B-Spline collocation method for numerical solution of the nonlinear two-point boundary value problems with applications to chemical reactor theory

M. Zarebnia*[1] and R.Parvaz†[1]

[1]Department of Mathematics, University of Mohaghegh Ardabili, 56199-11367 Ardabil, Iran.

October 4, 2014

Abstract

In this article, the cubic B-spline collocation method is implemented to find numerical solution of the problem arising from chemical reactor theory. The method is tested on some model problems from the literature, and the numerical results are compared with other methods.

Keywords : B-Spline Collocation method, Two-point boundary value problems, Chemical reactor theory.

1 Introduction

In this paper, we discuss a collocation method based on cubic B-splines for a class of the problem arising from chemical reactor theory. Consider the nonlinear differential equation

$$ay^{''}(x) + by^{'}(x) + G(x, y(x)) = 0, \qquad x \in [x_0, x_n], \tag{1}$$

with boundary conditions

$$c_0 y(x_0) + c_1 y^{'}(x_0) = 0, \qquad d_0 y(x_n) + d_1 y^{'}(x_n) = 0,$$

where a, b, c_0, c_1, d_0 and d_1 are given constants. The mathematical model for an adiabatic tubular chemical reactor which processes an irreversible exothermic chemical reaction can be reduced to

*zarebnia@uma.ac.ir
†rparvaz@uma.ac.ir

International Journal of Mathematical Engineering and Science (IJMES)
Volume 3 Issue 3 (Year 2014) ISSN : 2277-6982
http://www.ijmes.com/

the ordinary differential equation 1 with $a = 1, b = -\lambda$ and $G(x, y(x)) = \lambda\mu(\beta - y)exp(y)$. The parameters λ, μ and β represent the peclet number, the damkohler number and the dimensionless adiabatic temperature rise. Then we can write:

$$y^{''}(x) - \lambda y^{'}(x) + \lambda\mu(\beta - y)exp(y) = 0, \qquad x \in [0, 1], \tag{2}$$

with boundary conditions

$$-\lambda y(0) + y^{'}(0) = 0, \qquad y^{'}(1) = 0.$$

In recent years, many different methods have been used to estimate the solution of the the problem arising from chemical reactor theory, for example, see [1, 2].

The paper is organized as follows. In Section 2, cubic B-spline collocation method is explained. In Section 3, we develop an algorithm for the numerical solution of the problem. In Section 4, example is presented. Note that we have computed the numerical results by Mathematica-9 programming.

2 Cubic B-spline collocation method

The solution domain $0 \le x \le 1$ partitioned in to a mesh of uniform length $h = 1/N$, by the knots x_i where $i = 0, 1, 2, \ldots, N$ and $x_{i+1} = x_i + h$ such that $0 = x_0 < x_1 \ldots x_{N-1} < x_N = 1$. Our numerical treatment for the problem arising from chemical reactor theory using the collocation method with cubic B-spline is to find an approximate solution $Y(x)$ to the exact solution $y(x)$ in the form

$$Y(x) = \sum_{i=-3}^{N-1} c_i B_i(x). \tag{3}$$

We can determine c_i from boundary conditions and collocation form of the differential equations. Also $B_i(x)$ are the cubic B-spline basis functions at knots, given by [3, 4]

$$B_i(x) = \frac{1}{6h^3}\begin{cases} (x - x_i)^3, & x \in [x_i, x_{i+1}), \\ h^3 + 3h^2(x - x_{i+1}) + 3h(x - x_{i+1})^2 - 3(x - x_{i+1})^3, & x \in [x_{i+1}, x_{i+2}), \\ h^3 + 3h^2(x_{i+3} - x) + 3h(x_{i+3} - x)^2 - 3(x_{i+3} - x)^3, & x \in [x_{i+2}, x_{i+3}), \\ (x_{i+4} - x)^3, & x \in [x_{i+3}, x_{i+4}). \end{cases} \tag{4}$$

The values of $B_i(x)$ and its derivatives may be tabulated as in table 1.

International Journal of Mathematical Engineering and Science (IJMES)
Volume 3 Issue 3 (Year 2014) ISSN : 2277-6982
http://www.ijmes.com/

Table 1: B_i,$B_i^{'}$ and $B_i^{''}$ at the node points.

x	x_i	x_{i+1}	x_{i+2}	x_{i+3}	x_{i+4}
$B_i(x)$	0	$\frac{1}{6}$	$\frac{4}{6}$	$\frac{1}{6}$	0
$B_i'(x)$	0	$\frac{1}{2h}$	0	$-\frac{1}{2h}$	0
$B_i''(x)$	0	$\frac{1}{h^2}$	$-\frac{2}{h^2}$	$\frac{1}{h^2}$	0

3 Construction of the method

Substituting the approximate solution Y for y, we have

$$\sum_{i=-3}^{N-1} c_i B_i^{''}(x_j) - \lambda \sum_{i=-3}^{N-1} c_i B_i^{'}(x_j) + \lambda\mu(\beta - \sum_{i=-3}^{N-1} c_i B_i(x_j)) exp(\sum_{i=-3}^{N-1} c_i B_i(x_j)) = 0, \tag{5}$$

where $j = 0, \ldots, N$.

