A Numerical Method for Boundary Value Problems of Nonlinear Ordinary Differential Equations

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1. *Introduction*

Many problems in engineering are reduced to the form of boundary value problems of non-linear ordinary differential equations (abreviated in the followings as NLDE). The cut and try method as an initial value problem may succeed in some cases. At the present time Dynamic programming gives the solution not in practice but in principle. It seems rather 'an oracle' than a method.

The following is a numerical one which approximates the NLDE in the form of finite differences and solves them iteratively as a linear simulteneous equations. It is very effective, especially for the case of second or third order NLDE, which appears in chemical engineering or heat convection problem. In these cases the coefficient matrix of the reduced equations is a band matrix of width three and the solution is obtained by Gauss elimination method which is reduced to the recurrence form. The method is presented in the following with three examples.

2. *Chemical Reactor Problem*

The first example is a chemical reactor problem cited from a text of numerical methods [1] and is expressed as

$$\frac{1}{Pe}\frac{d^2f}{dz^2}-\frac{df}{dz}-Rf^m=0, \quad 0<z<1.0 \tag{2.1}$$

with boundary conditions

$$\left.\begin{aligned} &\text{at} \quad z=0:\ 1.0=f-\frac{1}{Pe}\frac{df}{dz},\\ &\text{at} \quad z=1.0:\ \frac{df}{dz}=0,\end{aligned}\right\} \tag{2.2}$$

where Pe: Peclect number,
R: constant involving reaction constant,
z: dimensionless axial-distance parameter,
f: fraction of reactant remaining.

We consider the case $m=2$. Dividing the interval of z (0, 1.0), we obtain the following finite-difference representations with mesh size h:

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$$\left.\begin{array}{l}\dfrac{1}{Pe}\dfrac{f_{n+1}-2f_n+f_{n-1}}{h^2}-\dfrac{f_{n+1}-f_{n-1}}{2h}\\ -Rf_n^2=0,\ (n=0,\ 1,\ \ldots,N)\end{array}\right\} \tag{2.3}$$

$$\left.\begin{array}{l}1.0=f_0-\dfrac{1}{2\,Peh}(f_1-f_{-1}),\\ f_{N+1}=f_{N-1}.\end{array}\right\} \tag{2.4}$$

The system to solve will now be a nonlinear set of algebraic simultaneous equations (quadratic equations in this case). The author of the text cited above tried to solve them from this point of view, but he could not obtain sufficient convergence. The number of iterations amounted to more than thousands especially for small mesh size h.

This is due to the lack of sense of order estimation which is important for the engineer or the numerical analysist. We shall now solve these equations reducing to the following linearized form:

$$\left.\begin{array}{l}f_0+b_0f_1=d_0,\\ f_0+a_1f_1+b_1f_2=d_1,\\ \quad\cdots\cdots\\ f_{n-1}+a_nf_n+b_nf_{n+1}=d_n,\\ \quad\cdots\cdots\\ f_{N-1}+a_Nf_N=d_N,\end{array}\right\} \tag{2.5}$$

where

$$\left.\begin{array}{l}a_0=1,\\ a_n=-(2+RPeh^2f_n)/(1+Peh/2),\\ \quad(n=1,\ 2,\ \ldots,\ N-1)\\ a_N=-(2+RPeh^2f_N)/2,\\ b_0=-2/(2+(1+Peh/2)\cdot 2\,Peh+RPeh^2f_0),\\ b_n=(1-Peh/2)/(1+Peh/2)\equiv b,\\ \quad(n=1,\ 2,\ \ldots,\ N=1)\\ d_0=(1+Peh/2)\cdot 2\,Peh/(2+(1+Peh/2)\cdot\\ \quad 2\,Peh+RPeh^2f_0),\\ d_n=0,\ (n=1,\ 2,\ \ldots,\ N)\end{array}\right\} \tag{2.6}$$

Since most of these coefficients do contain the variable f, these actully are not linear equations. From the point of physical considerations, however, it should be noted that the terms with f multiplied by h^2 would be sufficiently small in comparison with the other term, 1 or 2. Hence, substituting some assumed values for these terms, we solve the equations as a set of simultaneous linear equations.

