

Note

On the Solution of the Thomas–Fermi Equation by Differential Quadrature

Equations containing both partial derivatives and integrals which frequently arise in science and engineering are generally solved by numerical methods wherein the partial derivatives and integrals are replaced by their discrete analogs, such as Newton’s method for integrals and either finite differences or finite elements for derivatives. In this manner, solution of the resulting algebraic equations can be accomplished by well-developed, numerical techniques. Generally these methods require the use of a large number of discrete points to ensure stable numerical solutions even though the results at only a few points are of interest. In such cases the method of quadrature—either differential or integral—is particularly advantageous since stable solutions can be obtained with only a few points. In this paper the application of the method of differential quadrature is demonstrated by solving the Thomas–Fermi equation; these results are then compared with those presented by Krutter [7].

Since the basic concept of quadrature [1, 2] is to fit a polynomial to the integral or derivative of the function, it is subject to the limitations of the polynomial fit. Consequently, as the number of discrete sample points is increased, the accuracy of the quadrature method continues to improve, passes through a maximum and thereafter proceeds to diminish due to “ill-conditioning” [2, 4].

At the i th discrete point the quadrature approximation is given by

$$L\{f(x_i)\} \simeq \sum_{j=1}^N W_{ij}f(x_j), \quad i = 1, 2, \dots, N \quad (1)$$

in which L is a linear operator representing a differentiation of a function, $f(x)$, where x is the independent variable and x_i (where $i = 1, 2, \dots, N$) are the sample points obtained by dividing the x -variable into N discrete values; $f(x_i)$ are the function values at these points, and w_{ij} are the weights attached to these function values.

To determine the weighting coefficients, w_{ij} , Eq. (1) must be exact for all polynomials of degree less than or equal to $(N - 1)$. Thus the test function is [1]

$$f_k(x) = x^{k-1}, \quad k = 1, 2, \dots, N \quad (2)$$

so that Eq. (1) leads to

$$L\{x_i^{k-1}\} \simeq \sum_{j=1}^N w_{ij}x_j^{k-1}, \quad i \text{ and } k = 1, 2, \dots, N. \quad (3)$$

Equation (3) represents a set of linear algebraic equations which is solved simultaneously for the weighting coefficients w_{ij} . Note that this set has a unique solution for the weighting coefficients, w_{ij} , since the matrix of elements x_j^{k-1} compose a Vandermonde matrix whose inverse can be obtained analytically as described by Hamming [6]. The weighting coefficients, w_{ij} , obtained in this way are then used in Eq. (1) to express the derivative of a function at a discrete point in terms of all of the discrete function values.

For example, consider the linear operator $L \equiv x d/dx(x d/dx)$. The weighting coefficients, w_{ij} , for this operator can be obtained from Eq. (3) by replacing the term $L\{x_i^{k-1}\}$ in Eq. (3) with $(k-1)^2 x_i^{k-1}$. As a result the following set of N linear algebraic equations is obtained:

$$\sum_{j=1}^N w_{ij} x_j^{k-1} = (k-1)^2 x_i^{k-1}, \quad i \text{ and } k = 1, 2, \dots, N. \tag{4}$$

Solution of Eq. (4) for a set of prescribed $x_i, i = 1, 2, \dots, N$, discrete points produces the weighting coefficients. For example, for the case of $N = 4$ and equally spaced discrete points in the range of $0 \leq x \leq 1$ the weighting coefficients are

$$W = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 2/3 & -5/2 & 2 & -1/6 \\ 1/3 & 2 & -7 & 14/3 \\ -10 & 81/2 & -54 & 47/2 \end{bmatrix}. \tag{5}$$

Weighting coefficients for other values of N can be obtained similarly.

To generalize the quadrature approximation method for higher-order operations and multivariable functions consider a matrix F containing the function values at the sample points. Let W be the matrix containing the weighting coefficients attached to these function values for a given linear operator, L . Then Eq. (1) can be put into matrix form as

$$L\{F\} \simeq WF. \tag{6}$$

Higher-order approximation formulae can be obtained by iterating the linear transformation [1] given by Eq. (6). Thus, for an m th-order operator

$$L^m\{F\} \simeq W^m F \tag{7a}$$

or simply [4, 5]

$$L^m\{F\} \simeq \bar{W} F \tag{7b}$$

in which a new coefficient matrix is defined as $\bar{W} \equiv W^m$ whose elements can be obtained directly from the solutions of

$$L^m \{x_i^{k-1}\} \simeq \sum_{j=1}^N \bar{w}_{ij} x_j^{k-1}, \quad i \text{ and } k = 1, 2, \dots, N. \tag{8}$$

