JAERI-M
92-099

NUMERICAL EVALUATION OF GENERAL n-DIMENSIONAL INTEGRALS BY THE REPEATED USE OF NEWTON-COTES FORMULAS

July 1992

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編集兼発行　日本原子力研究所
印　　刷　日立高速印刷株式会社

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Numerical Evaluation of General n-Dimensional Integrals by the Repeated Use of Newton-Cotes Formulas

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(Received June 4, 1992)

The composite Simpson's rule is extended to n-dimensional integrals with variable limits. This extension is illustrated by means of the recursion relation of n-fold series. The structure of calculation by the Newton-Cotes formulas for n-dimensional integrals is clarified with this method. A quadrature formula corresponding to the Newton-Cotes formulas can be readily constructed. The results computed for some examples are given, and the error estimates for two or three dimensional integrals are described using the error term.

Keywords : Numerical Integration, Multiple Integral, Simpson's Rule, Newton-Cotes Formula

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Newton－Cotes式の繰り返し使用による一般多重積分の数値計算

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(1992年6月4日受理)

複合Simpson公式を積分の上下限が可変であるn次元積分に拡張した。この拡張はn次級数の漸化式によって示した。この方法により，n次元の積分に対し，Newton－Cotes式による計算構造を明らかにした。その結果，Newton－Cotes式に対応する求積式が容易に組み立てられるようになった。若干の計算例を示し，2次元および3次元積分に対する誤差の評価を誤差項を用いて記述した。

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1. Introduction

Since a paper giving two formulas for numerical integration in higher dimensions was published by Maxwell [17], the numerical evaluation of multiple integrals has been devised variously [1,10,12,14,19,20]. The most natural approach to the evaluation of n-dimensional integrals among them is through the repeated application of one dimensional quadrature formula to each variable [11,15]. There are two types in the quadrature formulas; the Newton-Cotes formulas and the Gauss formulas [1,3,5,7,9]. The former that contains the Simpson 3-point (closed) rule as a special case has convenient weights and uses function values at equally spaced points. The latter uses function values at unequally spaced points, determined by certain properties of orthogonal polynomials. In this paper we discuss the extension of the Newton-Cotes formulas to higher dimensions. Simpson's rule method has been employed for numerical integration with constant limits [3,4,6,7]. On the other hand, for numerical integration in which the domains of integral are variable, as far as we know, an application of Simpson's rule method to such integration is rarely seen in the library of computer programs [16,18], a book [7], and a paper [8]. Cadwell illustrated an algorithm by Simpson's rule for n-dimensional integrals [8]. However, it is difficult to construct the other Newton-Cotes formulas by analogy with them, because the domains of integration in higher dimensions are complicated. Fröberg has stated that it is possible, in principle at least, to construct a formula corresponding to the Newton-Cotes formulas and the Gauss formulas, but it is extremely clumsy and awkward [13].

The purpose of this work is to clarify, using the composite Simpson's rule, the structure of calculation by the Newton-Cotes formulas for n-dimensional iterated integrals. Its structure is illustrated by means of the recursion relation of n-fold series. This method is readily applicable to the other Newton-Cotes formulas (in the closed or the open ones). We give the numerical values computed for some examples and will estimate, using the error term of Simpson's rule or the Newton-Cotes 5-point rule, the error of numerical evaluation for two or three dimensional integrals.

We assume that the integrand of a given integral in higher dimensions is analytic over the range of integration except at the end points and the function which indicates the domain of integration is also analytic.

2. The one-dimensional definite integral

We begin our discussion with the definite integral of function of one variable, although known, for evaluating numerical integration in higher dimensions.

Let

$$(1) \qquad \int_a^b dx\ f(x)$$

be the integral to be evaluated.

If the interval (a, b) is divided into M equal subintervals, set $f_{2i-2} = f(x_{2i-2})$ for the function values at equally-spaced values of variable x:

$$(2) \qquad x_{2i-2} = a + (2i-2)h, \qquad (i=1,2,3,\dots,M)$$

where $h = \frac{1}{2M}(b - a)$. Then,

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where $h = \frac{1}{2M}(b - a)$. Then,

$$\int_a^b dx\ f(x) = \sum_{i=1}^{M} \frac{h}{3} \{f_{2i-2} + 4f_{2i-1} + f_{2i}\} + \sum_{i=1}^{M} E_i$$

$$= \sum_{i=1}^{M} F_i + \sum_{i=1}^{M} E_i, \tag{3}$$

where $F_i = \frac{h}{3} \{f_{2i-2} + 4f_{2i-1} + f_{2i}\}$ and E_i is the error term given by $-\frac{h^5}{90} f_x^{(4)}(\xi_i)$, where $x_{2i-2} \leq \xi_i \leq x_{2i}$. For the sake of simplicity, we discuss numerical integration in higher dimensions aside from the error term. The error of such integration is described in Section 8. Since the first term on the right side of (3) is of the form of series, let it be represented by the recursion relation. Then, we have the following formula

$$S_i = S_{i-1} + F_i, \tag{4}$$

where S_i gives a partial sum of the i-th, and the 0-th partial sum $S_0 = 0$. The integral of (1) is approximated by using eq.(4).

3. The two-dimensional integral with constant limits

Let

$$\int_a^b dx \int_c^d dy\ f(x,y) \tag{5}$$

be the integral to be evaluated.

Suppose that the interval (a, b) on the x-coordinate and the interval (c, d) on the y-coordinate are divided into M and N equal subintervals, respectively. To show how a quadrature formula for the integral of (5) could be constructed using Simpson's rule, we will use the recursion relation of a double series $\sum_{i=1}^{M} \sum_{j=1}^{N} F_{i,j}$. For that purpose, we associate the sum of

$$\int_a^b dx\, f(x) = \sum_{i=1}^{M} \frac{h}{3} \{f_{2i-2} + 4f_{2i-1} + f_{2i}\} + \sum_{i=1}^{M} E_i$$

$$= \sum_{i=1}^{M} F_i + \sum_{i=1}^{M} E_i, \qquad (3)$$

where $F_i = \frac{h}{3} \{f_{2i-2} + 4f_{2i-1} + f_{2i}\}$ and E_i is the error term given by $-\frac{h^5}{90} f_x^{(4)}(\xi_i)$, where $x_{2i-2} \le \xi_i \le x_{2i}$. For the sake of simplicity, we discuss numerical integration in higher dimensions aside from the error term. The error of such integration is described in Section 8. Since the first term on the right side of (3) is of the form of series, let it be represented by the recursion relation. Then, we have the following formula

