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NEW INSIGHTS IN SOLVING DISTRIBUTED SYSTEM EQUATIONS BY THE QUADRATURE METHOD—I. ANALYSIS

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Abstract—This paper provides new insights in solving distributed system equations by the method of differential quadrature (Bellman *et al.*, 1972). In this study, the method is shown to be essentially equivalent to the general collocation method (Finlayson and Scriven, 1966). Explicit formulae of the quadrature coefficients are derived for arbitrarily-distributed nodes and for nodes located at the zeros of an orthogonal polynomial. Due to their simplicity and flexibility, these formulae allow us to calculate the values of the coefficients accurately and efficiently. Since the accuracy of the equation solutions depends on the locations of the nodes, a systematic procedure for placing the grid points is developed. In Part II of this paper, this proposed approach is demonstrated to be superior than that of the orthogonal collocation. Methods for approximating partial derivatives in a symmetric problem are also proposed to minimize the computational effort. The above techniques are then extended to cases in which the given partial differential equation and associated constraints can not be transformed into an initial-value problem. Instead of the conventional approach of converting the problem into a large set of algebraic equations, a two-point boundary-value problem is formulated to reduce the number of iteration parameters. This strategy is especially suitable for cases with highly nonlinear equations.

INTRODUCTION

Partial differential equations (PDEs) are commonly used to formulate models of distributed-parameter systems. Except for a few cases, nonlinear PDEs cannot be solved analytically. Although effective numerical techniques are available in the literature, one problem in implementing these methods is that each of them is suitable for only a small class of PDEs and, thus, tends to be problem-specific. Therefore, there is a need for developing a reliable and efficient procedure that can be applied to a wide variety of problems.

The method of differential quadrature introduced by Bellman *et al.* (1972) seems to possess these desired properties. By approximating the partial derivatives in spatial coordinates as linear combinations of the values of the dependent variable at a finite number of grid points, the PDE can be transformed into a set of algebraic equations or ordinary differential equations. The solution can then be obtained by standard numerical methods. Excellent results have been reported in a number of application studies (Bellman and Kashef, 1974; Bellman, 1974; Bellman *et al.*, 1975a,b; Mingle, 1977; Bellman and Roth, 1979; Civan and Sliepcevich, 1983, 1984; Naadimuthu *et al.*, 1984; Bellman and Adomian, 1985; Bellman and Roth, 1986). However, it is also apparent from these studies that there are several undesirable characteristics associated with the original approach. One of the disadvantages of the quadrature method is that the accuracy of the approximate solution is difficult to determine. Normally, the number of grid points n necessary to guarantee a good numerical solution is not known. Thus, it is common to test several values of n, each one requiring the computation of a new set of quadrature coefficients, until the solution does not vary significantly with increasing value of n. For this reason, an efficient and reliable procedure for calculating these coefficients is highly desirable. If the grid points are arbitrarily distributed, the quadrature coefficients are usually obtained by inverting an ill-conditioned Vandermonde matrix (Bellman *et al.*, 1972; Civan and Sliepcevich, 1983). The numerical inversion procedure becomes unstable for large numbers of grid points. As a result, the accuracy of the solution deteriorates as the number of grid points increases. Thus, explicit formulae for quadrature coefficients are needed to overcome this problem. Bellman *et al.* (1975a) placed the grid points at the zeros of shifted Legendre polynomials to facilitate the calculation of the quadrature coefficients. Since the first and last shifted zeros were not located at the boundary points, extra approximations were introduced to satisfy the boundary conditions. Thus, solutions near the boundaries are not as accurate. To avoid the above problem, Bellman *et al.* (1975b) proposed the use of cardinal splines to calculate the differential quadrature coefficients. However, this technique is less efficient when compared with the previous approach due to the fact that explicit formulae can not be derived in this case.

Another closely related technique is the orthogonal collocation method. Lanczos (1956) was the first to place the collocation points at the zeros of orthogonal

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polynomials to improve the accuracy of the solutions of initial-value problems obtained by the general collocation method. Villadsen and Stewart (1967) extended the method to boundary-value problems. Since this technique is well-known, no attempt will be made here to present an exhaustive literature survey on this subject. A comprehensive review has been provided by Finlayson (1972). Numerous successful applications of this method in chemical engineering have also been reported (Villadsen and Michelsen, 1978, 1987; Finlayson, 1980).

This paper is the first of a series of papers. New insights in the differential quadrature method are presented in the present paper. First, the general collocation method is shown to be equivalent to the method of differential quadrature. Second, explicit formulae for the differential quadrature coefficients at arbitrarily located grid points are derived. Thus, the past problem of inverting an ill-conditioned matrix for determining the quadrature coefficients can be avoided. Third, simplified formulae are obtained by placing the grid points at the zeros of Jacobi polynomials. The formulae corresponding to the special cases of Jacobi polynomials, i.e. Legendre, Ultraspherical, Chebyshev of the first and second kind, are extremely simple and thus suitable for implementation. Fourth, formulae for approximating partial derivatives in symmetric problems are also provided for even and odd numbers of grid points. As a consequence, there is a substantial reduction in the number of equations to be solved. Fifth, a strategy for placing the grid points at the zeros of orthogonal polynomials is developed. As a result, boundary conditions can be satisfied without extra approximations. It is demonstrated in this work that the proposed strategy yields more accurate solutions when compared with the orthogonal collocation method. Sixth, techniques for handling boundary conditions are presented. Seventh, extensions of the differential quadrature method to problems which cannot be transformed into an initial-value problem are studied. Instead of solving algebraic equations, an alternative approach, which transforms the PDE and the associated constraints into a two-point boundary-value problem, is suggested to reduce the number of iteration parameters. Finally, all the new techniques developed in this work are summarized in a unified general procedure presented as the conclusion of this part of our study.

In the following paper, the results of a series of numerical experiments will be presented to support some of the important conclusions made in the first part. Also, several practical examples will be provided to demonstrate the capability of the suggested approach in typical chemical engineering applications.

