CUBATURE OF INTEGRANDS CONTAINING DERIVATIVES

J.N. LYNESS * AND U. RÜDE †

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Summary. We present a new technique for the numerical integration over $\mathcal{R}$, a square or triangle, of an integrand of the form $(\nabla u)^T B(\nabla v)$. This uses only function values of u, B, and v, avoiding explicit differentiation, but is suitable only when the integrand function is regular over $\mathcal{R}$. The technique is analogous to Romberg integration, since it is based on using a sequence of very simple discretizations $\mathrm{J}^{(m)}$, $m = 1, 2, 3, ...$, of the required integral and applying extrapolation in m to provide closer approximations. A general approach to the problem of constructing discretizations is given. We provide specific cost-effective discretizations satisfying familiar, but somewhat arbitrary guidelines. As in Romberg integration, when each component function in the integrand is a polynomial, this technique leads to an exact result.

Key words. Quadrature, Cubature, Numerical Differentiation, Two-Dimensional Integration, Richardson Extrapolation, Romberg Integration

AMS(MOS) subject classifications. 65B05, 65B15, 65D32

1. Introduction. The purpose of this article is to provide a numerical method for the evaluation of the two-dimensional integral

$$\int\int_{\mathcal{R}} (\nabla u)^T B(\nabla v)\, dxdy, \tag{1.1}$$

where $\mathcal{R}$ is either a parallelogram or a triangle and B is a 2×2 matrix of functions on $\mathcal{R}$. The method is effective in cases in which each of the constituent functions (from which the integrand is formed) is regular in and near $\mathcal{R}$. Using *finite difference* and *finite mean* operators (see, e.g., (3.5) or (3.6), below), we construct simple elementary discretizations $\mathrm{J}^{(m)}$ of (1.1) above. These discretizations use only function values of

$$u(\mathbf{x}), v(\mathbf{x}), \text{ and } b_{i,j}(\mathbf{x}), \quad i, j = 1, 2,$$

where abscissas $\mathbf{x} = (x, y) \in \mathbb{R}^2$, are located on grids fitted to $\mathcal{R}$ (see, for example, Figures 2.1, 2.2, and 4.1).

These discretizations are constructed in such a way that they enjoy an Euler-Maclaurin type expansion and so may be used in the context of extrapolation. This constitutes an application of Richardson's deferred approach to the limit [8] and a generalization of Romberg integration described in [9] and Bauer, Rutishauser, and Stiefel [1]. Specifically, it comprises a two-dimensional version of a method for calculating Stieltjes's integrals, as introduced by Lyness [4].

* Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439, USA. e-mail:lyness@mcs.anl.gov: This work was supported by the Mathematical, Information, and Computational Sciences Division subprogram of the Office of Computational and Technology Research, the U.S. Department of Energy, under Contract W-31-109-Eng-38.

† Institut für Mathematik, Universität Augsburg, D-86135 Augsburg, Germany, e-mail: ruede@math.uni-augsburg.de

The primary application of the results in this article is the evaluation of finite element stiffness matrices, which requires the computation of integrals of the form (1.1). The article thus presents a generalization of a prototype result of Rüde [10]. In this present article, however, both the underlying ideas and the detailed development provide the basis for the evaluation of similar integrals whose integrands may involve any specified mixture of functions and derivative functions of any order.

In the rest of this section, we discuss some preliminaries. In particular, we specify the coordinate system in which we develop the theory. In Section 2, we list some known results concerning minor generalizations of the Euler-Maclaurin expansion to numerical quadrature over squares and triangles. In Section 3, we provide the underlying theory and define a set of elementary discretizations $\mathrm{J}^{(m)}$ of (1.1), and in Section 4 we construct several special discretizations. While individually of only modest accuracy, these have the property that one may apply extrapolation to obtain successively better approximations. Finally, in Section 6, we illustrate the operation of some of these methods by means of a numerical example.

Our theory is restricted to the case in which $\mathcal{R}$ is a nondegenerate parallelogram $\square$ or a triangle $\triangle$. Without loss of generality, we assume that one vertex of $\mathcal{R}$ is located in the origin, so that the vertices of $\mathcal{R}$ are

$$\mathbf{0}, \mathbf{l}_1, \mathbf{l}_2, \text{ (and } \mathbf{l}_1 + \mathbf{l}_2 \text{ for the parallelogram)},$$

as illustrated in Figure 1.1.

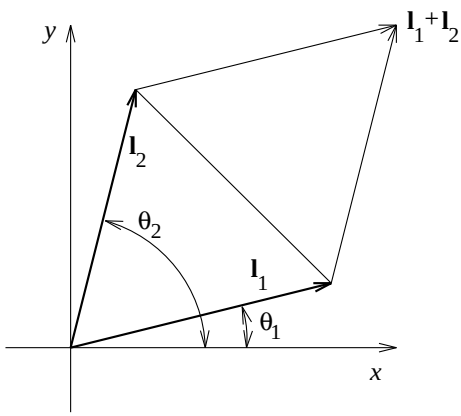

FIG. 1.1. *Basic parallelogram*

We define the unit vectors

$$n_i = \frac{1}{|\mathbf{l}_i|}\mathbf{l}_i = \begin{bmatrix} \cos\theta_i \\ \sin\theta_i \end{bmatrix} = \begin{bmatrix} c_i \\ s_i \end{bmatrix}, \quad \text{for } i = 1, 2,$$

and the directional derivatives satisfy

$$\frac{\partial}{\partial n_1} = c_1\frac{\partial}{\partial x} + s_1\frac{\partial}{\partial y}; \qquad \frac{\partial}{\partial n_2} = c_2\frac{\partial}{\partial x} + s_2\frac{\partial}{\partial y}.$$

Therefore, we can set

$$(\nabla u)^T B(\nabla u) = \left(\begin{bmatrix} \partial/\partial n_1 \\ \partial/\partial n_2 \end{bmatrix} u \right)^T A \begin{bmatrix} \partial/\partial n_1 \\ \partial/\partial n_2 \end{bmatrix} v,$$

where A is uniquely defined by

$$B = \begin{bmatrix} c_1 & c_2 \\ s_1 & s_2 \end{bmatrix} A \begin{bmatrix} c_1 & s_1 \\ c_2 & s_2 \end{bmatrix},$$

provided, of course, that $|\mathbf{l}_1 \times \mathbf{l}_2| \neq 0$, that is, the triangle or parallelogram is nondegenerate. It now remains to evaluate

$$\int\int_{\mathcal{R}} [\partial u/\partial n_1, \partial u/\partial n_2] \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} \partial v/\partial n_1 \\ \partial v/\partial n_2 \end{bmatrix} dxdy. \tag{1.2}$$

This comprises four terms. In most of the theory we shall treat each term separately. Thus we treat the numerical evaluation of

$$\mathrm{I}f_0 = \int\int_{\mathcal{R}} f_0(x,y)\, dxdy, \tag{1.3}$$

where

$$f_0(\mathbf{x}) = f_0(x,y) = \frac{\partial u}{\partial n_i}(\mathbf{x}) a_{ij}(\mathbf{x}) \frac{\partial v}{\partial n_j}(\mathbf{x}), \quad \text{for } i,j = 1,2. \tag{1.4}$$

We are looking for a discretization based on function values of a, u, and v.

2. Numerical Quadrature Error Expansions. In this section, we describe some of the underlying theory for using extrapolation integration over a parallelogram or triangle.

We denote the integral by

$$\mathrm{I}(\mathcal{R})\Phi := \int\int_{\mathcal{R}} \Phi\, dxdy \quad \text{for } \mathcal{R} = \square, \triangle.$$

For $\mathcal{R} = \square$, we restrict ourselves to quadrature rules of the form

$$\mathrm{Q}(\square)\Phi := \sum_{n=1}^{\nu} w_n \Phi(\mathbf{x}_n), \tag{2.1}$$

which integrate the constant function correctly. Thus

$$\sum_{n=1}^{\nu} w_n = \mathrm{A}(\square) = |\mathbf{l}_1 \times \mathbf{l}_2|, \tag{2.2}$$

where $\mathrm{A}(\mathcal{R})$ denotes the area of $\mathcal{R}$. For the parallelogram $\square$, the m^2-copy of (2.1) is obtained by subdividing $\square$ into m^2 congruent parallelograms and applying $\mathrm{Q}(\square)$ separately to each of its m^2 elements (see Figure 2.1). Thus

$$\mathrm{Q}^{(m)}(\square)\Phi := \sum_{n=1}^{\nu} \frac{w_n}{m^2} \sum_{k=0}^{m-1} \sum_{l=0}^{m-1} \Phi\left(\frac{1}{m}(\mathbf{x}_n + \mathbf{t}_{k,l}) \right), \tag{2.3}$$

where $\mathbf{t}_{k,l} = k\mathbf{l}_1 + l\mathbf{l}_2$.

