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Chebyshev finite difference method for a Two–Point Boundary Value Problems with Applications to Chemical Reactor Theory

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ABSTRACT

In this paper, a Chebyshev finite difference method has been proposed in order to solve nonlinear two-point boundary value problems for second order nonlinear differential equations. A problem arising from chemical reactor theory is then considered. The approach consists of reducing the problem to a set of algebraic equations. This method can be regarded as a non-uniform finite difference scheme. The method is computationally attractive and applications are demonstrated through an illustrative example. Also a comparison is made with existing results.

Keywords: Chemical reactor; Chebyshev finite difference method; Numerical methods; Boundary value problems; Gauss–Lobatto nodes.

1. INTRODUCTION

Consider the mathematical model for an adiabatic tubular chemical reactor which processes an irreversible exothermic chemical reaction. For steady state solutions, this model can be reduced to the ordinary differential equation [1,2,3].

$$u'' - \lambda u' + \lambda\mu(\beta - u)\exp(u) = 0, \tag{1}$$

with boundary conditions

$$u'(0) = \lambda u(0), \qquad u'(1) = 0. \tag{2}$$

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The unknown u represents the steady state temperature of the reaction, and the parameters λ, μ and β represent the Peclet number, the Damkohler number and the dimensionless adiabatic temperature rise, respectively. The existence of solutions (sometimes multiple solutions), for particular ranges, have been considered by several authors [1,2]. A numerical solution of (1) with boundary conditions in (2) is reported in [3,4]. In [3] the problem is converted into a Hammerstein integral equation, by using Green's function technique, and then the solution is obtained by using Adomian's method. The authors of [4] used Sinc-Galerkin method for solving (1)-(2). Sinc-Galerkin method consists of reducing the solution of (1)-(2) to a set of algebraic equations by expanding the $u(x)$ as Sinc function with unknown coefficients. The properties of Sinc function are then utilized to evaluate the unknown coefficients.
In the present paper, we first consider the nonlinear differential equations

$$u''(x) = F\left(x, u(x), u'(x)\right), \tag{3}$$

with boundary conditions

$$a_0\, u(0) + b_0\, u'(0) = c_0, \tag{4}$$

$$a_1\, u(1) + b_1\, u'(1) = c_1, \tag{5}$$

where a_0, a_1, b_0, b_1, c_0 and c_1 are given constants and F is an analytic function. We then solve a problem which falls into this category from chemical reactor theory. Our idea is to apply the Chebyshev finite difference method (ChFD) to discretize Equation (3) to get a nonlinear system of algebraic equations, thus greatly simplifying the problem. ChFD has proven to be successful in the numerical solution of various boundary value problems. This method can be regarded as a non-uniform finite difference scheme. In this method the derivatives of the function $u(t)$ at a point t_j is linear combination of the values of the function u at the Gauss–Lobatto points $t_k = \cos(k\pi / N)$, where $k = 0,1,2,...,N$, and j is an integer $0 \le j \le N$ [5-8]. The organization of this paper is as follows: In the next section we describe the basic formulation of ChFD method required for our subsequent development. In Section 3 the ChFD is used to approximate the solution for (3)-(5). In Section 4, we report our numerical finding for (1),(2) and demonstrate the accuracy of the proposed numerical scheme by considering a numerical example.

2. PRELIMINARIES

The well known Chebyshev polynomials of the first kind of degree n are defined on the interval $[-1,1]$ as

$$T_n(t) = \cos(n\cos^{-1}(t)), \qquad n = 0,1,....$$

Obviously $T_0(t) = 1$, $T_1(t) = t$ and they satisfy the recurrence relations:

$$T_{n+1}(t) = 2t\ T_n(t) - T_{n-1}(t), \qquad n = 1,2,...$$

We choose the grid (interpolation) points to be the extrema

$$t_k = \cos\left(\frac{k\pi}{N}\right), \quad k = 0,1,2,...,N$$

of the N th-order Chebyshev polynomial $T_N(t)$. These grids,

$$t_N = -1 < t_{N-1} < ... < t_1 < t_0 = 1$$

are also viewed as the zeros of $(1-t^2)\dot{T}(t)$ where $\dot{T}(t) = dT/dt$. Clenshaw and Curtis [9] introduced the following approximation of the function $u(t)$:

$$u_N(t) = \sum_{n=0}^{N}{}''\, a_n T_n(t), \quad a_n = \frac{2}{N}\sum_{j=0}^{N}{}''\, u(t_j)T_n(t_j) \tag{6}$$

