ v_{ii} \end{pmatrix} = \begin{pmatrix} \alpha_{ij} & \beta_{ij} \\ \gamma_{ij} & \delta_{ij} \end{pmatrix} \begin{pmatrix} 2^{-1} & 2^{-1} \\ h^{-1} & -h^{-1} \end{pmatrix} \begin{pmatrix} v_{ji} \\ v_{jj} \end{pmatrix}$$

This pair of equations may be solved for the values v_{ij} and v_{ji} at the virtual points in terms of the values v_{ii} and v_{jj} at the real points. This is true for each face of r_i. If the resulting expressions for each of the v_{ij} are substituted into the expression for the Laplacian at r_i, as given in equation (3.1), there results a partial difference equation relating v_{ii} with the values v_{jj} at the real points of the neighboring cubes. In this manner the virtual points may be eliminated in formulating the finite difference problem for numerical solution.

Solving equation (3.2) for the virtual values, one obtains

$$(3.3)\quad \begin{pmatrix} v_{ij} \\ v_{ji} \end{pmatrix} = \begin{pmatrix} a_{ij} & b_{ij} \\ b_{ji} & a_{ji} \end{pmatrix} \begin{pmatrix} v_{jj} \\ v_{ii} \end{pmatrix}$$

where

$$
(3.4)\qquad \begin{cases}
a_{ij} = \dfrac{4(\alpha_{ij}\,\delta_{ij} - \beta_{ij}\,\gamma_{ij})h}{\Delta_{ij}} \\[2ex]
b_{ij} = \dfrac{4\beta_{ij} + 2(\alpha_{ij} - \delta_{ij})h - \gamma_{ij}\,h^2}{\Delta_{ij}} \\[2ex]
a_{ji} = \dfrac{4h}{\Delta_{ij}} \\[2ex]
b_{ji} = \dfrac{4\beta_{ij} - 2(\alpha_{ij} - \delta_{ij})h - \gamma_{ij}\,h^2}{\Delta_{ij}}\ , \\[2ex]
\Delta_{ij} = 4\beta_{ij} + 2(\alpha_{ij} + \delta_{ij})h + \gamma_{ij}\,h^2\ .
\end{cases}
$$

The symmetry present in this solution is a consequence of the fact that the interface conditions (1.2) may also be written with u_j and $\nabla u_j \cdot n_j$ as functions of u_i. (Compare equations (1.7) and (1.8).) Note that the coefficients in (3.4) are well-behaved when $\beta_{ij} = 0$. In fact, when $\alpha_{ij} = \delta_{ij} = 1$ and $\beta_{ij} = \gamma_{ij} = 0$, then equation (3.3) reduces to

$$
(3.5)\qquad v_{ij} = v_{jj} \quad \text{and} \quad v_{ji} = v_{ii}\ .
$$

<u>Theorem</u> 3.4. <u>When the differential interface conditions</u> (1.2) <u>merely require that</u> v <u>and</u> $\partial v/\partial n$ <u>be continuous at the interface, then</u>

$$
a_{ij} = a_{ji} = 1 \quad \text{and} \quad b_{ij} = b_{ji} = 0
$$

<u>and hence the corresponding finite difference conditions are given by equations</u> (3.5).

The Boundary Condition

Let R be any region which is the union of a finite number of elementary lattice cubes $r_0, \ldots, r_{m-1}$. Lattice cubes lying in the complement of R shall have index $i \geq m$. Let r_i belong to R and let one of its neighbors r_j belong to the complement of R. The approximation to the boundary condition (1.4) which applies to the face between r_i and r_j is

$$\alpha_{ji} \frac{v_{ij} + v_{ii}}{2} + \beta_{ji} \frac{v_{ij} - v_{ii}}{h} = f_j \qquad (0 \leq i < m \leq j) \quad .$$

Solving for the virtual value,

$$v_{ij} = a_{ij} f_j + b_{ij} v_{ii} , \tag{3.6}$$

where

$$a_{ij} = \frac{2h}{2\beta_{ji} + h\alpha_{ji}} \quad \text{and} \quad b_{ij} = \frac{2\beta_{ji} - h\alpha_{ji}}{2\beta_{ji} + h\alpha_{ji}} \quad . \tag{3.7}$$

To verify that the a_{ij} and b_{ij} obtained here are in agreement with those given in (3.4), use the expressions for a_{ji} and b_{ji} given in (3.4) and then interchange the roles of i and j. If it is agreed that values of v_{jj} will be defined in the exterior of R such that

$$v_{jj} = f_j \qquad (m \leq j) \tag{3.8}$$

then, with this substitution, equation (3.6) has the same form as (3.3).

The Finite Difference Problem

In the partial difference equation (3.1) the virtual values may be eliminated in favor of real values by substitutions from equation (3.3).

The result is

$$(2N + D_i h^2 - \sum_{j \bar{N} i} b_{ij}) v_{ii} - \sum_{j \bar{N} i} a_{ij} v_{jj} = \rho_i h^2$$

or

$$v_{ii} = \sum_{j \bar{N} i} \tau_{ij} v_{jj} + \rho_i^* , \qquad (0 \le i < m) \tag{3.9}$$

where

$$\sigma_i = 2N + D_i h^2 - \sum_{k \bar{N} i} b_{ik}$$

$$\tau_{ij} = a_{ij}/\sigma_i \tag{3.10}$$

$$\rho_i^* = \rho_i h^2/\sigma_i ,$$

and where a_{ij} and b_{ij} are defined in (3.4). Only the expression for v_{ij} in equation (3.3) has been used. The expression for v_{ji} must be used, of course, to eliminate this virtual value in the finite difference equation expressed for the cube r_j.

The complete finite difference problem is formulated by the m equations in (3.9) plus the boundary conditions given in (3.8). By eliminating the virtual values, the interface conditions have been absorbed into the weights τ_{ij} assigned to the neighbors of any point.

Green's Identity for the Center Point Grid

Again, let R be any region which is the union of a finite number of elementary lattice cubes $r_0, \ldots, r_{m-1}$. Lattice cubes lying in the complement of R shall have index $i \ge m$. Let v and w be arbitrary grid

functions defined over the real and virtual points of R and consider the bilinear form B(v, w) defined by the following summation over R:

$$(3.11) \qquad B(v, w) \equiv \sum_{i=0}^{m-1} \left(\sum_{\substack{j=0 \\ jNi}}^{m-1} + \sum_{\substack{j \geq m \\ jNi}} \right) (v_{ij} - v_{ii}) w_{ii} .$$

By applying Lemma 2.1, B(v, w) may be rewritten in the form

$$(3.12) \qquad \begin{aligned} B(v, w) = & \sum_{i=0}^{m-1} \sum_{\substack{j=0 \\ jNi}}^{i-1} \left[(v_{ij} - v_{ii}) w_{ii} - (v_{jj} - v_{ji}) w_{jj} \right] \\ & + \sum_{i=0}^{m-1} \sum_{\substack{j \geq m \\ jNi}} (v_{ij} - v_{ii}) w_{ii} . \end{aligned}$$

This is a finite difference identity which, with some imagination, resembles Green's first integral identity.

In identity (3.12), no assumption has been made about the behavior of v and its first difference across the interfaces between the lattice cubes. Imposing conditions analogous to continuity of v and its normal derivative, as given in Theorem 3.4, a more easily recognizable result is obtained, namely

$$(3.13) \qquad B(v, w) = - \sum_{i=0}^{m-1} \sum_{\substack{j=0 \\ jNi}}^{i-1} (v_{jj} - v_{ii})(w_{jj} - w_{ii}) + \sum_{i=0}^{m-1} \sum_{\substack{j \geq m \\ jNi}} (v_{ij} - v_{ii}) w_{ii} .$$

An alternate form, which explicitly displays the approximate values of w on the exterior boundary, may be obtained from (3.13). It is

$$B(v, w) = -\sum_{i=0}^{m-1}\left[\sum_{\substack{j=0\\ jNi}}^{i-1}(v_{jj} - v_{ii})(w_{jj} - w_{ii})\right.$$

(3.14)

$$\left. + \frac{1}{2}\sum_{\substack{j\geq m\\ jNi}}(v_{ij} - v_{ii})(w_{jj} - w_{ii})\right] + \sum_{i=0}^{m-1}\sum_{\substack{j\geq m\\ jNi}}(v_{ij} - v_{ii})\left(\frac{w_{jj} + w_{ii}}{2}\right)$$

Since it has been assumed that v satisfies condition (3.5), the first double summation in (3.14) may be rewritten as

$$-\frac{1}{2}\sum_{i=0}^{m-1}\sum_{\substack{j=0\\ jNi}}^{i-1}\left[(v_{ij} - v_{ii})(w_{jj} - w_{ii}) + (v_{ji} - v_{jj})(w_{ii} - w_{jj})\right]$$

The use of Lemma 2.1 then produces the identity

$$B(v, w) = -\frac{1}{2}\sum_{i=0}^{m-1}\sum_{jNi}(v_{ij} - v_{ii})(w_{jj} - w_{ii})$$

(3.15)

$$+ \sum_{i=0}^{m-1}\sum_{\substack{j\geq m\\ jNi}}(v_{ij} - v_{ii})\left(\frac{w_{jj} + w_{ii}}{2}\right)$$

The remarkable property of this identity is that no assumption has to be made about the grid function w, except that it be defined over the real points of R and of those exterior lattice cubes adjoining R. There is no apparent purpose to be served, however, by exploring this property further. For symmetry, therefore, let it be assumed, henceforth, that w also satisfies condition (3.5). Then, after multiplying equation (3.15) by h^{N-2}, a very transparent finite difference analog of Green's identity is obtained. It is

$$h^N \sum_{i=0}^{m-1} w_{ii} \left[h^{-2} \sum_{jNi} (v_{ij}-v_{ii}) \right] + \frac{1}{2} h^N \sum_{i=0}^{m-1} \sum_{jNi} \left(\frac{v_{ij} - v_{ii}}{h} \right) \left(\frac{w_{ij} - w_{ii}}{h} \right)$$

(3.16)

$$= h^{N-1} \sum_{i=0}^{m-1} \sum_{\substack{j \geq m \\ jNi}} \left(\frac{v_{ij} - v_{ii}}{h} \right) \left(\frac{w_{ij} + w_{ii}}{2} \right) .$$

Theorem 3.5. Let v and w be grid functions defined over $R = \bigcup_{i=0}^{m-1} r_i$ and satisfying condition (3.5) across interfaces in R. Then equation (3.16) is an identity.

By combining Theorems 3.1 and 3.2 with this result, it is easy to prove Green's first integral identity for the region R.

There is one other member of this family of identities which will be needed in the next chapter. Subtract

$$\frac{1}{2} h^N \sum_{i=0}^{m-1} \sum_{\substack{j \geq m \\ jNi}} \left(\frac{v_{ij} - v_{ii}}{h} \right) \left(\frac{w_{ij} - w_{ii}}{h} \right)$$

from both sides of equation (3.16), to obtain

$$h^N \sum_{i=0}^{m-1} w_{ii} \left[h^{-2} \sum_{jNi} (v_{ij} - v_{ii}) \right] + \frac{1}{2} h^N \sum_{i=0}^{m-1} \sum_{\substack{j < m \\ jNi}} \left(\frac{v_{ij} - v_{ii}}{h} \right) \left(\frac{w_{ij} - w_{ii}}{h} \right)$$

(3.17)

$$= h^{N-1} \sum_{i=0}^{m-1} \sum_{\substack{j \geq m \\ jNi}} \left(\frac{v_{ij} - v_{ii}}{h} \right) w_{ii} .$$

The Divergence Theorem for the Center Point Grid

From the last theorem a finite difference analog of the divergence theorem can be obtained. Let f be a vector-valued function defined over the grid points of R, and let the components f_μ ($\mu = 1, \ldots, N$)

of f satisfy the conditions of Theorem 3.4 across the interface between any two cubes of R. Thus f behaves over R as an approximation of a vector-valued function which is continuous and has continuous normal derivatives in R. In equation (3.16) set

$$w_{ij} = f_{\mu ij}$$

and set

$$v_{ij} - v_{ii} = (e_\mu \cdot n_{ij})h ,$$

where n_{ij} is the exterior unit normal vector of the cube r_i directed into r_j, and e_μ is a unit vector in the μth coordinate direction. Since $e_\mu \cdot n_{ij} = 1, 0,$ or -1, the resulting expression is

$$\frac{1}{2} h^N \sum_{i=0}^{m-1} \sum_{jNi} \frac{f_{\mu ij}-f_{\mu ii}}{h} \left(e_\mu \cdot n_{ij}\right) = h^{N-1} \sum_{i=0}^{m-1} \sum_{\substack{j\geq m \\ jNi}} \frac{1}{2} (f_{\mu ij} + f_{\mu ii})(e_\mu \cdot n_{ij}) .$$

Now sum over all μ ($\mu = 1, \ldots, N$). Since $\sum_{\mu=1}^{N} f_\mu e_\mu = f$ the result is

$$(3.18) \qquad \frac{1}{2} h^N \sum_{i=0}^{m-1} \sum_{jNi} \left(\frac{f_{ij}-f_{ii}}{h}\right) \cdot n_{ij} = h^{N-1} \sum_{i=0}^{m-1} \sum_{\substack{j\geq m \\ jNi}} \frac{1}{2} (f_{ij} + f_{ii}) \cdot n_{ij} .$$

<u>Theorem</u> 3.6. <u>If</u> f <u>is a vector-valued function which is defined over the real and virtual points of</u> $R = \bigcup_{i=0}^{m-1} r_i$ <u>and if</u> f <u>satisfies the condition</u>

$$f_{ij} = f_{jj}$$

<u>for each</u> $i = 0, \ldots, m-1$ <u>and for all</u> $j = 0, \ldots, m-1$ <u>such that</u> jNi,

then equation (3.18) is exact, where n_{ij} is the exterior unit normal vector of r_i directed into r_j.

The Characteristic Value Problem

The finite difference problem formulated in this chapter is nonhomogeneous. The motivation for studying it has already been mentioned. It is the problem "solved" for each group in the inner iterations of a multigroup, multiregion, nuclear diffusion problem. This larger problem is a characteristic value problem. In this section, brief consideration is given to the one group, multiregion characteristic value problem. It may be described in the following manner:

In each subregion R_i, the function $u = u_i$ satisfies the equation

$$-\nabla^2 u_i + D_i u_i = \lambda \theta_i u_i , \tag{3.19}$$

where the θ_i's are real constants satisfying the auxiliary conditions

$$\theta_i \geq 0 \quad \text{and} \quad \sum_i \theta_i > 0 ,$$

and where the required characteristic value λ is the same for all R_i. This replaces equation (1.1). The interface conditions are exactly those given in (1.2). Around the boundary, a homogeneous condition is prescribed which has the form of (1.4a).

A definition of self-adjointness for such problems was given by Sangren (1953), and, for the case when the interfaces are topologically equivalent to concentric spheres, he obtained conditions on the coefficients of the interface conditions sufficient to ensure self-adjointness.

Hildebrandt (1956) showed that these conditions also are sufficient for the general multiregion problem. One of the consequences of self-adjointness is that the characteristic values are all real.

Such problems, in general, must be "solved" by finite difference methods. But it is not evident that the characteristic values remain real in the transition from differential problem to difference problem. Hopefully, the characteristic values will converge to real values as h approaches zero, but the choice of method for solving the finite difference problem is restricted if realness cannot be guaranteed for $h \neq 0$. For example, among the iterative techniques, the power method and the extrapolation method both require that the characteristic values are real.

For the particular finite difference formulation described in this chapter, it will be shown that the characteristic values are real if the coefficients of the interface conditions satisfy the conditions given by Sangren and by Hildebrandt for the differential problem.

The finite difference approximation for (3.19) is

$$u_{ii} - \sum_{jNi} \tau_{ij} u_{jj} = \lambda \theta_i u_{ii} . \tag{3.20}$$

(Compare equation (3.9).) In order to examine the possibility that λ may be real, proceed as follows: Multiply (3.20) by $\bar{u}_{ii}$, the complex conjugate of u_{ii}, and multiply the complex conjugate of equation (3.20) by u_{ii}. Then subtract and multiply both sides of the result by a positive, but as yet undetermined constant κ_i^2. The result applies to any grid cube r_i in R. Summing over all i, the resulting equation is

$$\sum_{i=0}^{m-1} \sum_{jNi} \kappa_i^2 \tau_{ij} (u_{ii} \bar{u}_{jj} - \bar{u}_{ii} u_{jj}) = (\lambda - \bar{\lambda}) \sum_{i=0}^{m-1} \kappa_i^2 \theta_i u_{ii} \bar{u}_{ii} .$$

Since the condition on the exterior boundary is homogeneous it follows from (3.8) that the inner summation vanishes for all $j \geq m$. Hence Lemma 2.1 may be applied directly to the left-hand side yielding

$$\sum_{i=0}^{m-1} \sum_{\substack{j=0 \\ jNi}}^{i-1} (\kappa_i^2 \tau_{ij} - \kappa_j^2 \tau_{ji})(u_{jj} \bar{u}_{ii} - u_{ii} \bar{u}_{jj}) = (\lambda - \bar{\lambda}) \sum_{i=0}^{m-1} \kappa_i^2 \theta_i |u_{ii}|^2.$$

It is evident that $\lambda - \bar{\lambda}$ will vanish - hence λ is real - if $\kappa_i^2 \tau_{ij} = \kappa_j^2 \tau_{ji}$ whenever jNi. Using the definition of τ_{ij} in (3.10) and in (3.4), it is easily shown that this relation is equivalent to the relation

$$\kappa_i^2 (\alpha_{ij} \delta_{ij} - \beta_{ij} \gamma_{ij}) = \kappa_j^2 \qquad (jNi) . \tag{3.21}$$

Thus a sufficient condition for the realness of the characteristic values λ is the existence of a set of positive constants κ_i^2 $(0 \leq i < n)$ satisfying (3.21).

This is precisely the condition obtained by Hildebrandt. Although there is a condition in (3.21) for each face of each grid cube, the system of conditions (3.21) actually reduces to conditions across interfaces. For if two neighboring cubes r_i and r_j belong to the same diffusing region then, by Theorem 3.4, $\alpha_{ij} \delta_{ij} - \beta_{ij} \gamma_{ij} = 1$ and hence the same κ_i^2 applies to both cubes.

Interfaces and Boundaries Not Parallel to Coordinate Planes

The preceding discussion applies to any collection of regions each of which is a union of grid cubes. But this is often not the situation of interest. Instead a general region R_i is merely approximated by a collection $R_i^{(h)}$ of grid cubes, and a surface S_{ij} of R_i is approximated by a surface $S_{ij}^{(h)}$ consisting of faces of grid cubes. One must then ask the question: What interface or boundary conditions are appropriate to apply on $S_{ij}^{(h)}$? That is, how should a condition imposed upon S_{ij} be modified — if at all* — when it is imposed upon $S_{ij}^{(h)}$? The answer given in this section is one that stays within the framework already discussed in this chapter. In fact, the coefficients of the modified conditions have the same form and the same properties as those discussed in the previous sections.

Basically, an interface or boundary condition imposed at a particular point on a surface is not as important as the integrated effect of the conditions imposed over all points of the surface. Otherwise, replacing a smooth surface S_{ij} by a surface with discontinuous normal derivatives would not be feasible. Thus the following discussion is concerned with integral properties of S_{ij} and $S_{ij}^{(h)}$.

Consider, for example, the one-region Neumann problem for Laplace's equation. If u is a harmonic function of class $C^{(2)}$ over some region with surface S_0, then it is a corollary of Green's identity that the integral of $\partial u/\partial n$ over the closed surface S_0 must vanish;

$$\iint_{S_0} \frac{\partial u}{\partial n}\, d\sigma = 0 .$$

*Shaw (1953, p. 114) suggests making no modifications.

Thus, for the Neumann problem where the condition

$$\frac{\partial u}{\partial n} = f \qquad \text{on } S_0 \tag{3.22}$$

is specified on the boundary S_0, there is the additional condition that

$$\iint_{S_0} f d\sigma = 0 .$$

Hence it is reasonable to require that

$$\lim_{h\to 0} \iint_{S_0^{(h)}} \frac{\partial u}{\partial n} d\sigma = 0 . \tag{3.23}$$

Can this be accomplished by setting $(\partial u/\partial n) = f$ on $S_0^{(h)}$?

For any portion S of a surface, the <u>total area</u> of S is a positive quantity denoted by

$$\sigma(S) = \iint_S d\sigma ;$$

and if n is a unit normal on one side of S, then the <u>directed area</u> of S is the vector quantity

$$a(S) = \iint_S n d\sigma .$$

In general, the total area of $S^{(h)}$ is not the same as the total area of S, but the directed area is the same, at least in the limit as h tends to zero; i.e.,

$$\lim_{h\to 0} a(S^{(h)}) = a(S) . \tag{3.24}$$

The validity of this relation is obvious if one considers the projections of S and $S^{(h)}$ onto each of the coordinate planes. Similarly, it is clear

that for all sufficiently small values of h,

$$\sigma(S) \leq \sigma(S^{(h)}) ,$$

and equality can occur only if S is parallel to a coordinate plane. If there exists a constant M_0 independent of h such that

$$\sigma(S^{(h)}) \leq M_0 \, \sigma(S) \tag{3.25}$$

then $S^{(h)}$ will be said to be a <u>reasonable approximation</u> of S.

Consider a constant vector p_0. By virtue of (3.24)

$$\lim_{h\to 0} \iint_{S^{(h)}} p_0 \cdot n d\sigma = p_0 \cdot \left(\lim_{h\to 0} a(S^{(h)})\right) = p_0 \cdot a(S) = \iint_S p_0 \cdot n d\sigma .$$

A similar result is true when $p = p(x)$ is a continuous vector-valued function.

The particular vectors p that are of interest here are functions of the normal direction on S — but never of the normal direction on $S^{(h)}$. The distinction between the two will henceforth be made by consistently using a bar to denote normals on S; e.g., $\bar{n}$, $\bar{n}_i$, and $\bar{n}_j$.

