REVIEW ON ORTHOGONAL COLLOCATION METHOD FOR SOLVING ORDINARY DIFFERENTIAL EQUATIONS

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Abstract

In this paper, the orthogonal collocation method is reviewed and used to solve the second order ordinary differential problems numerically. The trial function used here is discretized using Lagrange's interpolating polynomials. The collocation points used are the roots of Jacobi polynomial $P_n^{\alpha,\ \beta}$ *at* $= \beta = 0$ *. The results obtained from the method, is compared with results obtained from bvp4c solver in MATLAB.*

1. Introduction

A lot of physical world problems associated with different phenomenon can be mathematically described in the form of differential equations. The exact solutions of these differential equations are quite difficult to find. So numerical based methods and techniques are developed and applied to these differential equations to find the approximate solution of these problems. A variety of numerical techniques [4-8] has been developed and have been implemented to solve the differential equations.

The Weighted residual method is one of numerical technique which is widely used to find the approximate solution to the ordinary and partial differential equations. In these methods, the residual obtained from substituting the trial or approximate function in differential equation is set orthogonal to weight function of approximating polynomial. Orthogonal collocation method [1], Orthogonal Collocation on finite elements (OCFE) [3], Galerkin methods etc. are the types of weighted residual methods.

In this paper, Orthogonal Collocation Method is discussed and used to find the solution of second order differential equations arised in Tubular Reactor with Axial Mixing (TRAM) in which an irreversible second order reaction is carried out.

2. Description of the Method

An unknown approximate function $\psi(\xi)$ is chosen such that it satisfies a differential equation

$$\mathscr{L}^{\mathcal{V}}(\psi) = 0 \qquad (1)$$

in region $\mathcal{V}$ having the boundary $\mathscr{B}$ and the boundary condition

$$\mathscr{L}^{\mathscr{B}}(\psi) = 0 \text{ on } \mathscr{B}. \qquad (2)$$

The dependent variable ψ is written as the series expansion $\psi^{(k)}$ in k unknown parameters which are found by solving above equations at each of the k selected points. These points are known as Collocation points. The residual function is set to orthogonal to weight function of given base polynomial at Collocation points. So residual function becomes zero at Collocation points. The selection of Collocation points plays an important role in find the solution of differential equation using Collocation method. As the wrong choice of collocation points may lead to divergence from the solution. In this method, the roots of orthogonal polynomial like Legendre polynomial and Chebyshev polynomials are taken as Collocation points. In this paper, the roots of shifted Legendre polynomial which is the special case of Jacobi polynomial $P_n^{\alpha,\ \beta}$ at $\alpha = \beta = 0$ are used as Collocation points.

The approximate function $\psi(\xi)$ using $P_{n+2}(\xi)$ as nodal polynomial is given by

$$\psi(\xi) = \sum_{j=0}^{n+1} F_j(\xi)\, \psi_j \tag{3}$$

where $F_j(\xi) = P_{n+2}(\xi)/(\xi - \xi_j)P_{n+2}^{(1)}(\xi_j)$. In a convenient approach, combine like-powered terms in ξ in Equation 3 (note that $P_i(\xi)$ contains monomials: $1, \xi, \xi^2, \ldots, \xi^i$), and write the solution as:

$$\psi(\xi) = d_1 + d_2\,\xi + d_3\,\xi^2 + d_4\,\xi^3 + \cdots \ldots \ldots \ldots \ldots \ldots \ldots + d_{n+2}\,\xi^{n+1} \tag{4}$$

The $n+2$ coefficients, $d_i, i = 1, 2 \ldots n+2$, in Equation 4 are evaluated by satisfying the two boundary conditions at $\xi=\xi_1=0$, and $\xi=\xi_{n+2}=1$ (see Figure 1). In addition, make the residual, $R(\xi_i)$, zero at n distinct locations, $\xi_2, \xi_3, \ldots\ldots, \xi_{n+1}$, inside the interval, $0 < \xi < 1$. These points are referred to as collocation points. It is important to note that, in general, the internal collocation points are not equispaced. Here, take the n internal collocation points to be the roots of the n^{th} degree shifted Legendre polynomial, $P_n(\xi)$, given in Table 1. This is why this technique is now referred to as the orthogonal collocation (OC) technique. Such a choice of OC points leads to the error $|\psi_{exact}(\xi) - \psi(\xi)|$, being quite evenly distributed in the entire domain of x.