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(6) $$S_{M,N} = \sum_{j=1}^{N} \{(S_{M-1,j} - S_{M-1,j-1}) + F_{M,j}\},$$

where $F_{M,j}$ takes the form of $\frac{h}{3}$ $\{G_{2M-2,j} + 4G_{2M-1,j} + G_{2M,j}\}$, and $h = \frac{1}{2M}$ (b - a). The $G_{2M-2,j}$ has the form given by $\frac{k}{3}$ x x $\{f(x_{2M-2}, y_{2j-2}) + 4f(x_{2M-2}, y_{2j-1}) + f(x_{2M-2}, y_{2j})\}$ and $k = \frac{1}{2N}$ (d - c), and so on. By induction, we expand the right side of (6) with respect to j. If, in a formula obtained, we replace M, N by i, j, then (6) is given by

(7) $$S_{i,j} = S_{i-1,j} + S_{i,j-1} - S_{i-1,j-1} + F_{i,j}.$$

Equation (7) expresses the recursion relation for a double series. When the method of Section 2 is applied to this case, a quadrature formula for the integral of (5) can be immediately written down in the explicit form:

(8.1) $$h = \frac{1}{2M} (b - a)$$

$$x_1 = a + (2i - 2)h$$

(8.2) $$x_2 = a + (2i - 1)h$$

$$x_3 = a + 2ih$$

(8.3) $$k = \frac{1}{2N} (d - c)$$

$$y_1 = c + (2j - 2)k$$

(8.4) $$y_2 = c + (2j - 1)k$$

$$y_3 = c + 2jk$$

$$G_{2i-2,j} = \frac{k}{3}\{f(x_1,y_1) + 4f(x_1,y_2) + f(x_1,y_3)\}$$

(8.5) $$G_{2i-1,j} = \frac{k}{3}\{f(x_2,y_1) + 4f(x_2,y_2) + f(x_2,y_3)\}$$

$$G_{2i,j} = \frac{k}{3}\{f(x_3,y_1) + 4f(x_3,y_2) + f(x_3,y_3)\}$$

(8.6) $$F_{i,j} = \frac{h}{3}\{G_{2i-2,j} + 4G_{2i-1,j} + G_{2i,j}\}$$

$$S_{i,j} = S_{i-1,j} + S_{i,j-1} - S_{i-1,j-1} + F_{i,j},$$

where $S_{00} = S_{i0} = S_{0j} = 0$,

or

(9) $$S_{M,N} = \sum_{i=1}^{M} \sum_{j=1}^{N} F_{i,j}.$$

4. The two-dimensional integral with variable limits

Let

(10) $$\int_a^b dx \int_{F_1(x)}^{F_2(x)} dy\ f(x,y)$$

be the integral to be evaluated.

Suppose that the interval (a, b) on the x-coordinate and the interval $\{F_1(x),\ F_2(x)\}$ on the y-coordinate are divided into M and N subintervals, respectively. On taking note of the domain of the second integral of (10), we will attempt to change the formula of step size (8.3) in the following

$$k_1 = \frac{1}{2N}\{F_2(x_1) - F_1(x_1)\}$$

(11) $$k_2 = \frac{1}{2N}\{F_2(x_2) - F_1(x_2)\}$$

(8.4) $$y_2 = c + (2j - 1)k$$

$$y_3 = c + 2jk$$

$$G_{2i-2,j} = \frac{k}{3} \{f(x_1,y_1) + 4f(x_1,y_2) + f(x_1,y_3)\}$$

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(8.6) $$F_{i,j} = \frac{h}{3} \{G_{2i-2,j} + 4G_{2i-1,j} + G_{2i,j}\}$$

$$S_{i,j} = S_{i-1,j} + S_{i,j-1} - S_{i-1,j-1} + F_{i,j},$$

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$$k_3 = \frac{1}{2N} \{F_2(x_3) - F_1(x_3)\}.$$

Then, the arguments y_i in (8.4) and the G_{2i-2}, G_{2i-1}, etc. in (8.5) should also be rewritten in the following

$$y_{11} = F_1(x_1) + (2j - 2)k_1$$

$$y_{12} = F_1(x_1) + (2j - 1)k_1$$

$$y_{13} = F_1(x_1) + 2jk_1$$

$$y_{21} = F_1(x_2) + (2j - 2)k_2$$

(12) $$y_{22} = F_1(x_2) + (2j - 1)k_2$$

$$y_{23} = F_1(x_2) + 2jk_2$$

$$y_{31} = F_1(x_3) + (2j - 2)k_3$$

$$y_{32} = F_1(x_3) + (2j - 1)k_3$$

$$y_{33} = F_1(x_3) + 2jk_3$$

and

$$G_{2i-2,j} = \frac{k_1}{3} \{f(x_1,y_{11}) + 4f(x_1,y_{12}) + f(x_1,y_{13})\}$$

(13) $$G_{2i-1,j} = \frac{k_2}{3} \{f(x_2,y_{21}) + 4f(x_2,y_{22}) + f(x_2,y_{23})\}$$

$$G_{2i,j} = \frac{k_3}{3} \{f(x_3,y_{31}) + 4f(x_3,y_{32}) + f(x_3,y_{33})\}.$$

Substituting (13) into (8.6), we can evaluate numerically the integral of (10). One may now easily write down, using similar summation procedures, a quadrature formula of the other Newton-Cotes formulas for two-dimensional integrals.

5. The three-dimensional integral

Let

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y_{13} &= F_1(x_1) + 2jk_1 \\
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y_{22} &= F_1(x_2) + (2j - 1)k_2 \\
y_{23} &= F_1(x_2) + 2jk_2 \\
y_{31} &= F_1(x_3) + (2j - 2)k_3 \\
y_{32} &= F_1(x_3) + (2j - 1)k_3 \\
y_{33} &= F_1(x_3) + 2jk_3
\end{aligned} \tag{12}$$

and

$$\begin{aligned}
G_{2i-2,j} &= \frac{k_1}{3} \{f(x_1, y_{11}) + 4f(x_1, y_{12}) + f(x_1, y_{13})\} \\
G_{2i-1,j} &= \frac{k_2}{3} \{f(x_2, y_{21}) + 4f(x_2, y_{22}) + f(x_2, y_{23})\} \\
G_{2i,j} &= \frac{k_3}{3} \{f(x_3, y_{31}) + 4f(x_3, y_{32}) + f(x_3, y_{33})\}.
\end{aligned} \tag{13}$$

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5. The three-dimensional integral

Let

$$(14) \quad \int_a^b dx \int_{F_1(x)}^{F_2(x)} dy \int_{F_1(x,y)}^{F_2(x,y)} dz\ f(x,y,z)$$

be the integral to be evaluated.