<u>Lemma</u> 3.1. <u>Let</u> S <u>be a portion of</u> S_{ij} <u>contained in an open subset</u> Q <u>of</u> $R_i \cup R_j$. <u>If the vector-valued function</u> $p(x)$ <u>is continuous over</u> $\bar{Q}$, <u>then</u>

$$\lim_{h\to 0} \iint_{S^{(h)}} p \cdot n_i d\sigma = \iint_S p \cdot \bar{n}_i d\sigma ,$$

<u>where</u> n_i <u>and</u> $\bar{n}_i$ <u>are the exterior normals of</u> $R_i^{(h)}$ <u>and</u> R_i, <u>respectively</u>.

A proof is given at the end of this section.

Returning to the Neumann problem, consider the vector

$$p = \nabla u - f\bar{n} .$$

By Lemma 3.1, if $(\partial u/\partial \bar{n}) - f$ can be extended continuously over a compact region containing S, which is an element of S_0, then

$$\iint_S \left(\frac{\partial u}{\partial \bar{n}} - f\right) d\sigma = \iint_S [(\nabla u \cdot \bar{n}) - (f\bar{n} \cdot \bar{n})] d\sigma = \lim_{h \to 0} \iint_{S^{(h)}} (\nabla u - f\bar{n}) \cdot n d\sigma .$$

Since the left-hand side vanishes for any S, then the choice $(\nabla u - f\bar{n}) \cdot n = 0$ on $S^{(h)}$ is certainly appropriate and, hence, the Neumann condition corresponding to (3.22) is

$$\frac{\partial u}{\partial n} = (\bar{n} \cdot n) f \qquad \text{on } S_0^{(h)} .$$

It is easily verified that this choice satisfies (3.23).

Reasoning in this same manner one obtains from Lemma 3.1 the following:

<u>Rule</u>. <u>If an interface or boundary condition imposed across</u> S_{ij} <u>can be written in the form</u>

$$p \cdot \bar{n}_i = 0 = - p \cdot \bar{n}_j \qquad \text{on } S_{ij}$$

<u>then an appropriate choice for the corresponding condition to be imposed across</u> $S_{ij}^{(h)}$ <u>is</u>

$$p \cdot n_i = 0 = - p \cdot n_j .$$

For the first interface condition in (1.2), the vector p may be chosen to be

$$p = (\alpha_{ij} u_j - u_i) \bar{n}_j + \beta_{ij} \nabla u_j .$$

Thus the corresponding interface condition on $S_{ij}^{(h)}$ is

$$(\alpha_{ij}\, u_j - u_i)(\bar{n}_j \cdot n_j) + \beta_{ij}\, \nabla u_j \cdot n_j = 0 \qquad \text{on } S_{ij}^{(h)}.$$

Similarly, corresponding to the second condition in (1.2) one has

$$\gamma_{ij}(\bar{n}_j \cdot n_j) + (\delta_{ij}\, \nabla u_j - \nabla u_i) \cdot n_j = 0 \qquad \text{on } S_{ij}^{(h)}.$$

These conditions may be rewritten in the form

$$\text{(3.26)} \qquad \begin{pmatrix} u_i \\ -\nabla u_i \cdot n_i \end{pmatrix} = \begin{pmatrix} \alpha_{ij} & \beta'_{ij} \\ \gamma'_{ij} & \delta_{ij} \end{pmatrix} \begin{pmatrix} u_j \\ \nabla u_j \cdot n_j \end{pmatrix} \qquad \text{on } S_{ij}^{(h)}$$

where

$$\text{(3.27)} \qquad \beta'_{ij} = \beta_{ij}/(\bar{n}_j \cdot n_j) \quad \text{and} \quad \gamma'_{ij} = (\bar{n}_j \cdot n_j)\gamma_{ij}\,.$$

And for the general boundary condition

$$\alpha_{ni}\, u_i + \beta_{ni}\, \nabla u_i \cdot n_i = f_n \qquad \text{on } S_{ni},$$

the corresponding condition may be written in the form

$$\text{(3.28)} \qquad \alpha_{ni}\, u_i + \beta'_{ni}\, \nabla u_i \cdot n_i = f_n \qquad \text{on } S_{ni}^{(h)}$$

where β'_{ni} is defined in (3.27).

Note that difficulty in (3.27) because of the division by $(\bar{n}_j \cdot n_j)$ can be avoided since $S_{ij}^{(h)}$ may always be chosen such that $(\bar{n}_j \cdot n_j) > 0$.

Not only does (3.26) have the same form as the interface conditions (1.2), but also

$$\beta'_{ij}\, \gamma'_{ij} = \beta_{ij}\, \gamma_{ij}$$

because of (3.27). Hence, if the coefficients in (1.2) satisfy the conditions of the uniqueness theorem, then the modified coefficients in (3.26) also satisfy these conditions. Similarly, it is easily seen that the modified coefficients satisfy the conditions (1.6) if the original coefficients satisfy them. And the same applies to the coefficients of the boundary condition (3.28).

It should be observed that the conditions of Lemma 3.1 do not have to be satisfied to make the rule given above useful. Rather, the justification for the rule is simply this: If interface and boundary conditions on $S_{ij}^{(h)}$ are determined according to the rule given, then Lemma 3.1 implies the following theorem.

Theorem 3.7. *If u_i and ∇u_i are continuous on S and can be continued into a compact region $\overline{Q}$ containing S in its interior in such a manner that u_i and ∇u_i are continuous over $\overline{Q}$, then the linear differential forms*

$$\mathscr{L}(u_i) = \alpha u_i + \beta \nabla u_i \cdot \overline{n}_i$$

$$\mathscr{L}^{(h)}(u_i) = (\overline{n}_i \cdot n_i)\, \alpha u_i + \beta \nabla u_i \cdot n_i$$

have the property that

$$\lim_{h \to 0} \iint_{S^{(h)}} \mathscr{L}^{(h)}(u_i)\, d\sigma = \iint_S \mathscr{L}(u)\, d\sigma ,$$

where $\overline{n}_i$ is the normal on S and n_i is the normal on $S^{(h)}$.

Proof of Lemma 3.1. — Since $\overline{Q}$ is closed and bounded it is compact and hence p is uniformly continuous over $\overline{Q}$. Therefore, for any $\epsilon > 0$ there exists a finite set of spherical neighborhoods Q_λ covering

$\overline{Q}$ such that, if x and x_0 belong to Q_λ then

$$\|p(x) - p(x_0)\| < \epsilon ;$$

that is, there exists a vector-valued function q(x) such that

$$p(x) = p(x_0) + \epsilon q(x) ,$$

with

$$\|q(x)\| < 1 .$$

If $S_\lambda = S \cap Q_\lambda$ and $S_\lambda^{(h)} = S^{(h)} \cap Q_\lambda$, then it follows that

$$\left| \iint_{S_\lambda^{(h)}} p(x) \cdot n_i d\sigma - p(x_0) \cdot a(S_\lambda^{(h)}) \right| = \epsilon \left| \iint_{S_\lambda^{(h)}} q \cdot n_i d\sigma \right| < \epsilon M_0 \sigma(S_\lambda) ,$$

making use of the condition of reasonable approximation in (3.25). Similarly,

$$\left| \iint_{S_\lambda} p(x) \cdot \overline{n}_i d\sigma - p(x_0) \cdot a(S_\lambda) \right| = \epsilon \left| \iint_{S_\lambda} q \cdot \overline{n}_i d\sigma \right| < \epsilon \, \sigma(S_\lambda) .$$

Moreover, for this same ϵ one may determine an $h(\epsilon)$ such that if $0 < h < h(\epsilon)$ then

$$\|a(S_\lambda^{(h)}) - a(S_\lambda)\| < \epsilon \, \sigma(S_\lambda) .$$

Compare equation (3.24). The factor $\sigma(S_\lambda)$ on the right-hand side is justified because there is exact equality except when the (N-2)-dimensional curves bounding S_λ and $S_\lambda^{(h)}$ do not coincide. Thus the difference is proportional to $\epsilon h[\sigma(S_\lambda)]^{(N-2)/(N-1)}$ and this is less

than $\epsilon\ \sigma(S_\lambda)$ whenever $h^{(N-1)} < \sigma(S_\lambda)$. Combining these three estimates yields

$$\left| \iint_{S_\lambda^{(h)}} p(x) \cdot n_i d\sigma - \iint_{S_\lambda} p(x) \cdot \bar{n}_i d\sigma \right|$$

$$\leq \left| \iint_{S_\lambda^{(h)}} p(x) \cdot n_i d\sigma - p(x_0) \cdot a(S_\lambda^{(h)}) \right|$$

$$+ \ \|p(x_0)\| \|a(S_\lambda^{(h)}) - a(S_\lambda)\|$$

$$+ \left| p(x_0) \cdot a(S_\lambda) - \iint_{S_\lambda} p(x) \cdot \bar{n}_i d\sigma \right|$$

$$< \ \epsilon[M_0 + 2]\ \sigma(S_\lambda)\ .$$

Since this inequality is true for each λ and since there are only a finite number of the covering sets Q_λ, it follows immediately that

$$\left| \iint_{S^{(h)}} p(x) \cdot n_i d\sigma - \iint_{S} p(x) \cdot \bar{n}_i d\sigma \right| < \ \epsilon\ M_0'\ \sigma(S)\ ,$$

where M_0' is independent of h as h tends to zero. This completes the proof of Lemma 3.1.

It is a corollary of this proof that

$$\lim_{h \to 0} \frac{1}{\sigma(S)} \iint_{S^{(h)}} p \cdot n_i d\sigma \ = \ \frac{1}{\sigma(S)} \iint_{S} p \cdot \bar{n}_i d\sigma\ .$$

Moreover, since S is a portion of the surface of a regular region, S itself is regular. Consequently, $(p \cdot \bar{n}_i)$ is continuous over S, and as S shrinks to the point x'

$$\lim_{\sigma(S)\to 0} \left[\frac{1}{\sigma(S)} \iint_S p \cdot \bar{n}_i d\sigma \right] = p(x') \cdot \bar{n}_i(x') .$$

Chapter 4

CONVERGENCE IN THE INTERIOR

This chapter contains the proof that the family of finite difference solutions converges, in the limit as h approaches zero, to a function which satisfies the diffusion equation at every interior point. The convergence proofs of Weiner and Phillips (1923), of Courant, Friedrichs, and Lewy (1928), and of Petrovskiĭ (1941 and 1954) all depend upon showing that the solutions of the finite difference problem form a family of equicontinuous, bounded functions, and that any limit of this family satisfies the partial differential equation.

Each of the papers cited is concerned with Laplace's equation with a Dirichlet condition on the boundary. Weiner and Phillips obtain certain specialized results. Petrovskiĭ gives a proof of the existence of a solution using properties of superharmonic functions. It is not evident, however, that his boundary treatment can be generalized to include interfaces. The method of proof adopted for this multiregion study is that of Courant, Friedrichs, and Lewy.

The Method

In outline, their plan for proving equicontinuity is as follows: Let $v = v_h$ belong to the family of grid solutions. First show that there exist bounds, M_1 and M_2, independent of h, such that

$$\text{(A)} \qquad h^2 \sum_R v^2 < M_1$$

and

$$\text{(B)} \qquad h^2 \sum_R \left[\left(\frac{\Delta v}{\Delta x} \right)^2 + \left(\frac{\Delta v}{\Delta y} \right)^2 \right] < M_2 .$$

Second, let w be any finite difference quotient of v; e.g., $w = v$, $(\Delta v/\Delta x)$, $(\Delta v/\Delta y)$, $(\Delta^2 v/(\Delta x\ \Delta y))$, etc. If R^* is any interior subset of R ($R^* \subset R$), show that, if there exists an M_3, independent of h, such that

$$h^2 \sum_{R^*} w^2 < M_3 ,$$

then this implies that, for any $R^{**} \subset R^*$, there is an M_4, also independent of h, such that

$$\text{(C)} \qquad h^2 \sum_{R^{**}} \left[\left(\frac{\Delta w}{\Delta x} \right)^2 + \left(\frac{\Delta w}{\Delta y} \right)^2 \right] < M_4 .$$

With these results it is then shown that not only v, but all its partial difference quotients, are equicontinuous in any fixed interior region. Moreover, equicontinuity together with a bound such as (C) implies uniform boundedness over R^{**}. The convergence in any R^{**} of some subsequence of grid solutions then follows from Ascoli's theorem.

For Laplace's equation in a single region with Dirichlet conditions imposed on the boundary, the bound in (A) is a consequence of the theorem that maximum and minimum values can only be assumed on the boundary. Property (B) follows from the Dirichlet principle. The proof of (C) given in this paper is that of Courant, et al. extended to N-dimensions. Similarly, the equicontinuity demonstration is unchanged except for the complications of substituting N-dimensions for 2-dimensions.

The burden of the chapter is the obtaining of bounds for the grid

solutions and their partial difference quotients — bounds which are independent of h as h tends to zero. Some of the bounds developed are stronger than required to show convergence in the interior, but these stronger results are used in Chapter 5 in discussing the extent to which the limiting solution satisfies the interface and boundary conditions. In particular, some of the bounds will include values of the grid functions in the neighborhood of the interfaces and of the boundary.

The Finite Difference Solutions Are Square Integrable

Consider the multiregion problem defined over R. For a particular choice of the grid, let v be a grid function which is a solution of the corresponding finite difference problem. It will be shown that the summation

$$h^N \left(\sum_{r_i \in R} v_{ii}^2 \right)$$

over all grid cubes r_i in R is uniformly bounded with respect to grid size.

Two nonhomogeneous terms are present in the diffusion problem under consideration. One is the function ρ in the partial differential equation (1.1); the other is the function f in the boundary condition (1.4). Since the problem is linear, the solution may be expressed as the sum of the solutions of the following two problems:

$$\text{Problem I} \quad \begin{cases} -\nabla^2 u_i + D_i u_i = 0 & \text{in each } R_i \\ \alpha_{ni} u_i + \beta_{ni}(\nabla u_i \cdot n_i) = f & \text{on boundaries } S_{ni} \end{cases}$$

$$\text{Problem II} \quad \begin{cases} -\nabla^2 u_i + D_i u_i = \rho_i & \text{in each } R_i \\ \\ \alpha_{ni} u_i + \beta_{ni}(\nabla u_i \cdot n_i) = 0 & \text{on boundaries } S_{ni} . \end{cases}$$

The interface conditions (1.2) and (1.3) are to be satisfied in each of these problems. Both are homogeneous conditions.

For a particular grid, let $v^{(I)}$ and $v^{(II)}$ be finite difference solutions corresponding to Problems I and II, respectively. If it can be shown that both

$$h^N \sum_{r_i \epsilon R} \left[v_{ii}^{(I)} \right]^2 < B_I^2 \quad \text{and} \quad h^N \sum_{r_i \epsilon R} \left[v_{ii}^{(II)} \right]^2 < B_{II}^2$$

are bounded then by applying Cauchy's inequality, it follows that their sum is similarly bounded. Indeed,

$$h^N \sum_{r_i \epsilon R} \left[v_{ii}^{(I)} + v_{ii}^{(II)} \right]^2$$

$$< B_I^2 + B_{II}^2 + 2 \sum_{r_i \epsilon R} |h^{N/2} v_{ii}^{(I)}| \, |h^{N/2} v_{ii}^{(II)}|$$

$$< B_I^2 + B_{II}^2 + 2 B_I B_{II} .$$

Thus, it is sufficient to consider the two problems separately. (The inequality derived here is known as Minkowski's inequality.)

1. Problem I has the property that maximum values of $|v_{ii}|$ can only occur on the exterior boundary. This result depends upon a theorem which is due to Motzkin and Wasow (1953). This theorem makes use of the notion of effective linking between points. Consider an equation of the

form (3.9). If $\tau_{ij} \neq 0$, then the point x_j is said to be an <u>effective neighbor</u> of x_i relative to this equation. If a finite sequence of grid points exists such that each point after the first is an effective neighbor of its predecessor, then each point in the sequence is said to be <u>effectively linked</u> to all subsequent points. It is clear from equations (3.1) and (3.5) that, for the diffusion equation, any two interior points not separated by an interface are effectively linked. Moreover, it will be shown that even along an interface, each neighbor is an effective neighbor and, hence, any two points are effectively linked.

<u>Theorem</u> 4.1. <u>Let</u> x_i <u>be restricted to the points of a uniform orthogonal lattice of length</u> h, <u>and let</u> $f(x_i)$ <u>be a known, bounded function defined over the complement</u> C(R) <u>of</u> R. <u>Let</u> $v(x_i)$ <u>satisfy the equations</u>

$$(4.1) \qquad v(x_i) = \begin{cases} \sum_{jNi} \tau_{ij}(h)\, v(x_j) & \text{if } x_i \in R, \\ f(x_i) & \text{if } x_i \in C(R), \end{cases}$$

<u>where</u>

$$(4.2) \qquad \tau_{ij}(h) \geq 0 \qquad \text{for all } jNi,$$

<u>and</u>

$$(4.3) \qquad \sum_{jNi} \tau_{ij}(h) \leq 1 \qquad \text{for all } x_i \in R.$$

<u>If the extreme values of</u> $v(x_i)$ <u>in</u> R <u>are assumed at points which can be effectively linked to a point in</u> C(R), <u>then for all</u> x_i

$$(4.4) \qquad |v(x_i)| \leq \underset{x_k \in C(R)}{\text{maximum}} |f(x_k)| .$$

Motzkin and Wasow actually prove a more general result in which the notion of neighbor is not as restrictive as the one used here. Thus, the method of this section also can be used for higher order difference approximations. The proof of Theorem 4.1 is simple enough to be sketched briefly. Let $\bar{v} = \max |v(x_i)|$, $\bar{f} = \max |f(x_i)|$, and suppose there exists a point x_i in R such that $|v(x_i)| = \bar{v}$. Then

$$\bar{v} = |v(x_i)| \leq \sum_{x_j \epsilon R} \tau_{ij} |v(x_j)| + \sum_{x_j \epsilon C(R)} \tau_{ij} |f(x_j)|$$

and hence

$$(4.5) \qquad \bar{v} = |v(x_i)| \leq \bar{v} \sum_{\substack{x_j \epsilon R \\ jNi}} \tau_{ij} + \bar{f} \sum_{\substack{x_j \epsilon C(R) \\ jNi}} \tau_{ij} .$$

If the second sum does not vanish, then the conjecture $\bar{f} < \bar{v}$ leads to the contradiction

$$\bar{v} < \bar{v} \sum_{jNi} \tau_{ij} \leq \bar{v}$$

because of hypothesis (4.3). Hence, the inequality in (4.4) applies. If the second sum in (4.5) does vanish, then every neighbor x_j of x_i belongs to R and, again because of hypothesis (4.3), they all must have the value $v(x_j) = v(x_i)$. In this case inequality (4.5) may be applied to the successor of x_i and to each point in a sequence of grid points effectively linked to C(R), until a point is reached where the second sum in (4.5) is not zero.

The partial difference equation for Problem I is expressed by (3.9) with $\rho_i^* = 0$. Since the virtual values have been eliminated, this

is the form specified in Theorem 4.1. The demonstration that the coefficients τ_{ij} in (3.9) possess the properties (4.2) and (4.3) depends upon the following almost trivial lemma.

Lemma 4.1. *For any fixed i the coefficients τ_{ij} defined in (3.10) will satisfy conditions (4.2) and (4.3) provided that for each j such that jNi, it is true that*

$$a_{ij} \geq 0 \quad \text{and} \quad a_{ij} + b_{ij} \leq 1 \ .$$

By way of proof, it will only be remarked that every N-cube has 2N faces and neighbors.

Any face of the cube r_i must either be in the interior of a region, or be part of one of the prescribed interfaces, or else belong to the exterior boundary. In each case it will be shown that the inequalities of Lemma 4.1 are satisfied. The proof for the first case is contained in Theorem 3.4. For the second case, the following lemma will be proved.

Lemma 4.2. *If the prescribed interface conditions satisfy the restrictions (1.6), then the coefficients a_{ij} and b_{ij} defined in (3.4) will satisfy the inequalities of Lemma 4.1.*

For Δ_{ij} is positive and

$$(a_{ij} + b_{ij})\Delta_{ij} \leq 4\delta_{ij}h + 4\beta_{ij} + 2(\alpha_{ij} - \delta_{ij})h - \gamma_{ij}\, h^2$$

$$= \Delta_{ij} - 2\gamma_{ij}\, h^2 \leq \Delta_{ij} \ .$$

Finally, consider the case when some face of r_i belongs to the exterior boundary. It was observed in Chapter 3 that if one sets $v_{jj} = f_j$, when r_j is an exterior cube, then the boundary condition (3.6)

has precisely the form of equation (3.3), which relates the value at a virtual point to values at real points. Two boundary conditions have to be considered, equations (1.4a) and (1.4b). In the latter, $\alpha_{ni} = 1$ and the coefficients a_{ij} and b_{ij}, as given in (3.7), clearly satisfy Lemma 4.1. Moreover, $f_n = 0$ in condition (1.4a) so that equation (3.6) reduces to $v_{ij} = b_{ij}v_{ii}$. Hence, in effect, $a_{ij} = 0$ and $a_{ij} + b_{ij} = b_{ij} \leq 1$.

Thus it has been shown that equation (3.9) with ρ_i^* set equal to zero applies to any cube r_i not belonging to C(R), the complement of R, and that the coefficients τ_{ij}, by virtue of Lemma 4.1, satisfy conditions (4.2) and (4.3) of Theorem 4.1. Moreover, if j is replaced by i, then the definition of equation (3.8) has precisely the form of the second equality in (4.1). To complete the demonstration that Problem I satisfies the hypotheses of Theorem 4.1, it must be shown that any point in R can be effectively linked to C(R). But it is trivial to verify that $\tau_{ij} \neq 0$ in all cases and therefore, by definition, each neighbor is an effective neighbor. Hence, all points are effectively linked to points in C(R).

Since the extremum property expressed by inequality (4.4) applies to the solutions of the finite difference version of Problem I, one has

$$h^N \sum_{r_i \epsilon R} v_{ii}^2 \leq (\max |f|)^2 \sum_{r_i \epsilon R} h^N$$

(4.6)

$$< 2 (\max |f|)^2 (\text{volume } R) .$$

The factor 2 is included since an approximation of R by cubes may have

a volume slightly larger than that of R. The bound, however, is independent of h as h tends to zero.