PROPERTIES OF DIFFERENTIAL QUADRATURE

To facilitate the later discussion, some of the properties of differential quadrature are presented in this section. Let us consider the following general nonlinear PDE:

$$\frac{\partial u(t, y)}{\partial t} = g\left[t, y, u(t, y), \frac{\partial u(t, y)}{\partial y}, \frac{\partial^2 u(t, y)}{\partial y^2}\right], \tag{1a}$$

with initial condition:

$$u(0, y) = h(y). \tag{1b}$$

The basic idea of differential quadrature is the same as the quadrature methods used in numerical integration. The partial derivatives of the function $u(t, y)$ with respect to y are expressed as a linear combination of the values of this function at chosen grid points y_is (Bellman and Adomian, 1985):

$$\frac{\partial u(t, y_i)}{\partial y} \cong \sum_{j=1}^{n} \alpha_{ij} u(t, y_j), \quad \frac{\partial^2 u(t, y_i)}{\partial y^2} \cong \sum_{j=1}^{n} \beta_{ij} u(t, y_j)$$

$$i = 1, 2, \ldots, n, \tag{2}$$

where n is the number of grid points. The values of the differential quadrature coefficients, α_{ij}s and β_{ij}s, are dependent on the locations of the grid points. Methods for determining these values will be presented later. At this point let us assume that they are known.

After substitution of the above approximations in equation (1), we obtain the initial-value problem:

$$\frac{du(t, y_i)}{dt} \cong g\left[t, y_i, u(t, y_i), \sum_{j=1}^{n} \alpha_{ij} u(t, y_j), \sum_{j=1}^{n} \beta_{ij} u(t, y_j)\right], \tag{3a}$$

$$u(0, y_i) = h(y_i)$$

$$i = 1, 2, \ldots, n, \tag{3b}$$

which can be solved easily by a numerical integrator.

From equation (3) it is apparent that the success of the method of differential quadrature depends on the accurate determination of α_{ij}s and β_{ij}s. The calculation of the differential quadrature coefficients can be accomplished by several methods. In most of these methods, it is assumed that, at a given value of t and over a region in y, a set of test functions, $f_k(y)$, $k = 1, 2, \ldots, n$, can be chosen such that:

$$u(t, y) \cong \sum_{k=1}^{n} \vartheta_k(t) f_k(y) \tag{4}$$

where ϑ_k, $k = 1, 2, \ldots, n$, are constants to be determined. However, if the differential quadrature coefficients α_{ij}s and β_{ij}s, are chosen such that the equations:

$$\frac{df_k(y_i)}{dy} = \sum_{j=1}^{n} \alpha_{ij} f_k(y_j) \quad i, k = 1, 2, \ldots, n, \tag{5}$$

$$\frac{d^2 f_k(y_i)}{dy^2} = \sum_{j=1}^{n} \beta_{ij} f_k(y_j) \quad i, k = 1, 2, \ldots, n. \tag{6}$$

are satisfied, equation (2) should be valid without knowing the values of the ϑ_ks. As a result, a relationship between first- and second-order coefficients can be obtained:

$$\frac{d^2 f_k(y_i)}{dy^2} = \frac{d}{dy}\left[\frac{df_k(y_i)}{dy}\right] = \sum_{m=1}^{n} \alpha_{im} \sum_{j=1}^{n} \alpha_{mj} f_k(y_j)$$
$$= \sum_{j=1}^{n} \sum_{m=1}^{n} \alpha_{im}\alpha_{mj} f_k(y_j). \quad (7)$$

Thus,

$$\beta_{ij} = \sum_{m=1}^{n} \alpha_{im}\alpha_{mj} \quad i, j = 1, 2, \ldots, n. \quad (8)$$

In matrix notation:

$$\mathbb{B} = \mathbb{A}^2, \quad (9)$$

where

$$\mathbb{A} = (a_{ij})_{n \times n} \quad \mathbb{B} = (\beta_{ij})_{n \times n}.$$

Equation (9) implies that the values of β_{ij}s can be determined by two alternative (but equivalent) procedures, i.e. they can be obtained by directly solving equation (6) or by squaring the first-order matrix $\mathbb{A}$. One approach for calculating the entries of $\mathbb{A}$ and $\mathbb{B}$ (Mingle, 1977; Civan and Sliepcevich, 1984; Naadimuthu *et al.*, 1984; Bellman and Roth, 1986) is to use the test functions:

$$f_k(y) = y^{k-1} \quad k = 1, 2, \ldots, n. \quad (10)$$

From equations (5) and (6), we obtain:

$$\mathbb{V}\mathbf{a}_i = \frac{d\mathbf{z}(y_i)}{dy} \quad i = 1, 2, \ldots, n, \quad (11)$$

$$\mathbb{V}\mathbf{b}_i = \frac{d^2\mathbf{z}(y_i)}{dy^2} \quad i = 1, 2, \ldots, n, \quad (12)$$

where

$$\mathbf{a}_i = [\alpha_{i1}, \alpha_{i2}, \ldots, \alpha_{in}]^T \quad \mathbf{b}_i = [\beta_{i1}, \beta_{i2}, \ldots, \beta_{in}]^T$$

$$\mathbf{z} = [1, y, \ldots, y^{n-1}]^T,$$

$$\mathbb{V} = \begin{bmatrix} 1 & 1 & \ldots & 1 \\ y_1 & y_2 & \ldots & y_n \\ y_1^2 & y_2^2 & \ldots & y_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ y_1^{n-1} & y_2^{n-1} & \ldots & y_n^{n-1} \end{bmatrix}.$$

Since any polynomial of degree $(n-1)$ can be expressed as a linear combination of y^{k-1}, $k = 1, 2, \ldots, n$, the values of α_{ij}s and β_{ij}s determined by equations (11) and (12) should be the same as those obtained by adopting a set of n arbitrary linearly independent polynomials of degree $(n-1)$ as the test functions with the same grid points. Thus, the values of the differential quadrature coefficients are dependent only upon the locations of the grid points, if the test functions are polynomials. Also, notice that the matrix $\mathbb{V}$ on the left-hand side of equations (11) and (12) is a Vandermonde matrix, which is known to be ill-conditioned for large values of n (Press *et al.*, 1988). Although the inverse of $\mathbb{V}$ can be obtained analytically, significant errors can still be introduced by the multiplication of $\mathbb{V}^{-1}$ with the vectors on the right-hand side of equations (11) or (12). This phenomenon will be demonstrated in the second part of this paper. Thus, there is a definite need for obtaining explicit formulae of differential quadrature coefficients, α_{ij}s and β_{ij}s.