Suppose that the interval (a, b) on the x-coordinate, the interval $(F_1(x),\ F_2(x))$ on the y-coordinate and the interval $(F_1(x,y),\ F_2(x,y))$ on the z-coordinate are, respectively, divided into L, M and N subintervals.

We will use the recursion relation of a triple series $\sum_{i=1}^{M} \sum_{j=1}^{N} \sum_{k=1}^{L} F_{i,j,k}$. For that purpose, we associate the sum of functional value of $F_{i,j,k}$ at any grid point (i, j, k) in three dimensions to the partial sum of $S_{i,j,k}$, which is the sum of the value of $F_{i,j,k}$. Then, we make use of (7). Assuming that the partial sum of the L-, M-th terms in a triple series could be found, let us put the sum of k from 1 to N in the form

(15)

$$S_{L,M,N} = \sum_{k=1}^{N} \{(S_{L-1,M,k} - S_{L-1,M,k-1}) + (S_{L,M-1,k} - S_{L,M-1,k-1}) - - (S_{L-1,M-1,k} - S_{L-1,M-1,k-1}) + F_{L,M,k}\},$$

where $F_{L,M,k}$ takes the form of Simpson's rule. Proceeding as before, we obtain the formula analogous to (7),

(16)

$$S_{i,j,k} = S_{i-1,j,k} + S_{i,j-1,k} + S_{i,j,k-1} - S_{i-1,j-1,k} - S_{i-1,j,k-1} - S_{i,j-1,k-1} + S_{i-1,j-1,k-1} + F_{i,j,k}.$$

Equation (16) expresses the recursion relation for a triple series. When the method of Sections 2, 3 and 4 is applied to this case, we may write down a quadrature formula for the integral of (14) using Simpson's rule:

$$h = \frac{1}{2L}(b - a)$$

$$x_1 = a + (2i - 2)h$$

....

$$x_3 = a + 2ih$$

$$k_1 = \frac{1}{2M}\{F_2(x_1) - F_1(x_1)\}$$

$$k_2 = \frac{1}{2M}\{F_2(x_2) - F_1(x_2)\}$$

$$k_3 = \frac{1}{2M}\{F_2(x_3) - F_1(x_3)\}$$

$$y_{11} = F_1(x_1) + (2j - 2)k_1$$

$$y_{12} = F_1(x_1) + (2j - 1)k_1$$

$$y_{13} = F_1(x_1) + 2jk_1$$

....

$$y_{33} = F_1(x_3) + 2jk_3$$

$$k_{11} = \frac{1}{2N}\{F_2(x_1, y_{11}) - F_1(x_1, y_{11})\}$$

$$k_{12} = \frac{1}{2N}\{F_2(x_1, y_{12}) - F_1(x_1, y_{12})\}$$

$$k_{13} = \frac{1}{2N}\{F_2(x_1, y_{13}) - F_1(x_1, y_{13})\}$$

....

$$k_{33} = \frac{1}{2N}\{F_2(x_3, y_{33}) - F_1(x_3, y_{33})\}$$

$$z_{111} = F_1(x_1, y_{11}) + (2k - 2)k_{11}$$

$$z_{112} = F_1(x_1, y_{11}) + (2k - 1)k_{11}$$

$$z_{113} = F_1(x_1, y_{11}) + 2kk_{11}$$

$$z_{121} = F_1(x_1, y_{12}) + (2k - 2)k_{12}$$

$$z_{122} = F_1(x_1, y_{12}) + (2k - 1)k_{12}$$

$$z_{123} = F_1(x_1, y_{12}) + 2kk_{12}$$

....

$$z_{333} = F_1(x_3, y_{33}) + 2kk_{33}$$

$$G_{2i-2,2j-2,k} = \frac{k_{11}}{3} \{f(x_1, y_{11}, z_{111}) + 4f(x_1, y_{11}, z_{112}) + f(x_1, y_{11}, z_{113})\}$$

$$G_{2i-2,2j-1,k} = \frac{k_{12}}{3} \{f(x_1, y_{12}, z_{121}) + 4f(x_1, y_{12}, z_{122}) + f(x_1, y_{12}, z_{123})\}$$

$$G_{2i-2,2j,k} = \frac{k_{13}}{3} \{f(x_1, y_{13}, z_{131}) + 4f(x_1, y_{13}, z_{132}) + f(x_1, y_{13}, z_{133})\}$$

....

$$G_{2i,2j,k} = \frac{k_{33}}{3} \{f(x_3, y_{33}, z_{331}) + 4f(x_3, y_{33}, z_{332}) + f(x_3, y_{33}, z_{333})\}$$

$$H_{2i-2,j,k} = \frac{k_1}{3} \{G_{2i-2,2j-2,k} + 4G_{2i-2,2j-1,k} + G_{2i-2,2j,k}\}$$

$$H_{2i-1,j,k} = \frac{k_2}{3} \{G_{2i-1,2j-2,k} + 4G_{2i-1,2j-1,k} + G_{2i-1,2j,k}\}$$

$$H_{2i,j,k} = \frac{k_3}{3} \{G_{2i,2j-2,k} + 4G_{2i,2j-1,k} + G_{2i,2j,k}\}$$

$$F_{i,j,k} = \frac{h}{3} \{H_{2i-2,j,k} + 4H_{2i-1,j,k} + H_{2i,j,k}\}$$

$$S_{i,j,k} = S_{i-1,j,k} + S_{i,j-1,k} + S_{i,j,k-1} - S_{i-1,j-1,k} -$$

$$- S_{i-1,j,k-1} - S_{i,j-1,k-1} + S_{i-1,j-1,k-1} + F_{i,j,k},$$

where $S_{000} = S_{0jk} = S_{i0k} = S_{ij0} = S_{00k} = S_{i00} = S_{0j0} = 0$.

or

(18) $$S_{L,M,N} = \sum_{i=1}^{L} \sum_{j=1}^{M} \sum_{k=1}^{N} F_{i,j,k}.$$

6. The four-dimensional integral

Let

(19) $$\int_a^b dx^1 \int_{F_1(x^1)}^{F_2(x^1)} dx^2 \int_{F_1(x^1,x^2)}^{F_2(x^1,x^2)} dx^3 \int_{F_1(x^1,x^2,x^3)}^{F_2(x^1,x^2,x^3)} dx^4 \times$$
$$\times f(x^1,x^2,x^3,x^4)$$

be the integral to be evaluated.