Taken together, Lemmas 4.1 and 4.2 show that the restrictions upon the interface conditions expressed by the inequalities (1.6) are sufficient to guarantee that extreme values will not occur at an interface. These restrictions can also be shown to be necessary if the hypotheses of Theorem 4.1 are to be satisfied whenever the geometry is such that there exists at least one grid cube on each side of an interface which has 2N-1 faces across which u and $\partial u/\partial n$ are continuous.

2. In many of the preceding arguments, implicit use was made of the fact that a finite difference solution is a solution of a system of simultaneous, linear, algebraic equations. To obtain the desired bound for Problem II, explicit use will be made of the form of the system of equations.

For any particular choice of lattice, let the desired values $v(x_i) \equiv v_{ii}$ of the grid solution be formed into a column vector. This vector has as many components as there are grid points in the interior of R. Let the vector be denoted simply by v. Thus, if x_0, x_1, ... are grid points, then

$$v \equiv \begin{pmatrix} v(x_0) \\ v(x_1) \\ \cdots \\ v(x_i) \\ \cdots \end{pmatrix} .$$

Similarly, let ρ denote the vector whose components are $\rho_i = \rho(x_i)$. Let

equations (3.9) be written in the form

$$\sigma_i \, v_{ii} - \sum_{j \bar{N} i} a_{ij} \, v_{jj} = h^2 \rho_i \, . \qquad (0 \le i, \, j < m) \, . \tag{4.7}$$

This system may be written in the form

$$A \, v = h^2 \rho \, ,$$

where A is the square matrix whose coefficients are given in (4.7). The solution, of course, is

$$v = h^2 \, A^{-1} \, \rho \, . \tag{4.8}$$

The use of vector and matrix norms is not uncommon in numerical analysis. Although there have been substantial advances in the theory of matrix norms in recent years, the part of the theory to be used here is elementary (Householder, 1956a).

The vector norm which is particularly suited to the immediate discussion is the L^2 norm. If the vector v has m components, v_i, the L^2 norm is defined by

$$\|v\|_{L^2} = \left(\frac{1}{m} \sum_i v_i^{\,2} \right)^{1/2} \, .$$

That this is a valid vector norm follows immediately the fact that it is a constant multiple of the more familiar Euclidean norm. Since the lattice is uniform,

$$\lim_{h \to 0} \left(m \, h^N \right) = \text{vol. } R \, ,$$

and certainly for all values of h sufficiently small,

$$\frac{1}{2}\ m^{-1}\ (\text{vol. } R) < h^N < 2\ m^{-1}\ (\text{vol. } R)\ . \tag{4.9}$$

Hence, the desired bound can be obtained from the square of the L^2 norm of v:

$$h^N \sum_i v_i^{\ 2} \ < \ 2(\text{vol. } R) \left(\|v\|_{L^2} \right)^2 \ . \tag{4.10}$$

For any square matrix A, the matrix norm consistent with this vector norm is the spectral norm $\|A\|_{Sp}$. Consistent means $\|Av\| \leq \|A\|\ \|v\|$. The spectral norm of A is the square root of the largest characteristic value of the matrix $A^T A$. Henceforth, since only these two norms are used, the subscripts designating L^2 and spectral will be omitted.

Since these norms are consistent, they may be applied to equation (4.8) yielding

$$\|v\| \ \leq \ h^2\ \|A^{-1}\|\ \|\rho\|\ . \tag{4.11}$$

By inequality (4.9)

$$\|\rho\| \ \leq \ \left(\frac{1}{m} \sum_i \rho_i^{\ 2} \right)^{1/2}$$

$$\leq \ \left(\frac{2}{\text{vol. } R} \right)^{1/2} \left(h^N \sum_i \rho_i^{\ 2} \right)^{1/2} \tag{4.12}$$

$$\leq \ 2 \left(\frac{2}{\text{vol. } R} \right)^{1/2} \left(\int_R \rho^2\ d\sigma^N \right)^{1/2} \ .$$

Hence $\|\rho\|$ is bounded, independent of h as h tends to zero, if ρ is square

integrable over R.

An estimate for the spectral norm of A^{-1} — or more precisely, an upper bound — may be obtained by studying the form of A in some detail. In the ith row, the diagonal element is σ_i and the off-diagonal element in the jth column is $-a_{ij}$ if iNj; otherwise, it is zero. Similarly, the element in the jth row and ith column is $-a_{ji}$. Since the expressions for a_{ij} and a_{ji}, given in (3.4), are not the same, the matrix A is nonsymmetric. But, it is symmetrizable! This, in effect, was shown in Chapter 3 in the proof that the characteristic values are all real. Indeed, the symmetrizing matrix is the diagonal matrix $K = (\kappa_0, \kappa_1, \ldots, \kappa_{m-1})$ where

$$\kappa_j^{\,2} = (\alpha_{ij}\delta_{ij} - \beta_{ij}\gamma_{ij})\kappa_i^{\,2} . \qquad (jNi)$$

That is,

$$S = KAK^{-1}$$

is symmetric. The κ_i's are equal to the k_i's of the Uniqueness Theorem 2.1 because of the assumption that $\beta_{ij}\gamma_{ij} = 0$ on every interface. Clearly, the diagonal of S is the same as the diagonal of A. If $a_{ij} \neq 0$, then

$$s_{ij} = \kappa_i \, a_{ij} \, \kappa_j^{-1} .$$

But from (3.4), $a_{ij} = (\alpha_{ij}\delta_{ij} - \beta_{ij}\gamma_{ij})a_{ji}$. Hence

$$s_{ij} = \kappa_i(\kappa_j^{\,2} \, \kappa_i^{-2} \, a_{ji})\kappa_j^{-1} = s_{ji} .$$

Since A is symmetrizable, all its characteristic values are real. In fact, the characteristic values of S and of A are identical. Gerschgorin's theorem, moreover, provides the information that all the characteristic

roots are positive (Gerschgorin, 1931). For by Gerschgorin's theorem, all the characteristic values lie in the union of circles in the complex plane, with centers at σ_i and radii given by $\sum |a_{ij}|$, with summation over j for all jNi. The ith circle intersects the real axis nearest the origin at the point $\sigma_i - \sum a_{ij}$. By (3.10) and Lemma 4.2

$$\sigma_i - \sum_{jNi} a_{ij} = 2N + D_i h^2 - \sum_{jNi} (a_{ij} + b_{ij}) \geq D_i h^2 .$$

Thus, a lower bound for the characteristic values of S is $h^2 D_{min}$, and hence

$$\|S^{-1}\| \leq h^{-2}(D_{min})^{-1} .$$

Since $A^{-1} = K^{-1} S^{-1} K$,

$$\|A^{-1}\| \leq \|K^{-1}\| \, \|S^{-1}\| \, \|K\|$$

(4.13)

$$\leq \left(\frac{\max \kappa_i}{\min \kappa_i}\right)\left(\frac{1}{D_{min}}\right) h^{-2} .$$

Combining the estimates (4.12) and (4.13) with inequality (4.11) provides an upper bound for $\|v\|$, and this bound is independent of h as h tends to zero. Because of inequality (4.10), it has thus been shown that for Problem II, there exists a bound M, independent of h, such that

(4.14) $$h^N \sum_{r_i \epsilon R} v_{ii}^{\ 2} \leq M .$$

3. Since a similar bound exists for Problem I, it follows from the linearity of the equations and Cauchy's inequality — as already has

been demonstrated — that a bound of the type (4.14) also applies when both f and ρ are present in the diffusion problem.

Remark. The restriction that D_i be bounded away from zero is unpleasant. Further study of the matrix A may show that this condition can be dispensed with. This is true in the one-region problem. Indeed, it can be shown by the techniques of Householder (1956b and 1958) that $\|A^{-1}\| \leq (N \pi h^2)^{-1}$, assuming only that D is nonnegative.

Theorem 4.2. When the interface conditions satisfy the conditions of Theorem 2.1 as well as the conditions given in Chapter 1, then there exists a bound M, independent of h, such that inequality (4.14) applies to any grid solution of the multiregion diffusion problem.

Bounds for Difference Quotients of all Orders

Consider any region R and its complement C(R). If R^* is a subregion of R such that the distance from R^* to C(R) is greater than zero, then R^* is said to lie entirely in the interior of R or, simply, R^* is an interior subregion of R.

For any region R, once a particular lattice is chosen, there is a unique, smallest covering of R by cubes with centers at the grid points; i.e., by grid cubes. This minimal collection of grid cubes will be denoted by $G^+(h,R)$. Similarly, there is a maximal collection $G^-(h,R)$ of grid cubes which do not intersect C(R). For sufficiently small h, $G^-(h,R)$ will not be empty.

In this section the region R will not be, in general, a region bounded by interfaces and external boundaries. This is particularly the case when the grid function w is a high-order difference quotient of a

function v satisfying a finite difference equation.

Theorem 4.3. Consider any region R. Suppose that for any grid spacing h, there is a grid function w_h satisfying an equation of the form

$$-h^2 \sum_{j \bar{N} i} (w_{ij} - w_{ii}) + D_i w_{ii} = \zeta_i \tag{4.15}$$

at each point in $G^-(h,R)$. If there exist bounds B and M, independent of h, such that

$$h^N \sum_{G^-(h,R)} w_h^{\,2} < B \quad \text{and} \quad h^N \sum_{G^-(h,R)} \zeta_i^{\,2} < M$$

as h tends to zero, then for every interior subregion R^* of R, there exists a bound B^*, independent of h, such that

$$h^{N-2} \left[\sum_{r_i \epsilon G^+(h,R^*)} \sum_{j \bar{N} i} (w_{ij} - w_{ii})^2 \right] < B^* ,$$

as h tends to zero.

In fact, if α is the distance from R^* to C(R), the bound B^* does not increase faster than B/α^2. The following proof is due essentially to Courant, et al.

The region R^* can be covered by a finite number of N-dimensional rectangular parallelepipeds with sides parallel to the coordinate planes chosen such that the distance from any rectangle to C(R) is not less than $\alpha/2$. It is sufficient to prove the theorem for each of the covering

rectangles. Let R_1 be any one of them.

Consider an arbitrary lattice with fixed, uniform lattice spacing h. Let the minimum collection of grid cubes covering R_1, that is, let $G^+(h,R_1)$ be denoted simply as G_1. Let L_1 be the set of grid cubes in G_1, each of which has at least one face on the surface of G_1, i.e., L_1 is the layer of grid cubes along the inside surface of G_1. Let G_2 be a rectangle concentric with G_1 but having two more grid cubes in each coordinate direction. Then $G_2 - L_2 = G_1$. In this manner a nest of rectangles G_λ $(\lambda = 1, \ldots, \nu)$ may be constructed together with the layers L_λ $(\lambda = 1, \ldots, \nu)$. The last rectangle G_ν is determined by the condition that G_ν be contained in $G^-(h,R)$, whereas $G_{\nu+1}$ is not. Furthermore, let $L'_{\lambda+1}$ denote the subset of $L_{\lambda+1}$ obtained by removing those grid cubes of $L_{\lambda+1}$ which are not neighbors of some cube in G_λ. The deleted cubes will lie along edges or in corners of $G_{\lambda+1}$.

Since each G_λ is a region which is a union of grid cubes, the form of Green's identity given in equation (3.16) is applicable. To simplify displaying the following relations, the symbols

$$\sum_{G_\lambda} \varphi_{ij} \quad \text{and} \quad \sum_{L_\lambda} \varphi_{ii}$$

will be used as abbreviations for the summations

$$\sum_{r_i \in G_\lambda} \sum_{j N i} \varphi_{ij} \quad \text{and} \quad \sum_{r_i \in L_\lambda} \varphi_{ii} \quad ,$$

respectively, where the r_i are grid cubes belonging to G_λ or L_λ. Setting

v equal to w, equation (3.16) may be written in the form

$$\frac{1}{2} h^{N-2} \sum_{G_\lambda} (w_{ij} - w_{ii})^2 = \frac{1}{2} h^{N-2} \sum_{L'_{\lambda+1}} w_{ii}^{\ 2} - \frac{1}{2} h^{N-2} \sum_{L_\lambda} w_{ii}^{\ 2}$$

$$- h^{N-2} \sum_{G_\lambda} w_{ii}(w_{ij} - w_{ii}) \quad .$$

From this, an inequality may be obtained by restricting the summation on the left-hand side to G_1, by increasing the first summation on the right to include all of $L_{\lambda+1}$, and finally by replacing the last summation by one of equal or larger magnitude. Thus, for any λ, $1 \leq \lambda \leq \nu$,

$$\frac{1}{2} h^{N-2} \sum_{G_1} (w_{ij} - w_{ii})^2 \leq \frac{1}{2} h^{N-2} \sum_{L_{\lambda+1}} w_{ii}^{\ 2} - \frac{1}{2} h^{N-2} \sum_{L_\lambda} w_{ii}^{\ 2}$$

$$+ h^{N-2} \sum_{G_\nu} \left| w_{ii}(w_{ij} - w_{ii}) \right| .$$

Adding these inequalities for all λ from 1 through μ yields

$$\frac{1}{2} \mu h^{N-2} \sum_{G_1} (w_{ij} - w_{ii})^2 \leq \frac{1}{2} h^{N-2} \sum_{L_{\mu+1}} w_{ii}^{\ 2}$$

$$+ \mu h^{N-2} \sum_{G_\nu} \left| w_{ii}(w_{ij} - w_{ii}) \right| .$$

The omission of the summation over L_1 strengthens the inequality. The last inequality holds for all $1 \leq \mu \leq \nu - 1$; hence, a final summation

over μ yields

$$\frac{1}{2}\,\frac{\nu(\nu-1)}{2}\,h^{N-2}\sum_{G_1}(w_{ij}-w_{ii})^2$$

(4.16)

$$\leq \frac{1}{2}\,h^{N-2}\sum_{G_\nu} w_{ii}^{\;2} + \frac{\nu(\nu-1)}{2}\,h^{N-2}\sum_{G_\nu}\left|w_{ii}(w_{ij}-w_{ii})\right| .$$

It is a direct consequence of the manner in which ν is determined that

$$(\nu+1)\,h\sqrt{N} > \frac{1}{2}\,\alpha .$$

Therefore, for small enough values of h,

$$\nu h\sqrt{N} > (\nu-1)\,h\sqrt{N} > \frac{\alpha}{3}$$

and consequently

$$\frac{1}{\nu(\nu-1)h^2} < \frac{9N}{\alpha^2} .$$

Combining this with inequality (4.16) yields

$$(4.17)\quad \frac{1}{2}\,h^{N-2}\sum_{G_1}(w_{ij}-w_{ii})^2 < \frac{9N}{\alpha^2}\,h^N\sum_{G_\nu} w_{ii}^{\;2} + h^{N-2}\sum_{G_\nu}\left|w_{ii}(w_{ij}-w_{ii})\right| .$$

The conclusion of Theorem 4.3 follows from this inequality after substituting the partial difference equation into the last summation. For, by Cauchy's inequality,

$$h^N\sum_{G_\nu}\left|w_{ii}(D_i\,w_{ii}-\zeta_i)\right|$$

$$\leq h^N\sum_{G_\nu}|D_i|\,w_{ii}^{\;2} + \left(h^N\sum_{G_\nu}\zeta_i^{\;2}\right)^{1/2}\left(h^N\sum_{G_\nu} w_{ii}^{\;2}\right)^{1/2} ,$$

and this is bounded by hypothesis. Hence, the right-hand side of inequality (4.17) may be bounded independent of h. This completes the proof of Theorem 4.3.

The maximal collection $G^-(h,R)$ of grid cubes contained in R but not intersecting $C(R)$, and the minimal collection of grid cubes $G^+(h,R^*)$ containing R^* were introduced to point out that a distinction exists. If Theorem 4.4 required a bound for w_h^2 summed over $G^+(h,R)$ to conclude only that the first differences were similarly bounded over $G^-(h,R^*)$, there would be difficulty in using the theorem repeatedly for successively higher partial difference quotients over a nest of regions $R \supset R^* \supset R^{**} \supset \ldots$. Fortunately, this is not the case. In fact, since $G^-(h,R^*)$ either is identical with $G^+(h,R^*)$ or is a subset of it, the theorem can be weakened when applied to such a nest. Henceforth, the explicit distinction between $G^+(h,R)$ and $G^-(h,R)$ will not be made.

<u>Definition</u>. <u>A family $\mathcal{G}$ of grid functions defined over some region R will be said to belong to the class $\Sigma^2(R)$ if there exists a finite bound B, which may depend upon $\mathcal{G}$ and upon R but is independent of h as h tends to zero, such that any function $w_h \in \mathcal{G}$ satisfies the inequality</u>

$$h^N \sum_{G(h,R)} w_h^2 < B .$$

Theorem 4.3, together with Theorem 4.2, provides a bound over interior subregions for each of the first partial difference quotients of v_h. For – using the notation of 3-dimensions – if, for all h, the family of functions

$$\left[\left(\frac{\Delta v}{\Delta x}\right)^2 + \left(\frac{\Delta v}{\Delta y}\right)^2 + \left(\frac{\Delta v}{\Delta z}\right)^2\right]^{1/2}$$

belongs to the class $\Sigma^2(R^*)$ then $\left\{(\Delta v/\Delta x)\right\}$ also belongs to $\Sigma^2(R^*)$. In this case, referring to equation (4.15), $\zeta = \rho$. Next, let $w = (\Delta v/\Delta x)$. Theorem 4.3 then provides the information that $\left\{(\Delta^2 v/\Delta x\ \Delta x)\right\}$, $\left\{(\Delta^2 v/\Delta y\ \Delta x)\right\}$, etc. are of class $\Sigma^2(R^{**})$. The form of ζ in this case may be inferred from the corresponding differential equation satisfied by $\partial\mu/\partial x$, namely

$$-\nabla^2 u_x + D\, u_x = \rho_x - D_x\, u\ .$$

This process may be repeated as long as the required partial difference quotients (d.qs.) of D are bounded and the required d.qs. of ρ belong to $\Sigma^2(R)$. The conclusions obtained by continuing the argument in this direction are summarized in Theorem 4.4 below.

Before stating the theorem, certain definitions from Chapter 1 will be recalled. Equation (1.1), the diffusion equation, is to be satisfied in each of the regions R_i. If $D \equiv D_i(x)$, together with each of its partial derivatives of order not exceeding r, exists and is bounded over R_i, then this is denoted by $D \in M^{(r)}$. If $\rho \equiv \rho_i(x)$, together with each of its partial derivatives of order not exceeding r, exists and is square integrable over R_i, then this is denoted by $\rho \in L^2[M^{(r)}, R_i]$. Of course, if ρ has this property then ρ and each of its d.qs. through order r belong to the class $\Sigma^2(R_i)$.

<u>Theorem</u> 4.4. <u>Let</u> $D \in M^{(r)}$ <u>in</u> R_i, <u>let</u> $\rho \in L^2[M^{(r)}, R_i]$, <u>and let</u> w_h <u>be</u> v_h <u>or a</u> d.q. <u>of</u> v_h. <u>If the order of</u> w_h <u>is not greater than</u> $r + 1$, <u>then, for any interior subregion</u> R_i^* <u>of</u> R_i, $w_h \in \Sigma^2(R_i^*)$.

(To establish the equicontinuity of the family $\mathfrak{F}$ of grid solutions v_h, it is sufficient to show that only the mixed d.qs. of v_h are of class Σ^2. Hence, if establishing this were all that was desired, the conditions

on ρ and on D could be relaxed to involve only their mixed d.qs. But since equicontinuity of the first and second d.qs. of v_h is also desired, conditions on the mixed d.qs. of ρ_x, ρ_y, ..., ρ_{xx}, ρ_{xy}, ..., and similarly for D, are also needed.)

Equicontinuity of the Solutions

Let $\mathfrak{F}$ be the family of solutions whose members correspond to distinct choices of lattice size h. These solutions are grid functions. If some suitably smooth interpolation procedure is used to extend their domains so that all members of the family are defined over the same compact set, then the usual notion of equicontinuity may be applied. From the boundedness properties already obtained, it will be shown that $\mathfrak{F}$ is equicontinuous in any interior subregion R_i^* of any R_i. Moreover, it will be shown that the first and second d.qs. of v_h also form equicontinuous families in R_i^*. The theorem is proved in the following form:

Theorem 4.5. *Let $\mathfrak{G}$ be a family of grid functions w_h. Along with $\mathfrak{G}$, consider the families of the mixed d.qs. of all orders not exceeding N, formed from the functions w_h. If $\mathfrak{G}$ and each of these families are of class $\Sigma^2(R^*)$, then the family $\mathfrak{G}$ is equicontinuous over any R^{**} which is an interior subregion of R^*.*

In fact, for any two points p and q in R^{**}, it will be shown that

$$|w_h(p) - w_h(q)| < M\|p-q\|^{1/2} \tag{4.18}$$

for any w_h where M depends only upon the region R^*. To show that this Hölder condition is satisfied, it is sufficient to demonstrate it for any pair of points whose position vectors differ in only one component.

Furthermore, it may be assumed without jeopardizing the argument, that

$$p = q + \alpha_1 e_1 ,$$

i.e., that they differ in their first components.

Using p and q as two vertices, construct an N-dimensional rectangular parallelepiped which lies entirely in R^*. Denote it by $P_N(\alpha_1, \ldots, \alpha_N)$, where the α's indicate its linear dimensions. Specifically, $P_N(\alpha_1, \ldots, \alpha_N)$ is the set of points

$$x = q + \sum_{\nu=1}^{N} \xi_\nu e_\nu ,$$

where

$$0 \leq \xi_\nu \leq \alpha_\nu \qquad (\nu = 1, \ldots, N).$$

It must be noted that α_2 through α_N may be bounded away from zero since P_N is constructed in R^* while p and q are restricted to belong to R^{**}. Similarly, denote by $P_\mu(\alpha_1, \ldots, \alpha_\mu)$ the μ-dimensional face of P_N which consists of those points representable in the form

$$x = q + \sum_{\nu=1}^{\mu} \xi_\nu e_\nu .$$

A translation of such a face may be denoted by $P_\mu(\alpha_1, \ldots, \alpha_\mu) + \gamma_\lambda e_\lambda$. It is the set of points with the representation

$$x = q + \gamma_\lambda e_\lambda + P_\mu(\alpha_1, \ldots, \alpha_\mu) .$$

The desired estimate may be obtained by starting with the finite difference form of Green's first identity, as given in equation (3.17). To avoid obscuring the essence of the proof behind an array of multiple

summation signs, an integral analog of the proof will be given first.

