Numerical quadrature in n dimensions

By D. Mustard, J. N. Lyness and J. M. Blatt

We investigate a selection of integration rules based on the combination of third degree rules for elementary three-dimensional sub-domains. The practical problems associated with the application of these rules to domains bounded by planes of a certain type are discussed in detail. These include integration rules for less symmetrical domains which may occur near the boundary of the volume of integration, methods for combining integration coefficients from adjacent sub-domains, and methods for changing net size within the volume of integration.

Particular attention is paid to minimizing the number of points at which the function has to be evaluated, and error estimates in terms of computation time are given. A list of integration coefficients of general interest for three-dimensional integrations is presented. The discussion is generalized to n dimensions for hyper-cubic domains.

1. Introduction

To calculate the binding energy of the triton it is necessary to evaluate numerically a number of triple integrals. The domain of integration is defined by the inequalities

$$x + y \geqslant z \quad , \tag{1.1a}$$

$$y + z \geqslant x \quad , \tag{1.1b}$$

$$z + x \geqslant y \quad , \tag{1.1c}$$

$$x \geqslant r_0 \quad , \tag{1.2a}$$

$$y \geqslant r_0 \quad , \tag{1.2b}$$

$$z \geqslant r_0 \quad , \tag{1.2c}$$

where x, y and z are the three integrand variables and r_0 is a given constant (the nucleon hard core radius). The numerical integration is performed over the finite part of this infinite domain defined by the inequalities

$$x \leqslant R \quad , \tag{1.3a}$$

$$y \leqslant R \quad , \tag{1.3b}$$

$$z \leqslant R \quad , \tag{1.3c}$$

where R is a constant chosen to satisfy the requirements of both accuracy and economy. Since the integrands can be transformed into functions symmetric in x and y, the domain can be halved by the further inequality

$$x \geqslant y \quad . \tag{1.4}$$

This makes inequality (1.3b) superfluous.

Not only is the shape of the domain complicated but the integrands, although having the advantage of a form making tabulation over a cubic lattice convenient, have the disadvantage that some of them assume indefinite forms at points (termed "awkward points") where $x = y = z$. Many of the integrands are rapidly varying functions where at least one of x, y or z is small, but are slowly varying where x, y and z are all large, so changes in the fineness of the lattice of integration points are desirable. These are made suitably at boundaries defined by

$$\text{Min}\,(x, y, z) = r_i \tag{1.5}$$

where r_1, r_2, etc., are constants of magnitude between r_0 and R.

All of these boundary planes may be written

$$\Sigma \alpha_i x_i + \beta = 0$$

where α_i and β are small integers. The method of the final sections of this paper is *practical* only if the boundary planes are of this type.

We have described features of this particular problem because some of them, which led us to select and develop a particular method of integration, may be common to many other problems. There are three conventional methods, which treat the domain as a whole, and these are discussed briefly below.

(i) *Gaussian integration rules*

An integration rule is said to be of "degree of precision k" or a "k-th degree rule" if it computes exactly the integrals of all polynomials of at most degree k. The well-known Gaussian rules have the advantage that a given degree of precision can be achieved using about half the number of points required in other methods, but the disadvantage that unless the domain is simple the determination of the rule itself may be an enormous problem. To get sufficient accuracy in the triton calculation, for example, one would need more than one thousand points and so would have to find more than one thousand zeros of a complicated polynomial. This polynomial itself is difficult to determine since the Gram–Schmid process one uses for determining it (Courant and Hilbert, 1953) is numerically unstable with respect to rounding errors, and requires multiple-precision work after the twentieth polynomial. If having done all this one wanted to improve the accuracy by increasing the number of points or the value of R, one would have to start again *ab initio*.

(ii) *The Monte Carlo method*

This method is flexible, easily coded, and, if low accuracy is adequate, very efficient, so it is suitable for pilot calculations (it was, in fact, used in the triton problem (Derrick, 1959; Derrick and Blatt, 1960), but is unsuitable for final calculations partly because of its low accuracy.) If N is the number of trial points then the

error decreases as $N^{-\frac{1}{2}}$ or, in a modified method (Davis and Rabinowitz, 1956) as N^{-1}. In the triton problem the convenience of tabulating the functions over a cubic lattice, and the slightly better error law ultimately obtained, led to the use of other methods.*

(iii) *Product Simpson's rules*

In this method the integral is written as a repeated integral. In our case this has the form

$$\int_{r_0}^{R} dx \int_{r_0}^{x} dy\, K(x, y) \tag{1.6}$$

where $$K(x, y) = \int_{z_1}^{z_2} f(x, y, z)dz \tag{1.7}$$

and where $$z_1 = \max (r_0, x - y) \tag{1.8a}$$

$$z_2 = \min (R, x + y). \tag{1.8b}$$

Note that even if the integrand $f(x, y, z)$ is analytic the function $K(x, y)$ is *not*, since z_1 and z_2 are non-analytic.

The awkward boundaries create several difficulties. If one used the conventional Simpson's rule with interval h in the z dimension, one could define $K(x, y)$ only at intervals of $2h$ in x and y. The next integration would have to use an interval of $2h$ in the y dimension, and the resulting function of x would be defined only at intervals of $4h$, so the last integration would have to use an interval of $4h$. This choice of intervals would cope with the non-analytic nature of $K(x, y)$, but that of equal intervals in all three dimensions would not.

We discuss this asymmetric rule in Section 6 where we deal with the use of different intervals in different dimensions. There we mention that cases arise in which such a method is suitable.

There is no need for one to use different intervals if one makes some use of, for example, the Simpson's "$\frac{3}{8}$" rule if the number of points is even, or locates the lattice points differently according as this number is even or odd. However, in the following Sections we show that use of this rule without great modification is relatively inefficient.

In the method we develop for use in the triton problem the whole domain is dissected into elementary sub-domains, or *cells*, of relatively simple shape, and in each of which the integration rule is determined using the condition that it be of a specified degree of precision in that cell. Since each cell is small a low-degree rule suffices. This method is the natural extension to many dimensions of the usual method in one dimension.

Gaussian integration rules for the n-cube are known (Hammer and Stroud, 1958), but they are not the most efficient ones for our present purpose, for when cells are joined to form a larger domain the total number of integration points is not generally the sum of their numbers in each cell. The counting of integration points is discussed in Section 2; various integration rules are given and their errors discussed in Sections 3, 4, 5 and 6; non-cubic boundary cells are discussed in Section 7, and the joining of cells and changing of cell size are discussed in Section 8. For the sake of simplicity and concreteness the last two Sections are restricted to triple integrals of the type that interests us, but the methods used allow obvious generalization.

* The popular idea that the Monte Carlo method is generally better than a straightforward error estimate would indicate is, in our view, mistaken. Experiments have shown that if one is unlucky the actual error may greatly exceed the estimated error. Monte Carlo calculations are always rather a gamble.

2. Counting of points

Consider an n-dimensional domain of volume V which is dissected into cubic cells each of width $2h$ and volume $(2h)^n$. The number of cells, C, is given by

$$C = V/(2h)^n. \tag{2.1}$$

(We neglect, temporarily, possible non-cubic cells near the domain boundaries.)

Let x be the coordinate vector of any asymmetrically located point in the basic cell, whose centre we can take to be at the origin. By reflection, rotation and inversion symmetry this point is equivalent to many others (7 others in the square, 47 others in the 3-cube, etc.). Reasonable integration rules for this cell are symmetric and assign equal coefficients A_i to equivalent points, so it is best to use only points of high symmetry. Gaussian integration rules using this principle have been given before (Hammer and Wymore, 1957; Hammer and Stroud, 1958).

The counting of points is quite different, if a typical point is a boundary point of a cell, as, for example, is the vertex of the n-cube. There are 2^n vertices of an n-cube, and all of them have equal coefficients A_i. These 2^n points are effectively only *one* point since each point is a vertex of not only one particular cell but of all adjacent cells, i.e. the point is "shared" among 2^n cells, so if an integration rule uses only the cube centres and the cube vertices the number of integration points, N, in a hypercubic domain is given by:

$$N = C + (C^{1/n} + 1)^n \tag{2.2a}$$

and *not* $$N = (1 + 2^n)C.$$

If C is large, of the order 4,000 and n is small, say 3, (2.2a) may be approximated by*

$$N = 2C. \tag{2.2b}$$

This is the case for most practical applications. Since we use N only to estimate the error of a particular rule per number of points used, we shall be satisfied with (2.2b). We discuss the counting of points in this Section in the spirit of this rough approximation. When an accurate estimate of N is required the effect of the boundary cells must be calculated.

