ON THE CHEBYSHEV METHODS FOR THE NUMERICAL SOLUTION OF THE THIRD BOUNDARY VALUE PROBLEM FOR PARABOLIC EQUATIONS

by

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1. Introduction

The Chebyshev polynomial $T_n(x)$ of degree n appropriate to the range $[-1,1]$ of x is defined by the relation

$$T_n(\cos x) = \cos n\,\vartheta, \quad x = \cos\vartheta.$$

It is well-known that $T_n(x)$ differs from zero on $[-1,1]$ less than any other polynomial of degree n having the same coefficient of x^n, and hence a Chebyshev series can by expected to converge more rapidly then any other polynomial series. A Chebyshev series also generally converges more rapidly than a Fourier series, particularly for a function which is not truely periodic (See, Fox & Parker (1968)).

The solution of parabolic equations in Chebyshev series has been considered by many authors, among them Elliot (1961), Mason (1967, 1969), Boateng (1975), Fox & Parker (1968), Knibb & Scraton (1971), and Dew & Scraton (1972). Knibb & Scraton (1971) have considered the solution of the equation

$$(1) \qquad P(x) = \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

subject to the boundary conditions $u = 0$ when $x = \pm 1$, and $u = f(x)$ when $t = 0$. Dew & Scraton (1972) have developed an improved procedure for equation (1) with $P(x)$ reduced to a constant and with the slightly more general boundary conditions

$$u + \alpha \frac{\partial u}{\partial x} = 0, \; x = 1 \;\; \& \;\; u + \beta \frac{\partial u}{\partial x} = 0, \; x = -1,$$

and $u = f(x)$, $t = 0$.

In the present paper we develop a technique for solving (1) with $P = P(x)$ subject to the more general boundary conditions

(2) $$\alpha_1 u + \beta_1 \frac{\partial u}{\partial x} = \gamma_1(t), \quad x = 1,$$

(3) $$\alpha_2 u + \beta_2 \frac{\partial u}{\partial \alpha} = \gamma_2(t), \quad x = -1,$$

and

(4) $$u = f(x), \quad -1 \leq x \leq 1, \quad t = .$$

Throughout this paper we assume that $f(x)$ satisfies the boundary conditions (2) and (3) to make sure that the solution is free of discontinuities. We assume that $f(x)$ and $P(x)$ are known Chebyshev series

(5) $$f(x) = \sum_{n=0}^{\infty}{}' f_n T_n(x)$$

and

(6) $$P(x) = \sum_{n=0}^{\infty}{}' P_n T_n(x).$$

We also suppose that $u(x, t)$ can be expressed as a Chebyshev series in the form

(7) $$u(x, t) = \sum_{n=0}^{\infty}{}' a_n(t) T_n(x).$$

Here, Σ' denotes halving the first term in the series.

A numerical solution of equation (1) can be obtained by tabulating the coefficients $a_n(t)$ for a range values of t. This process may be accomplished by replacing the partial differential equation (1) with its boundary and initial conditions (2), (3) and (4) by a system of ordinary differential equations for the coefficients $a_n(t)$ and then solve this system of equations.

2. The system ordinary differencial equations for $a_n(t)$

Let $q_n(t)$ be the coefficient of $T_n(x)$ in the Chebyshev expansion of $P(x) \frac{\partial u}{\partial t}$, so that

(8) $$P(x) \frac{\partial u}{\partial t} = \sum_{n=0}^{\infty}{}' q_n(t) T_n(x).$$

We also assume the following expansions

(9) $$\frac{\partial u}{\partial t} = \sum_{n=0}^{\infty}{}' a_n'(t)\, T_n(x),$$

(10) $$\frac{\partial^2 u}{\partial x^2} = \sum_{n=0}^{\infty}{}' a_n^{(2)}(t)\, T_n(x).$$

From here on we shall write $a_n'(t) = \dfrac{d\, a_n(t)}{dt} = a_n'$. If we satisfy the differential equation (1) get

(11) $$q_n = a_n^{(2)}, \quad n \geq 0.$$

If we use the relation (Clenshaw, 1957)

(12) $$a_m^{(s)} - a_{m+2}^{(s)} = 2(m+1)\, a_{m+1}^{(s-1)},$$

and if we write (11), for $m = n$, $m = n+2$; subtract one from the other and use (12) with $s = 2$, we obtain