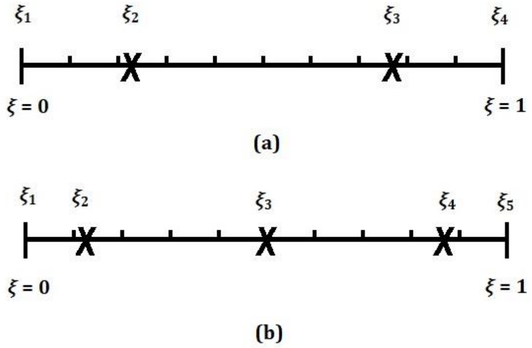

Figure 1: Location of the OC points when n = 2 and (b) for n = 3.

Moreover, such a choice of the OC points is optimal in the sense that values of the integral $\int_0^1 f(y)\, dx$ evaluated using quadratures, are very accurately estimated. The locations of the OC points are given in Tables 1 for some values of n. In order to evaluate the residuals, $R(\xi_i)$, the expressions for the first and second derivatives of ψ is needed. This is quite easy using the solution in Equation 4,

$$\psi_i = \psi\big|_{\xi_i} = 1d_1 + \xi_i\, d_2 + \xi_i^2\, d_3 + \xi_i^3\, d_4 + \xi_i^4\, d_5 + \cdots\cdots + \xi_i^{n+1}\, d_{n+2}$$

$$\psi_i' = \frac{d\psi}{d\xi}\bigg|_{\xi_i} = 0\,d_1 + 1d_2 + 2\xi_i\; d_3 + 3\xi_i^2\, d_4 + 4\xi_i^3\, d_5 + \cdots\cdots + (n+1)\xi_i^n\, d_{n+2}$$

$$\psi_i'' \equiv \frac{d^2 y}{d^2\xi}\bigg|_{\xi_I} = 0\,d_1 + 0\,d_2 + 2\,d_3 + 6\xi_i\; d_4 + 12\xi_i^2\, d_5 + \cdots\cdots + n(n+1)\xi_i^{n-1}\, d_{n+2} \tag{5}$$

The values of ψ and its derivatives at locations, $\xi_1, \xi_2, \xi_3, \ldots\ldots, \xi_{n+2}$ (note that the two boundary points are included) can be written in a matrix form as

$$\psi \equiv \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \psi_{n+2} \end{bmatrix} = \begin{bmatrix} 1 & \xi_1 & \xi_1^2 & \xi_1^3 & \cdots & \xi_1^{n+1} \\ 1 & \xi_2 & \xi_2^2 & \xi_2^3 & \cdots & \xi_2^{n+1} \\ \vdots & & & & & \\ \vdots & & & & & \\ \vdots & & & & & \\ \vdots & & & & & \\ \vdots & & & & & \\ 1 & \xi_{n+2} & \xi_{n+2}^2 & \xi_{n+2}^3 & \cdots & \xi_{n+2}^{n+1} \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ d_{n+2} \end{bmatrix} \equiv Qd \tag{6}$$

$$\psi' \equiv \begin{bmatrix} \psi'_1 \\ \psi'_2 \\ \psi'_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \psi'_{n+2} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 2\xi_1 & 3\xi_1^2 & \cdots & (n+1)\xi_1^n \\ 0 & 1 & 2\xi_2 & 3\xi_2^2 & \cdots & (n+1)\xi_2^n \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 0 & 1 & 2\xi_{n+2} & 3\xi_{n+2}^2 & \cdots & (n+1)\xi_{n+2}^n \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ d_{n+2} \end{bmatrix} \equiv Cd \tag{7}$$

$$\psi'' \equiv \begin{bmatrix} \psi''_1 \\ \psi''_2 \\ \psi''_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \psi''_{n+2} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 2 & 6\xi_1 & \cdots & n(n+1)\xi_1^{n-1} \\ 0 & 0 & 2 & 6\xi_2 & \cdots & n(n+1)\xi_2^{n-1} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ 0 & 01 & 2 & 6\xi_{n+2} & \cdots & n(n+1)\xi_{n+2}^{n-1} \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ d_{n+2} \end{bmatrix} \equiv Dd \tag{8}$$

where Q, C and D are (n+2) × (n+2) matrices of constants.