The definition of an m^2-copy version of a rule for the triangle is marginally more complicated. We define

$$\begin{aligned} \mathrm{Q}^{(m)}(\triangle)\Phi \quad &:= \quad \sum_{n=1}^{\nu} \frac{w_n}{m^2} \sum_{k=0}^{m-1} \sum_{l=0}^{m-1-k} \Phi\left(\frac{1}{m}(\mathbf{x}_n + \mathbf{t}_{k,l})\right) \\ &+ \quad \sum_{n=1}^{\bar{\nu}} \frac{\bar{w}_n}{m^2} \sum_{k=0}^{m-2} \sum_{l=0}^{m-2-k} \Phi\left(\frac{1}{m}(\bar{\mathbf{x}}_n + \mathbf{t}_{k,l})\right). \end{aligned} \tag{2.4}$$

This assigns properly scaled versions of one rule to each member of one set of elementary triangles and a properly scaled version of another rule to each member of another set. The first set comprises the $m(m+1)/2$ triangles similarly situated to $\triangle$, and the second set the other $m(m-1)/2$ triangles. The corresponding rules are respectively one involving only w_n and $\mathbf{x}_n$ and one involving only $\bar{w}_n$ and $\bar{\mathbf{x}}_n$.

It is convenient to restrict these abscissas to satisfy

$$\sum_{n=1}^{\nu} w_n + \sum_{n=1}^{\bar{\nu}} \bar{w}_n = A(\square). \tag{2.5}$$

This restriction ensures that, for a constant integrand f,

$$\lim_{m \longrightarrow \infty} \mathrm{Q}^{(m)} f = \mathrm{I} f.$$

Note that $\mathrm{Q}^{(1)}(\triangle)$ does not require the second set of terms in (2.4), but that these are required for other values of m to define the m^2-copy version. A brief description of the geometry and of some of the associated theorems is given in Lyness and Cools [6]. An asymptotic error expansion of the quadrature rule (2.3) or (2.4) is given by the following generalization of the Euler-Maclaurin asymptotic expansion.

THEOREM 2.1. *Let $\mathrm{Q}^{(m)}$ be given by (2.3) or (2.4) and the abscissas satisfy (2.2) and (2.5), respectively; let all derivatives of Φ of total order p or less be integrable over $\mathcal{R}$. Then*

$$\mathrm{Q}^{(m)}(\mathcal{R})\Phi - \mathrm{I}(\mathcal{R})\Phi = \sum_{\sigma=1}^{p-1} \frac{\mathcal{B}_\sigma(\mathrm{Q}, \mathcal{R}, \Phi)}{m^\sigma} + \frac{C_p(\mathrm{Q}, \mathcal{R}, \Phi, m)}{m^p}, \tag{2.6}$$

where $\mathcal{B}_\sigma$ is independent of m and C_p satisfies the uniform bound

$$C_p(\mathrm{Q}, \mathcal{R}, \Phi, m) \leq \bar{C}_p(\mathcal{R}) \quad \textit{for all } m. \tag{2.7}$$

The nature of the coefficients $\mathcal{B}_\sigma$ in this expansion is discussed in many places, including Lyness [5]. A detailed integral representation of the remainder term is given in Lyness and McHugh [7].

The following definitions are minor variants of standard definitions.

DEFINITION 2.2.

1. *The set of rules* $\mathrm{Q}^{(m)}(\mathcal{R})$ *is termed to be of* **polynomial degree** d *when every member of the set integrates all polynomials of degree* d *correctly.*
2. *The set of rules* $\mathrm{Q}^{(m)}(\mathcal{R})$ *is termed* **centrally symmetric** *when, for all* m,

$$\mathrm{Q}^{(m)}(\mathcal{R})\Phi = \mathrm{Q}^{(m)}(\mathcal{R})\Psi \text{ whenever } \Phi(\mathbf{x}) = \Psi(\mathbf{l}_1 + \mathbf{l}_2 - \mathbf{x})$$

for all $\mathbf{x} \in \mathcal{R}$.

When $\mathcal{R} = \square$, only one value of m is required to verify these properties. When $\mathcal{R} = \triangle$, two distinct values are required.

The reader may verify that, following Definition 2.2, the rules in (2.4) are centrally symmetric if $\nu = \bar{\nu}$, $w_n = \bar{w}_n$, and $x_n + \bar{x}_n = \mathbf{l}_1 + \mathbf{l}_2$ for all $n = 1, 2, \ldots, \nu$; moreover, all centrally symmetric rules may be expressed in a form satisfying these conditions.

We collect several known results in the following:

THEOREM 2.3. *Under the hypothesis of Theorem 2.1:*

1. *When* $\mathrm{Q}^{(m)}(\mathcal{R})$ *is centrally symmetric,* $\mathcal{B}_\sigma(\mathrm{Q}, \mathcal{R}, \Phi) = 0$ *for all* σ *odd.*
2. *When* $\mathrm{Q}^{(m)}(\mathcal{R})$ *is a rule of polynomial degree* d, $\mathcal{B}_\sigma(\mathrm{Q}, \mathcal{R}, \Phi) = 0$ *for* $\sigma = 1, 2, \ldots, d$.
3. *When* $\Phi(x, y)$ *is a polynomial of degree* d, $\mathcal{B}_\sigma(\mathrm{Q}, \square, \Phi) = 0$ *for* $\sigma > d$ *and* $\mathcal{B}_\sigma(\mathrm{Q}, \triangle, \Phi) = 0$ *for* $\sigma > d + 1$.

When $\mathcal{R}$ is the parallelogram $\square$, the definition of central symmetry is obvious. However, when $\mathcal{R}$ is the triangle $\triangle$, central symmetry relates the second set of terms in (2.4) with the first. It reduces to central symmetry about the midpoint of any edge of an elementary triangle. This property is related to the vanishing of the odd terms in the Euler-Maclaurin expansion. The rules illustrated in Figure 2.2 below are all centrally symmetric under this definition.

The theory above is wider than we need for immediate applications. For $\square$, we use only the *center* rule

$$\mathrm{Q}^{(m)}(\square)\Phi = \frac{\mathrm{A}(\square)}{m^2} \sum_{k=0}^{m-1} \sum_{l=0}^{m-1} \Phi\left(\frac{\mathbf{u}_{k,l}}{m}\right). \tag{2.8}$$

Here

$$\mathbf{u}_{k,l} = (k + 1/2)\mathbf{l}_1 + (l + 1/2)\mathbf{l}_2. \tag{2.9}$$

The points $\mathbf{x} = \frac{1}{m}\mathbf{u}_{k,l}, k, l = 0, 1, \ldots, m-1$, form the *center grid,* which is illustrated in Figure 2.1. The *vertex grid* consisting of $\mathbf{x} = \frac{1}{m}\mathbf{t}_{k,l}, k, l = 0, 1, \ldots, m$, is illustrated in Figure 4.1.

For the triangle, we employ three rules. The first is an adaption of the center rule (2.8) to the triangle:

$$\mathrm{Q}^{(m)}(\triangle)\Phi = \frac{\mathrm{A}(\square)}{m^2} \sum_{k,l=0}^{m-1} \theta_{m-k-l-1} \Phi\left(\frac{\mathbf{u}_{k,l}}{m}\right), \tag{2.10}$$

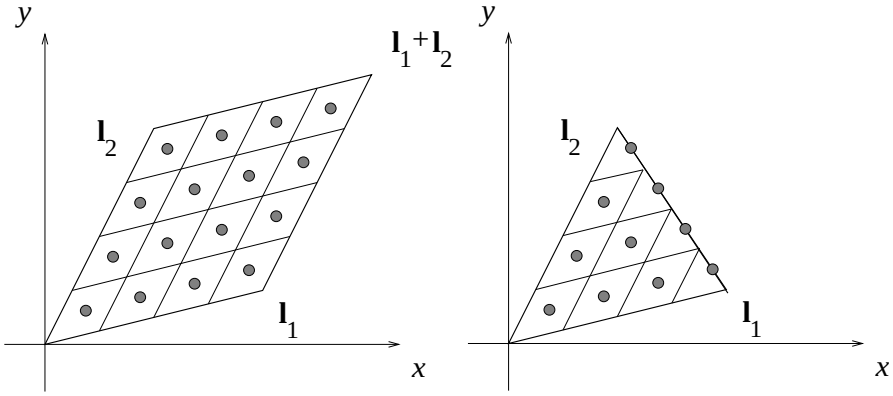

FIG. 2.1. *Center grid for* $\square$ *and* $\triangle$. *The points are abscissas used in (2.8) and (2.10), respectively.*

where

$$\theta_\mu = \begin{cases} 0 & \text{for} \quad \mu < 0 \\ 1/2 & \text{for} \quad \mu = 0 \\ 1 & \text{for} \quad \mu > 0 \end{cases} \tag{2.11}$$

is the Heaviside step function. This function is used here to eliminate points required in (2.8) that are outside the triangle $\triangle$ and to assign a factor of $1/2$ to those that lie on the boundary. (The upper limits of the summation over l and k may formally be replaced by ∞.) This rule assigns a function value to the midpoint of one of the three edges of each of the elementary triangles.