The summation symbol with double primes denotes a sum with both the first and last terms halved. The first and second derivatives of the function $u(t)$ at the point t_k are given by [7,8]

$$u_N^{(n)}(t_k) = \sum_{j=0}^{N} d_{k,j}^{(n)} u(t_j), \quad n = 1,2. \tag{7}$$

where

$$d_{k,j}^{(1)} = \frac{4\theta_j}{N}\sum_{n=0}^{N}\sum_{\substack{l=0 \\ (n+l)odd}}^{n-1}\frac{n\theta_n}{c_l}T_n(t_j)T_l(t_k), \quad k,j = 0,1,...,N.$$

$$d_{k,j}^{(2)} = \frac{2\theta_j}{N}\sum_{n=0}^{N}\sum_{\substack{l=0 \\ (n+l)even}}^{n-2}\frac{n(n^2-l^2)\theta_n}{c_l}T_n(t_j)T_l(t_k), \quad k,j = 0,1,...,N.$$

with $\theta_0 = \theta_n = 1/2$, $\theta_j = 1$ for $j = 1,2,...,N-1$, and $c_o = 2$, $c_i = 1$ for $i \geq 1$.

As we see from (7), the first and second derivatives of the function $u(x)$ at any point from the Gauss–Lobatto nodes are expanded as linear combination of the values of the function at these points.

3. DISCRETIZATION OF THE PROBLEM

In this section we solve the nonlinear second-order boundary value problems (3)-(5) by using ChFD method. For this purpose since the Gauss–Lobatto nodes lie in the computational interval $[-1,1]$ in the first step of this method, the transformation $t = 2x - 1$ is used to change equation (3) to the following form:

$$4u''(t) = F\left((t+1)/2,\, u(t),\, 2u'(t)\right), \tag{8}$$

also the boundary conditions (4) and (5) are changed to

$$a_0\, u(-1) + 2b_0\, u'(-1) = c_0, \tag{9}$$

$$a_1\, u(1) + 2b_1\, u'(1) = c_1, \tag{10}$$

Now, to find the solution $u(t)$ in (8) , by applying the ChFD method, a collocation scheme is defined by substituting (6) in (8) and evaluating the result at the Gauss–Lobatto nodes t_k for $k = 1, 2, ..., N-1$ and using equation (7) we obtain

$$4\sum_{j=0}^{N} d_{k,j}^{(2)} u(t_j) = F\left((t_k+1)/2,\, u(t_k),\, 2\sum_{j=0}^{N} d_{k,j}^{(1)} u(t_j)\right), \qquad k = 1, 2, ..., N-1, \tag{11}$$

for $k = 0$ and $k = N$ by using the boundary conditions (9) and (10) we obtain

$$a_0\, u(t_N) + 2b_0 \sum_{j=0}^{N} d_{N,j}^{(1)} u(t_j) = c_0, \tag{12}$$

$$a_1\, u(t_N) + 2b_1 \sum_{j=0}^{N} d_{0,j}^{(1)} u(t_j) = c_1, \tag{13}$$

Therefore equations (11) ,(12) and (13) generate a set of $N+1$ nonlinear algebraic equations, which can be solved for the unknown $u(t_k), k = 0, ..., N$. Consequently $u(t)$ given in equation (6) can be calculated.

4. ILLUSTRATIVE EXAMPLE

To validate the application of ChFD method to (1),(2), we use particular values of the parameters, $\lambda = 10, \beta = 3$ and $\mu = 0.02$ For such values for the parameters, a unique solution is guaranteed by the contraction mapping principle [3]. For this problem, by using the contraction mapping principle, the required integrations cannot be done analytically and are evaluated numerically using the trapezoidal rule. In order to use ChFD method, by using equations (11), (12) and (13) we have

$$4\sum_{j=0}^{N} d_{k,j}^{(2)} u(t_j) - 2\lambda \sum_{j=0}^{N} d_{k,j}^{(1)} u(t_j) + \lambda\mu(\beta - u(t_k))\exp(u(t_k)) = 0, \quad k = 1,2,...,N-1, \tag{14}$$

$$2\sum_{j=0}^{N} d_{N,j}^{(1)} u(t_j) - \lambda u(t_N) = 0, \tag{15}$$

$$\sum_{j=0}^{N} d_{0,j}^{(1)} u(t_j) = 0. \tag{16}$$

Thus by solving $N+1$ nonlinear algebraic equations (14),(15),(16) and by substituting the $u(t_k)$ for $k = 0,...,N$ to equation (6) the approximation solution can be found. Here we choose $N = 9$ and $N = 11$. Table 1 gives a comparison of the results from the contraction mapping principle [3], the shooting method [3], the Adomian's method [3], the Sinc-Galerkin method [4] and present method with $N = 9$ and $N = 11$.