(13) $$\frac{q_n - q_{n+2}}{2(n+1)} = a_{n+1}^{(1)}, \quad n \geq 0.$$

If we do the same again with (13), with $s = 1$, we have

$$\frac{1}{2(n+2)}\left\{\frac{q_n - q_{n+2} - q_{n+4}}{2(n+1)} - \frac{q_{n+2} - q_{n+4}}{2(n+3)}\right\} = a_{n+2}, \quad n \geq 0$$

rearranging this, and changing the subscripts, we get

(14) $$a_n = \frac{q_{n-2}}{4n(n-1)} - \frac{q_n}{2(n-1)(n+1)} + \frac{q_{n+2}}{4n(n+1)}, \quad n \geq 2.$$

From (6) and (9) have

$$P(x)\frac{\partial u}{\partial t} = \sum_{n=0}^{\infty}{}' a_n'\, T_n(x) \cdot \sum_{m=0}^{\infty}{}' P_m\, T_m(x) =$$

(15) $$= \frac{1}{2}\sum_{n=0}^{\infty}{}' a_n' \cdot \sum_{m=0}^{\infty}{}' P_m\left(T_{n+m}(x) + T_{n-m}(x)\right).$$

Equations (8) and (15) give

(16) $$q_m = \frac{1}{2}\sum_{n=0}^{\infty}{}' a_n'\left(P_{n+m} + P_{n-m}\right).$$

It is to be noted that $P_{-k} = P_k$, and similarly for all the other coefficients.

On making use of equation (16), equation (14) can be written as

(17) $$a_n(t) = \sum_{i=0}^{\infty}{}' A_{ni}\, a_i'(t), \quad n \geq 2,$$

or in the matrix form

$$A\,\mathbf{a}' = \mathbf{a}, \tag{18}$$

where

$$A_{ni} = \frac{1}{8n(n-1)}(P_{n-i-2}+P_{n+i-2}) - \frac{1}{4(n-1)(n+1)}(P_{n-i}+P_{n+i}) +$$

$$+\frac{1}{8n(n+1)}(P_{n+i+2}+P_{n-i+2}), \quad n \geq 2,\ i \geq 0. \tag{19}$$

The boundary conditions (2) and (3) can be written as

$$\frac{\alpha_1}{2}a_0(t)+(\alpha_1+\beta_1)\,a_1(t)+\sum_{n=2}^{\infty}[\alpha_1+n^2\beta_1]\,a_n(t) = \gamma_1(t), \tag{20}$$

$$\frac{\alpha_2}{2}a_0(t)-(\alpha_2-\delta_2)a_1(t)+\sum_{n=2}^{\infty}(-1)^n[\alpha_2-n^2\beta_2]\,a_n(t) = \gamma_2(t), \tag{21}$$

which, after some manipulation, can be put into the form

$$\frac{a_0(t)}{2}+\sum_{n=2}^{\infty}\mu_n\,a_n(t) = \lambda_1(t), \tag{22}$$

$$a_1(t)+\sum_{n=2}^{\infty}\nu_n\,a_n(t) = \lambda_2(t), \tag{23}$$

where

$$\mu_n = \{(\alpha_1+\beta_1 n^2)(\alpha_2-\beta_2)+ \tag{24}$$

$$+(-1)^n(\alpha_2-n^2\beta_2)(\alpha_1+\beta_1)\}/(2\alpha_1\alpha_2-\alpha_1\beta_2+\alpha_2\beta_1),$$

$$\nu_n = \{\alpha_2(\alpha_1+n^2\beta_1)-(-1)^n\alpha_1(\alpha_2-n^2\beta_2)\}/(2\alpha_1\alpha_2-\alpha_1\beta_2+\alpha_2\beta_1), \tag{25}$$

$$\lambda_1(t) = \{(\alpha_2-\beta_2)\gamma_1(t)+(\alpha_1+\beta_1)\gamma_2(t)\}/(2\alpha_1\alpha_2-\alpha_1\beta_2+\alpha_2\beta_1) \tag{26}$$

and

$$\lambda_2(t) = \{\alpha_2\gamma_1(t)-\alpha_1\gamma_2(t)\}/(2\alpha_1\alpha_2-\alpha_1\beta_2+\alpha_2\beta_1). \tag{27}$$