We shall also employ two rules that are effectively variants of this one; they assign the function value to the other two edges, respectively. These are

$$\mathrm{Q}^{(m)}(\triangle)\Phi = \frac{\mathrm{A}(\square)}{m^2} \sum_{k=0}^{m-1} \sum_{l=0}^{m-1-k} \theta_l \Phi \left(\frac{(k+\frac{1}{2})\mathbf{l}_1 + l\,\mathbf{l}_2}{m} \right) \tag{2.12}$$

and

$$\mathrm{Q}^{(m)}(\triangle)\Phi = \frac{\mathrm{A}(\square)}{m^2} \sum_{k=0}^{m-1} \sum_{l=0}^{m-1-k} \theta_k \Phi \left(\frac{(k\,\mathbf{l}_1 + (l+\frac{1}{2})\,\mathbf{l}_2}{m} \right). \tag{2.13}$$

These three rules, illustrated in Figure 2.2, are all of the form (2.4) and are all centrally symmetric.

3. Simple Integrand Discretizations and a Set of Elementary Integral Discretizations. In this section we return to the treatment of

$$\mathrm{I}f_0 = \int\int_{\mathcal{R}} f_0(x,y)\, dxdy,$$

where the integrand is given by

$$f_0(\mathbf{x}) = \frac{\partial u}{\partial n_i}(\mathbf{x}) a(\mathbf{x}) \frac{\partial v}{\partial n_j}(\mathbf{x}). \tag{3.1}$$

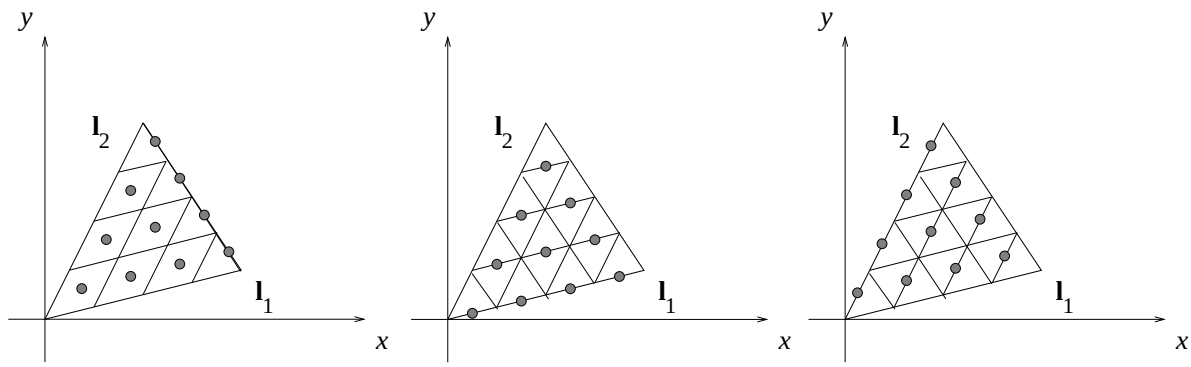

FIG. 2.2. *The abscissas used by quadrature rules (2.10), (2.12), and (2.13) for $m = 4$. These rules are affine transformations of one another.*

This integrand may be approximated by

$$F(\mathbf{x}, h) = \frac{1}{h^2}\left(u(\mathbf{x} + \mathbf{l}_i h) - u(\mathbf{x})\right) a(\mathbf{x}) \left(u(\mathbf{x} + \mathbf{l}_j h) - u(\mathbf{x})\right) \tag{3.2}$$

or many other expressions of similar form.

DEFINITION 3.1. *A* **simple discretization** $F(\mathbf{x}, h)$ *of* $f_0(\mathbf{x})$ *is a functional depending on u, v, and a in the form*

$$F(\mathbf{x}, h) = \sum_{\nu=1}^{\kappa} \frac{\rho_\nu}{h^2} u(\mathbf{x} + h\xi_\nu) a(\mathbf{x} + h\eta_\nu) v(\mathbf{x} + h\zeta_\nu), \tag{3.3}$$

where for $\nu = 1, \ldots, \kappa$ all of $\xi_\nu, \eta_\nu, \zeta_\nu \in \mathbb{R}^2$ are fixed vectors and $\rho_\nu \in \mathbb{R}$ are fixed numbers and where

$$\lim_{h \to 0} F(\mathbf{x}, h) = f_0(\mathbf{x}), \tag{3.4}$$

for all points $\mathbf{x}$ *and all functions u, v, and a for which the limit exists.*

The reader may verify that $F(\mathbf{x}, h)$ in (3.2) satisfies both (3.3) and (3.4). Additional simple discretizations appear in (3.9), (3.10), and (3.12), below.

In the remainder of this paper, we shall mainly consider *symmetric* simple discretizations. These satisfy $F(\mathbf{x}, h) = F(\mathbf{x}, -h)$. To define these, we use standard notation for mean and difference operators. Thus, for a general vector $\mathbf{p}$ and a function $g(\mathbf{x})$, we define

$$\mu(\mathbf{p}) g(\mathbf{x}) := \frac{1}{2}\left(g(\mathbf{x} + \mathbf{p}) + g(\mathbf{x} - \mathbf{p})\right) \tag{3.5}$$

and

$$\delta(\mathbf{p}) g(\mathbf{x}) := g(\mathbf{x} + \mathbf{p}) - g(\mathbf{x} - \mathbf{p}). \tag{3.6}$$

Where no confusion is likely to arise, we may suppress h, $\mathbf{l}_i$, and $\mathbf{x}$ and employ an abbreviated notation as follows:

$$\mathrm{M}_i a := \mu(h\mathbf{l}_i) a(\mathbf{x}) = \frac{a(\mathbf{x} + h\mathbf{l}_i) + a(\mathbf{x} - h\mathbf{l}_i)}{2}, \tag{3.7}$$

which is an approximation to $a(\mathbf{x})$, and

$$\mathrm{D}_i u := \frac{1}{2h|\mathbf{l}_i|}\delta(h\mathbf{l}_i)u(\mathbf{x}), \tag{3.8}$$

which is an approximation to $\partial u/\partial n_i$. Naturally, $\mathrm{D}_i\mathrm{M}_j u$ is also an approximation to $\partial u/\partial n_i$, and $\mathrm{M}_i\mathrm{M}_j a$ is also an approximation to a. We note that all these approximations depend on h, and for sufficiently smooth functions the approximation error is even in h.

There are many simple discretizations of $f_0(\mathbf{x})$ in (3.1) above. For example, when $i = 1$ and $j = 2$, the simplest symmetric discretization can be written in our abbreviated notation as

$$F(\mathbf{x}, h) = (\mathrm{D}_1 u)\, a\, (\mathrm{D}_2 v)\,, \tag{3.9}$$

and another simple discretization is

$$\begin{aligned} F(\mathbf{x}, h) &= \frac{1}{4h^2|\mathbf{l}_1||\mathbf{l}_2|}\,(\delta(h\mathbf{l}_1)\mu(h\mathbf{l}_2)u(\mathbf{x}))\ a(\mathbf{x})\ (\delta(h\mathbf{l}_2)\mu(h\mathbf{l}_1)v(\mathbf{x})) \\ &= (\mathrm{D}_1\mathrm{M}_2 u)\, a\, (\mathrm{D}_2\mathrm{M}_1 v)\,. \end{aligned} \tag{3.10}$$

Still another discretization of (3.1) is obtained when $a(\mathbf{x})$ in (3.10) is replaced by

$$\mu(h\mathbf{l}_1)\mu(h\mathbf{l}_2)a(\mathbf{x}). \tag{3.11}$$

In the abbreviated notation the latter function is written

$$F(\mathbf{x}, h) = (\mathrm{D}_1\mathrm{M}_2 u)\,(\mathrm{M}_1\mathrm{M}_2 a)\,(\mathrm{D}_2\mathrm{M}_1 v)\,. \tag{3.12}$$

All of these functions can be evaluated for nonzero h and reduce to $f_0(\mathbf{x})$ when h tends to zero.

In the following we shall use the standard definition of an ϵ-neighborhood of $\mathcal{R}$, namely,

$$\mathcal{R}_\epsilon = \{\mathbf{x} \in \mathbb{R}^2 |\ \exists \mathbf{y} \in \mathcal{R} : ||\mathbf{x} - \mathbf{y}|| < \epsilon\},$$

where $||\cdot||$ denotes the Euclidean norm, and we denote by $\mathcal{C}^p(\mathcal{R}_\epsilon)$ the space of p times continuously differentiable functions on $\mathcal{R}_\epsilon$.