Fortunately, the Gauss elimination method in this case is reduced to Thomas method as follows:

$$\left.\begin{array}{l} q_0=b_0,\ g_0=d_0, \\ w=a_n-q_{n-1},\ g_n=(d_n-g_{n-1})/w, \\ q_n=b_n/w,\ (n=1,\ 2,\ \ldots,\ N) \end{array}\right\} \quad (2.7)$$

$$\left.\begin{array}{l} f_N=g_N, \\ f_n=g_n-q_nf_{n+1},\ (n=N-1,\ N-2,\ \ldots,\ 1,\ 0) \end{array}\right\} \quad (2.8)$$

The new values of f are now substituted for the old ones. The iterations are repeated until the desired convergence is obtained.

Nnmerical results are shown in Table 1, where the reader will see that the number o iterations is very small compared with thousands. In all calculations the assumed values for f are 0.5. The result shows the method to be effective in practice.

3. *Natural Convection above a Horizontal Line Heat Source*

This problem in the laminar stationary flow is formulated in the form of non-linear partial differential equations with respect to the fluid velocity and temperature, which are derived from the equation of continuity of the fluid, Navier-Stokes equation and the energy balance. They, however, are reduced to the following form of boundary value problem of NLDE, when the stream function is introduced and similarity of the velocity field and the temperature field in the laminar boundary layer is assumed [2].

$$f'''+(3/5)ff''-(f')^2/5+h=0, \quad (3.1)$$

$$h''+(3/5)Pr(fh)'=0, \quad (3.2)$$

Table 1.

z \ h	0.1	0.05	0.02		0.01		0.005	
	f	f	f	Residuals	f	Residuals	f	Residuals
0	.6365360217	.6367261494	.6367745870	$.147\times10^{-8}$	.6367810170	$.218\times10^{-8}$	.6367796135	$.460\times10^{-10}$
0.1	.6024243277	.6025805761	.6026189805	.0	.6026239140	$-.100\times10^{-9}$	.6026218710	$-.800\times10^{-9}$
0.2	.5723627775	.5724965171	.5725281240	$-.100\times10^{-8}$	.5725320355	$-.700\times10^{-9}$	.5725295050	$.100\times10^{-9}$
0.3	.5460342254	.5461552162	.5461828115	$-.190\times10^{-8}$	.5461860760	$-.190\times10^{-8}$	.5461831875	$-.300\times10^{-9}$
0.4	.5232117201	.5233286422	.5233547030	$-.900\times10^{-9}$	.5233576795	$-.300\times10^{-9}$	.5233545695	$.200\times10^{-9}$
0.5	.5037505831	.5038714629	.5038982910	$.100\times10^{-9}$	.5039013210	.0	.5038981090	$-.160\times10^{-8}$
0.6	.4875838947	.4877164772	.4877463619	$-.300\times10^{-9}$	.4877497120	.0	.4877465146	$.100\times10^{-9}$
0.7	.4747210417	.4748731251	.4749081914	$-.200\times10^{9-}$	.4749123066	$-.100\times10^{-8}$	.4749092049	$.600\times10^{-9}$
0.8	.4652492107	.4654289766	.4654716419	$.100\times10^{-9}$	.4654766726	$-.320\times10^{-8}$	.4654738972	$.400\times10^{-9}$
0.9	.4593379166	.4595542730	.4596070997	$-.490\times10^{-8}$	.4596131785	$.710\times10^{-8}$	.4596110349	$-.160\times10^{-8}$
1.0	.4572468904	.4575098629	.4575754229	$.170\times15^{-6}$	.4575836573	$-.700\times10^{-9}$	.4575797316	$.338\times10^{-7}$
K	10	13	12		32		23	
EPS	10^{-4}	10^{-5}	10^{-6}		10^{-7}		10^{-7}	