EXPLICIT FORMULAE FOR DIFFERENTIAL QUADRATURE COEFFICIENTS

The explicit formulae for differential coefficients can be obtained by considering the sample polynomials introduced in a Lagrange interpolation process:

$$f_k(y) = \frac{\phi_n(y)}{(y - y_k)[d\phi_n(y_k)/dy]} = \sum_{j=1}^{n} c_{kj} y^{j-1}$$
$$k = 1, 2, \ldots, n, \quad (13)$$

where

$$\phi_n(y) = \prod_{m=1}^{n} (y - y_m). \quad (14)$$

Thus

$$\mathbf{f} = \mathbb{C}\mathbf{z}, \quad (15)$$

where

$$\mathbf{f}(y) = [f_1(y), f_2(y), \ldots, f_n(y)]^T \quad \mathbb{C} = (c_{ij})_{n \times n}.$$

Note the matrix $\mathbb{C}$ is the inverse of Vandermonde matrix $\mathbb{V}$ (Hamming, 1973). Next, let us consider the solution of equation (11) when the grid points are chosen at the zeros of $\phi_n(y)$, i.e.

$$\mathbf{a}_i = \mathbb{V}^{-1}\frac{d\mathbf{z}(y_i)}{dy} = \mathbb{C}\frac{d\mathbf{z}(y_i)}{dy} = \frac{d\mathbf{f}(y_i)}{dy}$$
$$i = 1, 2, \ldots, n. \quad (16)$$

Similarly,

$$\mathbf{b}_i = \frac{d^2\mathbf{f}(y_i)}{dy^2} \quad i = 1, 2, \ldots, n. \quad (17)$$

The method of differential quadrature was originally considered by Bellman to be a *new* approach for solving PDEs (Bellman *et al.*, 1972). Later, other researchers also published a number of theoretical and application studies (Bellman and Kashef, 1974; Bellman, 1974; Bellman *et al.*, 1975a, b; Mingle 1977; Bellman and Roth, 1979; Civan and Sliepcevich, 1983, 1984; Naadimuthu *et al.*, 1984; Bellman and Adomian, 1985; Bellman and Roth, 1986). However, a close examination of equations (16) and (17) shows that this method is essentially *equivalent* to the general collocation method (Finlayson and Scriven, 1966), i.e. the initial-value problems obtained by the above two approaches are identical. To the best of our knowledge, this fact has never been indicated in the literature.

From equations (13), (14), (16) and (17) it can be concluded that the values of the derivatives of the function ϕ_n at the grid points need to be calculated before determining the quadrature coefficients. A recursive procedure has been provided by Villadsen and Michelsen (1978) for this purpose. However, a more efficient and accurate approach can be obtained if analytical expressions are available. They can be derived by directly combining equations (13–17) i.e.

$$\alpha_{ij} = \frac{1}{y_j - y_i} \prod_{\substack{m=1 \\ m \neq i,j}}^{n} \frac{y_i - y_m}{y_j - y_m}, \tag{18}$$

$$\beta_{ij} = \frac{2}{y_j - y_i} \left(\prod_{\substack{m=1 \\ m \neq i,j}}^{n} \frac{y_i - y_m}{y_j - y_m} \right) \left(\sum_{\substack{k=1 \\ k \neq i,j}}^{n} \frac{1}{y_i - y_k} \right), \tag{19}$$

for $i \neq j$, and

$$\alpha_{ii} = \sum_{\substack{k=1 \\ k \neq i}}^{n} \frac{1}{y_i - y_k}, \tag{20}$$

$$\beta_{ii} = 2 \sum_{\substack{k=1 \\ k \neq i}}^{n-1} \left[\frac{1}{y_i - y_k} \left(\sum_{\substack{l=k+1 \\ l \neq i}}^{n} \frac{1}{y_i - y_l} \right) \right], \tag{21}$$

for $i = j$.

As far as the authors are aware, the results presented in equations (18–21) have not been published before. They will be referred as the general formulae. These formulae are valid for arbitrary location of grid points y_i, $i = 1, 2, \ldots, n$. More significantly, the differential quadrature coefficients can now be calculated directly and, therefore, accurate solutions can be obtained even for large values of n. Finally, it is interesting to note that equations (8) and (9) can be verified directly using these general fomulae.

Simplified formulae

In several previous studies (Bellman and Adomian, 1985; Bellman and Roth, 1986), the zeros of shifted Legendre polynomials were chosen as the grid points. This approach has two advantages: first, although the general formulae presented in equations (18–21) are sufficient for determining α_{ij}s and β_{ij}s, simpler expressions can be obtained if the properties of the orthogonal polynomials are utilized. Second, the accuracy of the solutions of PDEs can be improved when compared to the solutions with evenly-spaced grid points and those with grid points assigned by using the well-known orthogonal collocation method. Since only Legendre polynomials were used in the past, a system of general orthogonal polynomials (which includes Legendre) was studied in this work. Simplified formulae of the differential quadrature coefficients were also derived for several useful special cases. It should be pointed out that it is *not* possible to carry out the corresponding derivation for the orthogonal collocation method. This is due to the fact that the two boundary nodes used in the method are not zeros of the orthogonal polynomial (Finlayson, 1980). This issue of grid point placement will be addressed fully in the next section.

The classical orthogonal polynomials consist of three systems: Jacobi, Laguerre and Hermite (Szegö, 1975; Chihara, 1978). Of these systems, only the Jacobi polynomials, $P_n^{(r,s)}(x)$ with $-1 \leqslant x \leqslant 1$, have finite interval bounds. Because almost all applications problems are restricted to finite dimensions, we limited the derivation of quadrature coefficients to these polynomials. Since it is necessary to use some of the properties of Jacobi polynomials for obtaining the simplified formulae of the quadrature coefficients, these are included in Appendix A.

The differential quadrature coefficients will first be determined for the interval $[-1, 1]$. Although we are not usually interested in this interval, the derived formulae will be useful for the shifted polynomial case. Notice that, since their roots are real and within $[-1, 1]$, all Jacobi polynomials can be expressed in the form of equation (14). Substitution of the test function:

$$f_k(x) = \frac{P_n^{(r,s)}(x)}{(x - x_k)[\mathrm{d}P_n^{(r,s)}(x_k)/\mathrm{d}x]}, \tag{22}$$

into equations (16) and (17) gives:

$$\alpha_{ij} = \frac{\mathrm{d}P_n^{(r,s)}(x_i)/\mathrm{d}x}{(x_i - x_j)[\mathrm{d}P_n^{(r,s)}(x_j)/\mathrm{d}x]}, \tag{23}$$

$$\beta_{ij} = \frac{(x_i - x_j)[\mathrm{d}^2P_n^{(r,s)}(x_i)/\mathrm{d}x^2] - 2[\mathrm{d}P_n^{(r,s)}(x_i)/\mathrm{d}x]}{(x_i - x_j)^2[\mathrm{d}P_n^{(r,s)}(x_j)/\mathrm{d}x]}, \tag{24}$$

for $i \neq j = k$, and

$$\alpha_{ii} = \frac{\mathrm{d}^2P_n^{(r,s)}(x_i)/\mathrm{d}x^2}{2[\mathrm{d}P_n^{(r,s)}(x_i)/\mathrm{d}x]}, \tag{25}$$

$$\beta_{ii} = \frac{\mathrm{d}^3P_n^{(r,s)}(x_i)/\mathrm{d}x^3}{3[\mathrm{d}P_n^{(r,s)}(x_i)/\mathrm{d}x]}, \tag{26}$$

for $i = j = k$.