Apply Green's integral identity, equation (2.1), to any region $P_\mu(\gamma_\mu) \equiv P_\mu(\beta_1, \ldots, \beta_{\mu-1}, \gamma_\mu)$ contained in $P_\mu\ (\alpha_1, \ldots, \alpha_\mu)$, where $2 \leq \mu \leq N$. Let w be any arbitrary function $\varphi \in C'$. If the function u is chosen to be $u = \xi_\mu$, so that $\nabla u = \mathbf{e}_\mu$ and $\nabla^2 u = 0$, then the integral over the surface of $P_\mu(\gamma_\mu)$ vanishes except over the face $P_{\mu-1} \equiv P_{\mu-1}$ $(\beta_1, \ldots, \beta_{\mu-1})$ and the face $P_{\mu-1} + \gamma_\mu\, e_\mu$. The result is

$$(4.19) \qquad \int_{P_{\mu-1}} (-1)\ \varphi\ d\sigma^{(\mu-1)} + \int_{P_{\mu-1}+\gamma_\mu e_\mu} (+1)\ \varphi\ d\sigma^{(\mu-1)}$$

$$= \int_{P_\mu(\gamma_\mu)} (\nabla\varphi \cdot e_\mu)\ d\sigma^{(\mu)} \quad .$$

Integrating both sides of equation (4.19) with respect to γ_μ between the limits 0 and β_μ $(\beta_\mu \leq \alpha_\mu)$ and then rearranging the result slightly, one obtains

$$\beta_\mu \int_{P_{\mu-1}} \varphi\ d\sigma^{(\mu-1)} = \int_0^{\beta_\mu} \int_{P_{\mu-1}+\gamma_\mu e_\mu} \varphi\ d\sigma^{(\mu-1)} d\gamma_\mu$$

$$- \int_0^{\beta_\mu} \int_{P_\mu(\gamma_\mu)} D_\mu\ \varphi\ d\sigma^{(\mu)} d\gamma_\mu\ ,$$

where D_μ denotes differentiation with respect to ξ_μ. The first integral on the right is an integration over $P_\mu \equiv P_\mu\ (\beta_1, \ldots, \beta_\mu)$. Thus, the integral of φ over $P_{\mu-1}$ can be expressed in terms of integrals of φ and

$D_\mu \varphi$ over P_μ. Indeed,

$$\int_{P_{\mu-1}} \varphi \, d\sigma^{(\mu-1)} = \frac{1}{\beta_\mu} \int_{P_\mu} \varphi \, d\sigma^{(\mu)}$$

(4.20)

$$- \frac{1}{\beta_\mu} \int_0^{\beta_\mu} \int_{P_\mu(\gamma_\mu)} D_\mu \varphi \, d\sigma^{(\mu)} d\gamma_\mu \, .$$

Since this equality holds for any $\mu = 2, \ldots, N$ the integral of φ over $P_1(\alpha_1)$ can be represented in terms of integrals of φ and its mixed partial derivatives up to order N-1 over the region $P_N(\alpha_1, \ldots, \alpha_N)$ and certain of its N-dimensional subregions, simply by repeated substitutions using equation (4.20).

Consider the case of 3-dimensions. Set $\mu = 2$ in equation (4.20). The integrals on the right, over P_2 and $P_2(\gamma_2)$, can then be expressed by using (4.20) twice more, with $\mu = 3$. The result is

$$\int_{P_1} \varphi \, d\sigma^{(1)} = \frac{1}{\beta_1\beta_2} \left[\int_{P_3} \varphi \, d\sigma^{(3)} - \int_0^{\beta_3} \int_{P_3(\gamma_3)} D_3 \varphi \, d\sigma^{(3)} \right]$$

(4.21)

$$- \frac{1}{\beta_2\beta_3} \int_0^{\beta_2} \left[\int_{P_3(\gamma_2)} D_2 \varphi \, d\sigma^{(3)} - \int_0^{\beta_3} \int_{P_3(\gamma_2,\gamma_3)} D_3 D_2 \varphi \, d\sigma^{(3)} \right].$$

In this equation, if the substitution

$$\varphi = D_1 w$$

is made and if β_1, β_2, and β_3 are set equal to α_1, α_2, and α_3, respectively, then the left-hand side is exactly $w(p) - w(q)$. On the right-hand side, the absolute value of each of the integrals over P_3 or its subsets can be

bounded from above by applying Schwarz's inequality. For example,

$$\left| \int_{P_3(\gamma_2)} D_2 \varphi \, d\sigma^{(3)} \right| \leq \left[\int_{P_3(\gamma_2)} d\sigma^{(3)} \right]^{1/2} \left[\int_{P_3(\gamma_2)} (D_2 \varphi)^2 \, d\sigma^{(3)} \right]^{1/2}$$

$$\leq (\alpha_1 \alpha_2 \alpha_3)^{1/2} \left[\int_{P_3} (D_2 \varphi)^2 \, d\sigma^{(3)} \right]^{1/2} .$$

The domain of integration was extended over all of P_3 because the integrands are nonnegative. The last integral is bounded by hypothesis. That is, for the finite difference situation, which is actually the point under consideration, the boundedness is one of the assumptions of the theorem. Thus, with $\varphi = D_1 w$, it follows from (4.21) that

$$|w(p) - w(q)| \leq \alpha_1^{1/2} B = \|p - q\|^{1/2} B ,$$

where B is bounded. This relation implies that the family of functions w is equicontinuous.

To demonstrate the corresponding result for the family $\mathfrak{F}$ of grid functions w_h, it is sufficient to show that there is a finite difference relation corresponding to equation (4.20). The derivation proceeds exactly as in the continuous argument. Let all the dimensions of $P_\mu(\gamma_\mu) \equiv P_\mu(\beta_1, \ldots, \beta_{\mu-1}, \gamma_\mu)$ be multiples of h, so that $P_\mu(\gamma_\mu)$ may be constructed from grid cubes. Apply equation (3.17) to this region, replacing w_{ij} by φ_{ij} and choosing v_{ij} in such a manner that

$$v_{ij} - v_{ii} = (e_\mu \cdot n_{ij}) h .$$

With this choice, no matter what fixed value the index i is given, the

summation

$$h^{-2} \sum_{jNi} (v_{ij} - v_{ii})$$

vanishes. This corresponds to $\nabla^2 v = 0$ in the continuous case (see Theorem 3.2). Hence, equation (3.17) reduces to

$$h^{N-1} \sum_{i=0}^{m-1} \sum_{\substack{j \geq m \\ jNi}} (e_\mu \cdot n_{ij})\, \varphi_{ii}$$

$$= \frac{1}{2} h^{N-1} \sum_{i=0}^{m-1} \sum_{\substack{j<m \\ jNi}} (e_\mu \cdot n_{ij})(\varphi_{ij} - \varphi_{ii}) h^{-1} .$$

For the region $P_\mu(\gamma_\mu)$, the surface summation on the left reduces to summations over the faces $P_{\mu-1}$ and $P_{\mu-1} + \gamma_\mu e_\mu$. Indeed, the equation may be rewritten, with a slight change in notation, in the form

$$-h^{N-1} \sum_{P_{\mu-1}} \varphi_{ii} + h^{N-1} \sum_{P_{\mu-1}+\gamma_\mu e_\mu} \varphi_{ii}$$

$$= \frac{1}{2} h^{N-1} \sum_{P_\mu(\gamma_\mu)} \sum_{\substack{j<m \\ jNi}} (e_\mu \cdot n_{ij})(\varphi_{ij} - \varphi_{ii}) h^{-1} ,$$

where the summations on the left-hand side are understood to be over cubes belonging to $P_\mu(\gamma_\mu)$ but lying on the faces $P_{\mu-1}$ and $P_{\mu-1} + \gamma_\mu e_\mu$, respectively. (This equation corresponds to equation (4.19) in the continuous case.) Since γ_μ must be an integral multiple of h, let $\gamma_\mu = c_\mu h$. The smallest value for the integer c_μ is $c_\mu = 1$, and in this case $P_\mu(\gamma_\mu)$ is a single layer of cubes lying between the faces $P_{\mu-1}$ and $P_{\mu-1} + h\, e_\mu$. In the last relation, let c_μ $(= \gamma_\mu h^{-1})$ assume all

integral values from 1 to $\beta_\mu h^{-1}$. Multiply each of these equations by h and sum. The result can be written as

$$\beta_\mu h^{N-1} \sum_{P_{\mu-1}} \varphi_{ii} = h^N \sum_{c_\mu=1}^{\beta_\mu h^{-1}} \left[\sum_{P_{\mu-1}+c_\mu h e_\mu} \varphi_{ii} \right]$$

(4.22)

$$- \sum_{c_\mu=1}^{\beta_\mu h^{-1}} h \left[\frac{1}{2} h^{N-1} \sum_{P_\mu(c_\mu h)} \sum_{\substack{j<m \\ jNi}} (e_\mu \cdot n_{ij})(\varphi_{ij} - \varphi_{ii}) h^{-1} \right] .$$

The first double summation on the right-hand side is exactly the summation over all cubes in $P_\mu(\beta_\mu)$. Hence, after division by β_μ there results a finite difference expression corresponding to equation (4.20).

The remainder of the argument proceeds as in the continuous case. It involves only substitution and finally Cauchy's inequality for bounding the summations over P_N. The fact that higher order mixed difference quotients are involved does not create any new difficulties. These exist for cubes sufficiently far from boundaries. For example, corresponding to the substitution $\varphi = D_1 w$ used in the continuous case, one would define

$$\varphi_{ii} = \sum_{kNi} (n_{ik} \cdot e_1) \left(\frac{w_{ik} - w_{ii}}{2h} \right) .$$

Comparing Theorems 4.4 and 4.5, it is evident that if the integer r satisfies $r \geq N - 1$ then the equicontinuity of the family $\mathfrak{F}$ is ensured. While if w_h is a second d.q. of v_h, for each $v_h \in \mathfrak{F}$, then the family $\mathfrak{G}$ of functions w_h is equicontinuous if $r \geq N + 1$.

<u>Theorem</u> 4.6. <u>Let</u> $D \in M^{(N+1)}$ <u>in</u> R_i <u>and let</u> $\rho \in L^2[M^{(N+1)}, R_i]$. <u>Then, in any interior subregion</u> R_i^* <u>of</u> R_i, <u>the family</u> $\mathfrak{F}$ <u>of grid solutions</u>

v_h *is equicontinuous over* R_i^*. *Moreover, the several first and second order d.qs. of* v_h *also form families which are equicontinuous over* R_i^*.

Convergence

A family $\mathfrak{G}$ which is equicontinuous over a region R^* and belongs to the class $\Sigma^2(R^*)$ can be shown to be uniformly bounded over R^*. The convergence of the grid solutions is then a consequence of the following standard theorem.

Theorem 4.7. *If a family* $\mathfrak{G}$ *of functions* w *is uniformly bounded and equicontinuous on a compact set* R^*, *then* $\mathfrak{G}$ *contains a uniformly convergent subfamily.*

Combined with Theorem 4.7, this proves that in any R_i^* there is at least one uniformly convergent subfamily $\mathfrak{F}_0$ in $\mathfrak{F}$. Let u be the limiting function. From $\mathfrak{F}_0$, form the family $\mathfrak{G}$ consisting of the functions $w_h = \Delta v_h/\Delta\xi_1$, where $v_h \in \mathfrak{F}_0$ and where ξ_1 is the first coordinate direction. But $\mathfrak{G}$ also satisfies the conditions of Theorem 4.8 because of Theorem 4.7; hence it contains a uniformly convergent subfamily $\mathfrak{G}_0$, with a limiting function u_ξ. Recall that the *grid functions* v_h and w_h were extended over the region R_i^* by a "suitably smooth" interpolation so that the customary definition of equicontinuity applied. The criterion for "suitably smooth" can now be formulated. Let each v_h be interpolated so that it is differentiable and, moreover, so that at each grid point $\partial v_h/\partial\xi_1$ has the same value as w_h at that point. Since w_h converges to u_ξ uniformly, it follows that $u_\xi = \partial u/\partial\xi_1$. Continuing in this fashion, it can be shown that there is a subfamily of $\mathfrak{F}$ such that each of the first and second order d.qs. of v_h forms a uniformly convergent family whose only limit

function is the corresponding partial derivative of u. Moreover, for any $R_i^* \subset R_i$, u satisfies the diffusion equation (1.1) in R_i^*. Since any interior point p of R_i is contained in an interior subregion $R_i^* \subset R_i$, it follows that u satisfies equation (1.1) at any interior point of R_i.

Nothing has been assumed about the existence of a solution of the multiregion problem. Since the finite difference problem, for any $h > 0$, reduces to a finite system of simultaneous, linear, algebraic equations, the grid solutions do exist. Hence their limiting function u exists and, at least, satisfies the diffusion equation in the interior of each diffusing region. The behavior of u in the vicinity of interfaces and of boundary surfaces is discussed in the next chapter.

The results obtained so far do not prove that the limit function u is unique. If it could be shown, however, that any limit function u also satisfies the interface and boundary conditions in such a manner that Theorem 2.1 - the uniqueness theorem - could be applied, then the conclusion that the family $\mathfrak{F}$ has only one limit function would be valid. The uniqueness theorem assumed that u was of class $C^{(2)}$ over each region R_i. It cannot be expected that this will be the situation in general, however, since singular points may exist for the one region problem at which boundary conditions are not fulfilled.

Bounds Required in Chapter 5

The theorems in the next chapter on the behavior at interfaces and boundaries depend upon the following properties of the family $\{v_h\}$ of grid solutions in each diffusing region R_i:

(i) $\{v_h\}$ converges to u uniformly in any interior region $R_i^* \subset R_i$;

(ii) $\left\{v_h\right\}$ is of class $\Sigma^2(R_i)$;[‡]

(iii) the set of first difference quotients of the functions in $\left\{v_h\right\}$ form a family of class $\Sigma^2(R_i)$;

(iv) the set of second difference quotients of the functions in $\left\{v_h\right\}$ form a family of class $\Sigma^2(R_i)$.

Note that the required bounds are for entire diffusing regions and not just interior subregions. Thus the bounds extend to the surfaces of discontinuity.

Properties (ii), (iii), and (iv) may be relaxed somewhat by deleting from each region R_i an ϵ-neighborhood of the (N-2)-dimensional intersections of faces of R_i. That is, let $R_i(\epsilon)$ denote the region consisting of all those points p of R_i such that at most one face of R_i is a distance less than ϵ from p. Then in properties (ii), (iii), and (iv) the phrase "of class $\Sigma^2(R_i)$" may be replaced by "of class $\Sigma^2(R_i(\epsilon))$ for every $\epsilon > 0$."

Property (i) was proved in the last section, property (ii) is contained in Theorem 4.2, and property (iii) is proved in the next section. A demonstration for property (iv) has not been found.

The requirement of property (iv) seems to be unavoidable in this method of proof, although it will be observed in the next chapter that it can be weakened slightly. A need for this property does not arise in any of the papers already cited in the literature because they are

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[‡]The definition of $\Sigma^2(R)$ is given on page 64.

concerned only with the one region problem with a Dirichlet type condition imposed on the boundary. With mixed conditions or a Neumann condition, however, it comes in because of the presence of the normal derivative. Hence, it cannot be avoided in treating the interfaces of a multiregion problem even by further restricting the class of admissible interface conditions.

The First Difference Quotients Are Square Integrable

Let the prescribed interface and boundary conditions satisfy the uniqueness conditions of Theorem 2.1, and let v be the grid function which is a solution of the finite difference problem for some specified grid spacing. It will be shown that the summation

$$h^{N-2} \sum_{r_i \in R} \sum_{j \mathbb{N} i} (v_{ij} - v_{ii})^2 \tag{4.23}$$

over all grid cubes in R is uniformly bounded as h tends to zero.

As before, let the cubes r_i approximating the region of diffusion have indices $i = 0, \ldots, m-1$, and let those cubes outside this region have indices $i \geq m$. Start with the identity

$$v_{ii} \sum_{j \mathbb{N} i} (v_{ij} - v_{ii}) + \frac{1}{2} \sum_{j \mathbb{N} i} (v_{ij} - v_{ii})^2 = \frac{1}{2} \sum_{j \mathbb{N} i} (v_{ij} - v_{ii})(v_{ij} + v_{ii}) ,$$

which applies to any grid cube r_i $(0 \leq i < m)$. Since each cube belongs to one of the regions of the differential problem, multiply the identity for each cube r_i by the constant k_i^2 determined by the uniqueness conditions for the region R_ν containing the cube r_i. Moreover, use a set of constants k_i^2 such that each $k_i^2 \geq 1$ (see Remark 1, following Theorem

2.1). After multiplying each identity by the corresponding k_i^2, sum over all $r_i \in R$. Thus

$$h^{N-2} \sum_{i=0}^{m-1} k_i^2 v_{ii} \sum_{j \mathrm{N} i} (v_{ij} - v_{ii}) + \frac{1}{2} h^{N-2} \sum_{i=0}^{m-1} \sum_{j \mathrm{N} i} k_i^2 (v_{ij} - v_{ii})^2$$

(4.24)

$$= h^{N-1} \sum_{i=0}^{m-1} \left(\sum_{j=0}^{m-1} + \sum_{j \mathrm{N} i, j \geq m} \right) k_i^2 \eta_{ij} ,$$

where

$$\eta_{ij} = (1/2h)(v_{ij} - v_{ii})(v_{ij} + v_{ii}) .$$

By Lemma 2.1,

$$\sum_{i=0}^{m-1} \sum_{j=0}^{m-1} k_i^2 \eta_{ij} = \sum_{i=0}^{m-1} \sum_{\substack{j \mathrm{N} i \\ j<i}} (k_j^2 \eta_{ji} + k_i^2 \eta_{ij}) . \tag{4.25}$$

Expand η_{ij} in terms of v_{ji} and v_{jj} by using the finite difference interface equations (3.2). Then each term in the double summation can be rearranged – as in the proof of Theorem 2.1 – in the form

$$k_j^2 \eta_{ji} + k_i^2 \eta_{ij} = [k_j^2 - (\alpha_{ij}\delta_{ij} + \beta_{ij}\gamma_{ij})k_i^2]\eta_{ji}$$

(4.26)

$$- k_i^2 \alpha_{ij}\gamma_{ij} \left(\frac{v_{ji} + v_{jj}}{2} \right)^2 - k_i^2 \beta_{ij}\delta_{ij} \left(\frac{v_{ji} - v_{jj}}{h} \right)^2 .$$

The factor in brackets always vanishes. Indeed, if r_i and r_j belong to the same subregion, then $k_j^2 = k_i^2$ and the interface coefficients degenerate to

$$\alpha_{ij} = 1 = \delta_{ij} \text{ and } \beta_{ij} = 0 = \gamma_{ij} ,$$

while if r_i and r_j belong to different subregions then, by hypothesis, the conditions of the uniqueness theorem apply. Next combine equations (4.24), (4.25), and (4.26). The result, after using the partial difference equation (3.1) to eliminate the first summation over j in equation (4.24), is

$$h^N \sum_{i=0}^{m-1} k_i^2 v_{ii}(D_i v_{ii} - \rho_i) + h^{N-2} \sum_{i=0}^{m-1} \sum_{jNi} k_i^2 (v_{ij} - v_{ii})^2$$

$$+ h^{N-1} \sum_{i=0}^{m-1} \sum_{\substack{j<i \\ jNi}} k_i^2 \left[\alpha_{ij}\gamma_{ij} \left(\frac{v_{ji}+v_{jj}}{2} \right)^2 + \beta_{ij}\delta_{ij} \left(\frac{v_{ji}-v_{jj}}{h} \right)^2 \right]$$

$$= h^{N-1} \sum_{i=0}^{m-1} \sum_{\substack{j\geq m \\ jNi}} k_i^2 \eta_{ij} \quad .$$

Since all the terms on the left are nonnegative, except possibly the terms involving ρ_i, and since the $k_i^2 \geq 1$, it follows that

$$(4.27) \qquad h^{N-2} \sum_{i=0}^{m-1} \sum_{jNi} (v_{ij} - v_{ii})^2 \leq h^N \sum_{i=0}^{m-1} k_i^2 v_{ii}\rho_i + h^{N-1} \sum_{i=0}^{m-1} \sum_{\substack{j\geq m \\ jNi}} k_i^2 \eta_{ij}.$$

Cauchy's inequality provides a bound for the first summation on the right. Indeed,

$$h^N \sum_{i=0}^{m-1} k_i^2 v_{ii} \rho_i \leq (\max_i k_i^2) \left(h^N \sum_{i=0}^{m-1} v_{ii}^2 \right)^{1/2} \left(h^N \sum_{i=0}^{m-1} \rho_i^2 \right)^{1/2}$$

and all the factors on the right are uniformly bounded as h tends to zero. Consider next the second summation in (4.27), where the boundary

conditions must be brought into the argument. If condition (1.4a) applies on the jth face of the cube r_i, then η_{ij} cannot be positive. For, if $\alpha_{ji} > 0$ $(j \geq m)$, then $\frac{1}{2}(v_{ij} + v_{ii})$ may be eliminated from η_{ij} yielding

$$\eta_{ij} = \left(\frac{v_{ij} - v_{ii}}{h}\right)\left[-\frac{\beta_{ji}}{\alpha_{ji}}\left(\frac{v_{ij} - v_{ii}}{h}\right)\right] \leq 0 .$$

If $\alpha_{ji} = 0$ then $\beta_{ji} > 0$ and a similar result holds. When condition (1.4b) applies, then $\beta_{ji} > 0$ and hence

$$\eta_{ij} = \left(\frac{v_{ij} + v_{ii}}{2}\right)\left[\frac{f_j}{\beta_{ji}} - \frac{\alpha_{ji}}{\beta_{ji}}\left(\frac{v_{ij} + v_{ii}}{2}\right)\right] \leq \left(\frac{v_{ij} + v_{ii}}{2}\right)\frac{f_j}{\beta_{ji}} .$$

The linearity of the diffusion problem must be used at this point, as in the proof of Theorem 4.2. That is, the problem is decomposed into two problems, one having $f_n \equiv 0$ everywhere – as in the nuclear reactor problem – and the other problem having $\rho_i \equiv 0$ in every R_i. But it has been shown above that $\eta_{ij} \leq 0$ whenever $f_n = 0$. On the other hand, when $\rho_i = 0$ then v_{ii} satisfies the maximum principle – and $v_{ij} \equiv f_j$ – so that $\frac{1}{2}|v_{ij} + v_{ii}| \leq \max |f|$. Finally the assumption (1.5) that $|f_n(x)/\beta_{ni}(x)|$ is uniformly bounded yields the result

$$\eta_{ij} \leq M_0 \max |f| .$$

Since the second summation (4.27) is bounded for both problems, it follows from Minkowski's inequality that the sum is also bounded for the combined problem.