Table 1: Collocation points and Discretization Matrices for Shifted Legendre Polynomial

n	X	w	A	B
1	$\begin{pmatrix} 0 \\ 0.5 \\ 1.0 \end{pmatrix}$	$\begin{pmatrix} 0.1667 \\ 0.6667 \\ 0.1667 \end{pmatrix}$	$\begin{pmatrix} -3 & 4 & -1 \\ -1 & 0 & 1 \\ 1 & -4 & 3 \end{pmatrix}$	$\begin{pmatrix} 4 & -8 & 4 \\ 4 & -8 & 4 \\ 4 & -8 & 4 \end{pmatrix}$
2	$\begin{pmatrix} 0 \\ 0.21132 \\ 0.78868 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0.5 \\ 0.5 \\ 1 \end{pmatrix}$	$\begin{pmatrix} -7 & 8.196 & -2.196 & 1 \\ -2.732 & 1.732 & 1.732 & -0.7321 \\ 0.7321 & -1.732 & -1.732 & 2.732 \\ -1 & 2.196 & -8.196 & 7 \end{pmatrix}$	$\begin{pmatrix} 24 & -37.18 & 25.18 & -12 \\ 16.39 & -24 & 12 & -4.392 \\ -4.392 & 12 & -24 & 16.39 \\ -12 & 25.18 & -37.18 & 24 \end{pmatrix}$
3	$\begin{pmatrix} 0 \\ 0.11270 \\ 0.50000 \\ 0.88730 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0.27778 \\ 0.44444 \\ 0.27778 \\ 0 \end{pmatrix}$	Use Equation 5 to find the A & B	

Use Equations 6-8 to evaluate the residuals of the second- order ODE-BVP of Equation 1, and solve for the coefficients, d_i (there will be 2 equations from the boundary conditions, and n residual equations, for the $n+2$ coefficients, $d_1, d_2, \ldots\ldots\ldots\ldots\ldots\ldots. d_{n+2}$. It is convenient to transform equations 6-8 and express ψ_i' and ψ_i'' in terms of ψ, and then solve for $\psi_1, \psi_2, \ldots\ldots\ldots\ldots, \psi_{n+2}$. Equation 6 gives $d = Q^{-1}\psi$, which may be substituted in Equations 7 and 8 to give

$$\psi' \equiv \begin{bmatrix} \psi'_1 \\ \psi'_2 \\ \psi'_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \psi'_{n+2} \end{bmatrix} \equiv (CQ^{-1})\,\psi \equiv A\psi \quad \text{and} \quad \psi'' \equiv \begin{bmatrix} \psi''_1 \\ \psi''_2 \\ \psi''_3 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \psi''_{n+2} \end{bmatrix} \equiv (DQ^{-1})\psi \equiv B\psi \tag{9}$$

Q^{-1} exists if the OC points are distinct and the monomials 1, $\xi, \xi^2, \ldots, \xi^{n+1}$ are linearly independent, as indeed they are. The matrices *A* and *B* are also a set of (*n* + 2) × (*n* + 2) constants and can be easily computed. They are given in Table 1 for some values of N, and Villadsen and Michelsen [2] give computer programs which may be used to generate not only the location of the OC points, but these matrices as well.