At the zero x_i, the first derivative of the Jacobi polynomial can be obtained from equation (A12) in Appendix A, i.e.

$$\frac{\mathrm{d}P_n^{(r,s)}(x_i)}{\mathrm{d}x} = \frac{\psi_4(n)P_{n-1}^{(r,s)}(x_i)}{\psi_1(n)(1 - x_i^2)}, \tag{27}$$

where the functions $\psi_1(n)$ and $\psi_4(n)$ are defined by equations (A13) and (A16) in Appendix A. From the differential equation (A1) in Appendix A:

$$(1 - x_i^2)\frac{\mathrm{d}^2P_n^{(r,s)}(x_i)}{\mathrm{d}x^2} = -[s - r - (r + s + 2)x_i]\frac{\mathrm{d}P_n^{(r,s)}(x_i)}{\mathrm{d}x}. \tag{28}$$

Substitution of equation (27) into equation (28), gives:

$$\frac{d^2P_n^{(r,s)}(x_i)}{dx^2} = -\frac{\psi_4(n)[s-r-(r+s+2)x_i]P_{n-1}^{(r,s)}(x_i)}{\psi_1(n)(1-x_i^2)^2}. \quad (29)$$

Differentiation of equation (A1) with respect to x and using equation (29) to eliminate the second-order derivative, one obtains a relation between the first- and third-order derivative:

$$(1-x_j^2)^2\frac{d^3P_n^{(r,s)}(x_j)/dx^3}{dP_n^{(r,s)}(x_j)/dx} = [s-r-(r+s+2)x_j]^2 + (1-x_j^2)[r+s+2-n(n+r+s+1)] - 2x_j[s-r-(r+s+2)x_j]. \quad (30)$$

With these expressions for the derivatives, explicit formulae can be derived from equations (23–26), i.e.

$$\alpha_{ij} = \frac{(1-x_j^2)P_{n-1}^{(r,s)}(x_i)}{(x_i-x_j)(1-x_i^2)P_{n-1}^{(r,s)}(x_j)}, \quad (31)$$

$$\beta_{ij} = \frac{\{(x_i-x_j)[s-r-(r+s+2)x_i]+2(1-x_i^2)\}(1-x_j^2)P_{n-1}^{(r,s)}(x_i)}{(x_i-x_j)^2(1-x_i^2)^2P_{n-1}^{(r,s)}(x_j)}, \quad (32)$$

for $i \neq j$, and

$$\alpha_{ii} = \frac{(r+s+2)x_i+r-s}{2(1-x_i^2)}, \quad (33)$$

$$\beta_{ii} = \frac{1}{3(1-x_i^2)^2}\{[s-r-(r+s+2)x_i]^2 + (1-x_i^2)[r+s+2-n(n+r+s+1)] - 2x_i[s-r-(r+s+2)x_i]\}, \quad (34)$$

for $i = j$.

As mentioned before, it is often necessary to shift from the interval $-1 \leqslant x \leqslant 1$ to the interval $a \leqslant y \leqslant b$. This can be achieved by using the simple relation:

$$x = \frac{2}{b-a}y + \frac{b+a}{a-b}. \quad (35)$$

Explicit formulae for several special cases of the Jacobi polynomials are presented in Appendix B. These formulae are extremely simple and can be used in any finite interval $[a, b]$. They will be referred to as the simplified formulae.

Symmetrical systems

If the grid points are symmetrically distributed, equations (18–21) clearly imply that:

$$\alpha_{ij} = -\alpha_{(n+1-i)(n+1-j)}, \quad \beta_{ij} = \beta_{(n+1-i)(n+1-j)}, \quad i = 1, 2, \ldots, l \quad j = 1, 2, \ldots, n, \quad (36)$$

where

$$l = \begin{cases} n/2 & \text{if } n \text{ is even} \\ (n-1)/2 & \text{if } n \text{ is odd} \end{cases}. \quad (37)$$

Thus, not all the quadrature coefficients need to be calculated by the explicit formulae derived previously. In addition, more dramatical reduction in the computational effort can be realized if the distributed system model is symmetric in space, i.e.

$$u(t, y_i) = u(t, y_{n+1-i}) \quad i = 1, 2, \ldots, l, \quad (38)$$

where l is defined in equation (37). From equations (36) and (38), it can be shown (Quan, 1988) that:

$$\frac{\partial \tilde{\mathbf{u}}}{\partial y} = \tilde{\mathbb{A}}\tilde{\mathbf{u}}, \quad \frac{\partial^2 \tilde{\mathbf{u}}}{\partial y^2} = \tilde{\mathbb{B}}\tilde{\mathbf{u}}, \quad (39)$$

where

$$\tilde{\mathbb{A}} = (\tilde{\alpha}_{ij})_{l' \times l'}, \quad \tilde{\mathbb{B}} = (\tilde{\beta}_{ij})_{l' \times l'},$$

$$\tilde{\mathbf{u}} = [u(t, y_1), u(t, y_2), \ldots, u(t, y_{l'})]^T.$$

If the number of grid points n is even, then:

$$l' = l = n/2 \quad (40)$$

and

$$\tilde{\alpha}_{ij} = \alpha_{ij} + \alpha_{i(n+1-j)}, \quad \tilde{\beta}_{ij} = \beta_{ij} + \beta_{i(n+1-j)}, \quad i, j = 1, 2, \ldots, l. \quad (41)$$

The implication of equation (39) is that equation (3a) can be decoupled into two sets of identical ODEs. Thus, it is only necessary to integrate equation (3a) for $i = 1, 2, \ldots, n/2$ (or $i = n/2+1, n/2+2, \ldots, n$).