<u>Theorem</u> 4.8. <u>Let</u> $v = v_h$ <u>be any solution of the finite difference problem formulated with grid cubes. If the coefficients of the interface</u>

conditions satisfy the conditions of Theorem 2.1 — the uniqueness theorem — then the summation (4.23) is uniformly bounded as h tends to zero.

Without condition (1.5) this theorem is not true in general, as shown in the following example: Consider the region in the first quadrant bounded by the lines $x = 0$ and $y = 0$ and by the circular arc $x^2 + y^2 = 1$, as shown in figure 4.1. In this region — call it R — the function

$$u = \arctan \frac{y}{x}$$

is harmonic and on the boundary it satisfies the conditions

$$u(x,0) = 0$$

$$u(0,y) = \frac{1}{2}\pi$$

$$u(x, \sqrt{1-x^2}) = \theta \ .$$

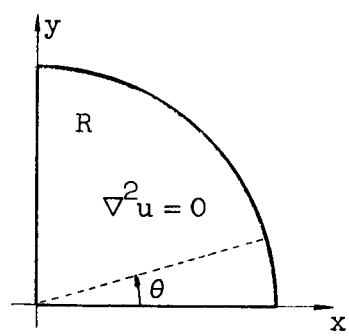


Figure 4.1

Since

$$\frac{\partial u}{\partial x} = - \frac{y}{x^2+y^2} \ ,$$

the integral

$$\iint_R \left(\frac{\partial u}{\partial x}\right)^2 dx\, dy = + \infty \ .$$

The fact that $\partial u/\partial x$ is unbounded at the origin is not surprising since this is a Dirichlet problem with a discontinuity in the prescribed boundary values.

Theorem 4.8 provides a bound in the large which is sufficient

but not necessary for the purposes of Chapter 5. A similar bound may be obtained in a local sense with less restrictions on the boundary conditions. The proof is included here because it suggests a possible approach to the problem of demonstrating bounds for the second partial difference quotients.

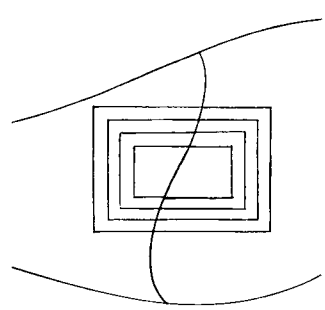
Since Theorem 4.8 is valid when f_n is identically zero, it is sufficient at this point to consider only the case where ρ_i is identically zero, i.e., the heat conduction problem.

Let $R_i(\epsilon)$ again denote the region consisting of those points p of R_i such that at most one face of R_i is a distance less than ϵ from p. Let s be any portion of the interface between $R_i(\epsilon)$ and $R_j(\epsilon)$, and let N(s) be a neighborhood of s whose distance from the complement of $R_i \cup R_j$ is greater than α. It will be shown that

$$\frac{1}{2} h^{N-2} \sum_{r_i \epsilon N(s)} \sum_{j N i} (v_{ij} - v_{ii})^2 \tag{4.28}$$

is uniformly bounded as h tends to zero.

The neighborhood N(s) can be covered by a finite number of rectangular parallelepipeds, each of which is a distance $\alpha/2$ from $C(R_i \cup R_j)$. It is sufficient to consider one of these rectangles. Call it G_1, and let it be imbedded in a nest of concentric rectangles G_λ $(\lambda = 1, \ldots, \nu)$ — as in the proof of Theorem 4.3 — lying in $R_i \cup R_j$, where $G_{\lambda+1} - G_\lambda = L_{\lambda+1}$ is the outer layer of grid cubes in $G_{\lambda+1}$.



In the proof of Theorem 4.8 it was shown that inequality (4.27) applies to any collection of grid cubes independent of the interface conditions between neighboring cubes, provided the uniqueness conditions of Theorem 2.1 are satisfied. Thus for any λ

$$\frac{1}{2} h^{N-2} \sum_{r_i \in G_1} \sum_{jNi} (v_{ij} - v_{ii})^2$$

$$\leq h^N \sum_{r_i \in G_\lambda} k_i^2 |v_{ii}\rho_i| + \frac{1}{2} h^{N-2} \sum_{r_i \in L_\lambda} \sum_{\substack{r_j \in L_{\lambda+1} \\ jNi}} k_i^2 (v_{ij}^2 - v_{ii}^2)$$

$$\leq h^N \sum_{G_\lambda} k_i^2 |v_{ii}\rho_i| + \frac{1}{2} h^{N-2} \sum_{r_j \in L_{\lambda+1}} k_j^2 v_{jj}^2 - \frac{1}{2} h^{N-2} \sum_{r_i \in L_\lambda} k_i^2 v_{ii}^2$$

(4.29)

$$+ \frac{1}{2} h^{N-2} \sum_{r_i \in L_\lambda} \sum_{\substack{r_j \in L_{\lambda+1} \\ jNi}} (k_i^2 v_{ij}^2 - k_j^2 v_{jj}^2) \quad .$$

Consider the last summation. If r_i and r_j belong to the same region, then $k_i^2 = k_j^2$ and $v_{ij} = v_{jj}$. Thus the only contributions to the sum come from that portion of the interface which coincides with the surface of G_λ. Since the intersection of G_λ and the actual interface is a set of dimension N-2, the number of cube faces in the intersection of G_λ and the approximation to the interface will be of the order h^{2-N}. This then is the number of nonzero terms in the summation. Since the maximum principle applies, the last summation in (4.29) cannot exceed

$$\gamma_0(\max k_i^2)(\max |f_n|^2) \equiv \Gamma_0 ,$$

where γ_0 and Γ_0 are constants independent of h. Summing inequality (4.29) over $\lambda = 1, 2, \ldots, \mu$ yields

$$\frac{1}{2}\mu h^{N-2} \sum_{r_i \in G_1} \sum_{j \mathrm{N} i} (v_{ij}-v_{ii})^2 < \mu h^N \sum_{G_\mu} k_i^2 |v_{ii}\rho_i| + \frac{1}{2} h^{N-2} \sum_{L_{\mu+1}} k_i^2 v_{ii}^2 + \mu \Gamma_0 .$$

A final summation — compare with inequalities (4.16) and (4.17) — over $\mu = 1, 2, \ldots, \nu-1$ yields the estimate

$$\frac{1}{2} h^{N-2} \sum_{r_i \in G_1} \sum_{j \mathrm{N} i} (v_{ij}-v_{ii})^2 < h^N \sum_{G_{\nu-1}} k_i^2 |v_{ii}\rho_i| + \frac{9N}{\alpha^2} h^N \sum_{G_\nu} k_i^2 v_{ii}^2 + \Gamma_0 .$$

The right-hand side of this inequality is uniformly bounded for all h because of Theorem 4.1 and the properties of ρ. Hence the summation (4.28) is uniformly bounded as h tends to zero.

The crucial point in this proof is the fact that the intersection of an interface with any of the rectangles consists of only $\gamma_0 h^{2-N}$ faces of grid cubes. Consequently, it is not necessary to restrict G_1 to be in the union of only two regions. In fact, (4.28) is uniformly bounded if N(s) is replaced by any open set belonging to the union of all R_i $(i = 0, \ldots, n-1)$ but lying at least a distance $\alpha > 0$ from the exterior. The use of the maximum principle means that the boundary condition was assumed to be of the form (1.4a) or (1.4b) but the restriction (1.5) was not used.

Chapter 5

BEHAVIOR AT INTERFACES AND BOUNDARIES

For second order, elliptic partial differential equations, the usual interface and boundary conditions are linear, differential conditions of first order. Thus, the condition or conditions imposed at a surface S_{ij} have the form

$$\mathcal{L}_i(u_i) = \mathcal{L}_j(u_j) , \tag{5.1}$$

where the expressions on the left and the right are differential expressions of the form

$$\mathcal{L}(u) = p \cdot \text{grad } u + \alpha u + \varphi . \tag{5.2}$$

In general, the vector p and the scalars α and φ are functions of position.

In the diffusion problem, the vector p is proportional to the normal to the surface and, hence, is not constant whenever curved surfaces are involved. The inhomogeneous term φ is usually absent in interface conditions, but generally occurs in boundary conditions, as in the Dirichlet problem.

This chapter is devoted to studying the behavior of sequences of finite difference solutions, v_h, in the vicinity of a boundary or an interface as the grid size, h, tends to zero. The results obtained are independent of any particular class of partial differential equations. The basic assumptions are (a) that there exists a sequence $\left\{v_h\right\}$ of grid functions converging uniformly to a function u in every interior subregion but not necessarily on S_{ij}, (b) that the surface S_{ij} is approximated by a

(possibly trivial) sequence of surfaces $\left\{S_{ij}^{(h)}\right\}$ tending to S_{ij}, (c) that at each surface $S_{ij}^{(h)}$ the corresponding grid function v_h satisfies a linear condition $L_i^{(h)}(v_h) = L_j^{(h)}(v_h)$, and (d) that the linear operators $L_i^{(h)}$ and $L_j^{(h)}$ converge to the differential operators $\mathscr{L}_i$ and $\mathscr{L}_j$ as h tends to zero. Note that conditions (a) and (d) imply that the sequence $\left\{L_i^{(h)}(v_h)\right\}$ converges uniformly to $\mathscr{L}_i(u)$ in every interior subregion. This is a consequence of the well-known iterated limits theorem.

These four conditions are satisfied for the multiregion diffusion problem. Condition (a) was demonstrated in Chapter 4; condition (b) is implicit in the grid cube approximation for the subregions. That condition (c) also holds may not be quite as obvious. Suppose, for example, that r_i and r_j are adjacent grid cubes whose common face is part of $S_{ij}^{(h)}$. Then one of the conditions imposed across this face is a finite difference approximation for

$$u_i = \alpha_{ij}\, u_j + \beta_{ij}\, \partial u_j/\partial n_j \ .$$

The approximation prescribed in equation (3.2) is

$$(v_{ij} + v_{ii})/2 = \alpha_{ij}(v_{ji} + v_{jj})/2 + \beta_{ij}(v_{ji} - v_{jj})/h \ .$$

The left-hand member is $L_i^{(h)}(v_h)$ and the right-hand member is $L_j^{(h)}(v_h)$. Although the virtual values v_{ij} and v_{ji} do not appear in the final numerical formulation given in Chapter 3, nevertheless, since the virtual values were eliminated by applying equation (3.3), the computed real values determine these virtual values by virtue of equation (3.3); and therefore the solution must satisfy the approximate interface conditions (3.2), since equations (3.3) and (3.2) are equivalent. Thus condition (c) above is

satisfied for the diffusion calculation as formulated in Chapter 3. Finally, Theorem 3.1 implies that condition (d) always holds; that is, that $L_i^{(h)}$ tends to $\mathscr{L}_i$ as h tends to zero.

Geometrical Considerations

Because of a necessity to single out some particular coordinate direction, the discussion in this chapter is phrased in the language of x, y, z coordinates. Nevertheless, the method is general in every respect.

Let $S = S_{ij}$ be any interface or boundary surface, and for any $\epsilon > 0$, let $S(\epsilon)$ be any open set of S with the property that the distance from $S(\epsilon)$ to the boundary of S is ϵ. This requirement serves to eliminate lines of intersection of two or more interfaces. Thus, the convergence behavior is only studied at interior points of the interfaces and the boundaries.

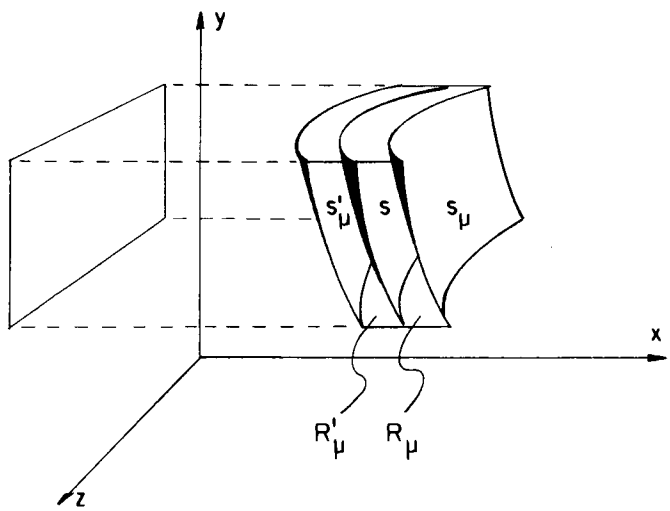
Given any fixed system of cartesian coordinates, the open surface $S(\epsilon)$ may be covered by a finite number of open surface elements each of which has the following properties: First, for at least one of the coordinate directions, which can be called the x direction without loss of generality, the surface element may be represented by an equation of the form

$$x = g(y,z) \quad ,$$

where g is single valued, continuous, and has a piecewise continuous derivative. Second, the maximum angle α_0, between the normals to the surface element and the coordinate lines parallel to the x axis, is bounded away from $\pi/2$.

Let s be one of these surface elements. If S_μ and S'_μ are the

loci of all points whose distance from S is exactly μ, then let s_μ and s'_μ be the portions of these loci lying inside the infinite cylinder determined by projecting s perpendicularly onto the plane $x = 0$. Moreover, let R_μ (or R'_μ) be the region bounded by the surfaces s and s_μ (or s'_μ) and this cylindrical surface. Henceforth in this chapter primes will be used in this fashion to distinguish between quantities



associated with the two sides of an interface. Moreover, it will be implicitly assumed that the direction of increasing x is from the primed side into the unprimed side. When ν satisfies the conditions $0 < \nu < \mu$, then the region $R_\mu - R_\nu$ may be defined. For simplicity, it will be denoted by $R_{\mu\nu}$. Since μ, in general, will be smaller than the dimensions of the surface element s, it is suggestive to refer to R_μ and $R_{\mu\nu}$ as layers.

For any fixed grid size, the surfaces s, s_ν, and s_μ will be approximated by surfaces $s^{(h)}$, $s_\nu^{(h)}$, and $s_\mu^{(h)}$ depending in some manner upon the lattice points. Note particularly that $s_\mu^{(h)}$ is determined

by s_μ and not by $s^{(h)}$. By G_μ will be understood the lattice points lying between $s^{(h)}$ and $s_\mu^{(h)}$ and the projection of $s^{(h)}$ onto the plane $x = 0$. $G_{\mu\nu}$ is similarly defined. In the following, the distinction will not always be made between s and $s^{(h)}$, etc. However, until h is allowed to approach zero, it will always be the approximating surfaces that are of interest, even though h is suppressed.

Let p and p' be arbitrary grid points belonging to G_μ and G'_μ. Then for any grid function w, the values w(p) and w(p') may be related to values at points q and q' near the interface s by means of relations of the form

$$w(p) = w(q) + h \sum_q^p w_x \tag{5.3}$$

$$w(p') = w(q') - h \sum_{q'}^{p'} w_x , \tag{5.3'}$$

where w_x denotes a first difference quotient of the grid function. The exact limits of summation depend upon whether forward or backward difference quotients are used. The choice is arbitrary and, indeed, for the developments of this chapter alone, it is not necessary to be specific. To be precise, however, let the summations in equation (5.3) and (5.3') be understood to mean

$$\sum_q^p w_x = \sum_{r=q}^{p-he_1} \left[w(r + he_1) - w(r) \right] h^{-1}$$

$$\sum_{q'}^{p'} w_x = \sum_{r=q'}^{p'+he_1} \left[w(r) - w(r - he_1) \right] h^{-1} .$$

Thus, the increment of x in the difference quotients is always directed away from the surface s. Note that there is nothing in the foregoing

to rule out the possibility that q might be a virtual point of the layer G_μ — in the sense of Chapter 3 — provided w is defined at q.

(Thus for the linear operator

$$L_i^{(h)}(v_h) = (v_{ij} + v_{ii})/2 ,$$

which - in another notation - can be written

$$L_i^{(h)}(v(r_i)) = \tfrac{1}{2}v(r_i + he_1) + \tfrac{1}{2}v(r_i) ,$$

the value at a point p away from the interface can be expressed in the form

$$\begin{aligned} L_i^{(h)}(v(p)) &= \tfrac{1}{2}v(p + he_1) + \tfrac{1}{2}v(p) \\ &= \tfrac{1}{2}v(q + he_1) + h \sum_{q+he_1}^{p+he_1} v_x \\ &\qquad + \tfrac{1}{2}v(q) + h \sum_{q}^{p} v_x \\ &= L_i^{(h)}(v(q)) + h \sum_{q}^{p} L_i^{(h)}(v_x) \end{aligned}$$

by applying relation (5.3) to v(p) and to $v(p + he_1)$.)

Consider next the line segment p, q and extend it to intersect s (not $s^{(h)}$). At this intersection the normal to s makes an angle α with the extended line segment, and by hypothesis, $|\alpha| \le \alpha_0 < \pi/2$. If $q \in s_\nu^{(h)}$ and $p \in s_\mu^{(h)}$, then the summation of h from q to p will certainly satisfy the inequality

$$\sum_{q}^{p} h \le (\mu - \nu)\gamma$$

where γ is some multiple of sec α_0, independent of ν, μ, or h. This estimate will be used repeatedly in subsequent sections.

Conditions with Variable Coefficients

The interface and the boundary conditions under consideration have the form

$$\mathcal{L}_i(u_i) = \mathcal{L}_j(u_j) ,$$

where $\mathcal{L}_i$ and $\mathcal{L}_j$ are linear differential operators with variable coefficients. For any h such a condition is approximated by a finite difference equation of the form

$$L_i^{(h)} (v_i^{(h)}) = L_j^{(h)} (v_j^{(h)}) .$$

In the limit as h tends to zero, the operator $L_i^{(h)}$ must converge to the operator $\mathcal{L}_i$.

But these finite difference and differential operators are only defined along the surface S_{ij}. Since s is a surface element of S_{ij} which can be represented in the form $x = g(y,z)$, it is possible to extend the domain of definition of $\mathcal{L}_i$ and $L_i^{(h)}$ to any layer R_μ in such a way that the variable coefficients of $\mathcal{L}_i$ and $L_i^{(h)}$ remain independent of x for any fixed choice of y and z. Geometrically, this means that at any point q of s the value of each coefficient of the operator is extended to all points along the coordinate line parallel to the x axis and passing through q.

When the definitions of the finite difference operators are extended in this manner, then, because they are linear operators whose

coefficients are independent of x, the grid function w in equation (5.3) may be replaced by $L^{(h)}(v)$. Thus

$$L^{(h)}(v(p)) = L^{(h)}(v(q)) + h \sum_{q}^{p} L^{(h)}(v_x) .$$

There will be no confusion if this identity and the corresponding one which applies to the other side of the interface are written in the abbreviated forms

$$L(p) = L(q) + h \sum_{q}^{p} L_x , \tag{5.4}$$

$$L'(p') = L'(q') - h \sum_{q'}^{p'} L'_x . \tag{5.4'}$$

<u>The Boundary Treatment of Courant, Friedrichs, and Lewy</u>

The analysis in this section follows very closely that given by Courant, Friedrichs, and Lewy in their classical treatment of the one region, two-dimensional Dirichlet problem.

Let the differential condition imposed along the boundary be $\mathcal{L}(u) = 0$. Then the corresponding condition in the finite difference problem is $L(\mathbf{v}) = 0$. It is only necessary, therefore, to consider one layer, say R_μ, which is chosen to lie along the inner surface of the boundary.

The following theorem is the principal result of this section. It applies to any surface element s representable in the form $x = g(y,z)$.

<u>Theorem</u> 5.1. <u>If the sequence</u> $\{v_h\} \to u$ <u>as</u> $h \to 0$, <u>then</u>

$$\lim_{\mu \to 0} \mu^{-1} \iiint_{R_\mu} [\mathscr{L}(u)]^2 \, dx \, dy \, dz = 0$$

<u>provided</u>

(i) $\left\{L(v_h)\right\} \to \mathscr{L}(u)$ <u>uniformly in every sublayer</u> $R_{\mu\nu}$, <u>and</u>

(ii) $h^3 \sum_{G_\mu} L_x^{\,2}$ <u>is uniformly bounded as</u> $h \to 0$.

Let the point q in the identity (5.4) be chosen such that $L(v(q)) = 0$. Thus, q is determined by the approximate boundary $S^{(h)}$. Squaring both sides of the result and applying Cauchy's inequality, one obtains

$$L(p)^2 = h \left(\sum_q^p h^{1/2} L_x \right)^2 \leq h \left(\sum_q^p h \right) \left(\sum_q^p L_x^{\,2} \right) .$$

Since h and $L_x^{\,2}$ are both positive, the range of summation may be extended to include all points lying on the segment of the line between the surfaces s and s_μ. The length of this line segment will never exceed $\gamma\mu$ for sufficiently small values of h. Hence

$$L(p)^2 \leq \gamma \mu h \sum_s^{s_\mu} L_x^{\,2} .$$

Summing this inequality over all points p on the line segment yields

$$h \sum_s^{s_\mu} L(p)^2 < \gamma^2 \mu^2 h \sum_s^{s_\mu} L_x^{\,2} .$$

Summing next in the y and z directions over the surface element s, one

obtains

$$h^3 \sum_{G_\mu} L^2 < \gamma^2 \mu^2 h^3 \sum_{G_\mu} L_x^{\ 2} .$$

In N-dimensional space this step is exactly the same — summation over the N-1 dimensional surface element s.