THEOREM 3.2. *Let the components of $f_0(x)$ satisfy*

$$a(\mathbf{x}) \in \mathcal{C}^{p'}(\mathcal{R}_\epsilon), u(\mathbf{x}) \in \mathcal{C}^{p+1}(\mathcal{R}_\epsilon), v(\mathbf{x}) \in \mathcal{C}^{p+1}(\mathcal{R}_\epsilon), \tag{3.13}$$

where $p' = p + 1$ for some $\epsilon > 0$ and some integer $p > 0$, and let $F(\mathbf{x}, h)$ be a simple discretization of $f_0(\mathbf{x})$. Then there exists $h_0 > 0$ such that, for all h satisfying $|h| < h_0$,

$$F(\mathbf{x}, h) = f_0(\mathbf{x}) + hf_1(\mathbf{x}) + \cdots + h^{p-1}f_{p-1}(\mathbf{x}) + h^p G_p(\mathbf{x}, h), \tag{3.14}$$

where

$$f_j(\mathbf{x}) = \frac{\dfrac{\partial^j}{\partial h^j} F(\mathbf{x}, h)|_{h=0}}{(j-1)!} \in \mathcal{C}^{p-j}(\mathcal{R}) \tag{3.15}$$

and where the remainder term has a finite bound of form

$$G_p(\mathbf{x}, h) < \bar{G}_p, \text{ for all } \mathbf{x} \in \mathcal{R}. \tag{3.16}$$

Proof. This theorem follows directly from the definition of simple discretizations and applying Taylor expansions to the component functions. □

In all the cases considered in this article, the conditions attached to $f_0(\mathbf{x})$ in this theorem are too stringent. We call $F(\mathbf{x}, h)$ factorizable when

$$F(\mathbf{x}, h) = \phi_1(\mathbf{x}, h)\phi_2(\mathbf{x}, h),$$

where $\phi_1(x)$ is a discretization for $a(\mathbf{x})$ and where $\phi_2(x)$ is a discretization for $\frac{\partial u}{\partial n_i}\frac{\partial v}{\partial n_j}$. Theorem 3.2 is valid with $p' = p$ under the additional hypothesis that $F(\mathbf{x}, h)$ is factorizable or may be expressed as the sum of factorizable components. Examples of non-factorizable simple discretizations do not seem to occur naturally, but they are readily contrived. When $F(\mathbf{x}, h)$ is any factorizable simple discretization, then

$$\tilde{F}(\mathbf{x}, h) = F(\mathbf{x}, h) + hD_1(a)D_1(u)D_2(v)$$

is of the form (3.3), and the specification $p' = p + 1$ is required to validate Theorem 3.2.

We now define the principal new concept in this paper.

DEFINITION 3.3. *Let $\mathrm{Q}^{(m)}(\mathcal{R})$ be any integration rule of form (2.3) or (2.4) above. Let $F(\mathbf{x}, h)$ be a simple discretiation of $f_0(\mathbf{x})$ as in Definition 3.1. Let λ be a fixed nonzero parameter. Then the set of quantities*

$$\mathrm{J}^{(m)} = \mathrm{Q}^{(m)}(\mathcal{R})F(\mathbf{x}, \lambda/m), \quad \textit{for } m = 1, 2, 3, \cdots$$

is called a **set of elementary discretizations of** $\mathrm{I}f_0(\mathbf{x})$.

Since $\mathrm{Q}^{(m)}(\mathcal{R})$ is simply a sum of function values of F, and each such function value has the form described in (3.3) above, it follows that $\mathrm{J}^{(m)}$ is also a weighted sum of function values of the form (3.3). $\mathrm{J}^{(m)}$ may be evaluated once one has available

1) a specification of rule $\mathrm{Q}(\mathcal{R})$;
2) a specification of $F(\mathbf{x}, h)$, which requires $u(\mathbf{x})$, $\mathrm{a}(\mathbf{x})$, and $v(\mathbf{x})$ to be specified individually; and
3) a specification of the parameter λ.

We come now to the fundamental theorem of this paper. All the results and methods described later in this paper are based on the following.

THEOREM 3.4. *Let $f_0(\mathbf{x})$ satisfy the conditions (3.13) given in Theorem 3.2. Let $F(\mathbf{x}, h)$ be a simple discretization of $f_0(\mathbf{x})$, and let $\mathrm{J}^{(m)}$ be the set of elementary discretizations defined in Definition 3.3.*

Then for a positive integer m

$$\mathrm{J}^{(m)} = \mathrm{I}f_0 + \sum_{q=1}^{p-1} \frac{D_q}{m^q} + \frac{E_p(m)}{m^p}, \tag{3.17}$$

where the constants D_q are independent of m and the remainder term $E_p(m)$ is uniformly bounded.

Proof. Let h_0 be defined as in Theorem 3.2. The expansion (3.17) is valid for $h < h_0$; hence trivially,

$$\mathrm{Q}^{(m)}(\mathcal{R})F(\mathbf{x}, h) = \sum_{k=0}^{p-1} \mathrm{Q}^{(m)}(\mathcal{R})f_k(\mathbf{x})h^k + \mathrm{Q}^{(m)}(\mathcal{R})G_p(\mathbf{x}, h)h^p. \tag{3.18}$$

But, since $f_k(\mathbf{x}) \in \mathcal{C}^{p-k}(\mathcal{R})$, we may apply the result of Theorem 2.1 to each term with p replaced with $p-k$; specifically,

$$\mathrm{Q}^{(m)}(\mathcal{R})f_k(\mathbf{x}) = \sum_{\sigma=0}^{p-1-k} \frac{\mathcal{B}_\sigma(\mathrm{Q}, \mathcal{R}, f_k)}{m^\sigma} + \frac{C_{p-k}(\mathrm{Q}, \mathcal{R}, f_k, m)}{m^{p-k}}. \tag{3.19}$$

Substituting (3.19) into (3.18), treating h and $1/m$ as terms of the same order, and assembling terms of the same order, we find

$$\begin{aligned} \mathrm{Q}^{(m)}(\mathcal{R})F(\mathbf{x}, h) &= \sum_{l=0}^{p-1} \left(\sum_{k+\sigma=l, k, \sigma \geq 0} \frac{\mathcal{B}_\sigma(\mathrm{Q}, \mathcal{R}, f_k)h^k}{m^\sigma} \right) \\ &+ \sum_{k=0}^{p-1} \frac{C_{p-k}(\mathrm{Q}, \mathcal{R}, f_k, m)h^k}{m^{p-k}} + \mathrm{Q}^{(m)}(\mathcal{R})G_p(\mathbf{x}, h)h^p. \end{aligned} \tag{3.20}$$

Finally, we set $h = \lambda/m$, where $\lambda \neq 0$. This reduces to

$$\mathrm{J}^{(m)} = \mathrm{I}f_0 + \sum_{l=0}^{p-1} \frac{D_l}{m^l} + \frac{E_p(m)}{m^p},$$

where

$$D_l = \sum_{k=0}^{l} \mathcal{B}_{l-k}(\mathrm{Q}, \mathcal{R}, f_k)\lambda^k \tag{3.21}$$

and

$$|E_p(m)| \leq \sum_{k=0}^{p-1} \bar{C}_{p-k,k}\lambda^k + \bar{G}_p\lambda^p.$$

Here $\bar{C}_{p-k,k}$ and $\bar{G}_p$ are bounds given by (2.7) and (3.16) to the corresponding term in (3.20) above. □

When $\mathcal{R} = \square$, an integral representation for each term of $\mathcal{B}_\sigma$ in (3.19) may be constructed by using (3.15) above. Corresponding integral representations also exist when $\mathcal{R} = \triangle$, but their structure is much more complicated. One of the advantages of the method based on this theory is that the knowledge of explicit representations of $\mathcal{B}_\sigma$ is not needed.

THEOREM 3.5. *Under the hypothesis of Theorem 3.4, if both $F(\mathbf{x},h)$ is even in h and $\mathrm{Q}(\mathcal{R})$ is centrally symmetric, then the expansion (3.17) is even in m^{-1}.*

Proof. When $\mathrm{Q}(\mathcal{R})$ is centrally symmetric, it follows from Theorem 2.3 that

$$\mathcal{B}_\sigma(\mathrm{Q}, \mathcal{R}, f_k) = 0 \quad \text{for all } \sigma \text{ odd;}$$

and when $F(\mathbf{x}, h)$ is even, then its Taylor expansion (3.14) is even, giving

$$f_k(\mathbf{x}) = 0 \quad \text{for all } k \text{ odd.}$$

In (3.21) we note that when l is odd, one of k and $l-k$ is odd, giving $D_l = 0$, establishing the result. $\square$

An interesting situation occurs in the case where $a(\mathbf{x})$, $u(\mathbf{x})$, and $v(\mathbf{x})$ are polynomials such that the integrand f_0 is itself a polynomial of degree d. An immediate consequence of (3.3) and (3.4) is that the coefficient functions $f_j(\mathbf{x})$ in (3.15) in the Taylor expansion (3.14) of $F(\mathbf{x}, h)$ now become polynomials of degree $d-j$ when $j \le d$ and vanish when $j > d$. It follows from Part 1 of Theorem 2.3 that

$$\mathcal{B}_\sigma(\mathrm{Q}, \square, f_j) = 0 \quad \text{for } \sigma > d-j \quad \text{and} \quad \mathcal{B}_\sigma(\mathrm{Q}, \triangle, f_j) = 0 \quad \text{for } \sigma > d-j+1.$$

Applying this in (3.21) gives the following theorem.