Notice that the same results can be obtained if polynomials of y^2 are used at the test functions. Values of $\tilde{\alpha}_{ij}$s and $\tilde{\beta}_{ij}$s corresponding to various orthogonal polynomials of y^2 have been published extensively in the literature (Villadsen and Stewart, 1967; Finlayson, 1980). However, it can be seen from equation (41) that these values can be actually determined from the entries of the original matrices $\mathbb{A}$ and $\mathbb{B}$. Furthermore, the published approach excludes the cases corresponding to odd number of grid points. If n is odd, then:

$$l' = l + 1 = (n+1)/2. \quad (42)$$

Equations (41) are still valid for $l = (n-1)/2$. The other entries in $\tilde{\mathbb{A}}$ and $\tilde{\mathbb{B}}$ can be determined by the following equations:

$$\tilde{\alpha}_{i(l+1)} = \alpha_{i(l+1)}, \quad \tilde{\beta}_{i(l+1)} = \beta_{i(l+1)} \quad i = 1, 2, \ldots, l+1, \quad (43a)$$

$$\tilde{\alpha}_{(l+1)j} = 0, \quad \tilde{\beta}_{(l+1)j} = 2\beta_{(l+1)j} \quad j = 1, 2, \ldots, l. \quad (43b)$$

Thus, only $(n+1)/2$ ordinary differential equations need to be solved in this situation.

PLACEMENT OF GRID POINTS

When there are no boundary conditions and the solution is sufficiently smooth, the method of

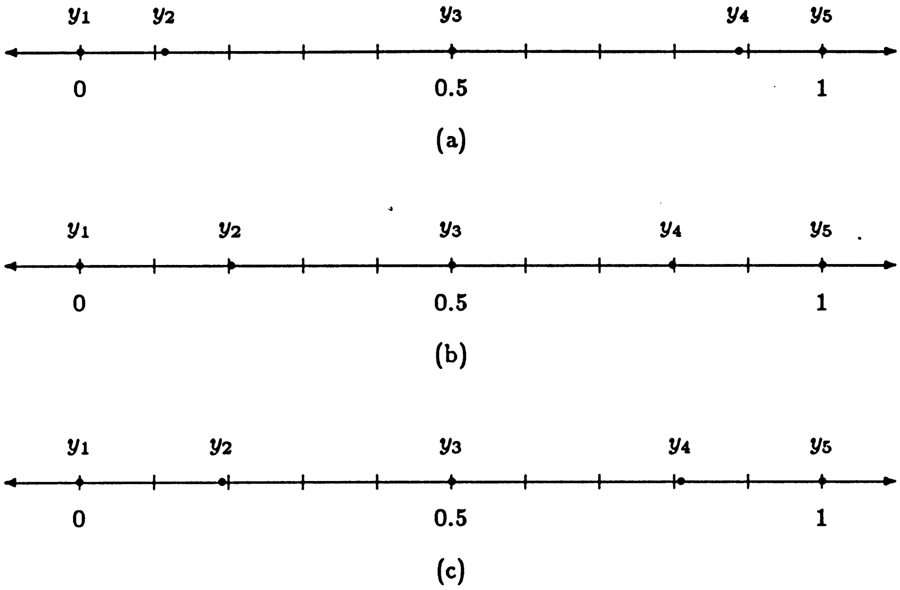

Fig. 1. Location of grid points: (a) orthogonal collocation (Legendre); (b) differential quadrature (Legendre); (c) differential quadrature (Chebyshev).

differential quadrature usually gives relatively good results, even with a small number of grid points (Bellman and Adomian, 1985). With the presence of boundary conditions, previous results obtained by placing the grid points at the zeros of a shifted Legendre polynomial have not been as satisfactory. This is due to the fact that the locations of the grid points are restricted to the zeros of the polynomials. Thus, additional approximations were introduced to satisfy the boundary conditions. The results obtained from the placement scheme of the orthogonal collocation method is better than those using evenly-spaced grid points. However, there is still room for improvement (Burka, 1982).

In this work, a new approach for placing the grid points has been developed to improve the accuracy of the numerical solutions. Depending on whether it is necessary to obtain solutions at desired locations, one of the following two strategies is recommended.

If accurate solutions at given locations are required, the general formulae in equations (18–21) should be adopted. In this case, the boundary points are assigned as the first and last grid points. To be more specific, let us consider the general PDE defined by equation (1a) with initial conditions, equation (1b), and proper boundary conditions stipulated at the two fixed boundary points on the y-axis, say C_1 and C_2. That is, the interval of interest is $C_1 \leqslant y \leqslant C_2$. Since the general formulae allow arbitrary placement of grid points, we can set $y_1 = C_1$, $y_n = C_2$ and choose the interior nodes at the desired locations.

On the other hand, if there is no preference in the locations of the numerical solutions, then it is better to select the grid points at the zeros of an orthogonal polynomial. In this case, care must be taken in selecting the domain of the shifted orthogonal polynomials. Since the zeros of these polynomials are located within an interval $[a, b]$, it is best to choose a and b such that $y_1 = C_1$ and $y_n = C_2$, i.e.

$$a = \frac{2[C_2(1 + x_1) - C_1(1 + x_n)]}{(1 - x_n)(1 + x_1) - (1 - x_1)(1 + x_n)} \tag{44}$$

and

$$b = \frac{2[C_1(1 - x_n) - C_2(1 - x_1)]}{(1 - x_n)(1 + x_1) - (1 - x_1)(1 + x_n)}, \tag{45}$$

where x_1 and x_n are the first and last unshifted zeros, respectively.

Notice that the latter strategy of assigning the grid points is different from that of the orthogonal collocation. The method of orthogonal collocation (Finlayson, 1980) selects, as grid points, the zeros of an orthogonal polynomial within a given interval $[C_1, C_2]$. Two additional grid points, located at C_1 and C_2, are then added for approximating the boundary conditions. To illustrate this difference in the placement of grid points, let us consider the case of selecting five points in the interval $0 \leqslant y \leqslant 1$. Figure 1a shows the locations of the nodes assigned by using the orthogonal collocation method. The positions of the interior points, y_2, y_3 and y_4, are chosen to be the zeros of a third-degree Legendre polynomial. The other two points, y_1 and y_5, coincide with the boundary points 0 and 1. Figures 1b and c represent the node assignments generated by using the proposed method. In these two cases, the grid points are located at the zeros of a fifth-degree Legendre (Fig. 1b) and Chebyshev polynomial (Fig. 1c), respectively.

As mentioned before, simplified formulae cannot be derived using the grid point placement scheme of orthogonal collocation. This is due to the fact that not all the grid points are the zeros of an orthogonal polynomial. In this study, this problem is solved by shifting the domain $[a, b]$ according to the locations of the boundary points, i.e. using equations (44) and (45). As a result, an extremely simple and accurate procedure for calculating the quadrature coefficients can be developed.

