The use of Lanczos τ-methods in the numerical solution of a Stefan problem

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Lanczos τ-methods are used to solve the ordinary differential equations with two-point boundary conditions which result from a finite-difference approximation to a Stefan problem. This technique, combined with the use of canonical polynomials, provides the basis of a computer program to solve the Stefan problem which, under certain conditions, is more efficient than the Douglas–Gallie method. Numerical results from the program are given.

1. Introduction

Mathematical models of physical processes such as the melting of ice and the recrystallization of metal which give rise to parabolic differential equations with moving boundaries are usually referred to as Stefan problems. Douglas (1961) describes a particular Stefan problem, defined by the equations

$$u_t = u_{xx},\ 0 < x < x(t),\ t > 0, \tag{1.1}$$

$$u_x(0, t) = -1,\ t > 0, \tag{1.2}$$

$$u(x(t), t) = 0,\ x = x(t),\ t > 0, \tag{1.3}$$

$$\frac{dx(t)}{dt} = -u_x(x(t), t),\ t > 0, \tag{1.4}$$

$$x(0) = 0. \tag{1.5}$$

Douglas and Gallie (1955) have discussed in detail a finite-difference technique for obtaining a numerical solution to this problem. This technique, with a slight modification to eliminate the need for iteration is also described by Douglas (1961). Equal intervals Δx are taken in the x-direction and variable intervals Δt_k in the t-direction. The boundary conditions (1.4) and (1.5) are replaced by an integrated form, the finite difference approximation of which is

$$t_{n+1} = x_{n+1} + \sum_{i=0}^{n} U_{i,n}\Delta x,$$

where

$$t_n = \sum_{k=0}^{n-1} \Delta t_k,\ \Delta t_n = t_{n+1} - t_n,\ x_i = i\Delta x,$$

and $U_{i,n}$ is an estimate of $u(x_i, t_n)$. If estimates of u are known at time t_n, then estimates of u at time t_{n+1} are found by solving the following tridiagonal system of simultaneous equations,

$$\frac{U_{i+1,n+1} - 2U_{i,n+1} + U_{i-1,n+1}}{(\Delta x)^2} = \frac{U_{i,n+1} - U_{i,n}}{\Delta t_n}, i = 1, 2, \ldots, n,$$

$$U_{1,n+1} - U_{0,n+1} = -\Delta x,$$

$$U_{n+1,n+1} = 0.$$

The whole process is easily programmed for a digital computer and provides successively better approximations to the moving boundary as Δx tends to zero. A minor disadvantage of the method is the need to provide storage for data arrays whose size is proportional to $(1/\Delta x)$. A more serious disadvantage is that the amount, and hence the speed, of calculation varies as $(1/(\Delta x)^2)$.

If equal intervals Δt are taken in the t-direction then the solution of (1.1) can be reduced to the solution of second-order ordinary differential equations. This approach, combined with the use of Clenshaw's method (Clenshaw, 1957), has been used by Elliott (1961) in the numerical solution of the heat conduction equation with linear boundary conditions on fixed boundaries.

It is shown in Section 2 of the present paper that the device of using the Lanczos τ-method (Lanczos, 1957), which is equivalent to Clenshaw's method (Fox, 1962), can be modified to deal with the moving boundaries occurring in the Stefan problem.

The use is extended in Section 3, canonical polynomials being introduced to facilitate variation of the degree of approximation, and a numerical method of solving the Stefan problem is obtained requiring an amount of calculation which varies as $(1/\Delta t)$.

Some programming details are given in Section 4, and numerical results are discussed in Section 5.

2. Lanczos τ-methods in the Stefan problem

Assume now that $U_0(x)$, $U_1(x)$ are approximations to $u(x, t_0)$, $u(x, t_1)$ and that the points (x_0, t_0), (x_1, t_1) lie on the moving boundary. If x_0 and $U_0(x)$ are known then finite-difference representations of (1.1), (1.2), (1.3) and (1.4) yield the following equations for x_1 and $U_1(x)$,

$$\frac{d^2U_1(x)}{dx^2} - \frac{U_1(x)}{\Delta t} + \frac{U_0(x)}{\Delta t} = 0, \tag{2.1}$$

$$\left[\frac{dU_1(x)}{dx}\right]_{x=0} = -1, \tag{2.2}$$

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$$[U_1(x)]_{x=x_1} = 0, \qquad (2.3)$$

$$\frac{x_1 - x_0}{\Delta t} = -\left[\frac{dU_0(x)}{dx}\right]_{x=x_0}. \qquad (2.4)$$