K: number of iterations, EPS: constant for convergence test with boundary conditions

at
$$\left.\begin{array}{l}\xi=0: f=0,\ f''=0,\ h'=0,\\ \xi=\infty: f'=0,\ \ h=0\end{array}\right\} \tag{3. 3a, b}$$

where the independent variable ξ is expressed by that of original partial equations and f and h are derived from the stream function and the temperature respectively, and Pr is the Prandtle number. Besides these homogeneous equations, the following quantity I is given by load condition of the heat source and it is normalized to

$$I=\int_{-\infty}^{\infty} hf'\ d\xi=1 \tag{3. 4}$$

By the law of conservation of momentum, the relation

$$\frac{4}{5}\int_{-\infty}^{\infty}(f')^2 d\xi=\int_{-\infty}^{\infty} h d\xi \tag{3. 5}$$

is obtained and it is useful for the check of accuracy.
Now, reformulating (3.1)~(3.4) by

$$f=(5/3)F,\ \ h=(5/3)H \tag{3. 6}$$

we have

$$F'''+FF''-(F')^2/3+H=0, \tag{3. 1'}$$
$$H'+Pr(FH)'=0, \tag{3. 2'}$$
$$\left.\begin{array}{l}\xi=0: F=0,\ \ F''=0,\ \ H'=0,\\ \xi=\infty: F'=0,\ \ H=0,\end{array}\right\} \tag{3. 3'a, b}$$
$$\int_{-\infty}^{\infty} F'\ H d\xi=\left(\frac{3}{5}\right)^2. \tag{3. 4'}$$

Put
$$\xi=aX,\ \ F=bY,\ \ H=cZ \tag{3. 7}$$

where a, b and c are constants. Replacing the variables in (3.1') (3.2') by (3.7), we have

$$\frac{b}{a^3}Y'''+\frac{b^2}{a^2}YY''-\frac{1}{3}\ \frac{b^2}{a^2}(Y')^2+cZ=0, \tag{3. 1''}$$

$$\frac{c}{a^2}Z''+Pr\cdot\frac{bc}{a}(YZ)'=0. \tag{3. 2''}$$

where ($'$) represents the differentiation with respect to X. If we assume the relations

$$ab=1,\ \ b^2=a^2c, \tag{3. 8}$$

then the set of equations (3.1'')~(3.3'') are reduced to the same form as (3.1')~(3.3'), besides that the variables ξ, F and H are replaced by X, Y and Z respectively.

$$Y'''+YY''-(Y')^2/3+Z=0, \tag{3. 9}$$
$$Z''+Pr(YZ)'=0, \tag{3. 10}$$
$$\left.\begin{array}{l}X=0:\ Y=0,\ \ Y''=0,\ \ Z=0,\\ X=\infty:\ Y'=0,\ \ Z=0.\end{array}\right\} \tag{3. 11a, b}$$

Since the combination of a, b and c is arbitrary, the solution of $(3.1'')\sim(3.3'')$ is not unique. Hence, choosing a relevant value of either $Y'(0)$ or $Z(0)$, if we could obtain a set of values Y and Z satisfying (3.11), then it is one of solutions. We, then, calculate the numerical value of the integral $\int_0^\infty Y'ZdX=J$ by just obtained values of Y and Z. From (3.4′) and (3.7) we have

$$\int_0^\infty F'\,Hd\xi=bc\int_0^\infty Y'\,ZdX=\frac{1}{2}\left(\frac{3}{5}\right)^2,$$

hence

$$bcJ=9/50 \tag{3.12}$$

and we have

$$a=(9/50\,J)^{-1/5},\ b=(9/50\,J)^{1/5},\ c=(9/50\,J)^{4/5}$$

The solution of $(3.1')\sim(3.3')$ is now written as

$$\left.\begin{aligned} \xi&=\left(\frac{9}{50\,J}\right)^{-1/5} X,\quad F=\left(\frac{9}{50\,J}\right)^{1/5} Y,\\ H&=\left(\frac{9}{50\,J}\right)^{4/5} Z,\quad F'=\left(\frac{9}{50\,J}\right)^{2/5} Y'. \end{aligned}\right\} \tag{3.13}$$