* For $N > 4096$ and $n = 3$, $2C < N < 2{\cdot}2C$. For large n this approximation is quite invalid. For $n = 10$ and $N = 1{,}000$, $N \simeq 18{\cdot}7C$. The authors are indebted to Dr. J. C. P. Miller for drawing their attention to this point. However, in a large number of dimensions, to obtain reasonable accuracy a larger number of points would be used; thus equation (2.2b) would still be not unreasonable.

For each value $\zeta\,(0 < \zeta < h)$ the n-cube contains $n+1$ different symmetry classes of points. The class j_ζ contains all points $\vec{x} = (x_1, x_2, \ldots, x_n)$ such that exactly j of the n coordinates x_i differ from zero and each non-zero x_i equals either $+\zeta$ or $-\zeta$. The number of points, G_j, in class j_ζ is given by

$$G_j = 2^j\binom{n}{j}. \tag{2.3}$$

When the cells are joined, each point in class j_h is shared between 2^j different cells, and so this class contributes an effective number of points per cell, N_j, given by

$$N_j = \binom{n}{j}. \tag{2.4}$$

If the integration rule uses all classes j_h $(j = 0, 1, \ldots n)$ and no others, then the total number of integration points is given by

$$N = \frac{V}{(2h)^n}\sum_{j=0}^{n} N_j = \frac{V}{h^n} \tag{2.5}$$

(as might be expected). If not all classes, j_h are used then the sum in (2.5) does not extend over all values of j. For example, a rule we call the "corner rule," using only body centres and vertices ($j = 0$ and $j = n$), uses a total number of points determined by (2.1) and (2.2*b*):

$$N = \frac{V}{2^{n-1}h^n} \quad \text{("corner rule")}. \tag{2.6}$$

The most efficient points are the ones with the lowest N_j, viz. the body centre and the vertices; next most efficient are those with $j = 1$ and $j = n - 1$; and so on. Less efficient than the points of class j_h are those of class $j_\zeta(\zeta < h)$ since the effective number of points of this class per cell is G_j not N_j. The most efficient of classes $j_\zeta(\zeta < h)$ are those with $j = 1$. An integration rule using the body centres, the vertices and points of a class 1_ζ $(\zeta < h)$ uses a total number of points given by

$$N = \frac{(n+1)V}{2^{n-1}h^n}. \tag{2.7}$$

We shall develop a fifth-degree rule of this type (error of order h^6) and several third-degree rules such as the corner rule (error of order h^4). These rules are more efficient and flexible than the conventional Gaussian rules applied to cells (Hammer and Stroud, 1958).

The integrals over the central n-cube of all monomials that have an odd power of a coordinate are zero, and many integrals of the others are related by symmetry (Hammer and Wymore, 1957; Miller, 1960). The only essentially different non-vanishing integrals of terms in a polynomial of degree 5 are those of

$$1,\ x_1^2,\ x_1^4,\ x_1^2x_2^2. \tag{2.8}$$

We write the general integration rule for the cell in the form

$$\int_h \vec{f(x)}d\tau \doteq (2h)^n\left\{\sum_{j=0}^{n} A_j \sum_{k=1}^{G_j} \vec{f(h_{jk})} + \sum_{l}\sum_{j=1}^{h} B_j^{(l)} \sum_{k=1}^{G_j} \vec{f(\zeta_{jk}^{(l)})}\right\}$$

where, $\vec{h_{jk}}$ are the points of class j_h and the $\vec{\zeta_{jk}^{(l)}}$ are those of class $j_\zeta(l)$.

3. The "corner rule" in *n* dimensions

In this Section we find a certain third-degree rule. By (2.8) the only essentially different integrals required are those of 1 and x_1^2, so two types of points are enough. According to Section 2 the best are the body centre $\vec{h_0}$ and the vertices $\vec{h_{nk}}$, so our rule reads

$$\int_h \vec{f(x)}d\tau \doteq (2h)^n\left\{A_0\vec{f(h_0)} + A_n\sum_k \vec{f(h_{nk})}\right\}. \tag{3.1}$$

Taking $f = 1$ and $f = x_1^2$ in turn we get the conditions

$$A_0 + 2^nA_n = 1 \quad (f = 1)$$
$$2^nA_n = 1/3 \quad (f = x_1^2)$$

with the solution

$$A_0 = 2/3 \qquad A_n = 1/(2^n3). \tag{3.2}$$

If we now join the cells the rule for use inside the domain, away from the boundaries, becomes very simple: Sum all body-centre function values with weight 2/3, and all vertex values with weight 1/3. We shall call (3.1) and (3.2) the "corner" rule. The small number of points it needs to cover the whole domain [see (2.6)], and their disposition on a body-centred cubic lattice, give this rule such an advantage that only in special circumstances would it be worth considering more accurate ones.

We make an estimate of the error made in using this rule. If we neglect all higher than fifth-order derivatives of the integrand $\vec{f(x)}$, we can replace $\vec{f(x)}$ inside each cell by some fifth-degree polynomial. By (2.8) the relevant terms for the central hypercubic cell form a polynomial $\vec{P(x)}$ of type given by

$$\vec{P(x)} = a_0 + \sum_{i=1}^{n}(b_ix_i^2 + c_ix_i^4) + \sum_{i>j=1}^{n} d_{ij}x_i^2x_j^2. \tag{3.3}$$

The integral, J, of this over the cell is given by

$$J = \int_h \vec{P(x)}d\tau = (2h)^n\left\{a_0 + \sum_{i=1}^{n}\left(\frac{h^2b_i}{3} + \frac{h^4c_i}{5}\right) + \frac{h^4}{9}\sum_{i>j=1}^{n} d_{ij}\right\}. \tag{3.4}$$

If we apply the corner rule (3.1)–(3.2) to $\vec{P(x)}$ the result of the approximation is

$$J_1 = (2h)^n\left\{a_0 + \sum_{i=1}^{n}(h^2b_i/3 + h^4c_i/3) + \frac{h^4}{3}\sum_{i>j=1}^{n} d_{ij}\right\}. \tag{3.5}$$

The error over a single cell, E_h, is given by

$$E_h = J_1 - J = (2h)^n\frac{2h^4}{45}\left(\sum_{i=1}^{n} 3c_i + \sum_{i>j=1}^{n} 5d_{ij}\right). \tag{3.6}$$

Table 1

Six third-degree rules for 3 dimensions

RULE NUMBER	A_0	A_1	A_2	A_3	$\bar{\nu}$	d_4	d_{22}	p_4	p_{22}
1	2/3	0	0	1/24	2	1/60	1/6	0·0026	0·0262
2	0	1/6	0	0	3	1/60	−1/12	0·0045	−0·0225
3	1/2	0	1/24	0	4	1/60	1/24	0·0066	0·0166
4	0	0	1/6	−1/8	4	1/60	−1/30	0·0066	−0·1333
5	2/9	1/9	0	1/72	5	1/60	0	0·0089	0
6	8/27	2/27	1/54	1/216	8	1/60	0	0·0166	0

Values of $\bar{\nu}$, d_4, d_{22}, p_4 and p_{22} for various third-degree rules for three dimensions. These numbers are defined in equations (4.1)–(4.5).

In order to get an error estimate for the original function $f(\vec{x})$ we observe that for the special case $f(\vec{x}) = P(\vec{x})$ the quantities c_i and d_{ij} can be written as derivatives evaluated at the origin:

$$c_i = \frac{1}{4!}\frac{\partial^4 f}{\partial x_i^4}, \qquad d_{ij} = \frac{1}{4}\frac{\partial^4 f}{\partial x_i^2 \partial x_j^2}. \tag{3.7}$$

For a general function f it is reasonable to replace these coefficients by the same derivatives, evaluated somewhere inside the hypercube. After this substitution our estimate of the error becomes

$$E_h \approx (2h)^n \frac{h^4}{180}\left\{\sum_{i=1}^{n}\frac{\partial^4 f}{\partial x_i^4} + 10\sum_{i>j=1}^{n}\frac{\partial^4 f}{\partial x_i^2 \partial x_j^2}\right\}. \tag{3.8}$$

The large number of different derivatives which enter this estimate makes any discussion difficult. In order to simplify matters we introduce the average direct fourth derivative

$$f^{(4)} = \frac{1}{n}\sum_{i=1}^{n}\frac{\partial^4 f}{\partial x_i^4} \tag{3.9}$$

and the average mixed fourth derivative

$$f^{(2,2)} = \frac{2}{n(n-1)}\sum_{i>j=1}^{n}\frac{\partial^4 f}{\partial x_i^2 \partial x_j^2}. \tag{3.10}$$

The error estimate (3.8) then takes the form

$$E_h \approx (2h)^n \frac{h^4}{180}\{nf^{(4)} + 5n(n-1)f^{(2,2)}\}. \tag{3.11}$$

We cannot make a fair comparison between different rules merely by finding E_h for each of them. For a given *total* error, E, it is not the quantity h alone which has practical significance but the computation time, which is proportional to N, the total number of points at which the integrand must be evaluated; so we must express E in terms of V (the volume of the domain) and N, rather than h.