THEOREM 3.6. *Let $a(\mathbf{x})$, $u(\mathbf{x})$, and $v(\mathbf{x})$ be polynomials such that $f_0(\mathbf{x})$ is a polynomial of degree d. Then, under the hypothesis of Theorem 3.4, the expansion (3.17) is finite, the final nonzero term being D_δ, where $\delta = d$ when $\mathcal{R} = \square$ and $\delta = d+1$ when $\mathcal{R} = \triangle$.*

4. Suitable Discretizations. In the preceding section we defined an elementary discretization $\mathrm{J}^{(m)}$ in some generality. This allowed an almost arbitrary choice for quadrature rule Q, many choices for the simple discretization $F(\mathbf{x}, h)$ (some of which have been mentioned), and any positive number for the incidental parameter λ. Naturally, it is possible to construct $\mathrm{J}^{(m)}$ by making these choices arbitrarily. The resulting $\mathrm{J}^{(m)}$ would have the expected asymptotic expansion in $1/m$ but might be unduly uneconomic in the number of function values required. For example, the use of (3.12) for $F(\mathbf{x}, h)$ requires four function values of each of u, a and v, located at points $\mathbf{x} \pm h\mathbf{l}_1 \pm h\mathbf{l}_2$. These values would be needed for each abscissa $\mathbf{x}$ required by the quadrature rule $\mathrm{Q}^{(m)}$.

Just as in standard quadrature rule design, the discretization $\mathrm{J}^{(m)}$ may be constructed to reduce the overall number of function values it requires. The reader will be familiar with the concept of economizing using point sharing. Here, if we choose $\mathrm{Q}^{(m)}$ to be either the product trapezoidal rule or the midpoint rule, and choose $\lambda = 1/2$, we find a situation in which nearly all the points mentioned above are shared, resulting in asymptotically only one function value of each constituent function per abscissa. This

would leave some points outside the region $\mathcal{R}$. When $\mathcal{R}$ is the parallelogram $\square$, this can be rectified by replacing the product trapezoidal rule by the center rule (2.8). It is less obvious how to do this and use only interior points in the case of the triangle.

This section is devoted to the construction of cost-effective self-contained discretizations. To this end we list three traditional guidelines.

(G1) The discretization $\mathrm{J}^{(m)}$ should require only $m^2 + O(m)$ function values of a, u, and v. In the limit this is only one function value per cell.

(G2) $\mathrm{J}^{(m)}$ should have an even expansion in m^{-1}.

(G3) The discretization $\mathrm{J}^{(m)}$ should be *self-contained* with respect to $\mathcal{R}$; that is, it should require function values only within the closure of $\mathcal{R}$.

We do not wish to imply that these are critical, or even desirable, properties in all applications. However, there are contexts in which these properties are desirable. The rest of this section briefly treats the simple discretizations (outlined above) for the parallelogram and then takes up the somewhat involved question of how to satisfy these guidelines in the case of the triangle.

4.1. Discretizations for $\square$.

Discretization 1. In this subsection we return to our original definition of $f_0(\mathbf{x})$, embracing all four components. One of the simplest discretizations for

$$\mathrm{I}f_0(\mathbf{x}) = \int\int_{\square} \sum_{i,j=1}^{2} \frac{\partial u}{\partial n_i} a_{i,j}(\mathbf{x}) \frac{\partial v}{\partial n_j}\, dxdy \tag{4.1}$$

may be obtained by using the center rule (2.8) and the simple discretization (3.10) in each of the four components and with $h = 1/2m$. Specifically, we employ

$$\mathrm{Q}^{(m)}(\square)\Phi = \frac{\mathrm{A}(\square)}{m^2} \sum_{k=0}^{m-1} \sum_{l=0}^{m-1} \Phi\left(\frac{\mathbf{u}_{k,l}}{m}\right) \tag{4.2}$$

and

$$F(\mathbf{x}, h) = \sum_{i,j=1}^{2} \left(\mathrm{D}_i \mathrm{M}_{3-i} u\right) a_{ij} \left(\mathrm{D}_j \mathrm{M}_{3-j} v\right) \tag{4.3}$$

to find

$$\begin{aligned} \mathrm{J}^{(m)} &= \mathrm{Q}^{(m)}(\square) F\left(\mathbf{x}, \frac{1}{2m}\right) \\ &= \sum_{i,j=1}^{2} \frac{\mathrm{A}(\square)}{|\mathbf{l}_i||\mathbf{l}_j|} \sum_{k,l=0}^{m-1} \left(\delta\left(\frac{\mathbf{l}_i}{2m}\right) \mu\left(\frac{\mathbf{l}_{3-i}}{2m}\right) u\left(\frac{\mathbf{u}_{k,l}}{m}\right)\right) \\ &\qquad a_{i,j}\left(\frac{\mathbf{u}_{k,l}}{m}\right) \left(\delta\left(\frac{\mathbf{l}_j}{2m}\right) \mu\left(\frac{\mathbf{l}_{3-j}}{2m}\right) v\left(\frac{\mathbf{u}_{k,l}}{m}\right)\right). \end{aligned} \tag{4.4}$$

This requires function values for $u(\mathbf{x})$ and $v(\mathbf{x})$ on the $(m+1)^2$ points of the vertex grid $\mathbf{x} = \mathbf{t}_{k,l}/m$, $k, l = 0, \ldots, m$ (see Figure 4.1) and function values for $a(\mathbf{x})$ on the center grid $\mathbf{x} = \mathbf{u}_{k,l}/m$, $k, l = 0, \ldots, m-1$ (see Figure 2.1).

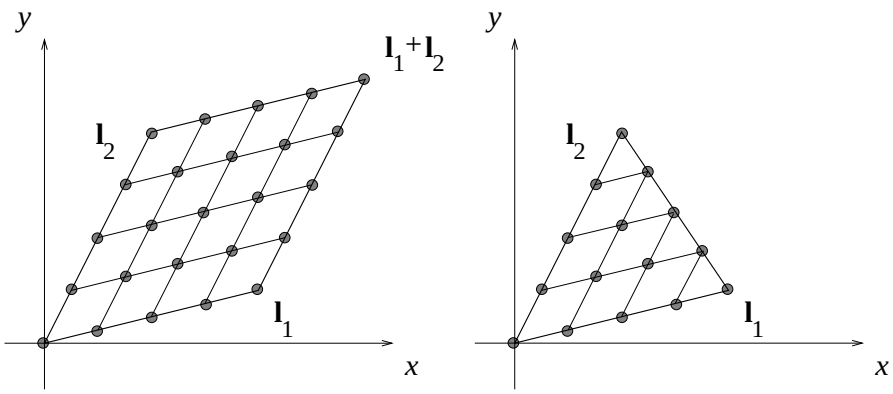

FIG. 4.1. *Vertex grid for* $\square$ *and* $\triangle$. *These points are used for the evaluation of* u *and* v *in Discretizations 1 and 8 and for the evaluation of* u, v, *and* a *in Discretizations 2, 3, 4, 5, 6, and 7.*

Many variants of the discretization are possible and may be obtained by different quadrature rules $\mathrm{Q}(\square)$ or different $F(\mathbf{x}, h)$ or both. We mention only one.

Discretization 2. This differs from Discretization 1 in that $F(\mathbf{x}, h)$ in (4.3) is replaced by (3.12). Thus, $a_{i,j}$ in (4.4) is replaced by $\mathrm{M}_1\mathrm{M}_2 a_{i,j}$. This replacement has the effect that all three component functions $u(\mathbf{x}), v(\mathbf{x}), a_{i,j}(\mathbf{x})$ are evaluated at the $(m+1)^2$ points of the vertex grid.

4.2. Discretizations for $\triangle$. The reason for the somewhat more complicated nature of the application in this section is that it appears that no general discretization for the triangle exists that satisfies all three guidelines (G1), (G2), and (G3).

To see the nature of the problem, the reader is invited to consider what happens when Discretization 2 for the parallelogram is modified for the triangle in an obvious way. To effect this, we replace the center rule $\mathrm{Q}^{(m)}(\square)$ in (4.2) by the corresponding rule for the triangle, $\mathrm{Q}^{(m)}(\triangle)$ given explicitly by (2.10). This rule differs from the rule (2.8) for the parallelogram (as used in Section 4.1) only by the factor $\theta_{m-k-l-1}$, which is inserted in the sum. This factor is the Heaviside step function defined in (2.11). Its effect is to curtail the sum so that instead of summing over all points in $\square$ on the center grid, we sum over only those in $\triangle$, applying a factor of $1/2$ to those on the boundary of $\triangle$.

When one inserts the coefficient $\theta_{m-k-l-1}$ into (4.4) and examines the remaining terms, one sees that most abscissas lie indeed within $\triangle$. However, a closer examination of those terms in the sum for which $\mathbf{u}_{k,l}$ lies on an edge (that is, for which $k+l=m-1$) reveals that of the four points required by $\mathrm{D}_i\mathrm{M}_{i+1}u(\mathbf{u}_{k,l}/m)$, two lie on the common edge, one interior to $\triangle$, and one outside. Consequently, this discretization for the triangle is not self-contained. But it does satisfy guidelines (G1) and (G2) above. For future reference, we term this Discretization 3.