Equations (22) and (23) are true for all t, and may be differentiated with respect to t; the resulting equations can be used to eliminate $a_0'(t)$ and $a_1'(t)$ from (17) to give

$$a_n(t) = A_{n0}\lambda_1'(t)+A_{n1}\lambda_2'(t)+\sum_{i=2}^{\infty}(A_{ni}-A_{n0}\mu_n-A_{n1}\nu_n)\,a_i'(t)$$

or

(28) $$a_n(t) = b_n(t) + \sum_{i=2}^{\infty} B_{ni}\, a'_i(t)$$

where

(29) $$b_n(t) = A_{n0}\, \lambda'_1(t) + A_{n1}\, \lambda'_2(t),$$

(30) $$B_{ni} = A_{ni} - A_{n0}\, \mu_n - A_{n1}\, \nu_n .$$

It is now necessary to assume that $a_n(t)$ and $a'_n(t)$ are negligable for $n > N$. Equation (28) can then be written in the matrix form as

(31) $$\mathbf{a} = B\,\mathbf{a}' + \mathbf{b},$$

where

$$\mathbf{a}(t) = \begin{bmatrix} a_2(t) \\ a_3(t) \\ \vdots \\ a_N(t) \end{bmatrix}, \quad B = \begin{bmatrix} B_{22} & B_{23} & \cdots & B_{2N} \\ B_{32} & B_{33} & \cdots & B_{3N} \\ \vdots & & & \\ B_{N2} & B_{N3} & \cdots & B_{NN} \end{bmatrix},$$

$$\mathbf{b} = \begin{bmatrix} b_2(t) \\ b_3(t) \\ \vdots \\ b_N(t) \end{bmatrix}.$$

Also, on making use of the initial condition (4), equation (7) yields $a_n(0) = f_n$ at once, so

(32) $$\mathbf{a}(0) = \mathbf{f} = \begin{bmatrix} f_2 \\ f_3 \\ \vdots \\ f_N \end{bmatrix}.$$

Equation (31), represents a system of nonhomogeneous linear differential equations with constant coefficients. It is then necessary to solve the matrix differential equations (31) subject to the initial condition (32).

3. Solution of the matrix differential equation

A formal solution of equation (31) is given by (see for exemple, Bellman & Cooke, 1963):

(33) $$\mathbf{a}(t) = e^{B^{-1}t}\left[\mathbf{a}(0) - B^{-1}\int_0^t e^{B^{-1}s}\,\mathbf{b}(s)\,ds\right],$$

where, as usual, $e^{At} = \sum_{k=0}^{\infty} (tA)^k/k!$; A being a square matrix.

If $\mathbf{b}(t)$ is composed, say, of exponential or oscillatory functions, a particular integral of equation (31) can be obtained by elementary means, and the complementary function can be tabulated by means of the step-by-step formula

$$\mathbf{a}^{m+1} = \Phi(-\Delta t\, B^{-1})\, \mathbf{a}^{m}, \tag{34}$$

where $t_m = m\Delta t$, $\mathbf{a}^m$ is an approximation to $\mathbf{a}(t_m)$, and $\Phi(-\Delta t\; B^{-1})$ is a rational approximation to $e^{-\Delta t\, B^{-1}}$ The best known rational approximations to e^{-z} are the Padé ones (See, Varga, 1962).
Another analytical solution to the matrix differential equation (31) can be expressed as (Fox & Parker, 1968):

$$\mathbf{a}(t) = \sum_{i=1}^{N} (\alpha_i\, e^{\lambda_i t} + \beta_i)\, \mathbf{u}_i\,, \tag{35}$$

where $\mathbf{u}_i$ are the eigenvectors of the matrix B^{-1} with eigenvalues λ_i, assumed distinct, $\bar{v}_i$ are the eigenvectors of the transposed matrix $(B^{-1})^T$, and

$$\alpha_i = \frac{v_i^T \cdot \mathbf{a}(0)}{v_i^T \cdot \mathbf{u}_i}\,, \quad \beta_i = \frac{v_i^T \cdot \mathbf{c}_i}{v_i^T \cdot \mathbf{u}_i}$$

where

$$\mathbf{c}_i = -B^{-1} \int_0^t e^{\lambda_i (t-s)}\, \mathbf{b}(s)\, ds.$$

Formula (33) is impractical if B is a large matrix, while formula (35) is probably the best when N is small, and the computation is not very difficult, and changes in the initial conditions, giving the vector $\mathbf{a}(0)$, are easily incorporated. For larger values of N the determination of the eigenvalues and eigenvectors can make formula (35) an uneconomical method of solution.