To estimate E for a hypercubic domain one needs $\sum (2h)^n f^{(4)}$ and $\sum (2h)^n f^{(2,2)}$, the summation being over all cells. These sums may be approximated by the quantities $F^{(4)}$ and $F^{(2,2)}$, respectively, defined by

$$F^{(4)} = \int f^{(4)}(x)d\tau \tag{3.12}$$

and

$$F^{(2,2)} = \int f^{(2,2)}(x)d\tau, \tag{3.13}$$

and which are independent both of h and the integration rule used.

The number of cells, C, is $V/(2h)^n$ [see (2.1)]; the number of integration points for the corner rule is about $2C$ [see (2.2*b*)] and each cell contributes an error E_h estimated in (3.11), so the total error E is estimated to be

$$E \approx \frac{n}{180 \cdot 2^{4(n-1)/n}}\{F^{(4)} + 5(n-1)F^{(2,2)}\}(V/N)^{4/n}. \tag{3.14}$$

For $n = 3$ we find that

$$E \approx 0{\cdot}00262\{F^{(4)} + 10F^{(2,2)}\}(V/N)^{4/3}. \tag{3.14'}$$

In *all* similar third-degree rules E varies as the $(4/n)$th power of the computation time, so the factors other than $(V/N)^{4/n}$ are the distinguishing ones.

4. Other third-degree rules in three dimensions

A similar analysis can be made of other rules we may invent. If a three-dimensional rule uses only the centre $\vec{h}_0$, face centres $\vec{h}_{1k}$, edge centres $\vec{h}_{21}$, and vertices $\vec{h}_{3m}$ of the cubic cell, we can write it in the form

$$\int_h f(\vec{x})d\tau \doteq (2h)^3\left\{A_0 f(\vec{h}_0) + A_1\sum_{k=1}^{6} f(\vec{h}_{1k}) + A_2\sum_{l=1}^{12} f(\vec{h}_{2l}) + A_3\sum_{m=1}^{8} f(\vec{h}_{3m})\right\}. \tag{4.1}$$

Six rules are listed in Table 1. Rule 2 (the "face-centre" rule) uses only face centres; rule 1 (the corner rule discussed before) and rules 3 and 4 each use only two of the other three types of point. Combinations of rules 1–4 may be used; two, including the three-dimensional product Simpson's rule (rule 6), are discussed here.

Table 2

Third-degree rules for n dimensions ($n \geqslant 2$)

RULE	A_0	A_1	A_{n-1}	A_n	$\bar{\nu}$	d_4	d_{22}	$2880p_4$	$2880p_{22}$	
1	$2/3$	0	0	$\frac{1}{3\cdot 2^n}$	2	$\frac{n}{180}$	$\frac{n(n-1)}{36}$	$n\cdot 24^{4/n}$	$5n(n-1)24^{4/n}$	
2	$1-\frac{n}{3}$	$\frac{1}{6}$	0	0	$n+1$	$\frac{n}{180}$	$\frac{-n(n-1)}{72}$	$n(n+1)^{4/n}$	$-\frac{5}{2}(n-1)n(n+1)^{4/n}$	$(n \neq 3)$
5	$\frac{8-2n}{9}$	$\frac{1}{9}$	0	$\frac{1}{9\cdot 2^n}$	$\begin{cases} n+2 \\ 5 \end{cases}$	$\frac{n}{180}$	0	$\begin{cases} n(n+2)^{4/n} \\ 20 \end{cases}$	$\begin{matrix} 0 \\ 0 \end{matrix}$	$\begin{matrix} n \neq 4 \\ n = 4 \end{matrix}$
6	$A_i = \left(\frac{2}{3}\right)^n \frac{1}{2^{2i}}$				2^n	$\frac{n}{180}$	0	$16n$	0	

Values of $\bar{\nu}$, d_4, d_{22}, p_4, p_{22} for certain n-dimensional third-degree rules. These numbers are directly analogous to those defined for 3 dimensions in equations (4.2)–(4.5).

Table 3

Some 5th-degree integration rules for three-dimensional cubic cells

RULE	INTEGRATION POINTS AND COEFFICIENTS							$\bar{\nu}$	ERROR ESTIMATE COEFFICIENTS			t
	A_0	A_1	A_2	A_3	B_1		B_3		p_6	p_{42}	p_{222}	
	h_0	h_{1k}	h_{2k}	h_{3k}	$\left(\frac{h}{2}\right)_{1k}$	$\left(\frac{2h}{5}\right)^{\frac{1}{2}}_{h_{1k}}$	$\left(\frac{h}{2}\right)_{3k}$					
1	$-\frac{7}{9}$	0	0	$\frac{1}{72}$	0	$\frac{5}{18}$	0	8	0·0000159	0·00556	0·00926	2·94
2	$-\frac{4}{3}$	0	$\frac{1}{90}$	$\frac{1}{120}$	$\frac{16}{45}$	0	0	11	0·000188	0·0105	0·00700	5·28
3	$-\frac{62}{45}$	$\frac{1}{45}$	0	$\frac{1}{72}$	$\frac{16}{45}$	0	0	11	0·000188	0·0105	0·0175	5·42
4	$-\frac{2}{45}$	$\frac{2}{45}$	0	$\frac{1}{120}$	0	0	$\frac{4}{45}$	13	0·000262	0·00367	0·0134	1·10
5	$\frac{2}{45}$	0	$\frac{1}{45}$	$-\frac{1}{360}$	0	0	$\frac{4}{45}$	13	0·000262	0·00367	−0·0159	1·08
6	−19/15	−1/30	$\frac{1}{36}$	0	$\frac{16}{45}$	0	0	13	0·000262	0·0147	−0·0122	5·60

We list in Table 3 several fifth-degree rules for three-dimensional cubic cells. Rule 1, which uses an irrational intermediate point, is the rule discussed above; the others all use intermediate points which lie on a cubic lattice of coordinate difference $h/2$, and so would not require interpolation if the function were tabulated at this regular interval. We see that although rule 1 has by far the lowest value of p_6, it does not have the lowest value of p_{42} or p_{222}, so if the mean direct sixth-order derivative of the integrand were very small compared with the other, mixed, mean derivatives, one of the other rules, such as 2 or 5, would be not only more convenient but more efficient.

Defining E_h, E, $f^{(4)}$, $f^{(2,2)}$, $F^{(4)}$, $F^{(2,2)}$, N and V as in Section 3, we again can find estimates of E_h and E in the forms

$$E_h \approx (2h)^3 h^4 \{d_4 f^{(4)} + d_{22} f^{(2,2)}\}; \tag{4.2}$$

$$E \approx h^4 \{d_4 F^{(4)} + d_{22} F^{(2,2)}\}; \tag{4.3}$$

where d_4 and d_{22} are coefficients dependent on the rule but independent of $f(\vec{x})$.

We define $\bar{\nu}$ to be the number of points used per cell when only a small proportion of the domain is occupied by boundary cells. Thus

$$N = \frac{V}{(2h)^3}\bar{\nu} \tag{4.4}$$

and we may write

$$E \approx \{p_4 F^{(4)} + p_{22} F^{(2,2)}\}\left(\frac{V}{N}\right)^{4/3} \tag{4.5}$$

where $$p_4 = d_4\left(\frac{\bar{\nu}}{8}\right)^{4/3} \text{ and } p_{22} = d_{22}\left(\frac{\bar{\nu}}{8}\right)^{4/3}. \tag{4.6}$$

In comparing rules the principal criterion that we use is that the rule should be efficient, i.e. have a low error per point used.

The rules easiest to code are the product Simpson's rule (rule 6), which uses a $1:4:2:4:\ldots 2:4:1$ ratio along each line, and the face-centre rule (rule 2), which uses a $1:2:2:\ldots 2:1$ ratio along each line; however, the other rules are only slightly harder to code. The important factor in the estimate of error per point is $\{p_4 F^{(4)} + p_{22} F^{(2,2)}\}$. If $F^{(2,2)}/F^{(4)}$ is small (in most of the domain) the corner rule (rule 1) is best; if it is close to some constant then either one of the rules 1–4 or a combination of rules 1 and 2 (with $p_4 = 0{\cdot}00890$) is best; and if it is large then rule 5 (a particular combination of rules 1 and 2) is best. It can be seen that the product Simpson's rule (rule 6) is always less efficient than rule 5. The asymmetric product Simpson's rule is discussed in Section 6. It is usually less efficient than the symmetric one.