Equations (13) and (14) suggest that equation (4) can be regarded as the approximation of the dependent variable u by the Lagrange interpolation if:

$$\vartheta_k(t) = u(t, y_k) \quad k = 1, 2, 3, \ldots, n. \tag{46}$$

Indeed, the same quadrature coefficient equations, equations (16) and (17), can be obtained by substituting equation (46) into equation (4) and differentiating the resulting equation. Also, it has been well-established that the absolute value of the error of interpolation is nearly minimized in the minimax sense, if the interpolation points are chosen to be the zeros of a Chebyshev polynomial of the first kind. Thus, although the minimization of the errors in approximating the partial derivatives of u by equation (2) can not be guaranteed, the zeros of the Chebyshev polynomials (first kind) still seems to be the most logical candidates among all the choices for grid points. As we will show in Part II, placement of grid points in the suggested fashion results in more accurate solutions than in the orthogonal collocation method. The results obtained by placing the nodes at the zeros of a Chebyshev polynomial of the first kind are consistently better than those obtained by any other means.

APPROXIMATION OF BOUNDARY CONDITIONS

After properly selecting the grid points, the boundary conditions can then be handled appropriately. Basically, the approach adopted here is the same as that of the orthogonal collocation method. For completeness, this subject is discussed briefly in this section.

Consider a 2-D PDE of the form of equation (1a) with initial condition, equation (1b), and appropriate boundary conditions. This problem can be transformed into a set of $(n-2)$ ordinary differential equations associated with the $(n-2)$ interior grid points, i.e. equations (3a) and (3b) with $i = 2, 3, \ldots, n-1$. In this initial-value problem, the values of the dependent variable at the first and last grid points, $u(t, y_1)$ and $u(t, y_n)$, need to be determined from the boundary conditions for each value of t. To illustrate the procedure used in this study for handling boundary conditions, let us consider one of the most commonly used boundary conditions, i.e.

$$u(t, C_1) + \gamma_1(t)\frac{\partial u(t, C_1)}{\partial y} = g_1(t), \tag{47a}$$

$$u(t, C_2) + \gamma_2(t)\frac{\partial u(t, C_2)}{\partial y} = g_2(t). \tag{47b}$$

Other types of boundary conditions can be treated in a similar way. Applying equation (3), we can approximate the boundary conditions in equations (47a) and (47b) by:

$$u(t, y_1) + \gamma_1(t)\left[\alpha_{11}u(t, y_1) + \sum_{j=2}^{n-1}\alpha_{1j}u(t, y_j) + a_{1n}u(t, y_n)\right] \cong g_1(t), \tag{48a}$$

$$u(t, y_n) + \gamma_2(t)\left[\alpha_{n1}u(t, y_1) + \sum_{j=2}^{n-1}\alpha_{nj}u(t, y_j) + \alpha_{nn}u(t, y_n)\right] \cong g_2(t). \tag{48b}$$

From these two expressions, the values of u at the initial and final grid points can be solved, in terms of the interior grid points, for any value of t.

EXTENSIONS

So far we have considered equations of the form of equation (1a) with given initial and boundary conditions. In this section, we are concerned with problems of the form:

$$\frac{\partial^2 u(y, z)}{\partial y^2} = g\left[y, z, u(y, z), \frac{\partial^2 u(y, z)}{\partial z^2}\right], \tag{49}$$

with appropriate boundary conditions. Clearly, this problem can not always be transformed into an initial-value problem. By approximating all the partial derivatives with their respective weighted linear summations, a set of algebraic equations is obtained (Finlayson, 1980; Civan and Sliepcevich, 1983). If the resulting problem is linear, very effective procedures for solving a system of linear algebraic equations exist (Fiedler, 1986). However, when the problem is nonlinear, time-consuming iterative procedures and/or the use of multiple intervals are needed.

An alternate approach is to transform the problem into an initial-value problem or a two-point boundary-value problem. For simplicity, let us consider equation (49) in a rectangular domain, i.e. $C_1 \leqslant y \leqslant C_2$ and $C_3 \leqslant z \leqslant C_4$, with given boundary conditions. The proposed method is illustrated in the remainder of this section by using two simple cases with different boundary conditions. Other types of boundary conditions can be handled in a similar fashion.

Case 1:

$$u(C_1, z) = g_1(z), \quad \frac{\partial u(C_1, z)}{\partial z} = g_2(z), \tag{50a}$$

$$u(y, C_3) = g_3(y), \quad u(y, C_4) = g_4(y). \tag{50b}$$

By approximating the second-order partial derivative with respect to z using equation (3), equation (49) can be transformed to:

$$\frac{d^2u(y, z_i)}{dy^2} \cong g\left[y, z_i, u(y, z_i), \frac{\partial^2 u(y, z_i)}{\partial z^2}\right]$$

$$i = 2, 3, \ldots, n-1. \quad (51a)$$

Let us define:

$$u_1(y, z_i) = \frac{du(y, z_i)}{dy} \quad i = 2, 3, \ldots, n-1. \quad (51b)$$

Note that the initial values of $u(y, z_i)$s and $u_1(y, z_i)$s can be determined by equation (50a), i.e.

$$u(C_1, z_i) = g_1(z_i), u_1(C_1, z_i) = g_2(z_i)$$

$$i = 2, 3, \ldots, n-1. \quad (51c)$$

Also, note that the values of $u(y, C_3)$ and $u(y, C_4)$ can be determined by the boundary conditions, equation (50b). Thus, equations (51a–c) form an initial-value problem, which can be solved easily without iteration.

Case 2:

$$u(C_1, z) = g_1(z), u(C_2, z) = g_2(z), \quad (52a)$$

$$u(y, C_3) = g_3(y), u(y, C_4) = g_4(y). \quad (52b)$$

Again, equation (3) can be used to convert equation (49) into a set of ordinary differential equations, which are the same as equations (51a) and (51b). Let us label them as equations (53a) and (53b). In this case, the initial and final values of $u(y, z_i)$s can be determined by equation (52a), i.e.

$$u(C_1, z_i) = g_1(z_i), \quad u(C_2, z_i) = g_2(z_i)$$

$$i = 2, 3, \ldots, n-1. \quad (53c)$$

Thus, equations (53a–c) form a two-point boundary-value problem. The values of $u(y, C_3)$ and $u(y, C_4)$ can be determined by using the boundary conditions, equation (52b). Note that there are $2 \times (n-2)$ ordinary differential equations and the number of parameters that require iteration is reduced from n^2, in the case of solving algebraic equations, to $(n-2)$.