The numerical procedure to solve (3.9) (3.11) is described in the following. Integration of (3.10) noting a condition of (3.11) yields

$$Z'+PrYZ=0,\ \text{or}\ Z'/Z=-PrY.$$

hence

$$Z=Z_0\exp\{-Pr\int_0^X YdX\}. \tag{3.14}$$

By substitution,

$$Y'=P\ \text{or}\ Y=\int_0^X PdX, \tag{3.15}$$

(3.9) becomes

$$P''+YP'-(P)^2/3+Z_0\exp(-YL)=0, \tag{3.16}$$

where

$$YL=Pr\int_0^X YdX. \tag{3.17}$$

Finite difference approximation is now obtained. From $Y''=0$ at $X=0$, we have $P_{-1}=P_1$,

hence

$$(2+(h^2/3)P_0)P_0-2\,P_1=Z_0h^2, \tag{3.18}$$

and generally at $X=nh$

$$\begin{aligned} &-(1-(h/2)Y_n)P_{n-1}+(2+(h^2/3)P_n)P_n\\ &\quad-(1+(h/2)Y_n)P_{n+1}=Z_0h^2\exp(-YL_n), \end{aligned} \tag{3.19}$$

with the condition for sufficiently large value of N, $P_N=0$. The method is now similar to the case for § 2 and the process will be briefly described below.

1) Assume sufficiently large integer value N for relevant mesh width h to satisfy $P_N=0$.

2) Assume the approximate values for P° and Z_0. We used $P^\circ=(1-\tanh^2(X/2))/2$* and $Z_0=0.3$.

3) Calculate Y_n, YL_n by (3.15) and (3.17).

* An analytical solution in the closed form is obtained for the case $P_r=2$.

4) Substitute them for the relevant terms in (3.19) and solve (3.18) and (3.19) by Thomas method and get new values of P.

5) Calculate Y_n and YL_n and compare them with the assumed or previous values in the preceding iteration. If the desired coincidence has been met, proceed to the following process and if not repeat the processes from 4) to 5).

6) Check the condition $|P_N|<\varepsilon$ (ε is a small positive number). If it is not satisfied, increase N and go to the process 4) supplementing the values P for the new mesh points.

7) If the condition is satisfied, calculate $J=\int_0^\infty Y'ZdX$ and normalize it. Then we have the solution ξ, f, h and f'.

The program was written in SIP, a symbolic input programming language, and later in ALGŌLIP, a subset of ALGŌL, prepared for HIPAC 101B and ŌKITAC 5090A respectively. Prior to the production run, the result for the case $Pr=2$ was compared with the one calculated according to the closed form solution:

the analytic solution: $F'(0)=0.502$, $H(0)=0.336$,

the numerical result: $F'(0)=0.503$, $H(0)=0.337$.

The coinsidence was satisfactory. For another cases the accuracy was checked by

Table 2.

P_r	Δ_x	N	EPS	K	Machine time (min.)	I_f	I_h
1.0	2^{-4}	200	10^{-5}	21	22	0.4695	0.4720
2.0	(2^{-3} 2^{-4}	80 200	2^{-13} 10^{-5}	8 20	26+34) 23		
3.0	2^{-4}	200	10^{-5}	19	22	0.4401	0.4376
5.0	2^{-4}	200	10^{-5}	17	19	0.4377	0.4317
10.0	(2^{-8} 2^{-4}	160 200	2^{-13} 10^{-5}	12 14	45+65) 15	0.4442	0.4313
30.0	2^{-4}	200	10^{-5}	16	15	0.4729	0.4423
100.0	2^{-4}	200	10^{-5}	14	15	0.5251	0.4591
300.0	2^{-4}	200	10^{-5}	17	13	0.5899	0.4650
1000.0	2^{-4}	200	10^{-5}	17	13	0.7060	0.4215
0.01	(1 2^{-1}	190 200	2^{-13} 10^{-5}	12 26	52+76) 26	0.7702	0.7850
0.03	2^{-1}	200	10^{-5}	25	25	0.6768	0.6957
0.1	2^{-4}	200	10^{-5}	29	25	0.6100	0.6157
0.3	2^{-4}	200	10^{-5}	24	25	0.5353	0.5404
0.7	(2^{-3} 2^{-4}	80 200	2^{-13} 10^{-5}	9 23	36+36) 26	0.4860	0.4896

