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NUMERICAL INTEGRATION (QUADRATURE) METHOD FOR STEADY –STATE CONVECTION-DIFFUSION PROBLEMS

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ABSTRACT

In this paper, a numerical integration method is presented for solving a general steady-state convection problem or singularly perturbed two-point boundary value problem. The governing second-order differential equation is replaced by an approximate first-order differential equation with a small deviating argument. Then the Simpson one-third formula is used to obtain the three term recurrence recurrence relationship. The proposed method is iterative on the deviating argument. To test and validity of this method we have solved several model linear problems with left-end boundary layer or right-end boundary layer or an internal layer and offered the computational results.

Keywords: Singular Perturbation; Boundary Layer; Peclet Number; Two-Point Boundary Value Problem..

I. INTRODUCTION

Convection-diffusion problems occur very frequently in the fields of science and engineering such as fluid dynamics, specifically the fluid flow problems involving large Reynolds number and other problems in the great world of fluid motion. The numerical treatment of singular perturbation problems is far from trivial because of the boundary layer behavior of the solution. However, the area of convection-diffusion problems is a field of increasing interest to applied mathematicians.

The survey paper by Kadalbajoo and Reddy [ ], gives an intellectual outline of the singular perturbation problems and their treatment starting from Prandtl's paper [ ] on fluid dynamical boundary layers. This survey paper will remain as one of the most readable source on convection-diffusion or singular perturbation problems.

For a detailed theory and analytical discussion on singular perturbation problems one may refer to the books and high level monographs: O'Malley [ ], Nayfeh [] , Bender and Orszag [ ] , Kevorkian and Cole.

In this paper , a numerical integration method is presented for solving general singularly perturbed two-point boundary value problems .The main advantage of this method is that it does not require very fine mesh size.

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The inventive second-order differential equation is replaced by an approximate first-order differential equation with a small differing argument. Then , the Simpson one-third formula is used to obtain the three term recurrence relationship. Thomas Algorithm is applied to solve the resulting tridiagonal algebraic system of equations. The proposed method is iterative on the deviating argument. The method is to be repeated for different choices of the deviating argument until the solution profile stabilizes. To examine the applicability of the proposed method, we have solved several model linear problems with left-end boundary layer or right –end boundary layer or an internal layer and presented the numerical results. It is observed that the numerical integration method approximates the exact solution extremely well.

II. NUMERICAL INTEGRATION METHOD

For the sake of convenience we call our method the ' Numerical Integration Method'. To set the stage for the numerical integration method , we consider the following Governing linear Convection-diffusion (singularly perturbed two-point boundary value problem:

$$\varepsilon\, y''(x) + a(x)\, y'(x) + b(x)y(x) = f(x);\ 0 \le x \le 1 \qquad (1)$$

With $y(0) = \alpha$ and $y(1) = \beta$ (2)

Where ε is a small positive parameter called diffusion parameter which lies in the interval $0 < \varepsilon \le 1$; α and β are given constants; a(x) , b(x) and f(x) considered to be sufficiently continuously differentiable functions in [0,1]. Furthermore , we assume that $a(x) \ge M > 0$ throughout the interval [0,1], where M is some positive constant. This assumption merely implies that the boundary layer will be in the neighborhood of x=0.

Let δ be a small positive deviating argument ($0 < \delta \le 1$). By applying Taylor series expansions in the neighborhood of the point x, we have

$$y(x-\delta) \approx y(x) - \delta\, y'(x) + \frac{\delta^2}{2} y''(x) \qquad (3)$$

And consequently, Eq. (1) is replaced by the following first-order differential equation with a small deviating argument.

$$\frac{\delta^2}{2} y''(x) = y(x-\delta) - y(x) + \delta\, y'(x) \Rightarrow y''(x) = \frac{2}{\delta^2}[\, y(x-\delta) - y(x) + \delta\, y'(x)] \text{ So that}$$

$$(1) \Rightarrow \frac{2\varepsilon}{\delta^2}[\, y(x-\delta) - y(x) + \delta\, y'(x)\,] + a(x)\, y'(x) + b(x)\, y(x) = f(x);\ 0 \le x \le 1$$

$$\Rightarrow 2\varepsilon\, y(x-\delta) - 2\varepsilon\, y(x) + 2\varepsilon\delta\, y'(x) + a(x)\, y'(x)\delta^2 + b(x)\, y(x)\delta^2 = \delta^2 f(x)$$