If $U_0(x)$ has a power series expansion

$$U_0(x) = \sum_{m=0}^{n+1} a_m \left(\frac{x}{x_0}\right)^m,$$

then in order to obtain $U_1(x)$ in the form

$$U_1(x) = \sum_{m=0}^{n+1} b_m \left(\frac{x}{x_1}\right)^m,$$

(2.1) is replaced by the perturbed equation

$$\frac{d^2U_1(x)}{dx^2} - \frac{U_1(x)}{\Delta t} + \frac{U_0(x)}{\Delta t} = \left(\tau_1 + \tau_2\frac{x}{x_1}\right)T_n^*\left(\frac{x}{x_1}\right), \qquad (2.5)$$

where

$$T_n^*(x) = \sum_{m=0}^{n} c_n^m x^m$$

and

$$c_n^0 = (-1)^n, \quad c_n^m = 2^{2m-1}\left[2\binom{n+m}{n-m} - \binom{n+m-1}{n-m}\right](-1)^{n+m}$$

for $m = 1, 2, \ldots, n$.

The perturbation

$$\left(\tau_1 + \tau_2\frac{x}{x_1}\right)T_n^*\left(\frac{x}{x_1}\right)$$

in (2.5) was chosen in preference to the more usual perturbation

$$\tau_1 T_n^*\left(\frac{x}{x_1}\right) + \tau_2 T_{n+1}^*\left(\frac{x}{x_1}\right)$$

in order to minimize the calculation of coefficients.

With these power series representations, (2.4) and (2.2) give

$$x_1 = x_0 - \frac{\Delta t}{x_0}\sum_{m=1}^{n+1} m a_m, \quad b_1 = -x_1, \qquad (2.6)$$

and (2.1) and (2.3) provide $(n+3)$ simultaneous equations for $b_0, b_2, b_3, \ldots, b_{n+1}, \tau_1, \tau_2$, which can be written as shown in (2.7).

The solution of (2.7) together with (2.6) determines x_1 and $U_1(x)$, which thus enables a step-by-step solution of the Stefan problem to be obtained.

3. Use of canonical polynomials

The possibility of varying the degree of the polynomial approximation to $U_1(x)$ in order to minimize $|\tau_1| + |\tau_2|$ leads in a natural manner to the introduction of canonical polynomials. The differential operator under consideration in the solution of the Stefan problem is

$$D \equiv \left(\frac{d^2}{dx^2} - \frac{1}{\Delta t}\right). \qquad (3.1)$$

The canonical polynomials $Q_m(x)$ are found by solving the differential equations

$$D\{U_1(x)\} = x^m, \; m = 0, 1, \ldots,$$

$$\begin{bmatrix}
1 & 1 & 1 & 1 & \cdots & 1 & 1 & & \\
-1 & \frac{2\Delta t}{x_1^2} & & & & & & -c_n^0\Delta t & \\
 & & \frac{6\Delta t}{x_1^2} & & & & & -c_n^1\Delta t & -c_n^0\Delta t \\
 & -1 & & \frac{12\Delta t}{x_1^2} & & & & -c_n^2\Delta t & -c_n^1\Delta t \\
 & & \ddots & & \ddots & & & \vdots & \vdots \\
 & & & -1 & & \frac{(n-1)n\Delta t}{x_1^2} & & -c_n^{n-2}\Delta t & -c_n^{n-3}\Delta t \\
 & & & & -1 & & \frac{n(n+1)\Delta t}{x_1^2} & -c_n^{n-1}\Delta t & -c_n^{n-2}\Delta t \\
 & & & & & -1 & & -c_n^n\Delta t & -c_n^{n-1}\Delta t \\
 & & & & & & -1 & & -c_n^n\Delta t
\end{bmatrix}
\begin{bmatrix} b_0 \\ b_2 \\ b_3 \\ b_4 \\ \vdots \\ b_n \\ b_{n+1} \\ \tau_1 \\ \tau_2 \end{bmatrix}
=
\begin{bmatrix} -b_1 \\ -a_0 \\ b_1 - a_1\left(\frac{x_1}{x_0}\right) \\ -a_2\left(\frac{x_1}{x_0}\right)^2 \\ \vdots \\ -a_{n-2}\left(\frac{x_1}{x_0}\right)^{n-2} \\ -a_{n-1}\left(\frac{x_1}{x_0}\right)^{n-1} \\ -a_n\left(\frac{x_1}{x_0}\right)^n \\ -a_{n+1}\left(\frac{x_1}{x_0}\right)^{n+1} \end{bmatrix}
\qquad (2.7)$$

to give

$$Q_m(x) = \sum_{s=0}^{m} q_{m,s}x^s \tag{3.2}$$

where

$$q_{m,s} = \begin{cases} 0, \text{ if } m < s \text{ or if } m + s \text{ is odd}, \\ -\dfrac{m!}{s!}(\Delta t)^{\left[\left(\frac{m-s}{2}\right)+1\right]}, \text{ otherwise.} \end{cases} \tag{3.3}$$