Discretization 3. This differs from Discretization 2 by the insertion of the factor $\theta_{m-k-l-1}$ in (4.4).

Having found (2.10) in Discretization 3 mildly unsatisfactory, we treat the triangle directly. We deal separately with each of the four components of (4.1).

Discretization 4.

$$\mathrm{I}f_0 = \int\int_{\triangle} \frac{\partial u}{\partial n_1} a(\mathbf{x}) \frac{\partial v}{\partial n_1}\, dxdy.$$

Using the rule (2.12) and the somewhat simpler simple discretization

$$F(\mathbf{x}, h) = (\mathrm{D}_1 u)(\mathrm{M}_1 a)(\mathrm{D}_1 v), \tag{4.5}$$

we find

$$\begin{aligned} \mathrm{J}^{(m)} &= \mathrm{Q}^{(m)}(\triangle) F\left(\mathbf{x}, \frac{1}{2m}\right) \\ &= \frac{\mathrm{A}(\square)}{|\mathbf{l}_1|^2} \sum_{k,l=0}^{m-1} \theta_l\, \delta\left(\frac{\mathbf{l}_1}{2m}\right) u\left(\frac{\mathbf{x}_{k,l}}{m}\right)\, \mu\left(\frac{\mathbf{l}_1}{2m}\right) a\left(\frac{\mathbf{x}_{k,l}}{m}\right)\, \delta\left(\frac{\mathbf{l}_1}{2m}\right) v\left(\frac{\mathbf{x}_{k,l}}{m}\right), \end{aligned} \tag{4.6}$$

where $\mathbf{x}_{k,l} = ((k+\frac{1}{2})\mathbf{l}_1 + l\mathbf{l}_2)$. This requires function evaluations of $u(\mathbf{x})$, $a(\mathbf{x})$, and $v(\mathbf{x})$ on all points of the vertex grid, except one; specifically, it requires all points of the form $\mathbf{t}_{k,l}/m$, $0 \le k + l \le m$ (with the trivial exception of the point $\mathbf{t}_{0,m} = \mathbf{l}_2$).

The reader will notice that this is hand tailored to the situation in which only derivatives in the direction of one of the edges of the triangle are required. In this case it is the direction $n_1 = \mathbf{l}_1/|\mathbf{l}_1|$. But the discretization satisfies the guidelines (G1), (G2), and (G3), and it requires function values of all quantities on the vertex grid $\mathbf{x} = \mathbf{t}_{k,l}/m$, $\mathbf{x} \in \triangle$.

We now examine other discretizations obtained naturally by using linear operations to transform the triangle $\triangle$ onto itself. One of these turns out to be the following.

Discretization 5.

$$\mathrm{I}f_0 = \int\int_{\triangle} \frac{\partial u}{\partial n_2} a(\mathbf{x}) \frac{\partial v}{\partial n_2}\, dxdy.$$

Here $\mathrm{J}^{(m)}$ is an obvious adjustment of (4.6), namely,

$$\mathrm{J}^{(m)} = \frac{\mathrm{A}(\square)}{|\mathbf{l}_2|^2} \sum_{k,l=0}^{m-1} \theta_k\, \delta\left(\frac{\mathbf{l}_2}{2m}\right) u\left(\frac{\mathbf{y}_{k,l}}{m}\right)\, \mu\left(\frac{\mathbf{l}_2}{2m}\right) a\left(\frac{\mathbf{y}_{k,l}}{m}\right)\, \delta\left(\frac{\mathbf{l}_2}{2m}\right) v\left(\frac{\mathbf{y}_{k,l}}{m}\right), \tag{4.7}$$

where $\mathbf{y}_{k,l} = (k\mathbf{l}_1 + (l+\frac{1}{2})\mathbf{l}_2)$. This again requires function evaluations of $u(\mathbf{x})$, $a(\mathbf{x})$, and $v(\mathbf{x})$ on the vertex grid.

Before we discuss the next discretization, we define $\mathbf{l}_3 = \mathbf{l}_2 - \mathbf{l}_1$, together with the subordinate definitions. Thus $n_3 = \mathbf{l}_3/|\mathbf{l}_3|$ and $\mathrm{M}_3 a(\mathbf{x})$ and $\mathrm{D}_3 u(\mathbf{x})$ are properly defined by (3.7) and (3.8), respectively. We note that

$$\frac{\partial}{\partial n_3} = \frac{|\mathbf{l}_2|}{|\mathbf{l}_3|}\frac{\partial}{\partial n_2} - \frac{|\mathbf{l}_1|}{|\mathbf{l}_3|}\frac{\partial}{\partial n_1}$$

and

$$\begin{aligned}\frac{\partial u}{\partial n_3} a \frac{\partial v}{\partial n_3} &= \frac{|\mathbf{l}_1|^2}{|\mathbf{l}_3|^2}\frac{\partial u}{\partial n_1} a \frac{\partial v}{\partial n_1} + \frac{|\mathbf{l}_2|^2}{|\mathbf{l}_3|^2}\frac{\partial u}{\partial n_2} a \frac{\partial v}{\partial n_2} \\ &- \frac{|\mathbf{l}_1|\,|\mathbf{l}_2|}{|\mathbf{l}_3|^2}\left(\frac{\partial u}{\partial n_2} a \frac{\partial v}{\partial n_1} + \frac{\partial u}{\partial n_1} a \frac{\partial v}{\partial n_2}\right).\end{aligned}$$

Discretization 6. Here

$$\mathrm{I}f_0 = \int\int_{\triangle} \left(\frac{\partial u(\mathbf{x})}{\partial n_3}\right) a(\mathbf{x}) \left(\frac{\partial v(\mathbf{x})}{\partial n_3}\right). \tag{4.8}$$

The discretization is given by

$$\mathrm{J}^{(m)} = \frac{\mathrm{A}(\square)}{|\mathbf{l}_3|^2} \sum_{k,l=0}^{m-1} \theta_{m-k-l-1}\, \delta\left(\frac{\mathbf{l}_3}{2m}\right) u\left(\frac{\mathbf{u}_{k,l}}{m}\right) \mu\left(\frac{\mathbf{l}_3}{2m}\right) a\left(\frac{\mathbf{u}_{k,l}}{m}\right) \delta\left(\frac{\mathbf{l}_3}{2m}\right) v\left(\frac{\mathbf{u}_{k,l}}{m}\right), \tag{4.9}$$

where $\mathbf{u}_{k,l} = (k+\frac{1}{2})\mathbf{l}_1 + (l+\frac{1}{2})\mathbf{l}_2$.

Note that Discretizations 4, 5, and 6 have isomorphic geometric properties and that all these satisfy (G1), (G2), and (G3). We have derived these by using the theory of Section 3 to develop Discretization 4 and then affine transformations. However, we could have equally well used the theory directly for Discretizations 5 and 6. We would have needed the two rules (2.12) and (2.13), respectively, and obvious variants of (4.5).

To obtain a discretization for $\mathrm{I}f_0$ in general, we still lack a discretization of the cross term

$$\frac{\partial u}{\partial n_1} a \frac{\partial v}{\partial n_2}.$$

In general, this cannot be constructed from the discretizations above. But when the matrix $A(\mathbf{x})$ is symmetric for all $\mathbf{x}$, we need only treat

$$\frac{\partial u}{\partial n_1} a \frac{\partial v}{\partial n_2} + \frac{\partial u}{\partial n_2} a \frac{\partial v}{\partial n_1},$$

with $a(\mathbf{x}) = a_{12}(\mathbf{x}) = a_{21}(\mathbf{x})$. We can provide such a discretization.

Discretization 7. (A symmetric) When B (and, by extension, A) is symmetric, one may proceed by setting (see also Lemma 2.1 in Rüde [10])

$$\begin{aligned}(\nabla u)^T B (\nabla v) = \sum_{i,j=1}^{2} \frac{\partial u}{\partial n_i} a_{i,j} \frac{\partial v}{\partial n_j} &= \left(a_{11}(\mathbf{x}) + \frac{|\mathbf{l}_1|}{|\mathbf{l}_2|} a_{12}(\mathbf{x})\right) \frac{\partial u}{\partial n_1}\frac{\partial v}{\partial n_1} \\ &+ \left(a_{22}(\mathbf{x}) + \frac{|\mathbf{l}_2|}{|\mathbf{l}_1|} a_{12}(\mathbf{x})\right) \frac{\partial u}{\partial n_2}\frac{\partial v}{\partial n_2} \\ &- \left(\frac{|\mathbf{l}_3|^2}{|\mathbf{l}_2|\,|\mathbf{l}_1|} a_{12}(\mathbf{x})\right) \frac{\partial u}{\partial n_3}\frac{\partial v}{\partial n_3}\end{aligned} \tag{4.10}$$

and constructing an overall discretization $\mathrm{J}^{(m)}$ as the sum of Discretizations 3, 4, and 5 applied to the respective terms in (4.10).

Each of the three discretizations used to compose Discretization 7 satisfies guidelines (G1)–(G3) separately. With trivial exceptions, the same $m(m+1)/2$ function values are used in each discretization. All function evaluations are located on the vertex grid.