Table 1. Comparison of $u(x)$ which has been found for $N = 9,11$.

x	Contraction Principle	Shooting Method	Adomian's Method	Sinc-Galerkin Method		ChFD Method	
				N = 10	N = 20	N = 9	N = 11
0.0	0.006079	0.006048	0.006048	0.006049	0.006048	0.006046	0.006048
0.2	0.018224	0.018192	0.018192	0.018197	0.018192	0.018190	0.018192
0.4	0.030456	0.030424	0.030424	0.030437	0.030424	0.030423	0.030424
0.6	0.042701	0.042669	0.042669	0.042649	0.042669	0.042666	0.042669
0.8	0.054401	0.054371	0.054371	0.054383	0.054371	0.054369	0.054371
1.0	0.061459	0.061458	0.061458	0.061459	0.061458	0.061459	0.061458

From Table 1 we see that the results using ChFD method with $N = 11$ agree with those of the Sinc Galerkin method, (with $N = 20$) shooting method and Adomian's method up to the sixth decimal place. It is worth to mention here that, in Sinc Galerkin method the result will be obtain by solving $(2N+1)$ nonlinear algebraic equations, but in ChFD method the result will be obtain by solving only $(N+1)$ nonlinear algebraic equations. Furtheremore in Figure1 the residual functions $\left|u_N''(x) - \lambda u_N'(x) + \lambda\mu(\beta - u_N(x))\exp(u_N(x))\right|$ are plotted for $N = 11$ and $N = 20$.

5. CONCLUSION

This paper described an efficient method for solving nonlinear two-point boundary value problems with applications to chemical reactor theory. Our approach was based on the Chebyshev finite difference method. This approach requires the definition of grid points and it can be applied to satisfy differential equation and the boundary conditions at these grid points. The method is computationally attractive and applications are demonstrated through an illustrative example.

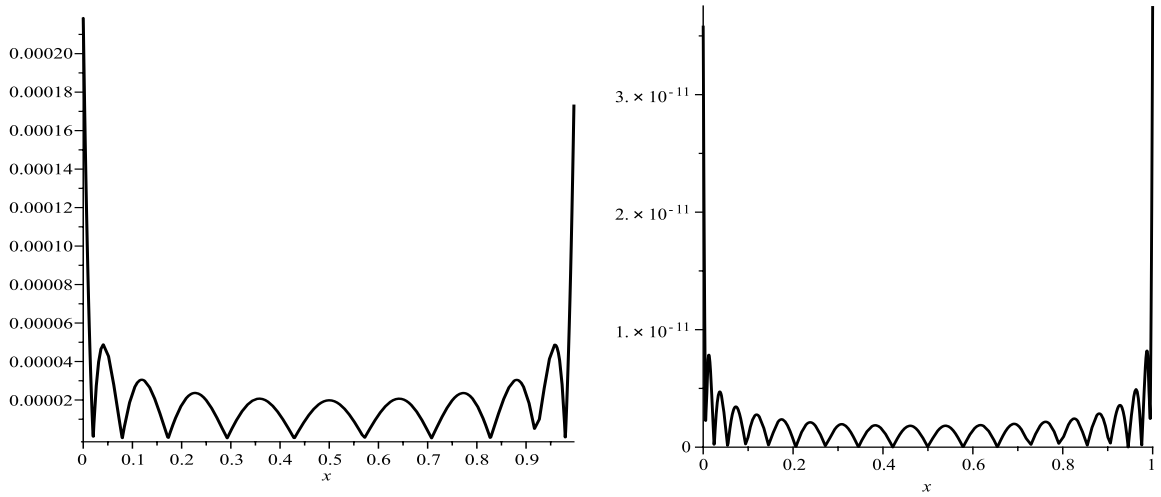

Figure 1. Plot of the Residual Functions for $N = 11$ (left) and $N = 20$ (right).

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