The values of ψ' and ψ'' can be written as

$$\psi_i' = A_{i1}\,\psi_1 + A_{i2}\,\psi_2 + \cdots \ldots \ldots \ldots + A_{i\,n+2}\,\psi_{n+2} = \sum_{j=1}^{n+2} A_{ij}\,\psi_j \tag{10}$$

$$\psi_i'' = B_{i1}\,\psi_1 + B_{i2}\,\psi_2 + \cdots \ldots \ldots \ldots + B_{i\,n+2}\,\psi_{n+2} = \sum_{j=1}^{n+2} B_{ij}\,\psi_j \tag{11}$$

Once again, we have expressed ψ_i' and ψ_i'' as weighted averages of values of ψ at several locations. It must be noted that in the OC technique, values of *y* at all OC locations are used in the expressions for ψ_i' and ψ_i'', while in the finite difference technique, values of ψ at only the neighboring locations are required.

3. Example

To understand more about orthogonal collocation method, the solution of differential equation used in isothermal Tubular reactor with axial mixing with an irreversible, second Order reaction taking place, described (in chemical engineering) by

$$\frac{1}{Pe}\frac{d^2c}{dz^2} - \frac{dc}{dz} - Da\ c^2 = 0 \qquad 0 \le z \le 1 \tag{12}$$

with boundary conditions

$$\frac{dc}{dz} = Pe(c-1) \ \text{ at } \ z = 0 \tag{13}$$

$$\frac{dc}{dz} = 0 \ \text{ at } \ z = 1 \tag{14}$$

here, c is the dimensionless reactant concentration , z is the dimensionless axial position, *Pe* is peclet number for mass transfer and *Da* is the Damkohler number. Take two orthogonal points (i.e. N=2). Then above equations reduces to

$$\frac{1}{Pe}c'' - c' - Da\ c^2 = 0 \tag{15}$$

$$c' = Pe(c-1) \ \text{ at } \ z = 0 \tag{16}$$

$$c' = 0 \ \text{ at } \ z = 1 \tag{17}$$

At the internal collocation points, we have

$$\frac{1}{Pe}\left[\sum_{j=1}^{4} B_{ij}c_j\right] - \sum_{j=1}^{4} A_{ij}c_j - Da\ c_i^2 = 0 \ ; \quad i = 2,3 \tag{18}$$

and at the two boundaries , we have

$$\sum_{j=1}^{4} A_{1j}c_j = Pe(c_1 - 1) \qquad \text{and} \qquad \sum_{j=1}^{4} A_{4j}c_j = 0 \tag{19}$$

Substituting the values of matrices A_{ij} and B_{ij} , we obtain

$$-7c_1 + 8.196c_2 - 2.196c_3 + c_4 = Pe(c_1 - 1) \qquad \text{for } (i = 1)$$

$$\frac{1}{Pe}[16.39c_1 - 24c_2 + 12c_3 - 4.392c_4] - [-2.732c_1 + 1.732c_2 + 1.732c_3 - 0.7321c_4] = Da\ c_2^2 \qquad \text{for } (i = 2)$$

$$\frac{1}{Pe}[-4.392c_1 + 12c_2 - 24c_3 + 16.39c_4] - [0.7321c_1 - 1.732c_2 - 1.732c_3 + 2.7321c_4] = Da\ c_3^2 \qquad \text{for } (i = 3)$$

$$-c_1 + 2.196c_2 - 8.196c_3 + 7c_4 = 0 \qquad \text{for } (i = 4)$$

or, in matrix form, *M C* =*D*, where

$$M = \begin{bmatrix} -7-Pe & 8.196 & -2.196 & 1 \\ \frac{16.39}{Pe}+2.732 & \frac{-24}{Pe}-1.732 & \frac{12}{Pe}-1.732 & \frac{-4.392}{Pe}+0.732 \\ \frac{-4.392}{Pe}-0.7321 & \frac{12}{Pe}+1.7321 & \frac{-24}{Pe}+1.7321 & \frac{16.39}{Pe}+2.7321 \\ -1 & 2.196 & -8.196 & 7 \end{bmatrix}$$

$$C = [c_1 \quad c_2 \quad c_3 \quad c_4]' \text{ , and } \qquad D = \begin{bmatrix} -Pe \\ Da\, c_2^2 \\ Da\, c_3^2 \\ 0 \end{bmatrix}$$

After solving the above system of equations, the solution at collocation points are obtained. In tables 1-4, the values of solution at collocation points for different Peclet Number *Pe* and Damkohler number *Da* are given.