Suppose that the interval on each direction in four-dimensional spaces is divided into N_1, N_2, N_3 and N_4 subintervals. Using similar summation procedures, we obtain the recursion relation of a quadruple series:

(20) $$S_{i,j,k,l} = \Sigma_{i-1,j,k,l} - \Sigma_{i-1,j-1,k,l} + \Sigma_{i-1,k-1,j-1,l} -$$
$$- S_{i-j,j-1,k-1,l-1} + F_{i,j,k,l},$$

where

$$\Sigma_{i-1,j,k,l} = S_{i-1,j,k,l} + S_{i.j-1,k,l} + S_{i,j,k-1,l} + S_{i,j,k,l-1},$$

$$\Sigma_{i-1,j-1,k,l} = S_{i-1,j-1,k,l} + S_{i-1,j,k-1,l} + S_{i-1,j,k,l-1} +$$
$$+ S_{i,j-1,k-1,l} + S_{i,j-1,k,l-1} + S_{i,j,k-1,l-1},$$

$$\Sigma_{i-1,j-1,k-1,l} = S_{i-1,j-1,k-1,l} + S_{i-1,j-1,k,l-1} +$$
$$+ S_{i-1,j,k-1,l-1} + S_{i,j-1,k-1,l-1},$$

$$- S_{i-1,j,k-1} - S_{i,j-1,k-1} + S_{i-1,j-1,k-1} + F_{i,j,k},$$

where $S_{000} = S_{0jk} = S_{i0k} = S_{ij0} = S_{00k} = S_{i00} = S_{0j0} = 0.$

or

(18) $$S_{L,M,N} = \sum_{i=1}^{L} \sum_{j=1}^{M} \sum_{k=1}^{N} F_{i,j,k}.$$

6. The four-dimensional integral

Let

(19) $$\int_a^b dx^1 \int_{F_1(x^1)}^{F_2(x^1)} dx^2 \int_{F_1(x^1,x^2)}^{F_2(x^1,x^2)} dx^3 \int_{F_1(x^1,x^2,x^3)}^{F_2(x^1,x^2,x^3)} dx^4 \times$$

$$\times f(x^1,x^2,x^3,x^4)$$

be the integral to be evaluated.

Suppose that the interval on each direction in four-dimensional spaces is divided into N_1, N_2, N_3 and N_4 subintervals. Using similar summation procedures, we obtain the recursion relation of a quadruple series:

(20) $$S_{i,j,k,l} = \Sigma_{i-1,j,k,l} - \Sigma_{i-1,j-1,k,l} + \Sigma_{i-1,k-1,j-1,l} -$$

$$- S_{i-j,j-1,k-1,l-1} + F_{i,j,k,l},$$

where

$$\Sigma_{i-1,j,k,l} = S_{i-1,j,k,l} + S_{i.j-1,k,l} + S_{i,j,k-1,l}$$

$$+ S_{i,j,k,l-1},$$

$$\Sigma_{i-1,j-1,k,l} = S_{i-1,j-1,k,l} + S_{i-1,j,k-1,l} + S_{i-1,j,k,l-1} +$$

$$+ S_{i,j-1,k-1,l} + S_{i,j-1,k,l-1} + S_{i,j,k-1,l-1},$$

$$\Sigma_{i-1,j-1,k-1,l} = S_{i-1,j-1,k-1,l} + S_{i-1,j-1,k,l-1} +$$

$$+ S_{i-1,j,k-1,l-1} + S_{i,j-1,k-1,l-1},$$

and $F_{i,j,k,l}$ takes the form of Simpson's rule. We may write down a quadrature formula for the integral of (19) using Simpson's rule:

$$h = \frac{1}{2N_1}(b - a)$$

$$x_1^1 = a + (2i - 2)h$$

$$x_2^1 = a + (2i - 1)h$$

$$x_3^1 = a + 2ih$$

$$k_1 = \frac{1}{2N_2}\{F_2(x_1^1) - F_1(x_1^1)\}$$

$$k_2 = \frac{1}{2N_2}\{F_2(x_2^1) - F_1(x_2^1)\}$$

$$k_3 = \frac{1}{2N_2}\{F_2(x_3^1) - F_1(x_3^1)\}$$

$$x_{11}^2 = F_1(x_1^1) + (2j - 2)k_1$$

$$x_{12}^2 = F_1(x_1^1) + (2j - 1)k_1$$

$$x_{13}^2 = F_1(x_1^1) + 2jk_1$$

....

$$x_{33}^2 = F_1(x_3^1) + 2jk_3$$

$$k_{11} = \frac{1}{2N_3}\{F_2(x_1^1, x_{11}^2) - F_1(x_1^1, x_{11}^2)\}$$

$$k_{12} = \frac{1}{2N_3}\{F_2(x_1^1, x_{12}^2) - F_1(x_1^1, x_{12}^2)\}$$

$$k_{13} = \frac{1}{2N_3}\{F_2(x_1^1, x_{13}^2) - F_1(x_1^1, x_{13}^2)\}$$

$$k_{21} = \frac{1}{2N_3}\{F_2(x_2^1, x_{21}^2) - F_1(x_2^1, x_{21}^2)\}$$

....

$$k_{33} = \frac{1}{2N_3} \{F_2(x_3^1, x_{33}^2) - F_1(x_3^1, x_{33}^2)\}$$

$$x_{111}^3 = F_1(x_1^1, x_{11}^2) + (2k - 2)k_{11}$$

$$x_{112}^3 = F_1(x_1^1, x_{11}^2) + (2k - 1)k_{11}$$

$$x_{113}^3 = F_1(x_1^1, x_{11}^2) + 2kk_{11}$$

$$x_{121}^3 = F_1(x_1^1, x_{12}^2) + (2k - 2)k_{12}$$

....