The values in parenthesis are computed by HIPAC-101B (drum machine) and they are shown in the form of the pure machine time plus the printing time.

I_f and I_h are the values to check the accuracy of the calculations by the law of conservation of momentum, equ. (3.5).

(3.5) and it was good too, except for large values of Pr. These are shown in Table 2.

In some cases the process had diverged, because the mesh size was not sufficiently small and it was restricted by memory capacity. The trouble was overcome by the trick that the average value of Y_n of old and new one just obtained in the preceeding iteration was adopted for the value to be substitued for (3.19) instead of new one as it was.

4. *Natural Convection above a Point Heat Source*

The following equations are to be solved:

$$\frac{f'''}{\xi}+\frac{f-1}{\xi}\left(\frac{f'}{\xi}\right)'+h=0, \tag{4.1}$$

$$(\xi h')'+Pr(fh)'=0, \tag{4.2}$$

$$\left.\begin{aligned}&\xi=0:\frac{f}{\xi}-\frac{f'}{2}=0,\left(\frac{f'}{2}\right)'=0,\ h'=0,\\ &\xi=\infty:\frac{f'}{\xi}=0,\ h=0.\end{aligned}\right\} \tag{4.3}$$

Since the fluid velocity at $\xi=0$ must be finite, f'/ξ is to be finite, too. Hence $f'(0)=0$ and $f(0)=0$. The normalizing condition is

$$\int_0^\infty hf'd\xi=1 \tag{4.4}$$

For an arbitrary solution, the integration for normalizing is

$$\int_0^\infty Y'ZdX=J \tag{4.5}$$

Then we have

$$\left.\begin{aligned}&\xi=J^{1/4}X,\ f=Y,\ h=J^{-1}Z,\\ &f'/\xi=J^{-1/2}Y/X,\end{aligned}\right\} \tag{4.6}$$

and the following equations of the same form as (4.1)~(4.3) are obtained

$$\frac{Y'''}{Y}+\frac{Y-1}{X}\left(\frac{Y'}{X}\right)'+Z=0, \tag{4.7}$$

$$(XZ')'+Pr(YZ)'=0, \tag{4.8}$$

$$\left.\begin{aligned}&X=0:\frac{Y}{X}-\frac{Y'}{2}=0,\left(\frac{Y'}{X}\right)'=0,\ Z'=0,\\ &X=\infty:\frac{Y'}{X}=0,\ Z=0.\end{aligned}\right\} \tag{4.9}$$

Since the procedure is similar to the case for line heat source, more explanations are deleted. The results were satisfactory, too.

5. *Conclusion and Discussion*

The method described here is essentially a finite difference method. The nonlinear equations are linearized according to the order estimation of the variable or parameters and are solved repeatedly as a linear simultaneous equations until the sufficient convergence is obtained. The results were satisfactory for all cases tested here. It shows that the sense of order estimation and the understanding of the physical meaning are important.

References

[1] Lapidus, L., Digital Computation for Chemical Engineers, McGraw-Hill, (1962), 318, Example 6.3.

[2] Fujii, T., Natural Convection above a Horizontal Line Heat Source and a Point Heat Source—Theory of the Steady Laminar Flow—. *The Reports of the Research Institute of Science and Industry,* Kyushu University, No. 33 (1962).