5. *n*-dimensional rules

The errors made by n-dimensional rules of this type increase quite seriously with n. Suppose one attempted to decrease the total error E by reducing the cell width from h to gh in a rule of degree $s-1$. The number of points used in the domain (and so also the computation time T) is increased by a factor g^{-n} and the error is decreased by a factor g^s, so the relation between error and computation time is

$$E \sim T^{-s/n}. \tag{5.1}$$

A third-degree rule in one dimension (Simpson's rule), for example, makes an error decreasing as T^{-4}, whereas one in three dimensions makes an error decreasing only as $T^{-4/3}$.

For $n \geqslant s$ the error decreases not faster than T^{-1}, whereas the modified Monte Carlo method makes an error decreasing as T^{-1}, and its simplicity and flexibility would usually compensate for any larger numerical factor in its error estimate. So *to evaluate an n-dimensional integral the modified Monte Carlo method is usually preferable to an integration rule of degree less than n.*

In view of this we list in Table 2 only four third-degree rules for n dimensions. Using the definition of classes of points $j_{\vec{\zeta}}$ given in Section 2, we call the $2n$ points of class 1_h "face centres" and the $n \cdot 2^{n-1}$ points of class $(n-1)_h$ "edge centres." The notation and general form of the error estimates are as in Section 4. The error estimate for rule 5 does not involve the mixed derivatives: if $n = 4$, rule 5 could be preferable to the corner rule if the magnitudes of these derivatives were significant. The conventional product Simpson's rule is again significantly inferior.

The best rule obtainable using points of class j_h alone is a third-degree rule that integrates exactly the mixed terms x^2y^2, etc., but not the terms x^4, etc. A fifth-degree rule uses points of at least one class $j_{\vec{\zeta}}(\zeta < h)$. According to Section 2 the rule

$$\int_h f(\vec{x})d\tau \doteq (2h)^n\Big\{A_0 f(\vec{h}_0) + A_n \sum_k^{2n} f(\vec{h}_{nk}) + B_1 \sum_{l=1}^{2n} f(\vec{\zeta}_{1l})\Big\}, \tag{5.2}$$

where the notation is that of (2.9), is the most economic rule having just the number of independent parameters (A_0, A_n, B_1, ζ) to satisfy the conditions that it be of fifth degree. These conditions, that integrals of all terms (2.8) be computed exactly, lead to the values

$$A_0 = (8-5n)/9;\ A_n = 2^{-n}/9;\ B_1 = 5/18;\quad \zeta/h = (2/5)^{\frac{1}{2}}. \tag{5.3}$$

For this rule, (5.2), $\bar{\nu} = 2n+2$ and N is given by (2.7). In three dimensions, then, this rule uses effectively 8 points per cell compared with 14 points per cell used by the most efficient fifth-degree rule given in Hammer and Stroud (1958). Compared with the corner rule the rule (5.2) has two disadvantages: (i) $n+1$ times as many points are needed, many of which are not cubic lattice points,* and (ii) one coefficient is negative.

To estimate the error we proceed as before. Making the definitions

$$F^{(6)} = \int f^{(6)}d\tau = \int \frac{1}{n}\sum_{i=1}^{n}\frac{\partial^6 f}{\partial x_i^6}d\tau, \tag{5.3a}$$

* If function values were known only at cubic lattice points some interpolation would be necessary, but the interpolation rule used must have degree of precision 5 at least, and so one would use altogether many more points per cell of width $2h$ than by applying, say, a fifth-degree integration rule developed specifically to use only the points of a cubic lattice having co-ordinate differences $\frac{1}{2}h$ instead of h.

Table 4

Lattice points and associated coefficients for a right-angled isosceles triangle

x/h	y/h	$\frac{1}{2h^2} \times$ COEFFICIENT
0	0	A_0
1	0	A_1
0	−1	A_1
1	−1	A_2
1	1	A_2
−1	−1	A_2

$$F^{(4,2)} = \int f^{(4,2)} d\tau = \int \frac{1}{n(n-1)} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \frac{\partial^6 f}{\partial x_i^4 \partial x_j^2}\, d\tau \quad (5.4)$$

$$F^{(2,2,2)} = \int f^{(2,2,2)} d\tau = \int \frac{6}{n(n-1)(n-2)} \sum_{i>j>k=1}^{n} \frac{\partial^6 f}{\partial x_i^2 \partial x_j^2 \partial x_k^2}\, d\tau \quad (5.5)$$

we find for a cell

$$E_h \approx (2h)^n \frac{nh^6}{189000} \left\{ f^{(6)} + 175(n-1) f^{(4,2)} + \frac{875}{3}(n-1)(n-2) f^{(2,2,2)} \right\} \quad (5.6)$$

and for the whole domain

$$E \approx \frac{n(2n+2)^{6/n}}{12096000} \left\{ F^{(6)} + 175(n-1) F^{(4,2)} + \frac{875}{3}(n-1)(n-2) F^{(2,2,2)} \right\} \left(\frac{V}{N}\right)^{6/n}. \quad (5.7)$$

For $n = 3$ the latter reduces to

$$E \approx \frac{1}{63000} \left\{ F^{(6)} + 350 F^{(4,2)} + \frac{1750}{3} F^{(2,2,2)} \right\} \left(\frac{V}{N}\right)^2. \quad (5.8)$$

As expected, the error from this rule is much smaller, and decreases with the computation time T as T^{-2} instead of as $T^{-4/3}$; however, the practical problems associated with the boundary cells are much more difficult than for third-degree rules.

In the discussion in Section 7 of integration over boundary cells in the three-dimensional case, we shall see that second-degree rules using only cubic lattice points are obtainable. Since the number of boundary cells is proportional to $V^{2/3}$ rather than to V, the total error still decreases with the total number of points N as $N^{-4/3}$. The numerical coefficient generally is larger than those obtained here, but since the boundary cells occupy only a small fraction of the domain this is not very serious.

6. The asymmetric product Simpson's rule

As mentioned in Section 2 the awkward boundaries of our (triton) domain suggest the use of an asymmetric-product Simpson's rule with different cells widths in different directions. As long as the boundaries are planes (or hyperplanes) passing through cubic lattice points, it is possible to use an asymmetric Simpson's product rule with cell width $g_1 h$ in the x_1 direction, $g_2 h$ in the x_2 direction and, in general, $g_i h$ in the x_i direction (where the g_i are integers). The volume of the cell is now $h^n \pi g_i$, and in terms of h the error per cell is estimated:

$$E_h \approx \pi g_i \,.\, h^{4+n} \left\{ \frac{1}{n} \sum_{i=1}^{n} \frac{d_4}{g_i^{-4}} \frac{\partial^4 f}{\partial x_i^4} + \frac{2}{n(n-1)} \sum_{i>j=1}^{n} \frac{d_{22}}{g_i^{-2} g_j^{-2}} \frac{\partial^4 f}{\partial x_i^2 \partial x_j^2} \right\}. \quad (6.1)$$

Cell width changes of this type are usually convenient only if the integration is carried out in each dimension in turn. The asymmetric product Simpson's rule of Section 2, where $n = 3$ and $g_i = 2^i$, leads to an estimate of total error

$$E \approx 0{\cdot}108 \left\{ \frac{1}{3} \int \left(\frac{\partial^4 f}{\partial x_3^4} + \frac{1}{16} \frac{\partial^4 f}{\partial x_2^4} + \frac{1}{256} \frac{\partial^4 f}{\partial x_1^4} \right) d\tau \right\} \left(\frac{V}{N}\right)^{4/3} \quad (6.2)$$

If the different partial derivatives are of the same magnitude, the figure 0·108 is directly comparable with the values of p_4 in Table 1, for example, with 0·0089 of rule 5 in that table.

Nevertheless, the asymmetric-product Simpson's rule is sometimes preferable. As one example, if the integrand varies much more slowly in one direction than in any other, then integrating last over that direction can improve the accuracy considerably. As another example, if the integrand is a product $k_1(x)\, k_2(y)\, k_3(z)$ the integration scheme (1.7) takes the form (for our domain)

$$J = \int_{r_0}^{R} dx\, k_1(x) \int_{r_0}^{x} dy\, k_2(y) \int_{Z_1}^{Z_2} d_z k_3(z) \quad (6.3)$$

where functions z_1 and z_2 are defined in (1.8); Simpson's rule can be used to tabulate the function

$$G(z) = \int_{r_0}^{z} k_3(\zeta) d\zeta \quad (6.4)$$

at intervals $2h$ in the variable z; then (6.3) is effectively a two-dimensional integral and can be evaluated more quickly than by a three-dimensional method. Product functions of this type do occur in the triton problem, and this method of evaluation has been used for them.