$$\Rightarrow [2\varepsilon\delta + a(x)\,\delta^2](y'(x)) + [b(x)\,\delta^2 - 2\varepsilon]\, y(x) = \delta^2 f(x) - 2\varepsilon\, y(x-\delta)$$

$$\Rightarrow y'(x) = \frac{\delta^2 f(x) - 2\varepsilon\, y(x-\delta)}{2\varepsilon\delta + a(x)\ \delta^2} y(x-\delta) + \frac{(2\varepsilon - b(x)\ \delta^2)}{2\varepsilon\delta + a(x)\ \delta^2}\ y(x)$$

$$\Rightarrow y'(x) = \frac{-2\varepsilon}{2\varepsilon\delta + a(x)\,\delta^2} y(x-\delta) + \frac{2\varepsilon - b(x)\,\delta^2}{2\varepsilon\delta + a(x)\,\delta^2} y(x) + \frac{\delta^2 f(x)}{2\ \varepsilon\delta + a(x)\,\delta^2} \qquad (4)$$

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(4) Can be re-written as

$$y'(x) = p(x)\, y(x-\delta) + q(x)\, y(x) + r(x) \text{ for } \delta \le x \le 1 \quad (5)$$

Where

$$p(x) = \frac{-2\varepsilon}{2\varepsilon\delta + \delta^2 a(x)} \quad (6)$$

$$q(x) = \frac{2\varepsilon - \delta^2 b(x)}{2\varepsilon\delta + \delta^2 a(x)} \quad (7)$$

$$r(x) = \frac{\delta^2 f(x)}{2\varepsilon\delta + \delta^2 a(x)} \quad (8)$$

We now divide the interval [0,1] in to N equal parts with mesh size h, i.e., h=1/N and $x_i = ih$ for i= 1,2,3…….N. Integrating equation (5) in [x_{i-1}, x_{i+1}] we get

$$y(x_{i+1}) - y(x_{i-1}) = \int_{x_{i-1}}^{x_{i+1}} [p(x)\, y(x-\delta) + q(x)\, y(x) + r(x)]\, dx \quad (9)$$

By making use of the Newton-Cotes formula when n=2 i.e. applying Simpson's 1/3 rule approximately, we obtain

$$y(x_{i+1}) - y(x_{i-1}) = \frac{h}{3}[p(x_{i+1})y(x_{i+1}-\delta) + 4\,p(x_i)\,y(x_i-\delta) + p(x_{i-1}-\delta) + (p_{i+1}+p_{i-1})\,[y(x_{i+1}-\delta) + y(x_{i-1}-\delta)] + q(x_{i+1})\,y(x_{i+1}) + q(x_{i-1})\,y(x_{i-1}) + q(x_{i+1})y(x_{i+1}) + 4q(x_i)y(x_i) + q(x_{i-1})y(x_{i-1}) + r(x_{i+1}) + 4r(x_i) + r(x_{i-1}) + r(x_{i+1}) + r(x_{i-1}) \quad (10)$$

Again by means of Taylor's series expansion, we have

$$y(x-\delta) \cong y(x) - \delta\, y'(x)$$

and then by approximating $y'(x)$ by Linear Interpolation method we get

$$y(x_i - \delta) \cong y(x_i) - \frac{\delta[y(x_{i+1}) - y(x_{i-1})]}{2h}$$

$$= y(x_i) + \frac{\delta}{2h} y(x_{i-1}) - \frac{\delta}{2h} y(x_{i+1}) \quad (11)$$

similarly

$$y(x_{i-1} - \delta) \cong (1 + \frac{\delta}{h})\, y(x_{i-1}) - \frac{\delta}{h} y(x_i) \quad (12)$$

$$y(x_{i+1} - \delta) = (1 - \frac{\delta}{h})\, y(x_{i+1}) + \frac{\delta}{h} y(x_i) \quad (13)$$