$$x_{333}^3 = F_1(x_3^1, x_{33}^2) + 2kk_{33}$$

$$k_{111} = \frac{1}{2N_4} \{F_2(x_1^1, x_{11}^2, x_{111}^3) - F_1(x_1^1, x_{11}^2, x_{111}^3)\}$$

$$k_{112} = \frac{1}{2N_4} \{F_2(x_1^1, x_{11}^2, x_{112}^3) - F_1(x_1^1, x_{11}^2, x_{112}^3)\}$$

$$k_{113} = \frac{1}{2N_4} \{F_2(x_1^1, x_{11}^2, x_{113}^3) - F_1(x_1^1, x_{11}^2, x_{113}^3)\}$$

....

$$k_{333} = \frac{1}{2N_4} \{F_2(x_3^1, x_{33}^2, x_{333}^3) - F_1(x_3^1, x_{33}^2, x_{333}^3)\}$$

$$x_{1111}^4 = F_1(x_1^1, x_{11}^2, x_{111}^3) + (2l - 2)k_{111}$$

$$x_{1112}^4 = F_1(x_1^1, x_{11}^2, x_{111}^3) + (2l - 1)k_{111}$$

$$x_{1113}^4 = F_1(x_1^1, x_{11}^2, x_{111}^3) + 2lk_{111}$$

$$x_{1121}^4 = F_1(x_1^1, x_{11}^2, x_{112}^3) + (2l - 2)k_{112}$$

....

$$x_{3333}^4 = F_1(x_3^1, x_{33}^2, x_{333}^3) + 2lk_{333}$$

$$G_{2i-2,2j-2,2k-2,l} = \frac{k_{111}}{3} \{f(x_1^1, x_{11}^2, x_{111}^3, x_{1111}^4) + 4f(x_1^1, x_{11}^2, x_{111}^3, x_{1112}^4) + f(x_1^1, x_{11}^2, x_{111}^3, x_{1113}^4)\}$$

$$G_{2i-2,2j-2,2k-1,l} = \frac{k_{112}}{3} \{f(x_1^1, x_{11}^2, x_{112}^3, x_{1121}^4) + 4f(x_1^1, x_{11}^2, x_{112}^3, x_{1122}^4) + f(x_1^1, x_{11}^2, x_{112}^3, x_{1123}^4)\}$$

$$G_{2i-2,2j-2,2k,l} = \frac{k_{113}}{3} \{f(x_1^1, x_{11}^2, x_{113}^3, x_{1131}^4) + 4f(x_1^1, x_{11}^2, x_{113}^3, x_{1132}^4) + f(x_1^1, x_{11}^2, x_{113}^3, x_{1133}^4)\}$$

....

$$G_{2i,2j,2k,l} = \frac{k_{333}}{3} \{f(x_3^1, x_{33}^2, x_{333}^3, x_{3331}^4) + 4f(x_3^1, x_{33}^2, x_{333}^3, x_{3332}^4) + f(x_3^1, x_{33}^2, x_{333}^3, x_{3333}^4)\}$$

$$H_{2i-2,2j-2,k,l} = \frac{k_{11}}{3} \{G_{2i-2,2j-2,2k-2,l} + 4G_{2i-2,2j-2,2k-1,l} + G_{2i-2,2j-2,2k,l}\}$$

$$H_{2i-2,2j-1,k,l} = \frac{k_{12}}{3} \{G_{2i-2,2j-1,2k-2,l} + 4G_{2i-2,2j-1,2k-1,l} + G_{2i-2,2j-1,2k,l}\}$$

$$H_{2i-2,2j,k,l} = \frac{k_{13}}{3} \{G_{2i-2,2j,2k-2,l} + 4G_{2i-2,2j,2k-1,l} + G_{2i-2,2j,2k,l}\}$$

. . . .

$$H_{2i,2j,k,l} = \frac{k_{33}}{3} \{G_{2i,2j,2k-2,l} + 4G_{2i,2j,2k-1,l} + + G_{2i,2j,2k,l}\}$$

$$I_{2i-2,j,k,l} = \frac{k_1}{3} \{H_{2i-2,2j-2,k,l} + 4H_{2i-2,2j-1,k,l} + + H_{2i-2,2j,k,l}\}$$

. . . .

$$I_{2i,j,k,l} = \frac{k_3}{3} \{H_{2i,2j-2,k,l} + 4H_{2i,2j-1,k,l} + H_{2i,2j,k,l}\}$$

$$F_{i,j,k,l} = \frac{h}{3} \{I_{2i-2,j,k,l} + 4I_{2i-1,j,k,l} + I_{2i,j,k,l}\}$$

$$S_{i,j,k,l} = \Sigma_{i-1,j,k,l} - \Sigma_{i-1,j-1,k,l} + \Sigma_{i-1,j-1,k-1,l} - - S_{i-1,j-1,k-1,l-1} + F_{i,j,k,l},$$

where

$$S_{0000} = S_{0jkl} = S_{i0kl} = S_{ij0l} = S_{ijk0} = S_{00kl} = S_{0j0l} = S_{0jk0} = = S_{i00l} = S_{i0k0} = S_{ij00} = S_{000l} = S_{00k0} = S_{0j00} = S_{i000} = 0$$

or

$$(21) \qquad S_{N_1,N_2,N_3,N_4} = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} \sum_{l=1}^{N_4} F_{i,j,k,l}.$$

7. The n-dimensional integral

Let

$$(22) \qquad \int_a^b dx^1 \int_{F_1(x^1)}^{F_2(x^1)} dx^2 \ \ldots \int_{F_1(x^1,x^2,\ldots,x^{n-1})}^{F_2(x^1,x^2,\ldots,x^{n-1})} dx^n \ f(x^1,x^2,\ldots,x^n)$$

be the integral to be evaluated.

. . . .

$$H_{2i,2j,k,l} = \frac{k_{33}}{3} \{G_{2i,2j,2k-2,l} + 4G_{2i,2j,2k-1,l} + G_{2i,2j,2k,l}\}$$

$$I_{2i-2,j,k,l} = \frac{k_1}{3} \{H_{2i-2,2j-2,k,l} + 4H_{2i-2,2j-1,k,l} + H_{2i-2,2j,k,l}\}$$

. . . .