7. Boundaries

Boundary cells present special problems. The way in which cells are joined to give the integration rule for the whole domain is discussed in Section 8, but the process is certainly simpler if all cells are cubes or portions of cubes of width $2h$, and so we restrict our rules to those satisfying this condition.

The simplest illustration is the two-dimensional triangular-cell, a half square, defined by: $|x| \leqslant h$; $|y| \leqslant h$; $y \leqslant x$. [This type of cell, in three dimensions, occurs in the triton problem—see (1.4).] Because of symmetry about the line $x + y = 0$, certain points are equivalent and must have equal coefficients in the integration rule. We give the square lattice points of the cell, and their associated coefficients, in Table 4.

Because of the symmetry of this cell, polynomials obtained from one another by interchanging x and y give identical conditions, not independent ones; for example, the two conditions obtained by requiring that the integrals of x and y be computed exactly are both (7.2) below.

The conditions that the integrals of $x^a y^b$, with $a \geqslant b$ and $a + b \leqslant 2$ be computed exactly are

$$A_0 + 2A_1 + A_2 + 2A_2' = 1 \quad (a = b = 0) \tag{7.1}$$

$$A_1 + A_2 = 1/3 \quad (a = 1, b = 0) \tag{7.2}$$

$$A_1 + A_2 + 2A_2' = 1/3 \quad (a = 2, b = 0) \tag{7.3}$$

$$A_2 - 2A_2' = 0 \quad (a = b = 1). \tag{7.4}$$

These are four equations in four unknowns, so we expect that the integrals of x^3 and x^2y (neither of which are zero for *this* cell) will not be computed exactly, and that the rule for this cell will be only a second-degree one.

Equations (7.1)–(7.4) have the solution

$$A_0 = A_1 = 1/3; \; A_2' = A_2 = 0, \tag{7.5}$$

so the integration rule is

$$\iint_h f(x, y)dx\,dy \doteq \tfrac{2}{3}h^2\{f(0, 0) + f(h, 0) + f(0, -h)\}. \tag{7.6}$$

The estimate of error, in the notation of Section 4, is

$$E_h \approx (2h^2)\frac{h^3}{45}\{2f^{(3)} - 3f^{(2,1)}\}. \tag{7.7}$$

Not only is the error of order h^3 instead of h^4, but also the numerical coefficient is larger than for the complete square.

As the next illustration we take the half-cube, corresponding to the half-square cell above, defined by $|x| \leqslant h$; $|y| \leqslant h$; $|z| \leqslant h$ and $y \leqslant x$. There are eighteen cubic lattice points in this cell, and these are listed in Table 5. In principle we could write down eighteen or more equations for the coefficients, from the conditions that the integrals of $x^a y^b z^c$ for various a, b and c be computed exactly. The exact computation of the integrals of the low-degree polynomials obviously has first priority. Now solutions do exist for the set of ten equations with $a + b + c \leqslant 2$; but of the twenty equations with $a + b + c \leqslant 3$ the largest consistent set that includes the first set is the set of those sixteen for which $a + b \neq 3$. We see then, that although there is no third-degree rule for this cell using only the given cubic lattice points, there exists a *family* of second-degree rules. The choice available among them may be exploited in various ways to give rules suitable for particular purposes.

Table 5

Lattice points and associated coefficients for the half cube, $|x| \leqslant h$, $|y| \leqslant h$, $|z| \leqslant h$, $y \leqslant x$

x/h	y/h	z/h	$\frac{1}{4h^3} \times$ COEFFICIENT
0	0	0	B_0
0	−1	0	B_1
1	0	0	B_1
1	−1	0	B_2
1	1	0	B_2'
−1	−1	0	B_2'
0	0	±1	A_0
0	−1	±1	A_1
1	0	±1	A_1
1	−1	±1	A_2
1	1	±1	A_2'
−1	−1	±1	A_2'

The problem can first be simplified by taking advantage of the symmetry of the cell. The cell is symmetric about the $z = 0$ plane, so we impose the restriction on the coefficients $A(x, y, z)$ that $A(x, y, z) = A(x, y, -z)$. This reduces the number of independent coefficients to twelve, and simultaneously ensures that the integrals of all functions $f(z) \cdot g(x, y)$, where $f(z)$ is any odd function, are computed exactly. Then it becomes superfluous to impose the conditions that integrals of z, zx, zy, zx^2, zxy, zy^2, etc., be computed exactly, since these conditions are satisfied identically. Similarly, since the cell is symmetric about the plane $x + y = 0$, we put $A(x.\ y,\ z) = A(-x, -y, z)$, and then the integrals of all functions of the type $f(x + y) \cdot g(x - y, z)$, where f is any odd function, are computed exactly.

There remain only eight distinct coefficients. With $a + b + c \leqslant 2$ there are only five independent equations, leaving three degrees of freedom which may be used in various ways. Any solution of these five equations will compute exactly all the cubic integrals involving an odd power of z and also the integrals of $z^2(x + y)$ and $(x - y)^2(x + y)$. Of the remaining cubic integrals, that is one of z^2y and z^2x and three of x^3, x^2y, xy^2 and y^3, at most three can be computed exactly. We list here these five equations

$$B_0 + 2B_1 + B_2 + 2B_2' + 2A_0 + 4A_1 + 2A_2 + 4A_2' = 1 \tag{7.8}$$

$$B_1 + B_2 + 2A_1 + 2A_2 = \tfrac{1}{3} \tag{7.9}$$

$$B_1 + B_2 + 2B_2' + 2A_1 + 2A_2 + 4A_2' = \tfrac{1}{3} \tag{7.10}$$

$$B_2 - 2B_2' + 2A_2 - 4A_2' = 0 \tag{7.11}$$

$$2A_0 + 4A_1 + 2A_2 + 4A_2' = \tfrac{1}{3}. \tag{7.12}$$

The values (a, b, c) for these five equations are (0, 0, 0), (1, 0, 0), (2, 0, 0), (1, 1, 0) and (0, 0, 2), respectively.

We may use the three degrees of freedom in several distinct ways depending on the particular problem. These various ways are discussed in turn.

(i) We may minimize the error in the classical way. We define $J(a, b, c)$ as the integral of $x^a y^b z^c$ over the domain, and $I(a, b, c; A_0, A_1, \ldots, B_2')$ as the approximation to this result obtained by using a rule which has the coefficients $A_0, A_1, \ldots B_2'$. We further introduce $\mu(a, b, c)$, a weighting function which is arbitrary and can be adjusted to suit the particular function. We then minimize the function

$$\sum_{a+b+c=3} \mu(a, b, c)[I(a, b, c; A_0, A_1, \ldots B_2') - J(a, b, c)]^2$$

subject to the five conditions (7.8)–(7.12). Using the method of Lagrange's undetermined multipliers, we have to solve thirteen equations in thirteen unknowns.

(ii) We may make various coefficients zero. The "awkward points" mentioned in the Introduction may occur in a cell of this type at points whose coefficients are B_0 and A_2'. If we put

$$B_0 = A_2' = B_2' = 0 \tag{7.13}$$

the set of equations (7.8)–(7.13) has the solution

$$A_0 = 1/6; A_1 = -1/18; A_2 = 1/9; B_1 = 4/9; B_2 = -2/9.$$

This rule computes exactly the integral of z^2x and so also that of z^2y, and the error is estimated by

$$E_h \approx (4h^3)\frac{h^3}{90}\left\{2\left(\frac{\partial^3 f}{\partial x^2} + \frac{\partial^3 f}{\partial y^2}\right) - 3\left(\frac{\partial^3 f}{\partial x^2 \partial y} + \frac{\partial^3 f}{\partial x \partial y^2}\right)\right\}. \tag{7.14}$$

(iii) We may assign the coefficient zero to points which are shared with adjacent cells and would have zero coefficient but for this cell. Doing this reduces the total number of points at which the functions have to be evaluated in the whole domain, thereby reducing the integration time.