If hypothesis (ii) of the theorem is satisfied, it follows that

$$\frac{1}{\mu} h^3 \sum_{G_\mu} [L(v)]^2 < \kappa\mu ,$$

where κ is a constant independent of μ, h, and of v. If the summation is limited to a closed layer $G_{\mu\nu}$ lying entirely in the interior, then the inequality still holds with the same constant κ. As h tends to zero, this inequality yields

$$\frac{1}{\mu} \iiint_{R_{\mu\nu}} [\mathscr{L}(u)]^2 \, dx \, dy \, dz < \kappa\mu .$$

This limiting process is valid because of hypothesis (i) of the theorem. Since this integral is bounded and monotonic as ν tends to zero, it implies the conclusion of Theorem 5.1.

For a Dirichlet problem $\mathscr{L}(u) = u - f$ and so the second hypothesis of Theorem 5.1 requires only that a bound be found for

$$h^3 \sum_{G_\mu} v_x^{\ 2}$$

while for a Neumann problem the boundedness of

$$h^3 \sum_{G_\mu} [v_{xx}^{\ 2} + v_{yx}^{\ 2} + v_{zx}^{\ 2}]$$

must be demonstrated.

Behavior at Interfaces and at Boundaries

If, for any fixed q, equation (5.4) is summed in the x direction over all points p belonging to the grid layer $G_{\mu\nu}$, the result is

$$h \sum_{s_\nu}^{s_\mu} L(p) = L(q) \sum_{s_\nu}^{s_\mu} h + h^2 \sum_{s_\nu}^{s_\mu} \sum_{q}^{p} L_x \ .$$

Since the number of grid points between s_ν and s_μ on the line through q may depend upon q, multiply this equation by the ratio

$$\theta_h(q) = (\mu - \nu) \left(\sum_{s_\nu}^{s_\mu} h \right)^{-1} .$$

Then summing in the y and z directions over the surface element s, one obtains

$$h^2 \sum_s \left(h\theta_h \sum_{s_\nu}^{s_\mu} L(p) \right) = (\mu - \nu) h^2 \sum_s L(q) + h^4 \sum_s \sum_{s_\nu}^{s_\mu} \sum_{q}^{p} \theta_h L_x \ .$$

Similarly, on the other side of the surface element

$$h^2 \sum_s \left(h\theta_h' \sum_{s_\nu'}^{s_\mu'} L'(p') \right) = (\mu - \nu) h^2 \sum_s L'(q') - h^4 \sum_s \sum_{s_\nu'}^{s_\mu'} \sum_{q'}^{p'} \theta_h' L_x' \ .$$

But for each point q there is a point q' such that $L'(q') = L(q)$.

Therefore when the last two equations are combined by subtracting and absolute values are introduced, the result is

$$(5.5) \qquad \left| h^3 \sum_{G_{\mu\nu}} \theta_h \, L(p) \; - \; h^3 \sum_{G'_{\mu\nu}} \theta'_h \, L'(p') \right|$$

$$\leq \sum_s h^2 \sum_{s_\nu}^{s_\mu} h \sum_q^p h|\theta_h \, L_x| \; + \; \sum_s h^2 \sum_{s'_\nu}^{s'_\mu} h \sum_{q'}^{p'} h|\theta'_h \, L'_x| .$$

In estimating the magnitude of the expressions on the right, certainly θ_h and θ'_h do not exceed 2. Moreover, by Cauchy's inequality, the inner summation has the bound

$$\sum_q^p h|\theta_h \, L_x| \leq 2 \left(\sum_q^p h \right)^{1/2} \left(\sum_q^p h \, L_x^{\,2} \right)^{1/2}$$

$$\leq 2 \left(\sum_q^{s_\mu} h \right)^{1/2} \left(\sum_q^{s_\mu} h \, L_x^{\,2} \right)^{1/2}$$

$$\leq 2 \, (\gamma\mu)^{1/2} \left(\sum_q^{s_\mu} h \, L_x^{\,2} \right)^{1/2} ,$$

because the length of any line segment parallel to the x axis and extending from q to s_μ (or $s_\mu^{(h)}$) will not exceed $\gamma\mu$. Similarly

$$\sum_{s_\nu}^{s_\mu} h \left(\sum_q^p h|\theta_h \, L_x| \right) \leq 2(\gamma\mu)^{1/2} \left(\sum_{s_\nu}^{s_\mu} h \right) \left(\sum_s^{s_\mu} h \, L_x^{\,2} \right)^{1/2}$$

$$\leq 2\gamma^{3/2} \, \mu^{1/2} \, (\mu - \nu) \left(\sum_s^{s_\mu} h \, L_x^{\,2} \right)^{1/2} ,$$

and hence, applying Cauchy's inequality to the summation over the surface

element s, one obtains the following estimate for the first term on the right side of inequality (5.5):

$$\sum_s h^2 \sum_{s_\nu}^{s_\mu} h \sum_q^p h|\theta_h L_x| \leq 2\gamma^{3/2}\mu^{1/2}(\mu - \nu)\sum_s \left[h \left(\sum_s^{s_\mu} h^3 L_x \right)^{1/2} \right]$$

$$\leq 2\gamma^{3/2}\mu^{1/2}(\mu - \nu)\left(\sum_s h^2\right)^{1/2}\left(\sum_s \sum^{s_\mu} h^3 L_x{}^2\right)^{1/2}$$

$$\leq 2\gamma^{3/2}(\mu - \nu)(\mu\sigma)^{1/2}\left(\sum_{G_\mu} h^3 L_x{}^2\right)^{1/2} ,$$

where σ is the area of the surface element s. A similar estimate applies to the triple summation on the other side of the surface.

If the summations

$$(5.6) \qquad h^3 \sum_{G_\mu} (L_x{}^2) \quad \text{and} \quad h^3 \sum_{G'_\mu} (L'_x)^2 ,$$

which occur in these estimates, are uniformly bounded as h tends to zero, then combining these estimates with inequality (5.5) yields

$$\left| h^3 \sum_{G_{\mu\nu}} \theta_h L - h^3 \sum_{G'_{\mu\nu}} \theta'_h L' \right| \leq \kappa(\mu - \nu)(\mu\sigma)^{1/2} .$$

Finally, allowing h to approach zero, the following theorem has been proved.

<u>Theorem</u> 5.2. <u>Let</u> s <u>be a surface element representable in the form</u> $x = g(y,z)$. <u>Suppose that the sequence</u> $\left\{L(v_h)\right\}$ <u>converges uniformly to</u> $\mathcal{L}(u)$ <u>in every interior layer</u> $R_{\mu\nu}$ $(0 < \nu < \mu)$, <u>and that</u> $\left\{L'(v_h)\right\}$

converges uniformly to $\mathscr{L}'(u)$ in every $R'_{\mu\nu}$. Suppose, moreover, that the summations (5.6) are uniformly bounded as h tends to zero. Then

$$(5.7) \qquad \left| \iiint_{R_{\mu\nu}} \mathscr{L}(u)\, dx\, dy\, dz - \iiint_{R'_{\mu\nu}} \mathscr{L}'(u)\, dx\, dy\, dz \right| \leq \kappa(\mu - \nu)(\mu\sigma)^{1/2} .$$

It does not appear possible to justify directly the process of allowing $R_{\mu\nu}$ to tend to R_μ in inequality (5.7) as was the case in the treatment of boundary conditions where there was a single integral with a nonnegative integrand. As an alternative procedure, the parameter μ will be allowed to tend to ν, so that the layer $R_{\mu\nu}$ degenerates into the surface s_ν. As a final step, ν will be allowed to approach zero and, hence, the integrals in inequality (5.7) will tend to surface integrals along the interface S. These limit processes may be carried out with the aid of a transformation of coordinates.

Let (ξ, η) be arbitrary coordinates defined over S and let τ be the oriented distance from S. The coordinates (ξ,η,τ) assigned to a point (x,y,z) are obtained by determining the length of τ of the shortest normal to S which passes through (x,y,z) and the coordinates (ξ,η) of the base of the normal on S. The new coordinates form a geodesic normal coordinate system. The Jacobian $J(x,y,z;\ \xi,\eta,\tau)$ of the transformation has the value $\sec\alpha$ on s_τ, where α is the angle between the normal to s_τ and a line parallel to the x axis. Thus $J\, d\xi\, d\eta \equiv d\sigma$ is an element of area of the surface s_τ.

Either integral in inequality (5.7) may, therefore, be written in the form

$$\iiint_{R_{\mu\nu}} \mathscr{L}(u)\, dx\, dy\, dz = \int_{\nu}^{\mu} \iint_{S_\tau} \mathscr{L} J\, d\xi\, d\eta\, d\tau = \int_{\nu}^{\mu} \iint_{S_\tau} \mathscr{L}\, d\sigma\, d\tau$$

$$= (\mu - \nu) \iint_{S_{\bar{\tau}}} \mathscr{L}\, d\sigma ,$$

where $\nu \leq \bar{\tau} \leq \mu$. The third equality results from an application of the mean-value theorem, which is valid provided $\mathscr{L}(u)$ is continuous in $R_{\mu\nu}$ for all $\nu \neq 0$. Hence, in the limit as μ tends to ν,

$$\lim_{\mu \to \nu} (\mu - \nu)^{-1} \iiint_{R_{\mu\nu}} \mathscr{L}\, dx\, dy\, dz = \iint_{S_\nu} \mathscr{L}\, d\sigma ,$$

and, hence, a new inequality is obtained from (5.7). It is

$$\left| \iint_{S_\nu} \mathscr{L}\, d\sigma - \iint_{S'_\nu} \mathscr{L}'\, d\sigma' \right| \leq \kappa(\nu\sigma)^{1/2} . \tag{5.8}$$

<u>Theorem</u> 5.3. <u>If</u> $\mathscr{L}(u)$ <u>and</u> $\mathscr{L}'(u)$ <u>are continuous in every</u> $R_{\mu\nu}$ <u>and</u> $R'_{\mu\nu}$, <u>respectively, for all</u> $\nu \neq 0$, <u>and if the conditions of Theorem</u> 5.2 <u>are satisfied, then inequality</u> (5.8) <u>is valid</u>.

<u>Corollary</u> 1.

$$\lim_{\nu \to 0} \iint_{S_\nu} \mathscr{L}(u)\, d\sigma = \lim_{\nu \to 0} \iint_{S'_\nu} \mathscr{L}'(u)\, d\sigma .$$

Consider inequality (5.8) again and let the sequence of surfaces s_ν be chosen so that the area, σ, of each is equal to $\sqrt{\nu}$. Since $\mathscr{L}(u)$ and $\mathscr{L}'(u)$ are continuous in the interior, the mean-value theorem may be applied to the integrals. This produces two sequences of points $p_\nu \in s_\nu$ and $p'_\nu \in s'_\nu$, converging to a common point q on S which possess the property

that

$$(5.9) \qquad \nu^{1/2}|\mathcal{L}(p_\nu) - \mathcal{L}'(p'_\nu)| \le \kappa\, \nu^{3/4} .$$

<u>Corollary</u> 2. <u>For any point</u> q <u>belonging to a surface element of</u> $S = S_{ij}$, <u>there exists a sequence of points</u> $\{p_\nu\}$ <u>converging to</u> q <u>from the interior of</u> R_μ <u>and a second sequence</u> $\{p'_\nu\}$ <u>converging to</u> q <u>from the interior of</u> R'_μ, <u>and these two sequences have the property that</u>

$$(5.10) \qquad \lim_{\nu\to 0} \mathcal{L}(p_\nu) = \lim_{\nu\to 0} \mathcal{L}'(p'_\nu) .$$

Figures 5.1 and 5.2 illustrate this corollary for two dimensions. The envelopes of the arcs $\{s_\nu\}$ and $\{s'_\nu\}$ are tangent to the interface because of the properties of $\sqrt{\nu}$. If the middle half of each arc in

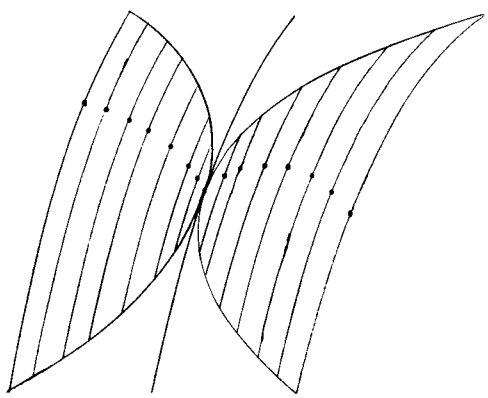


Figure 5.1

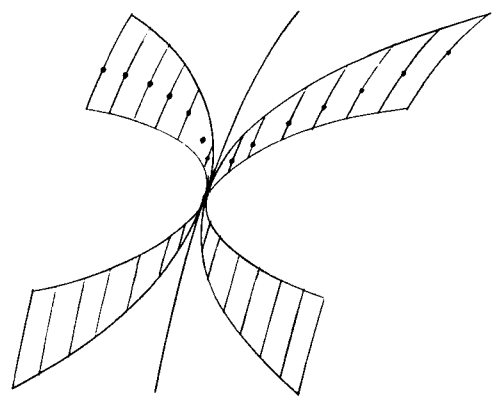


Figure 5.2

figure 5.1 is deleted, figure 5.2 results, where there are two sequences of arcs on each side. Consider just one of these. Again inequality (5.9) applies since each s_ν has length $\frac{1}{4}\sqrt{\nu}$. Moreover, the sequence $\{s_\nu\}$

is contained in a horn angle with vertex at q. For, using the normal through q and the tangent at q as basis vectors, the curves comprising the envelope of $\{s_\nu\}$ must ultimately coincide with the curves

$$t = +\frac{1}{4}\sqrt{\nu} \quad \text{and} \quad t = +\frac{1}{2}\sqrt{\nu} .$$

Hence, the sequences $\{p_\nu\}$ and $\{p'_\nu\}$ of Corollary 2 both approach q from a direction which is tangent to the interface. A similar argument applies in N-dimensions.

<u>Corollary</u> 3. <u>For any point</u> q <u>belonging to a surface element of</u> $S = S_{ij}$, <u>there exists a sequence of points</u> $\{p_\nu\}$ <u>converging to</u> q <u>from the interior of</u> R_μ <u>in a manner which is ultimately tangent to</u> S <u>at</u> q, <u>and a second sequence of points</u> $\{p'_\nu\}$ <u>converging to</u> q <u>in a similar manner from the interior of</u> R'_μ, <u>and these two sequences have the property expressed in relation</u> (5.10).

Similar theorems hold on the boundary. Indeed, if s is an element of a boundary surface S_{in}, then for each of the points q on or near $S_{in}^{(h)}$ there exists a point q' such that

$$L(q) = f(q')$$

where f is a specified function of class C' on S_{in}. In this case, inequality (5.5) may be replaced — compare the equations preceding (5.5) — by

$$\left| h^3 \sum_{G_{\mu\nu}} \theta_h L(p) - (\mu-\nu)h^2 \sum_s f(q') \right| \leq \sum_s h^2 \sum_{s_\nu}^{s_\mu} h \sum_q^p h|\theta_h L_x|.$$

The estimation of the right-hand side is exactly the same, and hence,

Theorem 5.2 applies with (5.7) replaced by

$$\left| \iiint_{R_{\mu\nu}} \mathcal{L}(u)\, dx\, dy\, dz - (\mu - \nu) \iint_{S} f\, d\sigma \right| \leq \kappa(\mu - \nu)(\mu\sigma)^{1/2} .$$

Finally, inequality (5.8) is replaced by

$$\left| \iint_{S_\nu} \mathcal{L}\, d\sigma - \iint_{S} f\, d\sigma \right| \leq \kappa(\nu\sigma)^{1/2} . \tag{5.11}$$

An alternative approach is also possible. Let $\mathcal{L}'(u) \equiv f$. Then recalling the convention for extending the domain of definition of variable coefficients in $\mathcal{L}'$, it is clear that f_x — the first difference quotient — is identically zero. Hence the summation

$$h^3 \sum_{G'_\mu} (L'_x)^2 = h^3 \sum_{G'_\mu} f_x^{\,2} = 0$$

vanishes for all h. Moreover, by hypothesis, $\mathcal{L}'(u) \equiv f$ is continuous for all R'_μ. Thus Theorem 5.3 applies with equation (5.8) replaced by

$$\left| \iint_{S_\nu} \mathcal{L}\, d\sigma - \iint_{S'_\nu} f\, d\sigma \right| \leq \kappa(\nu\sigma)^{1/2} . \tag{5.12}$$

By either method the following theorems may be obtained.

<u>Theorem</u> 5.4. <u>Let</u> s <u>be an element of a boundary surface</u> S_{in} <u>and let</u> s <u>be representable in the form</u> $x = g(y,z)$. <u>Suppose that the sequence</u> $\left\{L(v_h)\right\}$ <u>converges uniformly to</u> $\mathcal{L}(u)$ <u>in every interior layer</u>

$R_{\mu\nu}$ $(0 < \nu < \mu)$, that the summation

$$h^3 \sum_{G_\mu} L_x^{\,2}$$

is uniformly bounded as h tends to zero, and that $\mathscr{L}(u)$ is continuous in every $R_{\mu\nu}$, $\nu \neq 0$. Then inequalities (5.11) and (5.12) are valid.

Corollary 1.

$$\lim_{\nu \to 0} \iint_{S_\nu} \mathscr{L}(u)\, d\sigma = \iint_S f\, d\sigma .$$

Corollary 2. Let q be any point belonging to a surface element of S_{in}. Since, by hypothesis, f is continuous at q there exists a sequence of points $\left\{p_\nu\right\}$ converging to q from the interior of R_μ with the property that

$$\lim_{\nu \to 0} \mathscr{L}(p_\nu) = f(q) .$$

Corollary 3. Moreover, the sequence of Corollary 2 may be constrained so that it is ultimately tangent to S_{in} at q.

Chapter 6

A DISCRETE ANALOG OF THE DIVERGENCE THEOREM FOR POLYTOPIC REGIONS

Discrete Versus Finite Difference Analogs

In contrast to Chapter 3 where attention was focused entirely upon a particular choice for the finite difference approximation of the derivatives, the theorems to be developed here are independent of such a choice. They are based upon the assumption that the functions involved and their derivatives will only be known or approximated at a discrete set of points determined a priori by the geometry or other pertinent considerations. In Chapter 3 these points were the grid points and the centers of the faces of the cubes. Thus the results developed here involve derivatives evaluated at specific points. It seems appropriate to refer to these as discrete theorems.

By substituting finite difference approximations for the derivatives in these discrete theorems, the corresponding finite difference theorems can be obtained. This is carried out in the next chapter.

The regions considered in Chapter 3 were restricted to be the union of a finite number of N-dimensional cubes, one for each real grid point. To treat more general regions, it is necessary to distort the N-dimensional cubes. Thus in this chapter, regions may be the union of a finite number of closed, convex polytopes, each containing one real mesh point.

Statement of the Basic Theorem

Let P^N be such a closed polytope and let x_0 be the real grid point contained in P^N. The condition that P^N be convex can be relaxed. All that is required is that for any point $y \in P^N$ then the line segment joining x_0 and y — denoted by $L\,[x_0, y]$ — must lie entirely in P^N.

Definition. A domain D will be said to be convex about a point x_0 if for any point $y \in D$ the closed line segment $L\,[x_0, y]$ is contained in D.

An equivalent definition is provided by the theorem that D is convex about x_0 if and only if D is a union of convex sets, each of which contains x_0.

If P^N is any polytope, then its faces will be denoted, when necessary, by P_j^{N-1} $(j = 0, \ldots, M)$. Furthermore, the area of P_j^{N-1} and its exterior normal will be denoted by α_j and n_j, respectively, and its centroid by c_j. It is assumed in each of the following theorems that any polytope which is constrained to be convex about some point is also constrained to have at most a bounded number of faces. Thus $M + 1$ is less than some M_0 chosen in advance. For the applications in this paper, each P^N will be a distorted cube and hence will have exactly 2N faces.

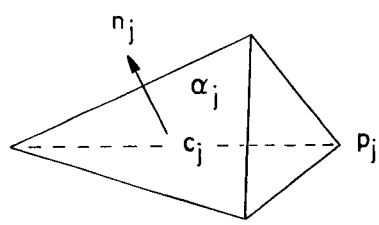
Theorem 6.1. Let f be a vector-valued function whose components are of class C' over R. Given any $\epsilon > 0$ then there exists a $\delta > 0$ such that for any point $x_0 \in R$ and any polytope P^N in R which is convex about x_0 and has diameter less than δ, then

$$\left| \sum_{j=0}^{M} \alpha_j\, n_j \cdot f(c_j) - (\text{volume of } P^N)\, \nabla \cdot f(x_0) \right| < (\text{vol. } P^N)\, \epsilon\ .$$

This basic theorem is a crude analog of Gauss' divergence theorem. It is valid for N-dimensional Euclidean space independent of any particular coordinate system. To prove it, however, it is sufficient to use the familiar rectangular cartesian coordinates. The proof rests primarily upon two geometric identities concerning polytopes.

Preliminary Lemmas

Any polytope may be triangulated so that it is the union of a finite number of closed simplexes, any two of which intersect at most in a common face. Briefly, this may be accomplished for a convex polytope, P^N, by triangulating each face into simplexes of dimension N-1 and then joining the vertices of each of these simplexes to an interior point of P^N. The desired identities will first be obtained for an arbitrary N-dimensional simplex S^N. Let the vertices of S^N be given by the position vectors $p_j (j = 0, 1, \ldots, N)$. Furthermore, let α_j be the area of the face not containing the vertex p_j, let c_j be the centroid of that face, and let the exterior unit normal to the face at c_j be denoted by n_j.



In the following, the vectors n_j, c_j, and p_j will be treated as column vectors with components $\eta_{\mu j}$, $\gamma_{\mu j}$, and $\pi_{\mu j}$ $(\mu = 1, \ldots, N)$, respectively.

<u>Lemma</u> 6.1. <u>For any simplex</u> S^N,

$$\sum_{j=0}^{N} \alpha_j \, \eta_{\mu j} = 0 , \qquad (\mu = 1, \ldots, N)$$

<u>Lemma</u> 6.2. <u>For any simplex</u> S^N,

$$\sum_{j=0}^{N} \alpha_j \, \eta_{\mu j} \, \gamma_{\nu j} = \delta_{\mu\nu}(\text{volume of } S^N), \qquad (\mu = 1, \ldots, N)$$

<u>where</u> $\delta_{\mu\nu}$ <u>is the Kronecker delta</u>.