$$I_{2i,j,k,l} = \frac{k_3}{3} \{H_{2i,2j-2,k,l} + 4H_{2i,2j-1,k,l} + H_{2i,2j,k,l}\}$$

$$F_{i,j,k,l} = \frac{h}{3} \{I_{2i-2,j,k,l} + 4I_{2i-1,j,k,l} + I_{2i,j,k,l}\}$$

$$S_{i,j,k,l} = \Sigma_{i-1,j,k,l} - \Sigma_{i-1,j-1,k,l} + \Sigma_{i-1,j-1,k-1,l} - S_{i-1,j-1,k-1,l-1} + F_{i,j,k,l},$$

where

$$S_{0000} = S_{0jkl} = S_{i0kl} = S_{ij0l} = S_{ijk0} = S_{00kl} = S_{0j0l} = S_{0jk0} = S_{i00l} = S_{i0k0} = S_{ij00} = S_{000l} = S_{00k0} = S_{0j00} = S_{i000} = 0$$

or

$$(21) \qquad S_{N_1,N_2,N_3,N_4} = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{k=1}^{N_3} \sum_{l=1}^{N_4} F_{i,j,k,l}.$$

7. The n-dimensional integral

Let

$$(22) \qquad \int_a^b dx^1 \int_{F_1(x^1)}^{F_2(x^1)} dx^2 \dots \int_{F_1(x^1,x^2,\dots,x^{n-1})}^{F_2(x^1,x^2,\dots,x^{n-1})} dx^n \, f(x^1,x^2,\dots,x^n)$$

be the integral to be evaluated.

Suppose that the interval on each direction in n-dimensional spaces is divided into $N_1, N_2, \ldots,$ and N_n subintervals. Using the above-mentioned method, we can put the partial sum of the recursion relation for n-fold series in the following

(23)

$$
\begin{aligned}
S_{i,j,k,\ldots,r,s} &= \Sigma_{i-1,j,k,\ldots,r,s} - \Sigma_{i-1,j-1,k,\ldots,r,s} + \\
&+ \Sigma_{i-1,j-1,k-1,\ldots,r,s} - \ldots + \\
&+ (-1)^{n-1} S_{i-1,j-1,k-1,\ldots,r-1,s-1} + \\
&+ F_{i,j,k,\ldots,r,s},
\end{aligned}
$$

where

$\Sigma_{i-1,j,k,\ldots,r,s}$ = the sum of such $\binom{n}{1}$ different partial sums as $S_{i-1,j,k,\ldots,r,s}$,

$\Sigma_{i-1,j-1,k,\ldots,r,s}$ = the sum of such $\binom{n}{2}$ different partial sums as $S_{i-1,j-1,k,\ldots,r,s}$,

$\Sigma_{i-1,j-1,k-1,\ldots,r,s}$ = the sum of such $\binom{n}{3}$ different partial sums as $S_{i-1,j-1,k-1,\ldots,r,s}$,

and $F_{i,j,k,\ldots,r,s}$ takes the form of Simpson's rule.

Since the structure of calculation in which Simpson's rule is used for the integral of (22) has been clarified using the recursion relation of n-fold series, we can now write down easily a quadrature formula by the repeated use of the Newton-Cotes formulas (of either open formulas or closed formulas) for the n-dimensional integral.

8. Error analysis

In this section we first consider the error estimates for two-dimensional integrals. For a double integral with constant limits the accuracy can be checked using the error term for function of one variable before integration is completed [7]. On the other hand, for the integral in which the domain of integration varies, we cannot check the accuracy before integration is completed, since the domain of each subinterval varies from step to step. However, if computations of integration and error estimates are carried out simultaneously, we may estimate the error. As can be given in the Appendix A, the error term of the composite Simpson's rule is obtained in the following

(24)

$$\left| E_{M,N} \right| \le$$

$$\sum_{i=1}^{M} \sum_{j=1}^{N} \max_{F_1(x_{2i-2}) \le \eta_j^1 \le F_2(x_{2i-2})} \frac{h}{3} \left| \frac{k_1^5}{90} f_y^{(4)}(x_{2i-2}, \eta_j^1) \right| +$$

$$+ \sum_{i=1}^{M} \sum_{j=1}^{N} \max_{F_1(x_{2i-1}) \le \eta_j^2 \le F_2(x_{2i-1})} \frac{4h}{3} \left| \frac{k_2^5}{90} f_y^{(4)}(x_{2i-1}, \eta_j^2) \right| +$$

$$+ \sum_{i=1}^{M} \sum_{j=1}^{N} \max_{F_1(x_{2i}) \le \eta_j^3 \le F_2(x_{2i})} \frac{h}{3} \left| \frac{k_3^5}{90} f_y^{(4)}(x_{2i}, \eta_j^3) \right| +$$

$$+ \sum_{i=1}^{M} \max_{\substack{x_{2i-2} \le \xi_i \le x_{2i} \\ F_1(\xi_i) \le \eta_i \le F_2(\xi_i)}} \left| \frac{h^5}{90} (F_2(\xi_i) - F_1(\xi_i)) \times \times f_x^{(4)}(\xi_i, \eta_i) \right| .$$

where $k_1 = \frac{1}{2N} (F_2(x_{2i-2}) - F_1(x_{2i-2}))$, $F_1(x_{2i-2}) \le \eta_j^1 \le F_2(x_{2i-2})$ and so on. The range of η_i is $F_1(\xi_i) \le \eta_i \le F_2(\xi_i)$. Thus, we may estimate the error of numerical integration for (10) using the error formula (24). Using the similar error term corresponding to the other Newton-Cotes formulas, we may also estimate the error of the integral of (10) or the error of higher dimensional integrals.

9. Numerical examples

In this section we will illustrate several examples for higher dimensional integrals which were computed by the method mentioned above. All computations reported below were performed in double-precision arithmetic.

Example 9.1

$$\int_0^{\frac{\pi}{2}} dx \int_0^x dy \sin(x + y)$$

The results computed by Simpson's rule method and the Newton-Cotes 5-point (closed) rule method are listed in Tables 1 and 2. The error from the error term are given in the fourth column of each table. When using Simpson's rule, the maximum error by the error term is given by eq.(24). However, it is difficult to find its error in the domain of each subinterval corresponding to the

$$+ \sum_{i=1}^{M} \max_{\substack{x_{2i-2} \le \xi_i \le x_{2i} \\ F_1(\xi_i) \le \eta_i \le F_2(\xi_i)}} \left| \frac{h^5}{90} (F_2(\xi_i) - F_1(\xi_i)) \times \times f_x^{(4)}(\xi_i, \eta_i) \right| .$$

where $k_1 = \frac{1}{2N} (F_2(x_{2i-2}) - F_1(x_{2i-2}))$, $F_1(x_{2i-2}) \le \eta_j^1 \le F_2(x_{2i-2})$ and so on. The range of η_i is $F_1(\xi_i) \le \eta_i \le F_2(\xi_i)$. Thus, we may estimate the error of numerical integration for (10) using the error formula (24). Using the similar error term corresponding to the other Newton-Cotes formulas, we may also estimate the error of the integral of (10) or the error of higher dimensional integrals.