(iv) We may reduce rounding errors in the computed results. To do this we need some measure by which we can compare the rounding error produced by different rules. Let the integration rule use N integration points x_i and corresponding coefficients a_i. We define a coefficient t by

$$t = \frac{1}{V}\left[N \sum_{i=1}^{N} a_i^2\right]^{\frac{1}{2}} \tag{7.15}$$

where $V = \Sigma a_i = \int d\tau$, the volume of the domain. Suppose that the computer registers work to base r and have p "decimal" places. It can be shown (Kopal, 1955) that the r.m.s. rounding error, $\hat{e}$, produced by this rule and computer is given by

$$\hat{e} = \frac{1}{2\sqrt{3}} r^{-p} \frac{V}{\sqrt{N}} t. \tag{7.16}$$

The minimum value of t is 1, for a rule whose integration coefficients are all equal. Such a rule is known as a Chebyshev rule so we refer to t as the "Chebyshev coefficient." Suppose a domain consists of a number of cells each of the same size, and that integration rules are applied to each cell, each using the same number of points and each having the same value of t. If the cells do not share integration points then the Chebyshev coefficient of the rule for the whole domain is the same as that of the rule for a single cell; however, if points are shared it may be different. For the rules listed in Table 3 we give their Chebyshev coefficients t, taking into account the sharing of points and neglecting the effect of boundary cells. Thus if rounding errors are likely to be important we may use any extra degrees of freedom to construct or select a rule with the lowest possible value of t.

If the function to be integrated has a particular symmetry we may start again and arrange the coefficients so that low-degree polynomials of that symmetry only are computed exactly. This is quite distinct from and additional to the symmetry discussed in the earlier part of this Section. The integrands occurring in the triton problem are symmetric about the plane $x - y = 0$. Indeed this is the reason for the appearance of this plane in the list of boundaries. So we need to compute exactly the integrals of the low-degree polynomials in $(x - y)^2$ and $(x + y)$, but not that of $(x - y)$ itself. The eight coefficients have to be chosen to compute exactly the integrals of $(x + y)^r(x - y)^s z^t$ with s even. This can be easily arranged for $r + s \leqslant 3$ and $t \leqslant 3$. Two solutions are:

$$B_0 = 1/3; \quad A_2' = 1/48; \quad A_2 = 1/24; \text{ or (other coefficients zero)} \tag{7.17}$$

$$A_1 = 1/12; \quad B_1 = 1/6; \text{ (other coefficients zero).} \tag{7.18}$$

These are in fact the corner rule and the face-centre rule, respectively, applied to this cell. The reason that it is possible to do this is a direct result of the symmetry of the integrands about $x - y = 0$. The error E_h is just half that made by the corresponding rule for the cubic cell, and so is of order h^4. It must be emphasized that these rules are appropriate only if the integrand has this symmetry. For example, the rule given by (7.17) does not compute exactly $\int x d\tau$ over the cell, and if it were applied to a function without this symmetry the error would be of order h.

The types of cell other than the complete cube are classified in the next Section. Possible sets of coefficients A_s for each type are given in the Appendix.

8. Joining cells and changing cell size

We suppose at first that cells of each type are all the same size, that is that the whole domain is dissected into cells by three sets of parallel planes each set parallel to one of the coordinate planes and with members separated

by distance $2h$. Most cells are cubes but some, at the boundaries of the domain, are cubes truncated in various ways. Each cell is specified uniquely by the coordinates (x_c, y_c, z_c) of its "centre," where these satisfy the following condition:

$$x_c/h,\ y_c/h \text{ and } z_c/h \text{ are all odd integers.} \qquad (8.1)$$

(Note that the "cell centre" so defined is not necessarily centrally placed in the cell, and may even lie outside it.)

The points with coordinates (x, y, z) such that x/h, y/h and z/h are all integers, form a cubic lattice. A lattice point (x, y, z) belongs to those cells (x_c, y_c, z_c) for which each of the differences

$$x_s = x - x_c,\ y_s = y - y_c,\ z_s = z - z_c \qquad (8.2)$$

is one of h, 0 or $-h$. A lattice point generally, then, belongs to several adjacent cells; for example, a face-centre point belongs to two adjacent cells, and a vertex point to eight. To avoid the labour of having to compute the integrand eight times at each vertex point, for example, *we first accumulate the coefficients for the integration rule* and then multiply by the integrand.

For a single integration, the time saved thereby is probably not very significant. But, in practice, runs are repeated with slightly altered parameters, each time integrating over the same domain. Thus, the integration coefficients at all contributing points are computed (in the way to be described) first, and this information is stored on magnetic tape. In addition to the values of x, y, z, and the integration coefficient, for each contributing point, the tape also contains other functions $g(x, y, z)$ which are the same from run to run, and whose numerical values are needed to compute some of the integrands. In a computer with tape buffering, the tape is read block by block, one block being employed in the computation at the same time that the next block is being transferred to core memory. Thus, the table look-up process does not cost any time at all.

Let us now describe the process of accumulating the integration coefficients. In one dimension the process is trivial: Simpson's rule, with coefficients 1/6, 4/6, 1/6 for a cell, gives coefficients 1/6, 4/6, 2/6, 4/6, . . ., 2/6, 4/6, 1/6 for a connected line; but for a complicated domain in three dimensions the process is best programmed for a computer.

To locate the cell centre of each cell to which the lattice point (x, y, z) belongs, one finds the coordinates of each of its 27 neighbouring points in turn (including itself), by subtracting h, 0 or $-h$ from x, y, and z, and then testing which of these 27 points satisfy the requirement (8.1) for a cell centre. The number of cell centres found in this way is between one and eight. Then one finds, as described below, to what type of cell this cell centre belongs. If it is one which forms part of the domain, one looks up the coefficient A_s for the point (x_s, y_s, z_s) of that type of cell. The total integration coefficient for the point (x, y, z) is the sum of the coefficient A_s contributed by each of the adjacent cells.

Let us now discuss the boundary conditions (1.1)–(1.4) in more detail.* The conditions (1.2) and (1.3) define boundary planes each of which is perpendicular to a coordinate axis. If we impose the following condition:

$$r_0/h \text{ and } R/h \text{ are even integers,} \qquad (8.3)$$

then it follows that if not all six conditions (1.2) and (1.3) are satisfied for the cell *centre* (x_c, y_c, z_c), the cell is a wholly excluded cube and contributes nothing to the integration coefficient; if all are satisfied the other conditions must be applied.

Only three of the four other conditions (1.1) and (1.4) are independent, namely:

$$x - y \geqslant 0 \qquad (8.4)$$

$$x + y - z \geqslant 0 \qquad (8.5)$$

$$y + z - x \geqslant 0. \qquad (8.6)$$

Using (8.2) we now rewrite these conditions in terms of the cell-centre coordinates. We define three integers m_1, m_2, and m_3 by:

$$x_c - y_c = m_1 h \qquad (8.7)$$

$$x_c + y_c - z_c = m_2 h \qquad (8.8)$$

$$y_c + z_c - x_c = m_3 h. \qquad (8.9)$$

These and (8.1) imply that m_2 and m_3 are odd and m_1 is even. In terms of these integers conditions (8.4), (8.5), and (8.6) become

$$(x_s - y_s)/h + m_1 \geqslant 0 \qquad (8.10)$$

$$(x_s + y_s - z_s)/h + m_2 \geqslant 0 \qquad (8.11)$$

$$(y_s + z_s - x_s)/h + m_3 \geqslant 0. \qquad (8.12)$$

The quantities x_s/h, y_s/h and z_s/h each assume only the values 1, 0 or -1.

Let us take the application of condition (8.11) as an illustration. Now $-3 \leqslant (x_s + y_s - z_s)/h \leqslant 3$; so if for a particular cell $m_2 = 5$, for example, then (8.11) is satisfied for *all* x_s, y_s, z_s; i.e. every point of the cell lies inside this boundary. For a cell with $m_1 = 3$, (8.11) is still satisfied for all x_s, y_s, z_s, but one of its vertices, the vertex $(x_s, y_s, z_s) = (-h, -h, +h)$, lies on the boundary surface. Cells with $m_2 = 1$ or -1 are cubes truncated by the boundary surface $x + y - z = 0$; i.e. some of the points (x_s, y_s, z_s), satisfying (8.11), are included in the domain while others are excluded. Cells with $m_2 \leqslant -3$ are cubes lying entirely outside the domain (except when $m_2 = -3$ for a single point) and contribute nothing to the integration coefficient. Hence there are only four essentially different values of m_2: $m_2 \leqslant -3$; $m_2 = -1$; $m_2 = 1$; and $m_2 \geqslant 3$. The first corresponds to a cube outside the domain, contributing nothing; the next two correspond to interior cells formed by

* This discussion is rather specialized, but the methods outlined can be generalized easily to other boundary conditions. The restriction to our particular domain makes the exposition more definite and, we hope, easier to follow than a more general treatment.

truncated cubes; the last corresponds (as far as this boundary is concerned) to an interior cubic cell.