Hence making use of (11),(12),(13) (10) can be written as

$$y_{i+1} - y_{i-1} = \frac{h}{3}[p_{i+1}[(1-\frac{\delta}{h})y_{i+1} + \frac{\delta}{h}y_i] + 4p_i[y_i - \frac{\delta}{2h}y_{i+1} + \frac{\delta}{2h}y_{i-1}] + p_{i-1}[(1+\frac{\delta}{h})y_{i-1} - \frac{\delta}{h}y_i]$$
$$+ (p_{i+1} + p_{i-1})[(1-\frac{\delta}{h})y_{i+1} + \frac{\delta}{h}y_i + (1+\frac{\delta}{h})y_{i-1} - \frac{\delta}{h}y_i + 2q_{i+1}y_{i+1} + 2q_{i-1}y_{i-1} + 4q_i y_i + 2r_{i+1} + 4r_i + 2r_{i-1}$$

$$[-1 - \frac{2p_i\delta}{3} - \frac{h}{3}p_{i-1}(1+\frac{\delta}{2h}) - \frac{h}{3}(p_{i+1}+p_{i-1})(1+\frac{\delta}{h}) - \frac{2h}{3}q_{i-1}]y_{i-1} + [\frac{\delta p_{i-1}}{3} - \frac{\delta}{3}p_{i+1} - \frac{4hp_i}{3}$$
$$- \frac{4hq_i}{3}]y_i + [1 - \frac{h}{3}p_{i+1}(1-\frac{\delta}{h}) + \frac{2p_i\delta}{3} - \frac{h}{3}(p_{i+1}+p_{i-1})(1-\frac{\delta}{h}) - \frac{2h}{3}q_{i+1}]y_{i+1}$$
$$= \frac{2h}{3}[r_{i+1} + 2r_i + r_{i-1}] \qquad (14)$$

can be written in the standard form as

$$A_i y_{i-1} + B_i y_i + C_i y_{i+1} = D_i \qquad (15)$$

where

$$A_i = -1 - \frac{2p_i\delta}{3} - \frac{h}{3}p_{i-1}(1+\frac{\delta}{2h}) - \frac{h}{3}(p_{i+1}+p_{i-1})(1+\frac{\delta}{h}) - \frac{2h}{3}q_{i-1} \qquad (16)$$

$$B_i = \frac{\delta p_{i-1}}{3} - \frac{\delta}{3}p_{i+1} - \frac{4hp_i}{3} - \frac{4hq_i}{3} \qquad (17)$$

$$C_i = 1 - \frac{h}{3}p_{i+1}(1-\frac{\delta}{h}) + \frac{2p_i\delta}{3} - \frac{h}{3}(p_{i+1}+p_{i-1})(1-\frac{\delta}{h}) - \frac{2h}{3}q_{i+1} \qquad (18)$$

$$D_i = \frac{2h}{3}[r_{i+1} + 2r_i + r_{i-1}] \qquad (19)$$

.

Here $y_i = y(x_i)$, $p_i = p(x_i)$, $q_i = q(x_i)$ and $r_i = r(x_i)$. Equation (16) gives a system of (N-1) equations with (N+1) unknowns y_0 to y_N. The two given boundary conditions ( ) together with these (N-1) equations are then sufficient to solve for the unknowns y_0 , y_N. The solution of the Tri-diagonal system (15) can be obtained by using an efficient algorithm called 'Thomas Algorithm. In this algorithm we set a difference relation of the form

$$y_i = W_i y_{i+1} + T_i \qquad (20)$$

Where W_i and T_i corresponding to $W(x_i)$ and $T(x_i)$ are to be determined from (20) we have

$$y_{i-1} = W_{i-1} y_i + T_{i-1} \qquad (21)$$

Substituting (21) in (15) we get

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$$y_i = \frac{C_i}{B_i - A_i W_{i-1}} y_{i+1} + \frac{A_i T_{i-1} - D_i}{B_i - A_i W_{i-1}} \qquad (22)$$

By compararing (20) and (22) , we can get

$$W_i = \frac{C_i}{B_i - A_i W_{i-1}} \qquad (23)$$

$$T_i = \frac{A_i T_{i-1} - D_i}{B_i - A_i W_{i-1}} \qquad (24)$$

To solve these recurrence relations for i=1,2,3,…….N-1; we need to know the initial conditions for W_0 and T_0 . This can be done by considering (2)

$$y_0 = \alpha = W_0 y_1 + T_0 \qquad (25)$$

If we choose W_0=0, then $T_0 = \alpha$. With these initial values , we compute sequentially W_i and T_i for i=1,2,3,….N-1;from (24) and (25) in the forward process and then obtain y_i in the backward process from (20) using (2).

Repeat the numerical scheme for different choices of δ (deviating argument, satisfying the conditions $(0 < \delta \leq 1)$, until the solution profiles do not differs significantly from iteration to iteration. For computational point of view, we use an absolute error criterion, namely

$$\left| y(x)^{m+1} - y(x)^m \right| \leq \rho, 0 \leq x \leq 1 \qquad (26)$$

Where $y(x)^m$ is the solution for the mth iterate of δ, and ρ is the prescribed tolerance bound.