CONCLUSIONS

Based on the previous analysis, it can be concluded that further improvements need to be introduced into the existing method of differential quadrature (or the orthogonal collocation method). All the new techniques developed in this study are summarized in a program-like procedure (Appendix C). This procedure represents a unified appraoch to solve partial differential equations in chemical engineering applications. It can be observed from Appendix C that, in addition to the calculation of quadratrue coefficients (procedure COEFF), it may be necessary to solve an initial-value problem (procedure IVP), a system of linear or nonlinear algebraic equations (procedure SYSALG) or a two point boundary-value problem (procedure TPBVP). Numerical solution techniques for solving these problems are readily available. Application examples and discussions will be presented in the following paper. Also, although only the scheme for placing grid points within one single interval is presented in this paper, the extension of this procedure to solutions with multiple intervals, in a way similar to that of the orthogonal collocation on finite elements (Villadsen and Michelsen, 1978; Finlayson, 1980; Gardini *et al.*, 1985) should be straightforward.

NOMENCLATURE

$\mathbb{A}$ = The first-order quadrature coefficient matrix
$\tilde{\mathbb{A}}$ = The first-order quadrature coefficient matrix for symmetric systems
$\mathbb{B}$ = The second-order quadrature coefficient matrix
$\tilde{\mathbb{B}}$ = The second-order quadrature coefficient matrix for symmetric systems
a, b = The lower and upper bound of a finite interval on y-axis
$\mathbf{a}_i$ = The vector $[\alpha_{i1}, \alpha_{i2}, \ldots, \alpha_{in}]^T$
$\mathbf{b}_i$ = The vecotr $[\beta_{i1}, \beta_{i2}, \ldots, \beta_{in}]^T$
$\mathbb{C}$ = The coefficient matrix of the sample polynomial in Lagrange interpolation
C_1, C_2 = The lower and upper bound of a finite interval on y-axis, $a \leqslant C_1 \leqslant C_2 \leqslant b$
C_3, C_4 = The lower and upper bound of a finite interval on z-axis
c_{ij} = The coefficient of the sample polynomial in Lagrange interpolation
$\mathbf{f}$ = The vector $[f_1, f_2, \ldots, f_n]^T$
f_k = The kth test function
g_1, g_2 = Two arbitrary functions of t
h = An arbitrary function of y
n = Total number of grid points
P_n = Legendre polynomial of degree n
$P_n^{(r,s)}$ = Jacobi polynomial of degree n
$P_n^{(\lambda)}$ = Ultraspherical polynomial of degree n
r, s = Parameters of the Jacobi polynomial
T_n = Chebyshev polynomial of the first kind of degree n
t = Independent variable, $0 \leqslant t < \infty$
U_n = Chebyshev polynomial of the second kind of degree n
u = Dependent variable
$\mathbb{V}$ = The Vandermonde matrix
x = Independent variable, distance in rectangular coordinates $-1 \leqslant x \leqslant 1$
y = Independent variable, shifted distance in rectangular coordinates $a \leqslant y \leqslant b$
z = Independent variable, distance in rectangular coordinates
$\mathbf{z}$ = The vector $[1, y, \ldots, y^{n-1}]^T$

Greek letters

α_{ij} = The first-order quadrature coefficients
$\tilde{\alpha}_{ij}$ = The first-order quadrature coefficients for symmetric systems
β_{ij} = The second-order quadrature coefficients
$\tilde{\beta}_{ij}$ = The second-order quadrature coefficients for symmetric systems
γ_1, γ_2 = Two arbitrary functions of t
ϑ_k = Coefficient of the kth test function
ϕ_n = A polynomial of y with n real roots
λ = Parameter of the Ultraspherical polynomial

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APPENDIX A

The Jacobi polynomials $P_n^{(r,s)}(x)$ satisfy the differential equation:

$$(1-x^2)\frac{d^2P_n^{(r,s)}(x)}{dx^2}+[s-r-(r+s+2)x]\frac{dP_n^{(r,s)}(x)}{dx}+n(n+r+s+1)P_n^{(r,s)}(x)=0 \quad \text{(A1)}$$

and contain, as special cases, the Legendre polynomials $P_n(x)$, the Chebyshev polynomials of the first kind $T_n(x)$, the Chebyshev polynomials of the second kind $U_n(x)$, and the Ultraspherical polynomials $P_n^{(\lambda)}(x)$. The relationships between these polynomials and the Jacobi polynomials are:

$$P_n(x)=P_n^{(0,0)}(x), \quad \text{(A2)}$$

$$T_n(x)=2^{2n}\binom{2n}{n}^{-1}P_n^{(-1/2,-1/2)}(x), \quad \text{(A3)}$$

$$U_n(x)=2^{2n}\binom{2n+1}{n+1}^{-1}P_n^{(1/2,1/2)}(x), \quad \text{(A4)}$$

$$P_n^{(\lambda)}(x)=\binom{2r}{r}^{-1}\binom{n+2r}{r}P_n^{(r,r)}(x), \quad \text{(A5)}$$

where

$$r=\lambda-1/2\neq-1/2.$$

Jacobi polynomials can be calculated through a three-term recurrence formula:

$$\varphi_1(n)P_n^{(r,s)}(x)=[\varphi_2(n)x+\varphi_3(n)]P_{n-1}^{(r,s)}(x)+\varphi_4(n)P_{n-2}^{(r,s)}(x), \quad \text{(A6)}$$

where

$$\varphi_1(n)=2n(n+r+s)(2n+r+s-2), \quad \text{(A7)}$$

$$\varphi_2(n)=(2n+r+s-1)(2n+r+s)(2n+r+s-2), \quad \text{(A8)}$$

$$\varphi_3(n)=(2n+r+s-1)(r^2-s^2), \quad \text{(A9)}$$

$$\varphi_4(n)=-2(n+r-1)(n+s-1)(2n+r+s), \quad \text{(A10)}$$

$$P_0^{(r,s)}(x)=1 \quad P_1^{(r,s)}(x)=[1+(1/2)(r+s)]x+(1/2)(r-s). \quad \text{(A11)}$$