Making use of the canonical polynomials, the solution of (2.5) can now be written

$$U_1(x) = -\frac{1}{\Delta t}\sum_{m=0}^{n+1}\frac{a_m}{x_0^m}Q_m(x) + \sum_{m=0}^{n}\frac{c_n^m}{x_1^m}\left(\tau_1 Q_m(x) + \frac{\tau_2}{x_1}Q_{m+1}(x)\right). \tag{3.4}$$

The boundary conditions (2.2) and (2.3) provide two linear algebraic equations for τ_1 and τ_2, namely

$$\left.\begin{aligned} \tau_1\left[\sum_{m=0}^{n}\frac{c_n^m}{x_1^m}Q_m(x_1)\right] + \tau_2\left[\sum_{m=0}^{n}\frac{c_n^m}{x_1^{m+1}}Q_{m+1}(x_1)\right] &= \frac{1}{\Delta t}\sum_{m=0}^{n+1}\frac{a_m}{x_0^m}Q_m(x_1), \\ \tau_1\left[\sum_{m=0}^{n}\frac{c_n^m}{x_1^m}\dot{Q}_m(0)\right] + \tau_2\left[\sum_{m=0}^{n}\frac{c_n^m}{x_1^{m+1}}\dot{Q}_{m+1}(0)\right] &= \frac{1}{\Delta t}\sum_{m=0}^{n+1}\frac{a_m}{x_0^m}\dot{Q}_m(0) - 1, \end{aligned}\right\} \tag{3.5}$$

where

$$\dot{Q}_m(0) \equiv \left[\frac{dQ_m(x)}{dx}\right]_{x=0} = \begin{cases} 0, \text{ if } m \text{ is even}, \\ -m!(\Delta t)^{\frac{m+1}{2}}, \text{ otherwise.} \end{cases} \tag{3.6}$$

The perturbation coefficients τ_1 and τ_2 having been found, the expression (3.4) for $U_1(x)$ can be rearranged as a power series of the required form, since if

$$\sum_{m=0}^{n+1}\alpha_m Q_m(x) = \sum_{m=0}^{n+1} b_m\left(\frac{x}{x_1}\right)^m,$$

then $b_0, b_1, \ldots, b_{n+1}$ are given by

$$b_m = x_1^m \sum_{s=m}^{n+1}\alpha_s q_{s,m},\ m = 0, 1, \ldots, n+1.$$

4. Program details

In order to keep the perturbations as small as possible it seems desirable to vary n for each time step and to choose n such that $|\tau_1| + |\tau_2|$ is a minimum. For this purpose a prescribed error ϵ is input with the initial data and at each step the smallest value of n within fixed limits n_{min} and n_{max} is selected which yields $|\tau_1| + |\tau_2| < \epsilon$. Note that the amount of storage required for data is dependent on n_{max}, and hence relatively small.

Table 1

Boundary values obtained using the Douglas–Gallie method

Δx	0·1	0·04	0·02	0·01	0·001
$x = 0{\cdot}4$	0·4542	0·4621	0·4646	0·4659	0·4670
$x = 0{\cdot}8$	1·0232	1·0350	1·0388	1·0408	1·0425
$x = 1{\cdot}2$	1·6837	1·6980	1·7027	1·7051	
$x = 1{\cdot}6$	2·4250	2·4409	2·4462	2·4488	
$x = 2{\cdot}0$	3·2401	3·2570	3·2626	3·2654	
$x = 2{\cdot}4$	4·1242	4·1416	4·1473	4·1502	
$x = 2{\cdot}8$	5·0735	5·0910	5·0967	5·0996	
$x = 3{\cdot}2$	6·0850	6·1022	6·1079	6·1107	
$x = 3{\cdot}6$	7·1564	7·1730	7·1785	7·1812	
$x = 4{\cdot}0$	8·2855	8·3012	8·3064	8·3090	
Time	1	5·5	18·25	72	285

When $b_0, b_1, \ldots, b_{n+1}$ are calculated, they are examined to see if the series can be truncated without loss of accuracy. A rough rule for this purpose is that a coefficient can be discarded if $i \times |b_i| < \epsilon/10$. The coefficient of the highest power is, of course, examined first, and if it is insignificant then the coefficient of the next highest power is examined. The examination terminates when either the minimum number of coefficients are left or a coefficient is reached which is significant. The range of variation of n for the next time step is then adjusted accordingly.