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The subroutine program used is given in the Appendix B.

Example 9.2

$$\int_0^{\frac{\pi}{2}} dx \int_0^{x} dy \int_0^{x+y} dz \sin(x + y + z)$$

The results computed by Simpson's rule method and Newton-Cotes 5-point (closed) rul^c method are listed in Tables 3 and 4. The ^{c}rror by the error term are given in the fifth column of each table.

Example 9.3

$$\int_{1.4}^{2.0} dx \int_{x^2}^{x^4} dy \int_{x^3+y^3}^{x^4+y^4} dz \ln(x + 2y + 2z)$$

The results computed by Simpson's rule method and the Newton-Cotes 5-point (closed) rule method are listed in Tables 5 and 6. For the exact value of this integral, we found it using the Newton-Cotes 7-point (closed) rule method. The error from the error term are given in the fifth column of each table.

Example 9.4

$$\int_0^{\frac{\pi}{2}} dx^1 \int_0^{x^1} dx^2 \int_0^{x^1+x^2} dx^3 \int_0^{x^1+x^2+x^3} dx^4 \sin(x^1 + x^2 + x^3 + x^4)$$

The results computed by Simpson's rule method are listed in Table 7.

Example 9.5

$$\int_0^{\frac{\pi}{2}} dx^1 \int_0^{x^1} dx^2 \int_0^{x^1+x^2} dx^3 \int_0^{x^1+x^2+x^3} dx^4 \int_0^{x^1+x^2+x^3+x^4} dx^5 \, x \cdot x \sin(x^1+x^2+x^3+x^4+x^5)$$

The results computed by Simpson's rule are listed in Tables 8.

10. Conclusions

The results of this study can be summarized as follows.

(i) The structure of calculation by the Newton-Cotes formulas for n-dimensional integrals with variable limits was clarified using Simpson's rule. Consequently, we became to be able to construct a quadrature formula corresponding to the Newton-Cotes formulas (closed formulas and open formulas).

(ii) The computations using the program of Simpson's rule constructed from the present method are far faster in the rate of convergence than the ones using the conventional program of Simpson's rule available from the present computer library.

(iii) The error estimates by the error term are very crude but give some indication of the order of magnitude.

(iv) The Newton-Cotes formulas will become a useful and powerful tool for carrying out numerical integration with variable limits in higher dimensions.

The results computed by Simpson's rule method are listed in Table 7.

Example 9.5

$$\int_0^{\frac{\pi}{2}} dx^1 \int_0^{x^1} dx^2 \int_0^{x^1+x^2} dx^3 \int_0^{x^1+x^2+x^3} dx^4 \int_0^{x^1+x^2+x^3+x^4} dx^5\, x \cdot x \sin(x^1+x^2+x^3+x^4+x^5)$$

The results computed by Simpson's rule are listed in Tables 8.

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Acknowledgments.

One of the authors (T. N) would like to thank the Information Processing Center of Ibaraki University for assistance from the staff. A part of the numerical calculation was carried out on M-880 of the Computer Center of the University of Tokyo.

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Acknowledgments.

One of the authors (T. N) would like to thank the Information Processing Center of Ibaraki University for assistance from the staff. A part of the numerical calculation was carried out on M-880 of the Computer Center of the University of Tokyo.

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Table 1 Results for Example 9.1 computed by Simpson's rule method. Exact Value = 1.000000000000

M	N	Approximate Value	Error	Actual Error
1	1	1.002976405572	9.5E-04	3.0E-03
2	2	1.000177898595	1.2E-04	1.8E-04
5	5	1.000004504636	4.1E-06	4.5E-06
10	10	1.000000280986	2.8E-07	2.8E-07
20	20	1.000000017553	1.8E-08	1.8E-08
30	30	1.000000003467	3.5E-09	3.5E-09
50	50	1.000000000449	4.6E-10	4.5E-10
100	100	1.000000000028	2.9E-11	2.8E-11

Table 2 Results for Example 9.1 computed by the Newton-Cotes 5-point (closed) rule method. Exact Value = 1.000000000000

M	N	Approximate Value	Error	Actual Error
1	1	0.9999896358656	2.3E-06	1.1E-05
2	2	0.9999998467837	1.0E-07	1.6E-07
5	5	0.9999999993826	5.6E-10	6.2E-10
10	10	0.9999999999904	9.4E-12	9.6E-12
20	20	0.9999999999998	2.0E-13	2.0E-13

Table 3 Results for Example 9.2 computed by Simpson's rule method. Exact Value = 0.5000000000000

L	M	N	Approximate Value	Error	Actual Error
1	1	1	0.5611079067930	7.0E-03	6.1E-02
2	2	2	0.5033951461125	2.8E-04	3.4E-03
5	5	5	0.5000820317546	1.1E-05	8.2E-05
10	10	10	0.5000050815660	1.3E-06	5.1E-06
20	20	20	0.5000003168956	1.6E-07	3.2E-07
30	30	30	0.5000000625709	4.7E-08	6.3E-08
50	50	50	0.5000000081070	1.0E-08	0.8E-08

Table 4 Results for Example 9.2 computed by the Newton-Cotes 5-point (closed) rule method. Exact Value = 0.5000000000000

L	M	N	Approximate Value	Error	Actual Error
1	1	1	0.4989404931725	5.6E-05	1.1E-03
2	2	2	0.4999873290126	1.8E-07	1.3E-05
5	5	5	0.4999999516284	3.5E-09	4.8E-08
10	10	10	0.4999999992515	8.8E-11	7.5E-10
20	20	20	0.4999999999883	2.2E-12	1.2E-11
30	30	30	0.4999999999989	2.6E-13	1.1E-12
50	50	50	0.4999999999994	1.8E-14	6.0E-13

Table 5 Results for Example 9.3 computed by Simpson's rule method. Exact Value = 171654.7094763

L	M	N	Approximate Value	Error	Actual Error
1	1	1	221702.6520213	1.4E+06	5.0E+04
2	2	2	176653.0147794	2.1E+04	5.0E+03
5	5	5	171798.8919232	1.8E+02	1.4E+02
10	10	10	171663.5511569	5.8E+00	8.8E+00
20	20	20	171655.2492011	2.1E-01	5.4E-01
30	30	30	171654.8152598	3.3E-02	1.1E-01
50	50	50	171654.7231187	3.5E-03	1.4E-02