By a similar argument we find that m_3 takes the same four values, and with similar significance. The essentially different values for m_1 are: $m_1 \leqslant -2$; $m_1 = 0$; and $m_1 \geqslant 2$. The first corresponds to an exterior cube, contributing nothing; the second to an interior truncated cubic cell (such as the one discussed in Section 5); the third to an interior cubic cell.

We can now outline the steps taken by the computer. Once it has found, for the given lattice point (x, y, z), an adjacent cell centre (x_c, y_c, z_c) which satisfies conditions (1.2) and (1.3), it then computes integers m_1, m_2, m_3. Only if all three integers are greater than or equal to -1 is the cell an interior, contributing cell. There are thus at most $3 \times 3 \times 2 = 18$ distinct types of cell included within the domain.* (In fact seven of these do not occur.) The computer then classifies the cell by assigning numbers m_1', m_2' and m_3' as follows:

$$m_1' = \min(m_1, 2) \tag{8.13}$$

$$m_2' = \min(m_2, 3) \tag{8.14}$$

$$m_3' = \min(m_3, 3). \tag{8.15}$$

Stored in the computer is a table (occupying 486 storage locations) of coefficients A_s for each type of cell (m_1', m_2', m_3'), and each of the 27 points (x_s, y_s, z_s) of the cube containing that cell. Points outside the cell, because of the boundary surface truncations, are assigned zero coefficients. The computer looks up the relevant coefficient A_s and accumulates the sum of these coefficients, one for each contributing cell adjacent to the point (x, y, z). The final sum is the integration coefficient for that point.

This procedure, although rather awkward to describe, is simple to code, takes little computation time, and can be adapted to deal easily with *changes of cell size*.

Suppose one wants cells of width $4h$ instead of $2h$ in that part of the domain where all x, y and z exceed some value r_1. If we call the original domain, defined by (1.1) (1.4), $D(r_0, R)$, then the domain $D(r_1, R)$ must be dissected into cells of width $4h$ and the remainder into cells of width $2h$. If we call the remainder $D'(r_0, r_1, R)$, then

$$D(r_0, R) = D'(r_0, r_1, R) + D(r_1, R). \tag{8.16}$$

The treatment of $D(r_1, R)$ is simple if we make the following condition:

$$r_1/2h \text{ and } R/2h \text{ are even integers.} \tag{8.17}$$

Points in $D(r_1, R)$ can be treated as before except that (i) lattice points are defined by the condition that $x/2h$, etc., are integers, and (ii) the integration coefficient A_s for the point (x_s, y_s, z_s) of a cell of width $4h$ is multiplied by 8 before adding (since each cell has eight times the volume of the corresponding one of width $2h$).

The treatment of the $D'(r_0, r_1, R)$ is equally simple. One need only add the condition:

$$\text{At least one of } x_c, y_c, z_c \text{ is less than } r_1. \tag{8.18}$$

Since the boundary planes defined by this condition are parallel to coordinate planes it does not introduce any new type of cell. This condition is applied at the same time as those of (1.2) and (1.3), before the computation of m_1, m_2, and m_3.

A second change of cell width, from $4h$ to $8h$, is easily accomplished by the same method.

For this process of joining cells and computing integration coefficients, it is essential that the whole domain be dissected into mutually exclusive elementary cells, and that the integral over each cell be expressed in terms of function values at points of that cell alone. It is not essential for the points to lie on a cubic lattice.*

9. Acknowledgements

In conclusion let us remark that the methods adopted in our calculation and described here represent only a first approach to the problem of accurate and efficient numerical integration over asymmetric regions in many-dimensional spaces. In many cases our selection of a certain procedure was influenced by the need to obtain a working code in the limited time at our disposal. Further work on many-dimensional integration rules is in progress.

We would like to thank Professor R. Richtmyer, Professor E. Isaacson and Mr. M. Goldstein of the Institute of Mathematical Sciences, New York University, and Mr. B. de Ferranti of IBM, Sydney, for valuable discussions. We are grateful to the U.S. Atomic Energy Commission for enabling two of us (J. B. and D. M.) to visit New York, where most of this work was done.

* It is necessary to emphasize that this small number of cells is a direct result of the fact that each plane is of the form

$$\Sigma\, \alpha_i x_i + \beta \quad 0$$

where α_i and β are integers. This means that each plane passes through many cubic lattice points, and leads to m_1, m_2 and m_3 being integers.

* In our particular problem the typical integrand had the form $g(x, y, z)\, k_1(x)\, k_2(y)\, k_3(z)$, where the $g(x, y, z)$ were only a few rather simple, functions, which needed to be tabulated only once, for the whole calculation. The parameters of the problem were all contained in the functions k_i, which were tabulated as functions of one variable. By using a cubic lattice of integration points we avoided the need for interpolation and thus saved considerable time.

References

COURANT, R., and HILBERT, D. (1953). *Methods of Mathematical Physics*, Vol. I, Interscience.

DAVIS, P., and RABINOWITZ, P. (1956). "Monte Carlo Experiments in Computing Multiple Integrals," *Math. Tables Aids Comput.*, Vol. 10, p. 1.

DERRICK, G. (1959). "The Ground State of H^3," Ph.D. Thesis, Sydney University.

DERRICK, G., and BLATT, J. M. (1960). "Tensor and L.S. Forces in the Triton," *Nuclear Physics*, Vol. 17, p. 67.
HAMMER, P. C., and WYMORE, A. W. (1957). "Numerical Evaluation of Multiple Integrals I," *Math. Tables Aids Comput.*, Vol. 11, p. 59.
HAMMER, P. C., and STROUD, A. H. (1958). "Numerical Evaluation of Multiple Integrals II," *Math. Tables Aids Comput.*, Vol. 12, p. 272.
KOPAL, Z. (1955). *Numerical Analysis*, London: Chapman and Hall.
MILLER, J. C. P. (1960). "Numerical Quadrature Over a Rectangular Domain in Two or More Dimensions," *Math. Tables Aids Comput.*, Vol. 14, p. 13; Vol. 14, p. 130; Vol. 14, p. 240.

Appendix

During our investigation we prepared three lists of coefficients, each list satisfying different criteria of Section 7. These "Memmo Lists" are:

(i) M_1, which applies to any regular function, and does not exclude the awkward points;

(ii) M_2, which applies to regular functions symmetric in x and y, and does not exclude the awkward points;

(iii) M_3, which applies to regular functions, symmetric in x and y, and assigns zero coefficients to the awkward points, i.e. those on the line $x = y = z$.

All three lists minimize the number of points assigned non-zero coefficients. M_1 and M_2 use the corner rule for all cubic cells, and M_3 uses it except where it would introduce an awkward point. M_1 and M_2 differ only for cells adjacent to the boundary plane $x - y = 0$, i.e. with $M_1 = 0$.

We list in Table 6 all of M_1, M_2 and M_3.

As mentioned before, the integration time depends on the number of distinct points at which the function has to be evaluated, that is points with non-zero coefficient. This is in fact the reason for choosing the corner rule, as is discussed in Section 2.

It is important to be able to calculate, at least approximately, the number of points with non-zero coefficients, taking into account the additional points introduced because of boundary domains. We have already done this, exactly, in Section 2, in the case where the total domain is a cube. Rewriting formulas (2.2*a*) and (2.2*b*), the number of points N required using the corner rule in a cubic volume V with a net size h is given by

$$N = \frac{V}{(2h)^3} + \left(\frac{V^{1/3}}{(2h)} + 1\right)^3 \approx \frac{2V}{(2h)^3}. \qquad \text{(A.1)}$$

It is tempting to apply this formula to the actual domain, calculating separately the number of net points in each of the three domains of net size $2h$, $4h$ and $8h$ on the basis of their volumes. We might even expect an overestimate, on the grounds that certain points on the boundaries of two domains would be counted twice. In fact, however, as we shall illustrate by example, even when the number of points is of the order of 10,000, an estimate based on (A.1) is too small by a factor of about 2, due to the large number of additional points introduced by the truncated cubes on the surface of the domain.