III. LINEAR PROBLEMS

Here we are considered the applicability of the numerical integration method, we have applied it to linear singular perturbation problems with left-end boundary layer. These examples have been chosen because they have been widely discussed in the literature and because approximate solution is available for comparison.

Example 1.

Consider the following homogeneous Singular value perturbation problem from Kevorkian and Cole [6, p.33,Eqs.(2.3.26) and (2.3.27)] with α =0:

$$\varepsilon y''(x) + y'(x) = 0, \ 0 \leq x \leq 1 \text{ with } y(0) = 0 \text{ and } y(1) = 1$$

The exact solution is given by

$$y(x) = \frac{(1 - \exp(-x/\varepsilon))}{(1 - \exp(-1/\varepsilon))}$$

The computational results are presented in Table 1(a) and (b) for ε = 10^{-3}, 10^{-4} respectively.

Table 1 Computational Result for Example 1

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X	y(x)			Exact solution
ε=0.001,h=0.01	δ=0.008	δ=0.009	δ=0.007	
0.00	**0.00000000**	**0.00000000**	**0.00000000**	**0.00000000**
0.02	**0.9876486**	**0.9899944**	**0.9917358**	**1.0000000**
0.04	**0.9998419**	**0.9998944**	**0.9999319**	**1.0000000**
0.06	**0.9999925**	**0.9999934**	**0.9999995**	**1.0000000**
0.08	**0.9999945**	**0.9999945**	**1.0000000**	**1.0000000**
0.10	**0.9999946**	**0.9999948**	**1.0000000**	**1.0000000**
0.20	**0.9999954**	**0.9999952**	**1.0000000**	**1.0000000**
0.40	**0.9999964**	**0.9999964**	**1.0000000**	**1.0000000**
0.60	**0.9999976**	**0.9999976**	**1.0000000**	**1.0000000**
0.80	**0.9999988**	**0.9999988**	**1.0000000**	**1.0000000**
1.00	**1.00000000**	**1.00000000**	**1.0000000**	**1.0000000**

(b) $\varepsilon = 10^{-4}$ and h= 0.01

0.00	**0.00000000**	**0.00000000**	**0.00000000**	**0.00000000**
0.02	**0.9998016**	**0.9998477**	**0.9998792**	**1.0000000**
0.04	**0.9999999**	**1.0000000**	**1.0000000**	**1.0000000**
0.06	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**
0.08	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**
0.10	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**
0.20	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**
0.40	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**
0.60	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**
0.80	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**
1.00	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**

Example 2

Consider the following homogeneous Spp from Bender and Orsag[2,p.480. problem 9.17] with α =0 :

$\varepsilon y''(x) + y'(x) - y(x) = 0,\ 0 \le x \le 1$ with $y(0) = 0$ and $y(1) = 1$

The exact solution is given by

$$y(x) = \frac{(e^{m_2} - 1)\ e^{m_1 x} + (1 - e^{m_1})\, e^{m_2 x}}{(e^{m_2} - e^{m_1})}$$ where

$$m_1 = \frac{-1 + \sqrt{1 + 4\varepsilon}}{2\varepsilon}\ ;$$

$$m_2 = \frac{-1 - \sqrt{1 + 4\varepsilon}}{2\varepsilon}$$

Table 2 Computational Results for Example 2 .

X	y(x)			Exact solution
ε=0.001,h=0.01	δ=0.008	δ=0.009	δ=0.007	
0.00	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**
0.02	**0.3834784**	**0.3819605**	**0.3808348**	**0.3756784**
0.04	**0.3834410**	**0.3833556**	**0.3832939**	**0.3832599**
0.06	**0.3910826**	**0.3910290**	**0.3909866**	**0.3909945**
0.08	**0.3989720**	**0.3989188**	**0.3988770**	**0.3988851**
0.10	**0.4070216**	**0.4069688**	**0.4069269**	**0.4069350**
0.20	**0.4497731**	**0.4497210**	**0.4496799**	**0.4496879**
0.40	**0.5492185**	**0.5491707**	**0.5491330**	**0.5491404**
0.60	**0.6706514**	**0.6706123**	**0.6705816**	**0.6705877**
0.80	**0.8189330**	**0.8189092**	**0.8188905**	**0.8188942**
1.00	**1.0000000**	**1.0000000**	**1.0000000**	**1.0000000**

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