It is pertinent to note that Rüde [10] has already published a discretization corresponding to Discretization 4. This is as follows.

Discretization 8. Like Discretization 4, this employs quadrature rule (2.12), but instead of (4.5) it uses the simpler

$$F(x,h) = (\mathrm{D}_1 u)a(\mathrm{D}_1 v).$$

As a rule for the 1-1 component only, it is apparently just as powerful as Discretization 4 above (as is illustrated below in the examples). However, it uses function values of $a(\mathbf{x})$ on a product center-vertex grid. Hence, variants formed by rotating the triangle into itself use a different set of function values. So, if one were to form a composite of this rule corresponding to Discretization 7 above, one would find that the number of function evaluation of $a(\mathbf{x})$ required is $3m^2 + O(m)$, violating guideline (G1).

In Table 4.1 we briefly summarize the features of the various discretizations introduced above.

TABLE 4.1
Summary of discretizations

#	$\mathcal{R}$	f_0	Quadrature rule Q	Discretization F
1	$\square$	A general	(2.8)	(4.3)
2	$\square$	A general	(2.8)	(4.3) with a_{ij} replaced by $\mathrm{M}_1\mathrm{M}_2 a_{ij}$
3	$\triangle$	A general	(2.10)	Discretization 2 truncated to triangle
4	$\triangle$	1-1 component only	(2.12)	$\mathrm{D}_1 u \mathrm{M}_1 a \mathrm{D}_1 v$, as in (4.5)
5	$\triangle$	2-2 component only	(2.13)	$\mathrm{D}_2 u \mathrm{M}_2 a \mathrm{D}_2 v$
6	$\triangle$	3-3 component only	(2.10)	$\mathrm{D}_3 u \mathrm{M}_3 a \mathrm{D}_3 v$
7	$\triangle$	A symmetric	composite of Discretizations 4, 5, and 6	
8	$\triangle$	1-1 component only	(2.12)	$\mathrm{D}_1 u a \mathrm{D}_1 v$

Additionally, we list the following features:

- All these discretizations satisfy guideline (G1) ($m^2 + O(m)$ function values) and (G2) (even expansion).
- All except Discretization 3 satisfy guideline (G3) (self-contained).
- Discretizations 2–7 use function values of u, a, and v located on the vertex grid.
- Discretizations 1 and 8 use function values of u and v on the vertex grid.

We remark that only in some applications are these guidelines likely to be important. For example, the guideline (G3) about the location of points for function evaluation is problem dependent. A user may prefer different grids. For some smooth functions the user may have no objections to using points well outside the specified region; indeed, in some cases, he may prefer to do this. There is nothing in the construction technique described above that prevents individual creativity of this sort. Even guideline (G1) is not sacrosanct. If one expects an extrapolation table of significant size, the early discretzations become relatively unimportant and are often discarded. However, these guidelines are traditional in character, and it is useful to see to what extent they can be accommodated.

The only guideline we have found to be of almost universal acceptance is that the expansion should be even. We know no instance in the application of Richardson extrapolation where a full expansion has been preferred to an even expansion.

5. Extrapolation. We follow the notation of the excellent description of Romberg integration given in the fundamental paper of Bauer, Rutishauser, and Stiefel [1]. Here we are dealing with a discretization $\mathrm{J}^{(m)}$ that satisfies an asymptotic expansion, even in m as follows:

$$\mathrm{J}^{(m)} = E_0 + \frac{E_1}{m^2} + \frac{E_2}{m^4} + \cdots \frac{E_p}{m^{2p}} + O(m^{-2p-2}), \tag{5.1}$$

and we are interested in obtaining numerical approximations to $E_0 = \mathrm{I}f_0$.

In general, $\mathrm{J}^{(m)}$ may be evaluated for any integer value of m, and extrapolation is particularly useful when the cost of evaluating $\mathrm{J}^{(m)}$ increases rapidly with m. The first step in an extrapolation process is to choose what is known as a *mesh ratio sequence*, a set of values of m for which $\mathrm{J}^{(m)}$ is to be evaluated. The classical sequence is (geometric)

$$\mathcal{G} = 1, 2, 4, 8, 16, \cdots. \tag{5.2}$$

Another sequence introduced by Bulirsch [2] and Bulirsch and Stoer [3] is

$$\mathcal{F} = 1, 2, 3, 4, 6, 8, 12, 16, \cdots,$$

and the most economic but ultimately unstable *harmonic sequence* (in $1/m$) is

$$\mathcal{H} = 1, 2, 3, 4, 5, 6, 7, 8, \cdots.$$

Different contexts are known in which any of these is more convenient than the other two.

Given $p+1$ values of $\mathrm{J}^{(m)}$ for $p+1$ distinct values of m, an approximation $\tilde{E}_0$ to E_0 may be defined as follows: One may drop the remainder term in (5.1) and substitute successively these $p+1$ values of m to obtain $p+1$ linear equations in $p+1$ unknowns $\tilde{E}_0, \tilde{E}_1, \tilde{E}_2, \ldots, \tilde{E}_p$, which are approximations to $E_0, E_1, \ldots, E_p$, respectively.

When the $p+1$ distinct values of m are $m_k, m_{k+1}, \ldots, m_{k+p}$, the solution $\tilde{E}_0$, which we denote by $T_{k,p}$, can be computed as part of the Romberg T-table, which is a table

containing distinct approximations to E_0.

$$\begin{array}{lllll}
T_{00} & & & & \\
 & T_{01} & & & \\
T_{10} & & T_{02} & & \\
 & T_{11} & & T_{03} & \\
T_{20} & & T_{12} & & \dots \\
 & T_{21} & & \dots & \\
T_{30} & & \dots & & \\
 & \dots & & & \\
\dots & & & &
\end{array}$$

The first column of this table has entries $T_{k,0} = \mathrm{J}^{(m_k)}$, and element $T_{k,p}$ is an extrapolant to E_0 based on $\mathrm{J}^{(m_i)}$, $i = k, k+1, \dots, k+p$. $T_{k,p}$ may be obtained by solving a linear set of equations $\mathbf{ME} = \mathbf{J}$, where the elements of $\mathbf{M}$ are $(m_i)^{(-2j)}$. In general, one needs to solve a different set of p linear equations for each individual extrapolant $T_{k,p}$, and it may be convenient to use a linear equation solver.

In our case, because (5.1) is such a simple expansion, an aesthetically satisfying alternative is to employ the Neville algorithm

$$T_{k,p} = \frac{T_{k+1,p-1} m_{k+p}^2 - T_{k,p-1} m_k^2}{m_{k+p}^2 - m_k^2}.$$

This is discussed in many places, including [1]. The entries in Tables 6.1–6.4 below are elements of the Romberg table, obtained by using $\mathrm{J}^{(m_i)} = T_{i,0}$, and the geometric mesh sequence (5.2).

The Romberg table is convenient because it provides a selection of approximations to E_0. This selection is widened as each new discretization $\mathrm{J}^{(m)}$ is calculated. The columns of such a table converge. Heuristic estimates of the numerical accuracy of the elements of the table can be made based on the numerical closeness of near-by elements.

A theoretical curiosity occurs when, as in Theorem 3.6, $a(\mathbf{x})$, $u(\mathbf{x})$, and $v(\mathbf{x})$ are polynomials such that $f_0(\mathbf{x})$ is a polynomial of degree d. Then the expansion (3.17) terminates, the final nonzero term being D_δ with $\delta = d$ or $\delta = d+1$. Thus the expansion (4.10) also terminates, the final nonzero term being E_μ with $\mu = \lfloor \delta/2 \rfloor$. This means that the procedure to compute E_0 is exact when $p \geq \mu$, since the dropped remainder term is zero. We summarize this property in the following theorem.

THEOREM 5.1. *When $a(x)$, $u(x)$, and $v(x)$ are polynomials such that $f_0(x)$ is a polynomial of degree d, the approximations $T_{k,p}$ (those in the pth column) are exact when $p \geq \lfloor \delta/2 \rfloor$, where*

$$\delta(\square) = d \quad \textit{and} \quad \delta(\triangle) = d + 1.$$

Naturally, any element $T_{k,p}$ can be expressed in a sum of the form

$$\sum_{n=1}^{\nu} w_n u(\mathbf{x}_n^1) a(\mathbf{x}_n^2) v(\mathbf{x}_n^3).$$

This demonstrates the character of $T_{k,p}$ as a quadrature rule; the theorem establishes that the quadrature rule is of polynomial degree $2p+1$ (or $2p$).