The first-order derivatives can be obtained from the relation (Chihara, 1978):

$$\psi_1(n)(1-x^2)\frac{dP_n^{(r,s)}(x)}{dx}=[\psi_2(n)x+\psi_3(n)]P_n^{(r,s)}(x)+\psi_4(n)P_{n-1}^{(r,s)}(x), \quad \text{(A12)}$$

where

$$\psi_1(n)=2n+r+s, \quad \text{(A13)}$$

$$\psi_2(n)=-n(2n+r+s), \quad \text{(A14)}$$

$$\psi_3(n)=n(r-s), \quad \text{(A15)}$$

$$\psi_4(n)=2(n+r)(n+s). \quad \text{(A16)}$$

APPENDIX B

Legendre Polynomials $[P_n(x), -1\leqslant x\leqslant 1]$

$$r=s=0$$

For $i \neq j$,

$$\alpha_{ij} = \frac{2(1 - x_j^2)P_{n-1}(x_i)}{(b-a)(x_i - x_j)(1 - x_i^2)P_{n-1}(x_j)}, \tag{B1}$$

$$\beta_{ij} = \frac{8[x_i(x_i - x_j) - (1 - x_i^2)](1 - x_j^2)P_{n-1}(x_i)}{(b-a)^2(x_i - x_j)^2(1 - x_i^2)^2P_{n-1}(x_j)}. \tag{B2}$$

For $i = j$,

$$\alpha_{ii} = \frac{2x_i}{(b-a)(1 - x_i^2)}, \tag{B3}$$

$$\beta_{ii} = \frac{4[8x_i^2 + (2 - n^2 - n)(1 - x_i^2)]}{3(b-a)^2(1 - x_i^2)^2}. \tag{B4}$$

Chebyshev polynomials of the first kind [$T_n(x)$, $-1 \leqslant x \leqslant 1$]

$$r = s = -1/2$$

For $i \neq j$,

$$\alpha_{ij} = \frac{2(1 - x_j^2)T_{n-1}(x_i)}{(b-a)(x_i - x_j)(1 - x_i^2)T_{n-1}(x_j)}, \tag{B5}$$

$$\beta_{ij} = \frac{4[x_i(x_i - x_j) - 2(1 - x_i^2)](1 - x_j^2)T_{n-1}(x_i)}{(b-a)^2(x_i - x_j)^2(1 - x_i^2)^2T_{n-1}(x_j)}. \tag{B6}$$

For $i = j$,

$$\alpha_{ii} = \frac{x_i}{(b-a)(1 - x_i^2)}, \tag{B7}$$

$$\beta_{ii} = \frac{4[(2 + n^2)x_i^2 + 1 - n^2]}{3(b-a)^2(1 - x_i^2)^2}. \tag{B8}$$

Chebyshev polynomials of the second kind [$U_n(x)$, $-1 \leqslant x \leqslant 1$]

$$r = s = 1/2$$

For $i \neq j$,

$$\alpha_{ij} = \frac{2(1 - x_j^2)U_{n-1}(x_i)}{(b-a)(x_i - x_j)(1 - x_i^2)U_{n-1}(x_j)}, \tag{B9}$$

$$\beta_{ij} = \frac{4\{3x_i(x_i - x_j) - 2(1 - x_i^2)\}(1 - x_j^2)U_{n-1}(x_i)}{(b-a)^2(x_i - x_j)^2(1 - x_i^2)^2U_{n-1}(x_j)}. \tag{B10}$$

For $i = j$,

$$\alpha_{ii} = \frac{3x_i}{(b-a)(1 - x_i^2)}, \tag{B11}$$

$$\beta_{ii} = \frac{4\{[12 + n(n+2)]x_i^2 + 3 - n(n+2)\}}{3(b-a)^2(1 - x_i^2)^2}. \tag{B12}$$

Ultraspherical polynomials [$P_n^{(\lambda)}(x)$, $-1 \leqslant x \leqslant 1$]

$$r = s = \lambda - 1/2 \neq -1/2$$

For $i \neq j$,

$$\alpha_{ij} = \frac{2(1 - x_j^2)P_{n-1}^{(\lambda)}(x_i)}{(b-a)(x_i - x_j)(1 - x_i^2)P_{n-1}^{(\lambda)}(x_j)}, \tag{B13}$$

$$\beta_{ij} = \frac{8\{-(\lambda + 1/2)x_i(x_i - x_j) + (1 - x_i^2)\}(1 - x_j^2)P_{n-1}^{(\lambda)}(x_i)}{(b-a)^2(x_i - x_j)^2(1 - x_i^2)P_{n-1}^{(\lambda)}(x_j)}. \tag{B14}$$

For $i = j$,

$$a_{ii} = \frac{2(\lambda + 1/2)x_i}{(b-a)(1 - x_i^2)}, \tag{B15}$$

$$\beta_{ii} = \frac{4}{3(b-a)^2(1 - x_i^2)^2}\{4x_i^2(\lambda + 1/2)(\lambda + 3/2) + (1 - x_i^2)[2(\lambda + 1/2) - n(n + 2\lambda)]\}. \tag{B16}$$

APPENDIX C

```
procedure GENERAL
  go to COEFF
  if there are only initial conditions then
    go to IVP
  else if there are boundary conditions
    if an initial-value problem can be formulated then
      go to IVP
    else
      if the number of grid points is small then
        go to SYSALG
      else
        go to TPBVP

procedure COEFF (differential quadrature coefficients)
  if there are no boundary conditions then
    if desired locations of the grid points are given then
      compute quadrature coefficients by the general
      formulae
    else
      place the grid points at the zeros of a shifted
      orthogonal polynomial
      compute the quadrature coefficients by the
      simplified formulae
  else
    if desired locations of the grid points are given then
      place the interior grid points at the desired locations
      place the first and last grid points at the boundaries
      compute the quadrature coefficients by the general
      formulae
    else
      determine the zeros of a unshifted orthogonal
      polynomial
      use Eqs. (44) and (45) to calculate a and b
      compute quadrature coefficients by the simplified
      formulae

procedure IVP (initial-value problem)
  if there are boundary conditions then
    if problem is symmetric then
      calculate new quadrature coefficients by Eqs. (41)
      and/or (43)
    approximate boundary conditions
  replace spatial partial derivatives by Eqs. (2) or (39)
  integrate the resulting ODEs

procedure SYSALG (system of algebraic equations)
  if problem is symmetric then
    calculate new quadrature coefficients by Eqs. (41)
    and/or (43)
  approximate boundary conditions
  replace all partial derivatives by Eqs. (2) or (39)
  solve the resulting system of algebraic equations

procedure TPBVP (two-point boundary-value problem)
  if problem is symmetric then
    calculate new quadrature coefficients by Eqs. (41)
    and/or (43)
  approximate boundary conditions
  replace spatial partial derivatives by Eqs. (2) or (39)
  solve the resulting two-point boundary-value problem
```