Since $d_j \equiv \sum_\mu \eta_{\mu j} \, \gamma_{\mu j}$ is the directed distance from the origin to the plane of the jth face, it is a corollary of Lemma 6.2 that

$$\sum_j \alpha_j \, d_j = N(\text{volume of } P^N) \; .$$

Lemma 6.1 and the last relation were given by Minkowski (1897). Lemma 6.2, itself, has not been located in the literature.

The first lemma is intuitively clear. The product $\alpha_j \, \eta_{\mu j}$ is the signed area of the projection of the jth face onto the μth coordinate plane. For any closed surface, however, the "upper" and "lower" portions with respect to any nonintersecting plane will have coinciding projections in that plane. The second lemma for the case $\mu \neq \nu$ asserts that the sum of the first moments of these projections also vanishes.

Once these lemmas have been established, it will be shown that they imply the same results for any polytope (because terms arising from the interface of two simplexes will cancel). In this sense, the case $\mu = \nu$ provides a generalization to N-dimensions of the familiar trapezoid rule for integration in two dimensions.

The following proof* for these lemmas is analytic and hence

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*I am indebted to A. S. Householder for suggesting this method of proof for the case of N-dimensions.

requires that some attention be given to the signs of the areas and volumes involved. It will be sufficient to show that an order for labeling the vertices of S^N may be established which guarantees that the volume of S^N is positive and that the normals to the faces of S^N are directed outward. In any rectangular cartesian coordinate system, regardless of the ordering of the vertices, the magnitude of the volume of S^N is given by the absolute value of the determinant

$$\frac{1}{N!}\begin{vmatrix} 1 & 1 & \cdots & 1 \\ \pi_{10} & \pi_{11} & & \pi_{1N} \\ \vdots & & & \\ \pi_{N0} & \pi_{N1} & & \pi_{NN} \end{vmatrix} .$$

It will be convenient to write such determinants in the abbreviated form

$$\frac{1}{N!}\begin{vmatrix} 1 & 1 & \cdots & 1 \\ p_0 & p_1 & & p_N \end{vmatrix}$$

which displays the position vectors of the vertices. The volume of a simplex is defined to be the value of this determinant and hence will be positive or negative depending upon the orientation of the vertices. Consider, however, the unit simplex whose vertices coincide with the origin, O, and with the end points of the unit coordinate vectors $e_1, \ldots, e_N$ (the μth component of e_j is $\delta_{\mu j}$). The volume of this unit simplex as given by the determinant is clearly positive. Now deform the unit simplex into the simplex S^N in a continuous manner such that all N+1 vertices never lie in an N-1 hyperplane; i.e., so that the volume always remains positive.

The vertices of S^N may now be labeled by assigning p_0 to the image of 0, and p_j to the image of e_j $(j = 1, \ldots, N)$. With this ordering, the volume of S^N will be positive.

Next the directed area of any face of S^N must be defined — first, however, some additional notation. The symbol $\vec{e}$ will be formally treated as a column vector whose components are the unit vectors e_j $(j = 1, \ldots, N)$. If $r_1, \ldots, r_{N-1}$ are linearly independent, then the determinant $|r_1 \ldots r_{N-1}\ \vec{e}|$ is a vector. This is a generalization of the cross product of two vectors in 3-dimensional space. Indeed,

$$|r\ s\ \vec{e}| \equiv \begin{vmatrix} \rho_1 & \sigma_1 & e_1 \\ \rho_2 & \sigma_2 & e_2 \\ \rho_3 & \sigma_3 & e_3 \end{vmatrix}$$

$$= (\rho_2\sigma_3 - \rho_3\sigma_2)e_1 + (\rho_3\sigma_1 - \rho_1\sigma_3)e_2 + (\rho_1\sigma_2 - \rho_2\sigma_1)e_3 .$$

The inner product of the vector $|r_1 \ldots r_{N-1}\ \vec{e}|$ with any vector q is the value of the determinant $|r_1 \ldots r_{N-1}\ q|$. The latter vanishes if q is a linear combination of $r_1, \ldots, r_{N-1}$ and therefore the vector $|r_1 \ldots r_{N-1}\ \vec{e}|$ is orthogonal to each of the r_j $(j = 1, \ldots, N-1)$.

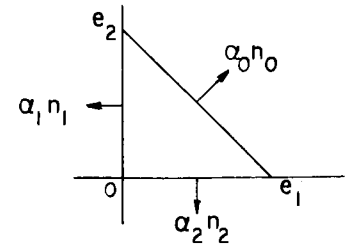
<u>Definition</u>. <u>If the vertices of S^N are treated in cyclic order so that $p_{j+N+1} \equiv p_j$, then the oriented area of the jth face is</u>

$$\alpha_j n_j = \frac{(-1)^{jN}}{(N-1)!} \left| p_{j+1} - p_{j+N},\ p_{j+2} - p_{j+N},\ \ldots,\ p_{j+N-1} - p_{j+N},\ \vec{e} \right| .$$

It is tedious, but not difficult, to verify that the areas of the faces of the unit simplex, as given by this definition are

$$\alpha_0 n_0 = \frac{1}{(N-1)!}(e_1 + e_2 + \dots + e_N) ,$$

$$\alpha_j n_j = \frac{-1}{(N-1)!} e_j, \qquad \text{for } j \neq 0 .$$



Using the continuous deformation argument again, it follows that the normals to the faces of S^N will be directed outward whenever the vertices are ordered in the manner already described.

The μth component of $\alpha_j n_j$ is

$$\alpha_j \eta_{\mu j} = \frac{(-1)^{jN}}{(N-1)!} \begin{vmatrix} p_{j+1} - p_{j+N} & \cdots & p_{j+N-1} - p_{j+N} & e_\mu \end{vmatrix} .$$

By applying μ-1 interchanges of adjacent rows, the μth row may be moved to the top, yielding

$$\alpha_j \eta_{\mu j} = \frac{(-1)^{jN+\mu-1}}{(N-1)!} \begin{vmatrix} \pi_{\mu,j+1} - \pi_{\mu,j+N} & \cdots & \pi_{\mu,j+N-1} - \pi_{\mu,j+N} & 1 \\ p'_{j+1} - p'_{j+N} & \cdots & p'_{j+N-1} - p'_{j+N} & 0 \end{vmatrix} ,$$

where primes denote that the vectors are of dimension N - 1 and are lacking a μth component. Let $\beta_{\nu j}$ ($j = 1, \dots, N$) be arbitrary scalars to be chosen later. Using the familiar rules for manipulating determinants,

$$(N-1)!\, \alpha_j \eta_{\mu j} \beta_{\nu j} = (-1)^{jN+\mu-1} \beta_{\nu j} \begin{vmatrix} 0 & \cdots & 0 & 1 \\ p'_{j+1} - p'_{j+N} & \cdots & p'_{j+N-1} - p'_{j+N} & 0 \end{vmatrix}$$

$$= (-1)^{jN+\mu-1} \beta_{\nu j} \begin{vmatrix} 1 & \cdots & 1 & 1 \\ p'_{j+1} & \cdots & p'_{j+N-1} & p'_{j+N} \end{vmatrix}$$

$$(N-1)!\ \alpha_j\ \eta_{\mu j}\ \beta_{\nu j} = (-1)^{jN+\mu-1} \begin{vmatrix} \beta_{\nu j} & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 1 & 1 \\ 0 & p'_{j+1} & \cdots & p'_{j+N-1} & p'_{j+N} \end{vmatrix}$$

$$= (-1)^{\mu-1} \begin{vmatrix} 0 & \cdots & 0 & \beta_{\nu j} & 0 & \cdots & 0 \\ 1 & \cdots & 1 & 0 & 1 & \cdots & 1 \\ p'_0 & \cdots & p'_{j-1} & 0 & p'_{j+1} & \cdots & p'_N \end{vmatrix} .$$

The last expression is obtained after jN interchanges of adjacent columns. Finally, summing over all j, the result is

$$(N-1)!\ \sum_{j=0}^{N} \alpha_j\ \eta_{\mu j}\ \beta_{\nu j} = (-1)^{\mu-1} \begin{vmatrix} \beta_{\nu 0} & \beta_{\nu 1} & \cdots & \beta_{\nu N} \\ 1 & 1 & \cdots & 1 \\ p'_0 & p'_1 & \cdots & p'_N \end{vmatrix} .$$

Lemma 6.1 follows directly from this result by setting $\beta_{\nu j} = 1$ for all j. To obtain Lemma 6.2, let

$$\beta_{\nu j} = -\ \pi_{\nu j} + \sum_{k=0}^{N} \pi_{\nu k} = N\ \gamma_{\nu j}$$

and then multiply the second row of the last determinant by $\sum_{k=0}^{N} \pi_{\nu k}$ and subtract from the first row. The result is

$$N!\ \sum_{j=0}^{N} \alpha_j\ \eta_{\mu j}\ \gamma_{\nu j} = (-1)^{\mu-1} \begin{vmatrix} -\pi_{\nu 0} & -\pi_{\nu 1} & \cdots & -\pi_{\nu N} \\ 1 & 1 & \cdots & 1 \\ p'_0 & p'_1 & \cdots & p'_N \end{vmatrix}$$

But if $\nu \neq \mu$, the determinant has two identical rows and, hence, vanishes. This proves part of Lemma 6.2. The remaining assertion may be obtained

from the last expression by multiplying the first row by -1 and then performing μ interchanges of adjacent rows. The resultant determinant is N! times the volume of S^N. This completes the proof of Lemmas 6.1 and 6.2.

Consider next an arbitrary polytope P^N which has been triangulated. Apply the previous lemmas to each simplex and then add. The two terms arising from an interior face common to two simplexes will cancel, since the areas are equal, but the normals are opposite. Hence, only the summation over exterior faces of the simplexes will remain. Let $S_{k,1}^{N-1}, \ldots, S_{k,r}^{N-1}$ be the faces which comprise P_k^{N-1}, the kth face of the polytope. The area, α_k, of P_k^{N-1} is

$$\alpha_k = \alpha_{k,1} + \ldots + \alpha_{k,r} ,$$

and the centroid, c_k, of P_k^{N-1} is the weighted mean of the centroids of the $S_{k,j}^{N-1}$. That is,

$$c_k = \frac{\alpha_{k,1} c_{k,1} + \ldots + \alpha_{k,r} c_{k,r}}{\alpha_k} .$$

Therefore, since the exterior normal to P_k^{N-1} is also the exterior normal for each $S_{k,j}^{N-1}$ $(j = 1, \ldots, r)$, the identities of Lemmas 6.1 and 6.2 are also true for arbitrary polytopes.

<u>Lemma</u> 6.3. <u>If</u> P^N <u>is an arbitrary polytope with faces</u> P_j^{N-1} $(j = 0, \ldots, M)$, <u>then</u>

$$\sum_{j=0}^{M} \alpha_j \eta_{\mu j} = 0 \qquad (\mu = 1, \ldots, N)$$

and

$$\sum_{j=0}^{M} \alpha_j \eta_{\mu j} \gamma_{\nu j} = \delta_{\mu\nu} \text{ (volume of } P^N) \qquad (\mu, \nu = 1, \ldots, N)$$

where α_j is the (unsigned) area of P_j^{N-1} and $\eta_{\mu j}$ and $\gamma_{\mu j}$ are the components of the exterior normal and the centroid, respectively, of P_j^{N-1}.

It is convenient in subsequent developments to define the $\gamma_{\nu j}$ to be the components of the vector $c_j - x_0$, where x_0 is some fixed reference vector in the polytope.

Corollary. Lemma 6.3 is also valid when the $\gamma_{\nu j}$ are the components of the position vector c_j relative to any fixed vector.

If x_0 and all the centroids c_j are interior points of R, then, with these lemmas, the proof of Theorem 6.1 requires only an application of the standard mean-value theorem for functions of several variables.

Before proceeding with the proof, however, it is desirable to call attention to the fact that it is not sufficient to prove the weaker theorem in which the polytope P^N is contained in the interior of the region R. For it is precisely to handle irregular boundaries that the polytopes have been introduced. It is therefore necessary to admit the possibility that c_j and x_0 may be points on the boundary of the region R beyond which there is no guarantee that f has continuous partial derivatives. In fact, the line joining them may lie in a face of P^N which forms part of the boundary of R. To admit these boundary situations the following extension of the mean-value theorem is used. A proof is given by Downing (1960).

Lemma 6.4. Let K be a convex, open set in E^N and let ψ be a

real-valued function of class C' over $\bar{K}$, the closure of K. Let x and y be distinct points of $\bar{K}$. Then there exists a point p on the open line segment joining x and y such that

$$\psi(y) = \psi(x) + \nabla\psi(p) \cdot (y - x) \quad .$$

The mention of both K and $\bar{K}$ insures that $\bar{K}$ is an N-dimensional body and not merely an (N-1) disc.

The Discrete Divergence Theorem

With these preliminary results, the proof of Theorem 6.1 is simple and direct. Since the components f_μ of the vector field f are of class C' over R, then the first partial derivatives of f_μ are, in fact, uniformly continuous over R. By definition, this means that for any $\epsilon' > 0$ there exists a $\delta > 0$ such that if ξ_ν is any coordinate, and if x and y are any two points in R, then

$$(6.1) \qquad |D_\nu f_\mu(x) - D_\nu f_\mu(y)| < \epsilon'$$

whenever $\|x - y\| < \delta$. By the extension of the mean-value theorem to closed, convex sets (Lemma 6.4)

$$(6.2) \qquad f_\mu(c_j) = f_\mu(x_0) + \sum_\nu \gamma_{\nu j} D_\nu f_\mu(x_0 + \lambda c_j - \lambda x_0) ,$$

where the $\gamma_{\nu j}$ are components of $c_j - x_0$ and where $0 < \lambda < 1$. Here, and subsequently, summations over μ and ν range from 1 to N. Summations over the faces of P^N have the range $j = 0, \ldots, M$. Because of the uniform

continuity of $D_\nu f_\mu$, equation (6.2) may be rewritten in the form

$$(6.3) \qquad f_\mu(c_j) = f_\mu(x_0) + \sum_\nu \gamma_{\nu j} [D_\nu f_\mu(x_0) + \epsilon'_{\mu\nu j}] ,$$

where

$$|\epsilon'_{\mu\nu j}| < \epsilon' .$$

By definition

$$\alpha_j n_j \cdot f = \sum_\mu \alpha_j \eta_{\mu j} f_\mu .$$

Hence, summing over j and applying equation (6.3), one obtains

$$\sum_j \alpha_j n_j \cdot f(c_j) = \sum_\mu f_\mu(x_0) \sum_j \alpha_j \eta_{\mu j} + \sum_\mu \sum_\nu D_\nu f_\mu \sum_j \alpha_j \eta_{\mu j} \gamma_{\nu j} + \kappa ,$$

where

$$\kappa = \sum_\mu \sum_\nu \sum_j \alpha_j \eta_{\mu j} \gamma_{\nu j} \epsilon'_{\mu\nu j} .$$

Applying Lemmas 6.1 and 6.2, this reduces to

$$(6.4) \qquad \sum_j \alpha_j n_j \cdot f(c_j) = (\text{vol. } P^N) \nabla \cdot f(x_0) + \kappa .$$

In estimating κ, note that

$$|\alpha_j \gamma_{\nu j}| \leq (\text{vol. } P^N) ,$$

for any choice of j and ν. Hence, estimating crudely

$$(6.5) \qquad |\kappa| < (\text{vol. } P^N) N^2 M_0 \epsilon' ,$$

where use has been made of the assumption that M is bounded by some M_0, which is at most a function of N. Since the dimension is fixed, it is evident, therefore, that given any $\epsilon > 0$, one may choose

$$\epsilon' = \epsilon/N^2(M_0 + 1) \quad . \tag{6.6}$$

And ϵ' determines δ. Hence, the conclusion of Theorem 6.1 follows by combining equations (6.4) and (6.6) with inequality (6.5).

Consider next a polytopic region (i.e., a closed, bounded polytope) that has been subdivided into a finite number of closed polytopes P_i^N $(i = 0, \ldots, n-1)$. The subdivision need not be a triangulation; however, the only subdivisions of interest in this paper are those which have the following property, which is also a property of any triangulation. The intersection $P_i^N \cap P_j^N$ is either the empty set or is some P^{N-r} $(1 \leq r \leq N)$ which is an (N-r)-face of P_i^N and of P_j^N.

Definition. A subdivision of a polytopic region R will be called an admissible subdivision if it has the property described in the preceding paragraph.

Definition. An admissible δ-subdivision of a polytopic region R is a collection of polytopes, denoted by $\Psi(\delta,R)$, which forms an admissible subdivision of R and has the following additional properties: Each $P_i^N \in \Psi(\delta,R)$

(i) has diameter less than δ,

(ii) is convex about some point x_i, and

(iii) has less than M_0 faces, where M_0 is independent of δ.

Theorem 6.2. Let R be any polytopic region and let f be a vector-valued function of class C' over R. Given any $\epsilon > 0$, then there

exists a $\delta > 0$ such that for any admissible δ-subdivision $\Psi(\delta,R)$, then

$$(6.7) \qquad \left| \sum_{\substack{\text{surface}\\ \text{of } R}} \alpha_j n_j \cdot f(c_j) - \sum_{i=0}^{n-1} (\text{vol. } P_i^N) \nabla \cdot f(x_i) \right| < (\text{vol. } R)\epsilon ,$$

where the second summation is over all P_i^N in $\Psi(\delta,R)$, and the first summation is over the faces P_j^{N-1} of $\Psi(\delta,R)$ which form the surface of R. The symbols α_j, n_j, and c_j denote the area, the exterior normal, and the centroid, respectively, of each P_j^{N-1}.

For any prescribed ϵ, let δ be determined so that Theorem 6.1 applies. For any $\Psi(\delta,R)$ let the area of the jth face of P_i^N be denoted by α_j^i, and similarly denote the exterior normal and centroid of P_i^N. Consider then the double summation

$$J = \sum_{i=0}^{n-1} \sum_j \alpha_j^i \, n_j^i \cdot f(c_j^i) .$$

For each interface, there will be two terms which will cancel because the exterior normals are oppositely directed. There remain, therefore, only terms involving the faces P_j^{N-1} which lie on the surface of R. Indeed, the union of these P_j^{N-1} is the surface of R. Hence

$$(6.8) \qquad J = \sum_{\substack{\text{surface}\\ \text{of } R}} \alpha_j \, n_j \cdot f(c_j) .$$

On the other hand, Theorem 6.1 provides the estimate

$$\left| J - \sum_{i=0}^{n-1} (\text{vol. } P_i^N) \nabla \cdot f(x_i) \right| < (\text{vol. } R)\epsilon .$$

The desired result is then obtained by substituting equation (6.8) into this estimate.

It might be recalled here that in Chapter 3 the subdivision into cubes had the property that two cubes intersected in at most one face. This is not necessarily the case for an arbitrary Ψ (δ,R).

Theorem 6.2 is a discrete analog of the divergence theorem.

Discrete Analogs of Green's Identities

Discrete analogs of Green's first and second identities may be obtained from Theorem 6.2 in precisely the same manner as the integral identities are derived from the divergence theorem. They are included here for completeness.

Theorem 6.3. *Let R be any polytopic region and let w and u be real-valued functions of class C' and $C^{(2)}$, respectively, over R. Then the conclusion of Theorem 6.2 holds for the inequality*

$$\left| \sum_{\substack{\text{surface}\\ \text{of } R}} \alpha_j \, w(c_j) \, n_j \cdot \nabla u(c_j) - \sum_{i=0}^{n-1} (\text{vol. } P_i^N)[w(x_i)\nabla^2 u(x_i) + \nabla w(x_i) \cdot \nabla u(x_i)] \right| < (\text{vol. } R)\epsilon \, . \tag{6.9}$$

This is obtained by setting $f = w\nabla u$. To obtain the second identity, let $w \in C^{(2)}$ over R and interchange the roles of u and w in relation (6.9). Combining the two relations, one obtains

$$\left| \sum_{\substack{\text{surface}\\ \text{of } R}} \alpha_j \, [w(c_j) \, n_j \cdot \nabla u(c_j) - u(c_j) \, n_j \cdot \nabla w(c_j)] - \sum_{i=0}^{n-1} (\text{vol. } P_i^N)[w(x_i)\nabla^2 u(x_i) - u(x_i)\nabla^2 w(x_i)] \right| < 2(\text{vol. } R)\epsilon \, . \tag{6.10}$$

Theorem 6.4. Let R be a polytopic region and let w and u be real-valued functions of class $C^{(2)}$ over R. Then the conclusion of Theorem 6.2 holds for inequality (6.10).

Chapter 7

FINITE DIFFERENCE ANALOGS FOR POLYTOPIC REGIONS

In this chapter finite difference theorems will be obtained which correspond to the discrete theorems of the previous chapter, but with an important difference. The error estimate obtained there, namely (vol R)ϵ, will be replaced by one which is proportional to the mesh size, h. To achieve this, a further restriction must be imposed upon the admissible subdivisions.

Well-Selected Subdivisions

In the class of all admissible δ-subdivisions, those which are nearly cubical are of special interest. For if the interior of a region is subdivided into cubes and the boundary layer into suitable polytopes, then the strict identities obtained in Chapter 3 will apply to the interior, and δ, ϵ results, analogous to those obtained in the previous chapter, will apply to the boundary layer. The volume of this layer, however, is clearly proportional to h, the mesh size. Hence, in the limit as h tends to zero, the errors introduced by the finite difference approximations will vanish. The term "nearly cubical" used above is roughly descriptive of a well-selected subdivision.