We suppose that the domain $D(r_0, R)$ is divided into the three regions $D'(r_0, r_1, R)$, $D'(r_1, r_2, R)$ and $D(r_2, R)$ (see eqn. 8.16) with $r_0 < r_1 < r_2 < R$, by surfaces of the type (1.5), and that in these three regions we use cells of width $2h$, $4h$ and $8h$, respectively. We define by $N(r_i, R; nh)$ the number of points used within and on the surface of $D(r_i, R)$ when the cell width is nh, and by $S(r_i, R, nh)$ the number of these which lie on the net-change boundary, i.e. which are common to $D(r_i, R)$ and $D'(r_0, r_i, R)$. In this case the total number of points used is given by

$$\begin{aligned} N = {} & N(r_0, R; 2h) - N(r_1, R; 2h) + S(r_1, R; 2h) \\ & + N(r_1, R; 4h) - N(r_2, R; 4h) + S(r_2, R; 4h) \\ & + N(r_2, R; 8h) - S(r_1, R; 4h) - S(r_2, R; 8h). \end{aligned} \qquad \text{(A.2)}$$

The first three terms are the number in $D'(r_0, r_1, R)$, the second three the number in $D'(r_1, r_2, R)$, the seventh the number in $D(r_2, R)$, and the final two terms subtract the number of points on net-change boundaries counted twice.

The functions N and S depend on the Memmo list used. If we write

$$j = \frac{R - r}{nh}; \qquad k = \max\left(\frac{R - 2r}{nh}, 0\right), \qquad \text{(A.3)}$$

these functions for M_3 with $r_0 \neq 0$ are given by

$$\begin{aligned} S(r, R; nh) &= [(2j + 1)(j + 1) - \tfrac{1}{2}k(3k + 1)] \\ N(r, R; nh) &= \tfrac{1}{2}[(2j^2 + 3j + 2)(j + 1) - k(k + 1)^2] \\ &\quad + \tfrac{1}{2}(9k^2 + 19k) + 11j - 18. \end{aligned} \qquad \text{(A.4)}$$

(The terms in square brackets are in fact the exact number of block vertex and centre points in the region, whether with zero coefficient or not. The final terms in (A.4) are quadratically correct, and refer to M_3 with $r_0 \neq 0$.)

As an illustration we apply this formula to calculate the number of points when $(r_0, r_1, r_2, R) = (6, 12, 24, 96)h$. In this case equation (A.1) reads $N = 6{,}196 \approx 5{,}319$ and (A.2) to (A.4) give $N = 11{,}653$. Using a previous Memmo list, which instead of minimizing the number of points, used criterion (i) of Section 7, the same domain used $N = 14{,}000$ points. These figures illustrate the importance of making a valid estimate of the number of points used, and the importance of using a Memmo list which minimizes the number of points.

Table 6

The "Memmo" lists

The coefficients are "normalized" so that the volume of a cube of side $2h$ is $8640 = 18 \times 480 = 2^6 \times 3^3 \times 5$. Lists M_1 and M_2 may be read directly from the table.

List M_3 may be obtained from the lists M_2 and M_3' of the table. The coefficients in list M_2 should be used, unless the condition in the final column is satisfied. In these cases the coefficients of list M_2 would assign a non-zero coefficient to an awkward point, and the coefficients in list M_3' should be used instead.

BLOCK	POINT	COEFFICIENT			
$m_1'\ m_2'\ m_3'$	$\frac{x}{h}\ \frac{y}{h}\ \frac{z}{h}$	M_1	M_2	M_3'	CONDITION THAT M_3' BE USED INSTEAD OF M_2 TO FORM M_3
0 −1 3	0 0 −1	180	144	180	if centre is (1, 1, 3)
	1 −1 −1	−15	−72	−72	
	1 0 −1	162	288	216	
	1 0 0	228	288	288	
	1 1 −1	0	−36	0	
	1 1 0	198	144	144	
	1 1 1	−33	−36	− 36	
0 1 1	−1 −1 −1	−90	0	0	if centre is (1, 1, 1) i.e. always
	0 −1 0	504	0	288	
	0 0 −1	108	0	324	
	0 0 0	864	1584	0	
	0 0 1	−36	0	684	
	1 −1 1	−108	216	−72	
	1 0 0	216	0	1008	
	1 0 1	576	0	−144	
	1 1 −1	90	108	−216	
	1 1 0	0	0	288	
	1 1 1	36	252	0	
0 1 3	−1 −1 −1	−162	396	236	if centre is (3, 3, 5)
	0 −1 −1	0	−576	−192	
	0 −1 0	1080	−480	−224	
	0 0 −1	972	0	0	
	0 0 0	0	3504	2736	
	0 0 1	252	−240	−112	
	1 −1 −1	72	840	456	
	1 −1 0	0	−576	−192	
	1 −1 1	−36	792	472	
	1 0 −1	0	0	256	
	1 0 0	1368	0	0	
	1 0 1	0	−576	−192	
	1 1 −1	−126	96	0	
	1 1 0	0	0	128	
	1 1 1	180	420	228	
0 3 1	−1 −1 −1	36	36	0	if centre is (3, 3, 1)
	−1 −1 1	36	252	0	
	0 −1 0	432	0	1152	
	0 −1 1	432	0	0	
	0 0 −1	0	0	72	
	0 0 0	1152	2016	−288	
	0 0 1	0	0	1080	
	1 −1 1	−144	288	−288	
	1 0 0	432	0	1152	
	1 0 1	432	0	0	
	1 1 −1	36	36	0	
	1 1 1	36	252	0	
0 3 3	−1 −1 −1	0	180	0	if $\lvert m_2 - m_3 \rvert \leqslant 4$
	−1 −1 1	0	180	0	
	0 −1 0	1440	0	1440	
	0 0 −1	720	0	720	
	0 0 0	0	2880	0	
	0 0 1	720	0	720	
	1 −1 −1	0	360	0	
	1 −1 1	0	360	0	
	1 0 0	1440	0	1440	
	1 1 −1	0	180	0	
	1 1 1	0	180	0	
2 −1 3	−1 1 −1		−72		
	0 0 −1		288		
	0 1 −1		288		
	0 1 0		288		
	1 −1 −1		−72		
	1 0 −1		288		
2 −1 3	1 0 0		288		
	1 1 −1		−72		
	1 1 0		288		
	1 1 1		−72		
2 1 1	−1 −1 −1		72	576	if centre is (3, 1, 3)
	−1 1 −1		504	0	
	−1 1 1		288	288	
	0 −1 0		0	−1008	
	0 0 0		4032	4032	
	0 1 0		0	1008	
	1 −1 1		72	576	
	1 1 −1		288	288	
	1 1 1		504	0	
2 1 3	−1 −1 −1		792		
	−1 0 −1		−576		
	−1 0 0		−480		
	−1 1 −1		840		
	−1 1 0		−576		
	−1 1 1		792		
	0 −1 −1		−576		
	0 −1 0		−480		
	0 0 0		7008		
	0 0 1		−480		
	0 1 1		−576		
	1 −1 −1		840		
	1 −1 0		−576		
	1 −1 1		792		
	1 0 1		−576		
	1 1 −1		192		
	1 1 1		840		
2 3 −1	−1 −1 1		−72	36	if centre is (3, 1, 1)
	−1 0 0		288	0	
	−1 0 1		288	144	
	−1 1 −1		−72	−72	
	−1 1 0		288	864	
	−1 1 1		−72	0	
	0 0 1		288	288	
	0 1 0		288	0	
	0 1 1		288	144	
	1 1 1		−72	36	
2 3 1	−1 −1 −1		792	472	if centre is (5, 3, 3)
	−1 −1 0		−576	−192	
	−1 −1 1		840	456	
	−1 0 −1		−576	−192	
	−1 0 1		0	256	
	−1 1 −1		840	456	
	−1 1 0		0	256	
	−1 1 1		192	0	
	0 −1 0		−480	−224	
	0 −1 1		−576	−192	
	0 0 −1		−480	−224	
	0 0 0		7008	5472	
	0 1 −1		−576	−192	
	0 1 1		0	256	
	1 −1 1		792	472	
	1 0 0		−480	−224	
	1 0 1		−576	−192	
	1 1 −1		792	472	
	1 1 0		−576	−192	
	1 1 1		840	456	
2 3 3	−1 −1 −1		360	0	if both $m_1 = 2$ and $\lvert m_2 - m_3 - 2 \rvert \leqslant 2$
	−1 −1 1		360	0	
	−1 0 0		0	1440	
	−1 1 −1		360	0	
	−1 1 1		360	0	
	0 −1 0		0	1440	
	0 0 −1		0	1440	
	0 0 0		5760	0	
	0 0 1		0	1440	
	0 1 0		0	1440	
	1 −1 −1		360	0	
	1 −1 1		360	0	
	1 0 0		0	1440	
	1 1 −1		360	0	
	1 1 1		360	0	