In the following we consider some schemes for approximating the solution of (31) in which the time variable is discretized. The first discrete method is obtained by approximating (31) by the difference equations

$$\mathbf{a}^{m+\frac{1}{2}} = B\, \frac{\mathbf{a}^{m+1} - \mathbf{a}^{m}}{\Delta t} + \mathbf{b}^{m+\frac{1}{2}}, \quad m \geq 0 \tag{36}$$

$$\mathbf{a}^{0} = \mathbf{a}(0),$$

where

$$\mathbf{a}^{m+\frac{1}{2}} = \frac{\mathbf{a}^{m} + \mathbf{a}^{m+1}}{2}\,. \quad \mathbf{b}^{m+\frac{1}{2}} = \frac{\mathbf{b}^{m} + \mathbf{b}^{m+1}}{2}\,.$$

Solution of (36) for $\mathbf{a}^{m+1}$ gives:

$$\begin{aligned} \mathbf{a}^{m+1} &= -[2I - \Delta t\, B^{-1}]^{-1}\, [2I + \Delta t\, B^{-1}]\, \mathbf{a}^{m} + \\ &+ \Delta t[2I - \Delta t\, B^{-1}]^{-1}\, B^{-1}[\mathbf{b}^{m} + \mathbf{b}^{m+1}] + 0(\Delta t)^{3}. \end{aligned} \tag{37}$$

It is to be noted that this approximate solution is equivalent of using a (1.1) Padé approcimant for $\Phi(-\Delta t\ B^{-1}.)$ Also it is worth mentioning that in the actual computer implementation of (37), it is more economical to solve the equations (36) in the form

$$(37') \qquad \left(B - \frac{1}{2}\,\Delta t\, I\right)\varepsilon^{m+1} = \Delta t\, I\, \mathbf{a}^m + \Delta t\, I(\mathbf{b}^m + \mathbf{b}^{m+1}),$$

then

$$\mathbf{a}^{m+1} = \mathbf{a}^m + \varepsilon^{m+1}.$$

This formulation saves arithmetic operations as well as round-off errors. Formula (37) is a suitable one to use, notably, if $\mathbf{b}(t)$ is a more complicated function of time.

It is also worth noting, that if $\mathbf{b}$ is independent of time, then the solution of (31) is given explicitly by

$$\mathbf{a}(t) = e^{B^{-1}t}\{\mathbf{a}(0) - \mathbf{b}\} + \mathbf{b},$$

and hence

$$(38) \qquad \mathbf{a}^{m+1} = \Phi(-\Delta t\, B^{-1})\{\mathbf{a}^m - \mathbf{b}\} + \mathbf{b}.$$

Here a (2.3) Padé approximant can be used to approximate the matrix $\Phi(-\Delta t\ B^{-1})$, and this requires the determination of the matrix

$$\Phi(-\Delta t\, B^{-1}) = \left[B^3 - \frac{3}{5}\,\Delta t\, B^2 + \frac{3}{20}\,(\Delta t)^2 B - \right.$$

$$(39) \qquad \left. - \frac{1}{60}\,(\Delta t)^3 I\right]^{-1}\left[B^3 + \frac{2}{5}\,\Delta t\, B^2 + \frac{1}{20}\,(\Delta t)^2 B\right].$$

If Δt is small, it is obvious that the matrix to be inverted approximates to B^3, and this is less wellconditioned than B. Therefore, it is preferable to write equation (39) in the alternative form

$$\Phi(-\Delta t\, B^{-1}) = I + \Delta t\left\{B - \frac{1}{2}\,\Delta t\, I + \right.$$

$$(40) \qquad \left. + \frac{1}{12}\,(\Delta t)^2\left[B + \frac{1}{60}\,(\Delta t)^2\left(B - \frac{1}{10}\,\Delta t\, I\right)^{-1}\right]^{-1}\right\}^{-1},$$

which requires no more arithetic.

If Φ is taken as a Padé approcimant with denominator of higher degree than the numerator, tabulation using equations (34) and (38) is necessarly stable. Knibb & Scraton (1971) have reported that the use of a (1.1) Padé approximant to $\Phi(-\Delta t B^{-1})$ may cause some oscillation in the tabulation of $\mathbf{a}^m$, but this oscillation can be avoided completely by using a more satisfactory Padé approximant in which the denominator is of higher degree than the numerator (See for example, formula (39)).

To sum up the method, we first find the matrix B from equation (30); then form the matrix $\Phi(-\Delta t\, B^{-1})$ by means of equations (37) or (39); then tabulate $\mathbf{a}(t)$ for the required values of t, and finally $a_0(t)$ and $a_1(t)$ for each t from equations (22) and (23) respectively.

To conclude this paper, we wish to report that the previous method has been applied by the author to the boundary value problem for parabolic problems is two-space variables; the results will be published in a forthcoming paper.

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