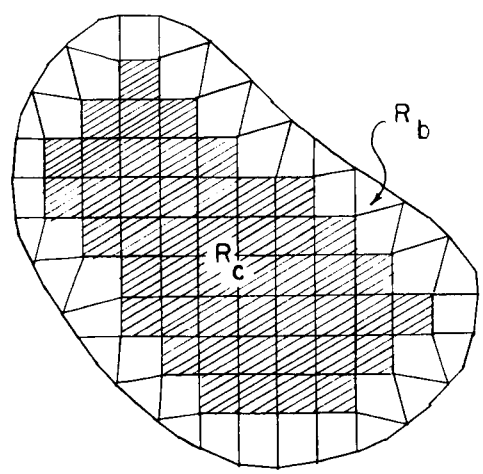
For any region R, a well-selected subdivision may be constructed as follows: Superimpose on R a uniform lattice of points with spacing h in each coordinate direction. Let each lattice point be the center of a cube with sides parallel to the coordinate axes and of length h. Approximate the region R by the union of those cubes associated with lattice points lying in R. Next, distort the cubes near the boundary of

R until the boundary of R is approximated by a suitable polyhedron, under the restrictions that the distorted cubes remain polytopes, that the number of faces remains invariant, and that the new subdivision is an admissible δ-subdivision in which each polytope is convex about its own lattice point. In general, δ will be larger than h but need not be more than a relatively small multiple of it. Indeed, for the sake of a concrete definition of a well-selected subdivision, it may be stipulated, without real restriction, that $\delta < 3h\sqrt{N}$, where N is the dimension of the space.

If R is a union of two or more regions, the same procedure is applicable with one exception. When a lattice point lies on an interface, it must be assigned, arbitrarily, to one and only one of the regions meeting at the interface. Cubes near the boundary and the interfaces may then be distorted as already described to obtain polyhedral approximations of these surfaces.

Well-selected subdivisions will be denoted by $\Psi(h,\delta,R)$.

Consider now a region R and a well-selected subdivision $\Psi(h,\delta,R)$. Let the polytopes of $\Psi(h,\delta,R)$ be grouped into a boundary region, R_b, and an interior region, R_c, such that the latter is a union of lattice cubes only. Let the surface of the polyhedrons approximating R, R_b, and R_c, respectively, be denoted by S, S_b, and S_c. The ratio S_c/S is certainly bounded from above for any fixed dimension N. Moreover, the thickness of the



boundary layer of polytopes will be a small multiple of δ for any particular region. Hence, for any fixed R, there exist constants k_1 and k_2 such that

$$S_c < k_1 S \tag{7.1}$$

$$(\text{volume of } R_b) < k_2 \delta S. \tag{7.2}$$

The Finite Difference Divergence Theorem

To apply Theorem 6.2 to a finite difference scheme over R_b, it is necessary to approximate the vector-valued function f at the centroids of the faces in terms of known values of f at the lattice points. Let the polytope containing the centroid c_j be convex about the lattice point x_i. The value of $f(c_j)$ may then be approximated by a linear combination — not necessarily unique — of the values

$$f(x_i) \quad \text{and} \quad f(x_i \pm h\, e_\mu)\,, \qquad (\mu = 1, \ldots, N)\,.$$

An acceptable approximation, $f^*(c_j)$, of $f(c_j)$ is given by any linear combination of the form

$$f^*(c_j) = \beta_0\, f(x_i) + \sum_{\mu=1} \left[\beta_\mu\, f(x_i + h\, e_\mu) + \beta'_\mu\, f(x_i - h\, e_\mu) \right]\,, \tag{7.3}$$

provided the β's satisfy the conditions

$$\left\{ \begin{aligned} &\beta_0 + \sum_{\mu=1}^{N} (\beta_\mu + \beta'_\mu) = 1\,, \\ &\sum_{\mu=1}^{N} (\beta_\mu - \beta'_\mu)\, h\, e_\mu = c_j - x_i\,, \\ &\sum_{\mu=1}^{N} (|\beta_\mu| + |\beta'_\mu|) h < 3\, n\, \delta\,. \end{aligned} \right. \tag{7.4}$$

The last condition ensures that the β's remain bounded. (If f were of class C'' it would be desirable to replace this condition by the conditions

$$\beta_\mu + \beta'_\mu = \gamma_\mu^2/h^2 \qquad (\mu = 1, \ldots, N) ,$$

where γ_μ is the μth component of $c_j - x_i$.) These conditions are sufficient because, by hypothesis, each component of f is of class C' and therefore, for any component, f_ν, of f, there exist numbers θ_ν, $\theta_{\mu\nu}$, and $\theta'_{\mu\nu}$ $(0 < \theta_\nu, \theta_{\mu\nu}, \theta'_{\mu\nu} < 1)$ such that

$$(7.5) \quad \begin{cases} f_\nu(c_j) = f_\nu(x_i) + (c_j - x_i) \cdot \nabla f_\nu(x_i + \theta_\nu(c_j - x_i)) \\ f_\nu(x_i + h\, e_\mu) = f_\nu(x_i) + h\, e_\mu \cdot \nabla f_\nu(x_i + \theta_{\mu\nu}\, h\, e_\mu) \\ f_\nu(x_i - h\, e_\mu) = f_\nu(x_i) - h\, e_\mu \cdot \nabla f_\nu(x_i - \theta'_{\mu\nu}\, h\, e_\mu) \end{cases}$$

for all $\mu = 1, 2, \ldots, N$. By direct substitution it follows that

$$\begin{aligned} f_\nu^*(c_j) &= \left[\beta_0 + \sum_{\mu=1}^{N} (\beta_\mu + \beta'_\mu)\right] f_\nu(x_i) \\ &\quad + \sum_{\mu=1}^{N} \beta_\mu\, h\, D_\mu\, f_\nu(x_i + \theta_{\mu\nu}\, h\, e_\mu) \\ &\quad - \sum_{\mu=1}^{N} \beta'_\mu\, h\, D_\mu\, f_\nu(x_i - \theta_{\mu\nu}\, h\, e_\mu) \\ &= f_\nu(c_j) + \kappa_\nu \end{aligned}$$

where

$$\kappa_\nu = \sum_{\mu=1}^{N} \beta_\mu h \left[D_\mu f_\nu(x_i + \theta_{\mu\nu} h e_\mu) - D_\mu f_\nu(x_i + \theta_\nu(c_j - x_i)) \right]$$

$$- \sum_{\mu=1}^{N} \beta'_\mu h \left[D_\mu f_\nu(x_i - \theta_{\mu\nu} h e_\mu) - D_\mu f_\nu(x_i + \theta_\nu(c_j - x_i)) \right] .$$

Since the diameter of the polytope is less than δ, inequality (6.1) may be used to estimate κ_ν. Indeed

$$|\kappa_\nu| < \sum_{\mu=1}^{N} (|\beta_\mu| + |\beta'_\mu|) h \epsilon' < 3 \epsilon' N \delta .$$

Since each component of $f(c_j)$ is approximated to within $3 \epsilon' N \delta$, it follows that

$$\|f(c_j) - f^*(c_j)\| < 3 \epsilon' N^{3/2} \delta .$$

Consequently, summing over all faces of R_b, one obtains

$$\left| \sum_{S_b} \alpha_j n_j \cdot [f(c_j) - f^*(c_j)] \right| < 3 \epsilon' N^{3/2} \delta S_b . \tag{7.6}$$

Likewise

$$\nabla^* \cdot f(x_i) = \sum_{\mu=1}^{N} \rho_\mu e_\mu \cdot \left[f(x_i + h e_\mu) - f(x_i) \right] + \sum_{\mu=1}^{N} \rho'_\mu e_\mu \cdot \left[f(x_i - h e_\mu) - f(x_i) \right] \tag{7.7}$$

is a satisfactory approximation for $\nabla \cdot f(x_i)$ provided the ρ's satisfy the conditions

$$(\rho_\mu - \rho'_\mu)h = 1 , \qquad (\mu = 1, \ldots, N)$$

(7.8)

$$\sum_{\mu=1}^{N} (|\rho_\mu| + |\rho'_\mu|)h < 3N.$$

Indeed,

$$\nabla^* \cdot f(x_i) = \sum_{\mu=1}^{N} \rho_\mu \left[f_\mu(x_i + h\, e_\mu) - f(x_i) \right]$$

$$+ \sum_{\mu=1}^{N} \rho'_\mu \left[f_\mu(x_i - h\, e_\mu) - f(x_i) \right] ,$$

or, after substitution from equations (7.5)

$$\nabla^* \cdot f(x_i) = \sum_{\mu=1}^{N} \rho_\mu\, h\, e_\mu \cdot \nabla f_\mu(x_i + \theta_{\mu\mu}\, h\, e_\mu)$$

$$- \sum_{\mu=1}^{N} \rho'_\mu\, h\, e_\mu \cdot \nabla f_\mu(x_i - \theta'_{\mu\mu}\, h\, e_\mu)$$

$$= \sum_{\mu=1}^{N} (\rho_\mu - \rho'_\mu)h\, D_\mu\, f_\mu(x_i)$$

$$+ \sum_{\mu=1}^{N} \rho_\mu\, h[D_\mu\, f_\mu(x_i + \theta_{\mu\mu}\, h\, e_\mu) - D_\mu\, f_\mu(x_i)]$$

$$- \sum_{\mu=1} \rho'_\mu\, h[D_\mu\, f_\mu(x_i - \theta'_{\mu\mu}\, h\, e_\mu) - D_\mu\, f_\mu(x_i)]$$

$$= \nabla \cdot f(x_i) + \kappa ,$$

where

$$|\kappa| < \sum_{\mu=1}^{N} (|\rho_\mu| + |\rho'_\mu|)h\,\epsilon' < 3\,N\,\epsilon' .$$

Therefore, after summing over all the polytopes, P_i^N, forming R_b, one obtains the inequality

$$(7.9) \qquad \left| \sum_{R_b} (\text{vol. } P_i^N)[\nabla \cdot f(x_i) - \nabla^* \cdot f(x_i)] \right| < (\text{vol. } R_b)\, 3\,\epsilon'\, N .$$

Combining inequalities (7.6) and (7.9) with the inequality of Theorem 6.2 yields

$$(7.10) \qquad \left| \sum_{S_b} \alpha_j\, n_j \cdot f^*(c_j) - \sum_{R_b} (\text{vol. } P_i^N)\, \nabla^* \cdot f(x_i) \right|$$

$$< (\text{vol. } R_b)\epsilon + (\text{vol. } R_b)\, 3\,\epsilon'\, N + 3\,\delta\, S_b\, \epsilon'\, N^{3/2} .$$

The relation between ϵ and ϵ', given in equation (6.6), is

$$\epsilon = N^2(2N + 1)\,\epsilon' .$$

The expression on the right-hand side of inequality (7.10) may be bounded from above by applying the simple properties of well-selected subdivisions given by relations (7.1) and (7.2). Indeed

$$(\text{vol. } R_b)(\epsilon + 3\,\epsilon'\, N) + 3\,\delta\, S_b\, \epsilon'\, N^{3/2} < \epsilon^*\, h\, S ,$$

where

$$\epsilon^* = (\delta/h)[(\epsilon + 3\,\epsilon'\, N)k_2 + 3\,\epsilon'\, N^{3/2}(1 + k_1)] .$$

It is convenient to summarize these results in the form of a lemma. Compare

Theorem 6.2.

Lemma 7.1. Let R be any polytopic region and let f be a vector-valued function with components of class C' over R. Given any $\epsilon^* > 0$, then there exists an $h > 0$ such that for any well-selected subdivision $\Psi(h,\delta,R)$, then

$$(7.11) \quad \left| \sum_{S_b} \alpha_j \, n_j \cdot f^*(c_j) - \sum_{R_b} (\text{vol. } P_i^N) \, \nabla^* \cdot f(x_i) \right| < \epsilon^* \, h \, S \, ,$$

where R_b is the collection of noncubical polytopes in $\Psi(h,\delta,R)$, S_b is the collection of exterior faces of R_b, and where $f^*(c_j)$ and $\nabla^* \cdot f(x_i)$ are finite difference approximations satisfying conditions (7.1) and (7.4).

The existence of a positive grid size satisfying this lemma is justified by the following argument: Given any R, then the dimension N is fixed and k_1 and k_2 may be determined. Therefore, for any ϵ^*, a corresponding ϵ' is determined. The existence of an $h > 0$ then follows by the hypothesis that each component of f has a continuous first differential.

This lemma can be combined with Theorem 3.6 which states a corresponding result for the cubical region R_c. The latter result is an identity which depends upon the use of a particular choice for the approximations $f^*(c_j)$ and $\nabla^* \cdot f(x_i)$. To convert the identity to the notation of this chapter, recall that for each cube r_i, the position vector of its center is x_i, and hence, the position vector of the centroid of the jth face of r_i, denoted by $c_j^{(i)}$, is $\frac{1}{2}(x_i + x_j)$. Moreover,

$$f^*(c_j^{(i)}) = \frac{1}{2}(f_{ij} + f_{ii}) = \frac{1}{2}[f(x_j) + f(x_i)]$$

because this is the interior of R. Thus, the coefficients β_0, β_μ, β'_μ are chosen to be

$$(7.12)\qquad \begin{cases} \beta_0 = \frac{1}{2} N; \\ \beta_\mu = \begin{cases} \frac{1}{2}, \text{ if } (x_j - x_i)/h = e_\mu, \\ 0, \text{ otherwise;} \end{cases} \\ \beta'_\mu = \begin{cases} \frac{1}{2}, \text{ if } (x_j - x_i)/h = -e_\mu, \\ 0, \text{ otherwise .} \end{cases} \end{cases}$$

The approximation for the divergence of f at x_i is

$$\nabla^* \cdot f(x_i) = \frac{1}{2} \sum_{j N i} \left(\frac{f_{ij} - f_{ii}}{h} \right) \cdot n_{ij}$$

$$= \sum_{j N i} \frac{1}{2h} n_{ij} \cdot [f(x_j) - f(x_i)]$$

and so

$$(7.13)\qquad \rho_\mu = \frac{1}{2h} = -\rho'_\mu . \qquad (\mu = 1, \ldots, N)$$

Let the particular approximations defined by equations (7.12) and (7.13), respectively, be denoted by $f^{**}(c_j)$ and $\nabla^{**} \cdot f(x_i)$. Then Theorem 3.6 states that

$$(7.14)\qquad \sum_{S_c} \alpha_j n_j \cdot f^{**}(c_j) - \sum_{R_c} (\text{vol. } P_i^N) \nabla^{**} \cdot f(x_i) = 0 .$$

Two approximations for $f(c_j)$ have been defined on the surface

between R_b and R_c. If the symbols S, S_b, and S_c are used, for the present, as oriented surfaces, then the portion of the surface of R_b in contact with R_c is given by $S_b - S = -S_c$. Thus, by simple manipulation

$$\sum_{S_b-S} \alpha_j n_j \cdot f^* + \sum_{S_c} \alpha_j n_j \cdot f^{**}$$

$$= \sum_{S_b-S} \alpha_j n_j \cdot f^* - \sum_{S_b-S} \alpha_j n_j \cdot f^{**}$$

$$= \sum_{S_b} \alpha_j n_j \cdot f^* - \sum_{S} \alpha_j n_j \cdot f^* - \sum_{S_b-S} \alpha_j n_j \cdot f^{**}$$

$$= \left[\sum_{S_b} \alpha_j n_j \cdot f^* - \sum_{R_b}(\text{vol. } P_i)\, \nabla^* \cdot f\right]$$

$$- \left[\sum_{S} \alpha_j n_j \cdot f^* + \sum_{S_b-S} \alpha_j n_j \cdot f^{**} - \sum_{R_b}(\text{vol. } P_i)\nabla^* \cdot f\right].$$

Lemma 7.1 applies to each term in square brackets, and hence

$$\left|\sum_{S_b-S} \alpha_j n_j \cdot f^* + \sum_{S_c} \alpha_j n_j \cdot f^{**}\right| < 2\,\epsilon^*\, h\, S. \tag{7.15}$$

In actual practice the probability is nearly one that the same approximation for $f(c_j)$ would be used on S_c and on $S_b - S$.

When combined with inequalities (7.10) and (7.11), Lemma 7.1 provides a proof of a finite difference analog of the divergence theorem which is applicable to arbitrary polyhedral regions.

<u>Theorem</u> 7.1. <u>Let</u> R <u>be any polytopic region and let</u> f <u>be a vector-valued function with components of class</u> C' <u>over</u> R. <u>Given any</u> $\epsilon^* > 0$,

then there exists a grid size $h > 0$ *such that for any well-selected subdivision* $\Psi(h,\delta,R)$, *and any choice of approximations* $f^*(c_j)$ *and* $\nabla^* \cdot f(x_i)$ *of the form* (7.3) *and* (7.7), *respectively, satisfying conditions* (7.4) *and* (7.8) *in* R_b, *then*

$$(7.16) \qquad \left| \sum_S \alpha_j n_j \cdot f^*(c_j) - \sum_{R_b} (\text{vol. } P_i^N) \nabla^* \cdot f(x_i) - \sum_{R_c} h^N \nabla^{**} \cdot f(x_i) \right| < \epsilon^* h S$$

where R_b *is the collection of noncubical polytopes in* $\Psi(h,\delta,R)$, *where* $R_c = R - R_b$, *and where* $\nabla^{**} \cdot f(x_i)$ *is defined by* (7.13) *and* (7.7).

Green's Identity

The procedure employed in the previous section can also be used to obtain a finite difference analog of Green's identity. Thus, the result in this section is based upon Theorem 6.3, the discrete version of Green's first identity, and upon Theorem 3.5 which applies to cubical regions. In applying Theorem 3.5, however, there is difficulty in approximating the normal derivative on the surface S, at least under the restriction that there be only 2N neighbors for each real lattice point. The resulting theorem is not as sharp as the one obtained in the previous section.

In the polytope P_i^N, which contains the lattice point x_i, suppose that $\nabla u(c_j)$ is approximated by the gradient of u at x_i, and suppose that $\nabla u(x_i)$, in turn, is approximated by a finite difference expression. That is, let the approximation for $\nabla u(c_j)$ be

$$\nabla^* u(c_j) \equiv \frac{1}{2h} \sum_{\nu=1}^{N} [u(x_i + h\, e_\nu) - u(x_i - h\, e_\nu)] e_\nu \ .$$

Since

$$\|\nabla u(c_j) - \nabla u(x_i)\| < \|c_j - x_i\| \max_{x \in R_b} \left(\max_{\mu,\nu} |D_{\mu\nu} u(x)| \right)$$

$$< \delta \max. |D_{\mu\nu} u|$$

$$< 3h\, N^{1/2} \max. |D_{\mu\nu} u|$$

and

$$\|\nabla u(x_i) - \nabla^* u(c_j)\| < N^{1/2} \frac{h}{2} \max. |D_{\nu\nu} u| \ ,$$

the error in approximating $\nabla u(c_j)$ may be estimated from

$$\|\nabla u(c_j) - \nabla^* u(x_i)\| < 4h\, N^{1/2} \max. |D_{\mu\nu} u| \ .$$

Combining this with Theorem 3.5, the resulting error estimate for the sum over the entire surface S_b is

$$4\, N^{1/2} (h\, S_b) \max. |D_{\mu\nu} u| \max. |w| \ .$$

To obtain a result corresponding to Lemma 7.1, error estimates for additional terms must be added to this expression. The expression above, however, is proportional to h S while Lemma 7.1 guarantees an error less than h S times some ϵ^*, which can be made as small as is desired by choosing h sufficiently small. Since the argument, in all respects, proceeds as in the previous section, the details are omitted here.

The choice for $\nabla^* u(c_j)$ on the surface of S need not be as restricted as given above. Indeed it is sufficient to choose

$$(7.17) \qquad \nabla^* u(c_j) = \sum_{\mu=1}^{N} e_\mu D_\mu^* u(c_j)$$

where

$$(7.18) \qquad D_\mu^* u(c_j) = \sum_{\nu=1}^{N} \sigma_{\mu\nu} [u(x_i + h e_\nu) - u(x_i)] + \sum_{\nu=1}^{N} \sigma'_{\mu\nu} [u(x_i - h e_\nu) - u(x_i)] ,$$

provided the σ's satisfy the conditions

$$(7.19) \qquad \begin{aligned} & h(\sigma_{\mu\nu} - \sigma'_{\mu\nu}) = \delta_{\mu\nu} \\ & \frac{1}{2} h^2 \sum_{\nu=1}^{N} (|\sigma_{\mu\nu}| + |\sigma'_{\mu\nu}|) < 3 \sum_{\nu=1}^{N} |(c_j - x_i) \cdot e_\nu|, \quad (\mu = 1, \ldots, N). \end{aligned}$$

The approximations for $\nabla u(x_i)$ and $\nabla w(x_i)$ in R_b will be of the same form, satisfying the same conditions.

In the cubical region R_c, the approximations for $\nabla u(x_i)$ and $\nabla w(x_i)$ must satisfy the conditions

$$(7.20) \qquad \sigma_{\mu\nu} = \frac{1}{2h} = -\sigma'_{\mu\nu} , \qquad (\mu,\nu = 1, \ldots, N).$$

There is no choice in the approximation for $\nabla^2 u(x_i)$. Everywhere in R, both in R_b and R_c, the approximation must be

$$(7.21) \qquad (\nabla^2)^* u(x_i) = \frac{1}{h^2} \sum_{\nu} [u(x_i + h e_\nu) - 2u(x_i) + u(x_i - h e_\nu)] .$$

<u>Theorem</u> 7.2. <u>Let</u> R <u>be any polytopic region and let</u> w <u>and</u> u <u>be real-valued functions of class</u> C' <u>and</u> $C^{(2)}$, <u>respectively, over</u> R. <u>If</u>

$\Psi(h,\delta,R)$ <u>is any well-selected subdivision, then</u>

$$\Bigg| \sum_S \alpha_j \, w(c_j) \, n_j \cdot \nabla^* u(c_j)$$

$$- \sum_{R_b} (\text{vol. } P_i^N)[w(x_i)(\nabla^2)^* \, u(x_i) + \nabla^* w(x_i) \cdot \nabla^* u(x_i)]$$

$$- \sum_{R_c} h^N [w(x_i)(\nabla^2)^* \, u(x_i) + \nabla^{**} \, w(x_i) \cdot \nabla^{**} \, u(x_i)] \Bigg| < h \, S \, B \, ,$$

<u>where</u> B <u>is proportional to the maximum of</u> $|D_{\mu\nu} \, u|$ <u>over</u> R_b, <u>and where the finite difference approximations satisfy the conditions given in the preceding paragraphs</u>.

A similar result holds for Green's second identity.

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