Approximation formulae for mixed operators can be obtained similarly as

$$L_1^m L_2^n \dots L_k^p \{F\} \simeq \bar{W}_1 \bar{W}_2 \dots \bar{W}_k F \tag{9a}$$

where $L_1^m, L_2^n, \dots, L_k^p$ denote separate operators applied m, n, \dots, p times and $\bar{W}_1, \bar{W}_2, \dots, \bar{W}_k$ are the corresponding matrices of the weighting coefficients, respectively. Equation (9a) can also be written as

$$L_1^m L_2^n \dots L_k^p \{F\} \simeq \bar{\bar{W}} F \tag{9b}$$

in which $\bar{\bar{W}} = \bar{W}_1 \bar{W}_2 \dots \bar{W}_k$. Therefore, the number of sample points for each of the independent variables must be selected in such a way that the sizes of the weighting matrices are adequate for consecutive matrix multiplications.

By way of demonstration, the Thomas-Fermi equation as given below will be solved

$$\frac{d^2 f}{dx^2} = \frac{f^{3/2}}{x^{1/2}} \tag{10}$$

subject to the boundary conditions

$$f = 1 \quad \text{at } x = 0 \tag{11}$$

$$f = 0 \quad \text{at } x = \infty. \tag{12}$$

To avoid the uncertainty in representing infinity the semi-infinite domain can be converted to a finite domain by defining a new variable as

$$t = e^{-\alpha x} \tag{13}$$

where α is some arbitrary scaling factor which should be selected such that better resolution is achieved in the region of immediate interest. Thus Eqs. (10) through (12) become

$$t \frac{d}{dt} \left(t \frac{df}{dt} \right) = f^{3/2} / [\alpha^3 \ln(1/t)]^{1/2} \tag{14}$$

$$f = 0 \quad \text{at } t = 0 \tag{15}$$

$$f = 1 \quad \text{at } t = 1. \tag{16}$$

For a numerical solution via differential quadrature replacing the term on the left of Eq. (14) by Eq. (1) results in

$$\sum_{j=1}^N w_{ij} f_j = f_i^{3/2} / [\alpha^3 \ln(1/t_i)]^{1/2}, \quad i = 2, 3, \dots, (N-1). \quad (17)$$

The boundary function values are given by Eqs. (15) and (16) which in terms of the first and N th grid point become

$$f_1 = 0, \quad t_1 = 0 \quad (18)$$

$$f_N = 1, \quad t_N = 1. \quad (19)$$

Equation (17) represents a set of $(N-2)$ nonlinear algebraic equations which needs to be solved for $(N-2)$ unknown discrete function values f_i , $i = 2, 3, \dots, (N-1)$, using an appropriate iterative method such as Newton-Raphson.

In the present study the Newton-Raphson computer program (N one dimensional) presented by Carnahan *et al.* [3] was used to generate solutions to Eq. (17). For this purpose, substituting the boundary conditions given by Eqs. (18) and (19) into Eq. (17) and rearranging,

$$g_i \equiv \sum_{j=2}^{(N-1)} w_{ij} f_j + w_{iN} - f_i^{3/2} / [\alpha^3 \ln(1/t_i)]^{1/2} = 0, \quad i = 2, 3, \dots, (N-1) \quad (20)$$

from which the elements of the Jacobian matrix are calculated as

$$\frac{\partial g_i}{\partial f_j} = w_{ij} - (3/2) \delta_{ij} f_i^{1/2} / [\alpha^3 \ln(1/t_i)]^{1/2}, \quad i \text{ and } j = 2, 3, \dots, (N-1) \quad (21)$$

in which δ_{ij} is the Kronecker delta whose value is 1 when $i=j$ but is 0 when $i \neq j$.

Calculations have been carried out using $N=7$ and $N=15$ and equally spaced discrete points for various values of the scaling factor α on an IBM 3081 computer with double precision. The solutions with $N=7$ were almost identical to $N=15$. The results obtained for $N=15$, using α values of 1.0, 0.75, 0.50, 0.25, 0.10, 0.075, and 0.05, are presented in Fig. 1 for comparison with the numerical results published by Krutter [7]. Table I shows some typical numerical values obtained in the present study and those generated from Krutter's results by a Hermite cubic interpolation method [8]—after converting the x -variable to $\ln x$ -variable—as well as the absolute value of the relative deviation defined by

$$\varepsilon = |[f(x)_{\text{present}} - f(x)_{\text{Krutter}}] / f(x)_{\text{present}}|. \quad (22)$$

As can be seen the deviation is on the order of 10^{-2} .