From table 1, we calculate Y, $Y^{'}$ and $Y^{''}$ at node points as

$$Y_i = \frac{1}{6}[c_{i-3} + 4c_{i-2} + c_{i-1}], \tag{6}$$

$$Y_i' = \frac{1}{2h}[c_{i-1} - c_{i-3}], \tag{7}$$

$$Y_i'' = \frac{1}{h^2}[c_{i-3} - 2c_{i-2} + c_{i-1}]. \tag{8}$$

Using equations 6,7 and 8 at the knots and equation 5 we get:

$$\frac{1}{h^2}[c_{j-3}-2c_{j-2}+c_{j-1}]-\lambda\frac{1}{2h}[c_{j-1}-c_{j-3}]+\lambda\mu(\beta-\frac{1}{6}[c_{j-3}+4c_{j-2}+c_{j-1}])exp(\frac{1}{6}[c_{j-3}+4c_{j-2}+c_{j-1}]) = 0, \tag{9}$$

equation 9 can be written as

$$k_1 c_{j-3}+k_2 c_{j-2}+k_3 c_{j-1}+\lambda\mu(\beta-\frac{1}{6}[c_{j-3}+4c_{j-2}+c_{j-1}])exp(\frac{1}{6}[c_{j-3}+4c_{j-2}+c_{j-1}]) = 0, \ \ j = 0, \ldots, N, \tag{10}$$

where $k_1 = \frac{1}{h^2} + \frac{\lambda}{2h}$, $k_2 = \frac{-2}{h^2}$ and $k_3 = \frac{1}{h^2} - \frac{\lambda}{2h}$.

The system 10 consists of $N+1$ nonlinear equations in $N+3$ unknowns $\{c_{-3}, \ldots, c_{N-1}\}$. To obtain a unique solution for $\{c_{-3}, \ldots, c_{N-1}\}$, we must use the boundary conditions. From boundary conditions, we can write

$$(\frac{-\lambda}{6} - \frac{1}{2h})c_{-3} + (\frac{-2\lambda}{3})c_{-2} + (\frac{-\lambda}{6} + \frac{1}{2h})c_{-1} = 0, \tag{11}$$

International Journal of Mathematical Engineering and Science (IJMES)
Volume 3 Issue 3 (Year 2014) ISSN : 2277-6982
http://www.ijmes.com/

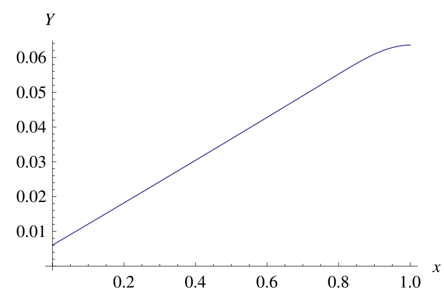

Figure 1: Numerical solution for Example with N=5.

$$c_{N-1} - c_{N-3} = 0. \tag{12}$$

Then we obtain The system consists of $N + 3$ nonlinear equations in $N + 3$ unknowns. The above system has been solved using the computer algebra system package, Mathematica-9.

4 Numerical examples

In order to illustrate the performance of the cubic B-spline collocation method in solving problem, we consider the following example. In this example, we assume that $\lambda = 10, \beta = 3$ and $\mu = 0.02$. For such values for the parameters, a unique solution is guaranteed by the contraction mapping principle [5]. Table 2 gives a comparison of the results by present method with method in [5], shooting method [5] and contraction principle [5]. Also figures show the numerical results.

Table 2: Comparison of the results by present method with method in [5].

x	Contraction principle	Shooting method	method in [5]	Present method	
				$n = 10$	$n = 50$
0.0	0.006079	0.006048	0.006048	0.00604856	0.00604838
0.2	0.018224	0.018192	0.018192	0.0181942	0.018193
0.4	0.030456	0.030424	0.030424	0.0304325	0.030425
0.6	0.042701	0.042669	0.042669	0.0427138	0.0426711
0.8	0.054401	0.054371	0.054371	0.0545839	0.0543802
1.0	0.061459	0.061458	0.061458	0.0619841	0.0614797

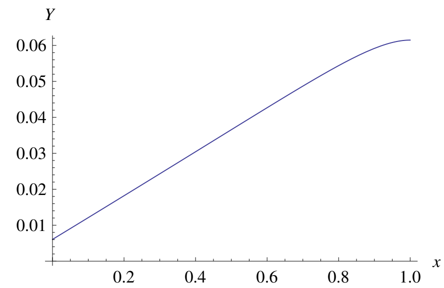

Figure 2: Numerical solution for Example with N=50.

5 Conclusion

In this paper, the cubic B-spline collocation method is used to solve the nonlinear two-point boundary value problems with applications to chemical reactor theory. The numerical results given in the previous section. Also the numerical results are compared with other methods.

References

[1] A. Saadatmandi, M. Razzaghi, and M. Deghan, "Sinc-galerkin solution for nonlinear two-point boundary value problems with applications to chemical reactor theory," *Mathematical and Computer Modelling*, vol. 42, pp. 1237 –1244, 2005.

[2] A. Saadatmandi and M.R.Azizi, "Chebyshev finite difference method for a two-point boundary value problems with applications to chemical reactor theory," *Iranian Journal of Mathematical Chemistry*, vol. 3, no. 1, pp. 1–7, 2012.

[3] P. Prenter, "Spline and variational methods," *Wiley, New York*, 1975.

[4] J. Stoer and R. Bulirsch, "Introduction to numerical analysis," *third edition ,Springer-Verlg*, 2002.

[5] N. Madbouly, D. McGhee, and G. Roach, "Adomian's method for hammerstein integral equations arising from chemical reactor theory," *Applied Mathematics and Computation*, vol. 117, pp. 249 – 341, 2001.