6. Examples. The four numerical examples in this section are included simply to illustrate this method in operation and to draw attention to some of its features. We have not compared our results with those obtained using other methods. In all examples we obtain an approximation to

$$f_0(\mathbf{x}) = \frac{\partial u}{\partial x} a \frac{\partial v}{\partial x},$$

where $\triangle$ is the unit triangle with vertices

$$P_1 = (0,0),\ P_2 = (1,0),\ P_3 = (1,1)$$

and

$$a(x,y;\epsilon) = \frac{1}{\sqrt{(x-1/2)^2 + (y+\epsilon)^2}},\ u(x,y) = x^3y^2,\ v(x,y) = x^3 + y^2. \tag{6.1}$$

The incidental parameter ϵ was set to $1/2$ in Example 1, and to $\epsilon = 1/32$ in the other three. In Examples 1 and 2, we used Discretization 4. In Example 3 we used Discretization 8. In Example 4 we evaluated the derivatives analytically which has the effect of reducing the calculation to an application of Romberg integration to the integrand

$$f_0(x,y) = 9x^4y^2a(x,y;\epsilon).$$

In all examples we used the geometric mesh sequence (5.2) with $m = 1, 2, 4, \ldots$. In the tables, we have listed the absolute errors

$$\mathcal{E}_{k,p} = T_{k,p} - \mathrm{I}f_0$$

and the observed convergence rates $\mathcal{E}_{k,p}/\mathcal{E}_{k+1,p}$.

For $\mathrm{I}f_0$ we used values determined by symbolic integration with respect to x and numerical integration with respect to y using the symbolic mathematics package Maple with 20 digits prescribed accuracy. For $\epsilon = 1/2$, $\mathrm{I}f_0 = 0.31230355389424416$, and for $\epsilon = 1/32$, $\mathrm{I}f_0 = 0.49635872127087894$.

We note that $a(x,y;\epsilon)$ has a singularity at $(1/2, -\epsilon)$. In the second integrand (Examples 2, 3, and 4), this is uncomfortably close to the triangle $\triangle$. The results indicate that this method (as would most other numerical quadrature methods) finds the second integrand more difficult than the first. Like the first, the second integral is properly evaluated, however, at a greater expense. It is well known that a singularity close to the region of integration perturbs the observed convergence rates for small m, that is, when the elementary triangles are still large. Naturally, the correct asymptotics should be observed when the discretization becomes sufficiently fine (m large enough).

TABLE 6.1
Romberg table for Example 1 ($\epsilon = 1/2$) (Discretization 4)

m	$\mathcal{E}_{k,0}$		$\mathcal{E}_{k,1}$		$\mathcal{E}_{k,2}$		$\mathcal{E}_{k,3}$	
1	3.123E-01							
2	1.310E-01	2.38	7.057E-02					
4	3.621E-02	3.62	4.613E-03	15.30	2.156E-04			
8	9.273E-03	3.90	2.937E-04	15.71	5.759E-06	37.44	2.428E-06	
16	2.332E-03	3.98	1.847E-05	15.90	1.204E-07	47.83	3.089E-08	78.59
32	5.839E-04	3.99	1.156E-06	15.97	2.149E-09	56.04	2.716E-10	113.74
64	1.460E-04	4.00	7.230E-08	15.99	3.492E-11	61.53	1.370E-12	198.31
128	3.651E-05	4.00	4.519E-09	16.00	5.512E-13	63.36	5.638E-15	242.92

TABLE 6.2
Romberg table for Example 2 ($\epsilon = 1/32$) (Discretization 4)

m	$\mathcal{E}_{k,0}$		$\mathcal{E}_{k,1}$		$\mathcal{E}_{k,2}$		$\mathcal{E}_{k,3}$	
1	4.964E-01							
2	1.850E-01	2.68	8.125E-02					
4	4.709E-02	3.93	1.116E-03	72.79	-4.226E-03			
8	1.186E-02	3.97	1.102E-04	10.13	4.308E-05	-98.10	1.108E-04	
16	2.969E-03	3.99	6.550E-06	16.82	-3.568E-07	-120.75	-1.046E-06	-105.95
32	7.424E-04	4.00	2.238E-07	29.26	-1.979E-07	1.80	-1.954E-07	5.36
64	1.856E-04	4.00	2.775E-09	80.65	-1.196E-08	16.54	-9.011E-09	21.68
128	4.640E-05	4.00	-1.953E-10	-14.21	-3.933E-10	30.41	-2.097E-10	42.97
256	1.160E-05	4.00	-2.042E-11	9.56	-8.759E-12	44.90	-2.655E-12	78.98
512	2.900E-06	4.00	-1.422E-12	14.36	-1.558E-13	56.24	-1.920E-14	138.30

TABLE 6.3
Romberg table for Example 3 ($\epsilon = 1/32$) (Discretization 8)

m	$\mathcal{E}_{k,0}$		$\mathcal{E}_{k,1}$		$\mathcal{E}_{k,2}$		$\mathcal{E}_{k,3}$	
1	4.964E-01							
2	1.704E-01	2.91	6.169E-02					
4	4.565E-02	3.73	4.085E-03	15.10	2.442E-04			
8	1.160E-02	3.94	2.494E-04	16.38	-6.292E-06	-38.82	-1.027E-05	
16	2.910E-03	3.99	1.281E-05	19.47	-2.964E-06	2.12	-2.912E-06	3.53
32	7.278E-04	4.00	5.699E-07	22.47	-2.459E-07	12.05	-2.028E-07	14.36
64	1.820E-04	4.00	2.386E-08	23.89	-1.255E-08	19.60	-8.844E-09	22.93
128	4.550E-05	4.00	1.104E-09	21.60	-4.125E-10	30.42	-2.199E-10	40.22

TABLE 6.4
Romberg table for Example 4 ($\epsilon = 1/32$) (Analytic derivatives)

m	$\mathcal{E}_{k,0}$		$\mathcal{E}_{k,1}$		$\mathcal{E}_{k,2}$		$\mathcal{E}_{k,3}$	
1	4.964E-01							
2	7.775E-02	6.38	-6.178E-02					
4	1.614E-02	4.82	-4.393E-03	14.06	-5.667E-04			
8	3.803E-03	4.25	-3.111E-04	14.12	-3.897E-05	14.54	-3.059E-05	
16	9.341E-04	4.07	-2.204E-05	14.12	-2.767E-06	14.08	-2.192E-06	13.95
32	2.323E-04	4.02	-1.618E-06	13.62	-2.567E-07	10.78	-2.169E-07	10.11
64	5.799E-05	4.01	-1.136E-07	14.24	-1.331E-08	19.29	-9.445E-09	22.96
128	1.449E-05	4.00	-7.493E-09	15.16	-4.197E-10	31.71	-2.152E-10	43.90

Reference to Examples 2, 3, and 4 reveals that the cost-effectiveness of the method is not particularly sensitive to the details of the discretization. The drawback of Discretization 8 does not reveal itself here: If other derivatives were required with Discretization 8, a different set of locations for the function evaluation of $a(\mathbf{x})$ would be required.

The use of the mean operator to approximate $a(\mathbf{x})$ by (3.11) in cases when the function values are readily available may appear to be introducing an unnecessary component in the error. However, if the result is to be integrated by using an equally spaced formula, this extra error may well be illusory. As a trivial example, suppose that at the points $x = (j - \frac{1}{2})h$, the function $f(x)$ is approximated by the mean

$$\tilde{f}(x) = \frac{1}{2}\left(f(x + \frac{h}{2}) + f(x - \frac{h}{2})\right)$$

and the integral $\mathrm{I}f$ is approximated by $\mathrm{M}f$, a midpoint m panel rule with $m = \frac{1}{h}$. Clearly,

$$\mathrm{M}\tilde{f} = \frac{1}{m}\sum_{j=1}^{m} \tilde{f}\left(\frac{j - \frac{1}{2}}{m}\right) = \frac{1}{m}\sum_{j=0}^{m}{}'' f\left(\frac{j}{m}\right).$$

The effect of the mean operator is to replace the midpoint rule approximation by the endpoint rule approximation. Both these rules have similar characteristics, and the quality of the results is generally the same.

7. Concluding Remarks. The construction of numerical quadrature techniques for the integral $\mathrm{I}\nabla u B \nabla v$ is intrinsically as wide a research area as is numerical quadrature over squares and triangles. However, at the present time, applications are far less widespread. Here, we have covered a significant part of the theory, that which corresponds to extrapolation quadrature in standard numerical quadrature.

Sections 2 and 3 cover the theory in a somewhat general way. In Section 3 the new definitions and theorems are given. These include a definition of a discretization of the integrand $f_0(\mathbf{x})$ by $F(\mathbf{x}, h)$, its use in constructing an elementary discretization $\mathrm{J}^{(m)}$, and the basic theorem that allows extrapolation.

The main results are in Section 4, where several elementary discretizations $\mathrm{J}^{(m)}$ are discussed. These approximations to the integral $\mathrm{I}f_0$ are designed to be used in extrapolation quadrature, where they would appear in the initial column of a Romberg table. These particular discretizations conform, as far as is feasible, to three stated guidelines of a traditional nature, which prescribe economy in terms of function values, and containment of abscissas in the integration region.

However, we have kept in mind the user with a special problem who may need to construct a variant of the method described here. For this reason, we have presented a somewhat general theory, which in Section 4 is specialized to a conventional problem context. Such an unconventional user may exploit the results given in Sections 2 and 3 to construct a specialized discretization that conforms to his problem specification.

The final sections comprise a brief summary of the extrapolation technique and its subsequent use in four simple illustrative numerical examples.

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