Table 6 Results for Example 9.3 computed by the Newton-Cotes 5-point (closed) rule method. Exact Value = 171654.7094763

L	M	N	Approximate Value	Error	Actual Error
1	1	1	173691.4139897	3.1E+06	2.0E+04
2	2	2	171695.1634843	1.9E+04	4.1E+01
5	5	5	171654.5268374	3.1E+01	1.8E-01
10	10	10	171654.6957218	2.4E-01	1.4E-02
20	20	20	171654.7090801	2.0E-03	3.9E-04
30	30	30	171654.7094353	1.3E-04	4.1E-05
50	50	50	171654.7094741	4.4E-06	2.2E-06

Table 7 Results for Example 9.4 computed by Simpson's rule method. Exact Value = -1.000000000000

N_1	N_2	N_3	N_4	Approximate Value
1	1	1	1	-0.301606619191
2	2	2	2	-1.070946748664
5	5	5	5	-1.000120749446
10	10	10	10	-1.000007464750
20	20	20	20	-1.000000465531
30	30	30	30	-1.000000091921
50	50	50	50	-1.000000011911

Table 8 Results for Example 9.5 computed by Simpson's rule method. Exact Value = -0.8750000000000

N_1	N_2	N_3	N_4	N_5	Approximate Value
1	1	1	1	1	-0.1518271451815
5	5	5	5	5	-0.9074006283430
10	10	10	10	10	-0.8749806808405
15	15	15	15	15	-0.8749961503998
20	20	20	20	20	-0.8749987787813

Appendix A

As seen in Sections 3, 4 and 5, the calculation for numerical integration has been proceeded from the first integral. So, we may write down using the error formula of Simpson's rule in the following

(A.1)

$$\int_a^b dx \int_{F_1(x)}^{F_2(x)} dy\ f(x,y) = \frac{h}{3} \sum_{i=1}^{M} \int_{F_1(x_{2i-2})}^{F_2(x_{2i-2})} dy\ f(x_{2i-2},y) +$$

$$+ \frac{4h}{3} \sum_{i=1}^{M} \int_{F_1(x_{2i-1})}^{F_2(x_{2i-1})} dy\ f(x_{2i-1},y) +$$

$$+ \frac{h}{3} \sum_{i=1}^{M} \int_{F_1(x_{2i})}^{F_2(x_{2i})} dy\ f(x_{2i},y) -$$

$$- \frac{h^5}{90} \sum_{i=1}^{M} \int_{F_1(\xi_i)}^{F_2(\xi_i)} dy\ f_x^{(4)}(\xi_i,\ y)$$

$$= \frac{h}{3} \sum_{i=1}^{M} \sum_{j=1}^{N} \frac{k_1}{3} \{f(x_{2i-2},y_{2j-2}) + 4f(x_{2i-2},y_{2j-1}) +$$

$$+ f(x_{2i-2},y_{2j})\} - \frac{h}{3} \sum_{i=1}^{M} \sum_{j=1}^{N} \frac{k_1^5}{90} f_y^{(4)}(x_{2i-2},\ \eta_j^1) +$$

$$+ \frac{4h}{3} \sum_{i=1}^{M} \sum_{j=1}^{N} \frac{k_2}{3} \{f(x_{2i-1},y_{2j-2}) + 4f(x_{2i-1},y_{2j-1}) +$$

$$+ f(x_{2i-1},y_{2j})\} - \frac{4h}{3} \sum_{i=1}^{M} \sum_{j=1}^{N} \frac{k_2^5}{90} f_y^{(4)}(x_{2i-1},\ \eta_j^2) +$$

$$+ \frac{h}{3} \sum_{i=1}^{M} \sum_{j=1}^{N} \frac{k_3}{3} \{f(x_{2i},y_{2j-2}) + 4f(x_{2i},y_{2j-1}) +$$

$$+ f(x_{2i}, y_{2j})\} -$$

$$- \frac{h}{3} \sum_{i=1}^{M} \sum_{j=1}^{N} \frac{k_3^5}{90} f_y^{(4)}(x_{2i}, \eta_j^3) -$$

$$- \frac{h^5}{90} \sum_{i=1}^{M} \{F_2(\xi_i) - F_1(\xi_i)\} f_x^{(4)}(\xi_i, \eta_i).$$

Here we applied the integral mean-value theorem [7,9]. On collecting the error terms in (A.1), we have eq.(24). Similarly, we may derive the error formulas corresponding to the Newton-Cotes formulas for higher dimensional integrals.

Appendix B

```
      SUBROUTINE SQUAD(F,FL1,FL2,A,B,MM,NN,SUM)
C     DOUBLE INTEGRAL OF F(X,Y), DOMAIN (A,B),(FL1(X),FL2(X))
C     NUMBER OF ORDINATES MM,NN
C     QUADRATURE BY SIMPSON'S RULE
      IMPLICIT REAL*8(A-H,O-Z)
      HM=2.0D0*MM
      HN=2.0D0*NN
      HH=(B-A)/HM
      HHK=HH/9.0D0
      SUM=0.0D0
      DO 10 I=1,MM
      HI=2.0D0*(I-1)
      X1=A+HI*HH
      X2=X1+HH
      X3=X2+HH
      HY1=(FL2(X1)-FL1(X1))/HN
      HY2=(FL2(X2)-FL1(X2))/HN
      HY3=(FL2(X3)-FL1(X3))/HN
      DO 20 J=1,NN
      HJ=2.0D0*(J-1)
      Y11=FL1(X1)+HJ*HY1
      Y12=Y11+HY1
      Y13=Y12+HY1
      Y21=FL1(X2)+HJ*HY2
      Y22=Y21+HY2
      Y23=Y22+HY2
      Y31=FL1(X3)+HJ*HY3
      Y32=Y31+HY3
      Y33=Y32+HY3
      F1=HY1*(F(X1,Y11)+4.0D0*F(X1,Y12)+F(X1,Y13))
      F2=HY2*(F(X2,Y21)+4.0D0*F(X2,Y22)+F(X2,Y23))
      F3=HY3*(F(X3,Y31)+4.0D0*F(X3,Y32)+F(X3,Y33))
      FS=HHK*(F1+4.0D0*F2+F3)
      SUM=SUM+FS
20    CONTINUE
10    CONTINUE
      RETURN
      END
```