Table 1: *Concentration values 'c' at Collocation Points for Da = 2 at different Pe*

x	*Pe*=5	*Pe* =10	*Pe* =15	*Pe* =20	*Pe* =25	*Pe* =40	*Pe* = 50	*Pe* =100
0	0.823757	0.891544	0.921516	0.938474	0.949395	0.966967	0.973173	0.986165
0.2113	0.658606	0.68907	0.702154	0.709448	0.714103	0.721524	0.724124	0.729531
0.7887	0.413522	0.392692	0.383252	0.377853	0.374355	0.368694	0.366685	0.362464
1	0.395237	0.370975	0.360098	0.353911	0.349915	0.343469	0.341188	0.336405

Table 2: *Concentration values 'c' at Collocation Points for Da = 4 at different Pe*

x	*Pe*=5	*Pe* =10	*Pe* =15	*Pe* =20	*Pe* =25	*Pe* =40	*Pe* = 50	*Pe* =100
0	0.756819	0.842681	0.883336	0.907214	0.922954	0.948914	0.958278	0.978226
0.2113	0.540159	0.565945	0.577187	0.583542	0.587638	0.594246	0.596588	0.601506
0.7887	0.277007	0.249478	0.236418	0.228723	0.223636	0.215213	0.212162	0.205638
1	0.262993	0.234937	0.221926	0.214334	0.209341	0.201114	0.198145	0.191812

Table 3: *Concentration values 'c' at Collocation Points for Da = 10 at different Pe*

x	*Pe*=5	*Pe* =10	*Pe* =15	*Pe* =20	*Pe* =25	*Pe* =40	*Pe* = 50	*Pe* =100
0	0.690663	0.793647	0.844828	0.87561	0.896189	0.930615	0.943176	0.970176
0.2113	0.426378	0.44616	0.455011	0.460118	0.463462	0.468956	0.470937	0.475166
0.7887	0.167327	0.134733	0.118033	0.107669	0.100562	0.088266	0.083627	0.073323
1	0.160818	0.13116	0.116141	0.106802	0.100371	0.089168	0.08491	0.075375

Table 4: *Concentration values 'c' at Collocation Points for Pe = 6 at different Da*

x	*Da* =4	*Da* =6	*Da* =8	*Da* =10	*Da* =12
0	0.780989	0.744205	0.718964	0.700156	0.685396
0.2113	0.547724	0.478823	0.432138	0.39763	0.370693
0.7887	0.269258	0.20081	0.158428	0.128974	0.106973
1	0.255	0.191217	0.152633	0.126286	0.106868

Table 5: *Absolute Error between Solutions using OCM and bvp4c Solver*

Pe	*Da* =4	*Da* =8	*Da* =12
4	0.03×10^{-2}	0.19×10^{-2}	0.39×10^{-2}
6	0.10×10^{-2}	0.55×10^{-2}	0.94×10^{-2}
8	0.24×10^{-2}	0.89×10^{-2}	1.48×10^{-2}
10	0.36×10^{-2}	1.19×10^{-2}	1.98×10^{-2}
12	0.46×10^{-2}	1.46×10^{-2}	2.43×10^{-2}
14	0.55×10^{-2}	1.69×10^{-2}	2.84×10^{-2}
16	0.62×10^{-2}	1.89×10^{-2}	3.21×10^{-2}
18	0.69×10^{-2}	2.07×10^{-2}	3.55×10^{-2}

And Table 5 gives the absolute error between solutions obtained from OCM method and bvp4c solver of MATLAB.

4. Conclusion

Orthogonal Collocation method is a useful method to solve ordinary differential equations. In this paper, the ordinary differential equation using OCM method is solved. The results obtained using OCM method is compared with MATLAB *bvp4c* solver for different Peclet Number *Pe* and Damkohler number *Da*. As the table 5 shows the results obtained using Orthogonal Collocation method is almost same (of order 10^{-2}) as solution obtained using MATLAB *bvp4c* solver. Further, Orthogonal Collocation method can also be applied to solve partial differential equations.

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