For the Stefan problem considered here it is possible to obtain, by analytical techniques, power series expansions for both the function $u(x, t)$ and the boundary $x(t)$ which are valid for small x and t. Expansions of this type have been derived by Evans, Isaacson and MacDonald (1950) and the series

$$x(t) = t - \frac{1}{2!}t^2 + \frac{5}{3!}t^3 - \frac{51}{4!}t^4 + \frac{827}{5!}t^5 - \ldots,$$

$$u(x, t) = (t - x) + \left(-t^2 + \frac{1}{2}x^2\right) + \left(\frac{7}{3}t^3 - x^2t\right) + \left(-\frac{15}{2}t^4 + \frac{7}{2}x^2t^2 - \frac{1}{12}x^4\right) + \left(29\frac{1}{10}t^5 - 15x^2t^3 + \frac{7}{12}x^4t\right) + \ldots,$$

can be obtained directly from their results. These expressions provide a convenient means of obtaining starting values for the program.

5. Numerical results

Table 1 shows the time coordinates of the moving boundary corresponding to $x = 0{\cdot}4(0{\cdot}4)4{\cdot}0$, for several values of Δx, working with the Douglas-Gallie discretization.

Table 2

Boundary values obtained using the method of Section 3

Δt	0·1	0·04	0·02	0·01
$x = 0 \cdot 4$	0·4576	0·4635	0·4653	0·4662
$x = 0 \cdot 8$	1·0304	1·0378	1·0403	1·0415
$x = 1 \cdot 2$	1·6940	1·7021	1·7048	1·7061
$x = 1 \cdot 6$	2·4376	2·4459	2·4487	2·4500
$x = 2 \cdot 0$	3·2542	3·2626	3·2654	3·2668
$x = 2 \cdot 4$	4·1391	4·1475	4·1503	4·1517
$x = 2 \cdot 8$	5·0887	5·0970	5·0998	5·1011
$x = 3 \cdot 2$	6·1000	6·1082	6·1109	6·1122
$x = 3 \cdot 6$	7·1705	7·1786	7·1813	7·1826
$x = 4 \cdot 0$	8·2984	8·3063	8·3089	8·3102
Time	4·5	10·5	20·5	44·25

Table 2 shows the corresponding values, after inverse interpolation, obtained when working with the method described in Section 3 and the values $n_{min} = 3$, $n_{max} = 8$, $\epsilon = 10^{-5}$.

It will be seen that the results from the two methods are in good agreement, and a comparison of the time factors shows that for small increments the method of Section 3 is more efficient than the Douglas–Gallie method.

Table 3

The effect of using different prescribed errors, $\Delta t = 0 \cdot 01$

ϵ	10^{-3}	10^{-4}	10^{-5}	10^{-6}
$t = 0 \cdot 4$	0·348911	0·348911	0·348911	0·348911
$t = 0 \cdot 8$	0·640077	0·640077	0·640078	0·640078
$t = 1 \cdot 2$	0·900171	0·900175	0·900176	0·900176
$t = 1 \cdot 6$	1·139336	1·139346	1·139347	1·139347
$t = 2 \cdot 0$	1·362938	1·362957	1·362958	1·362958
$t = 2 \cdot 4$	1·574281	1·574312	1·574314	1·574314
$t = 2 \cdot 8$	1·775590	1·775637	1·775640	1·775640
$t = 3 \cdot 2$	1·968458	1·968525	1·968529	1·968529
$t = 3 \cdot 6$	2·154078	2·154167	2·154174	2·154173
$t = 4 \cdot 0$	2·333373	2·333488	2·333496	2·333496
Time	12	15	18	21·5

Table 3 shows the effect of varying ϵ with a fixed time increment $\Delta t = 0 \cdot 01$. The small variation of the results indicates that the choice of $\epsilon = 10^{-5}$ for the results in Table 2 was perhaps too conservative. However, questions of this nature, together with the possibility of automatically choosing optimum intervals will be considered in a further paper.

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