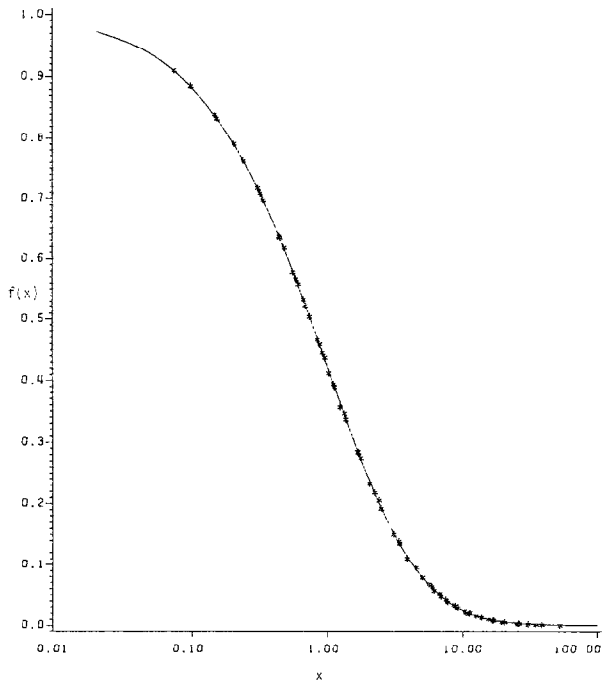


FIG. 1. Comparison of results of this study with those of Krutter.
 (*) This study for $N = 15$ and $0.05 \leq \alpha \leq 1.0$; (—) Krutter [7].

TABLE I
 Comparison of Results from This Study with Krutter [7]

x	$f(x)$ this study	$f(x)$ interpolated from Krutter	ε , absolute relative deviation
0.09881	0.88465	0.88436	0.00032
0.24116	0.76206	0.76307	0.00132
0.48232	0.61737	0.61628	0.00177
0.74615	0.50361	0.50364	0.00007
0.96465	0.43680	0.43445	0.00537
2.50552	0.19188	0.19249	0.00319
5.01105	0.07877	0.07855	0.00277
10.29619	0.02331	0.02307	0.01032
19.45911	0.00615	0.00611	0.00709
30.80888	0.00212	0.00216	0.01733

Krutter used a Runge–Kutta method for forward numerical integration from $x = 0$ and backward integration from $x = \infty$ ($u = 1/x$) which required fitting of the two solutions near $x = 30$. In return for the investment in substantial computational effort, his method lends itself to a high degree of accuracy which can be prescribed.

By comparison, in this study differential quadrature is applied to a transformed version of the Thomas–Fermi equation to obtain numerical solutions at relatively few discrete points. The computing time on the IBM 3081 (for double precision) was less than two seconds.

ACKNOWLEDGMENTS

The authors acknowledge the support of the University of Oklahoma Graduate College and the Computer Laboratory, as well as University Technologists, Inc.

REFERENCES

1. R. E. BELLMAN, B. G. KASHEF, AND J. CASTI, Differential quadrature: A technique for the rapid solution of nonlinear partial differential equations, *J. Comput. Phys.* **10** (1972), 40–52.
2. R. E. BELLMAN, "Methods of Nonlinear Analysis," Vol. II, Chap. 16, Academic Press, New York, 1973.
3. B. CARNAHAN, H. A. LUTHER, AND J. O. WILKES, "Applied Numerical Methods," pp. 322–327, Wiley, New York, 1969.
4. F. CIVAN AND C. M. SLIEPCEVICH, Application of differential quadrature to transport processes, *J. Math. Anal. Appl.* **93** (1983), 206–221.
5. F. CIVAN AND C. M. SLIEPCEVICH, Differential quadrature for multidimensional problems, *J. Math. Anal. Appl.* **101** (1984), 423–443.
6. R. W. HAMMING, "Numerical Methods for Scientists and Engineers," 2nd ed, McGraw–Hill, New York, 1973.
7. H. KRUTTER, Numerical integration of the Thomas–Fermi equation from zero to infinity, *J. Comput. Phys.* **47** (1982), 308–312.
8. J. R. RICE, "Numerical Methods, Software and Analysis," IMSL Reference Edition, McGraw–Hill, New York, 1983.

RECEIVED July 19, 1983; REVISED February 13, 1984

FARUK CIVAN

*School of Petroleum and Geological Engineering
University of Oklahoma, Felgar Hall 236
865 Asp Avenue, Norman, Oklahoma 73019*

C. M. SLIEPCEVICH

*School of Chemical Engineering and Materials Science
University of Oklahoma, 1215 Westheimer Drive
Norman, Oklahoma 73069*