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A Comparison of Crank–Nicolson and Chebyshev Rational Methods for Numerically Solving Linear Parabolic Equations

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A numerical comparison of the Crank–Nicolson and Chebyshev rational method is presented for problems involving a specific class of linear parabolic differential equations. The numerical results indicate that the Chebyshev rational method possesses a significant computational advantage over the standard Crank–Nicolson finite difference method. Numerical results are also used to demonstrate the usefulness of the Chebyshev rational method for solving problems involving piecewise-constant, as a function of time, boundary conditions and/or source terms. In addition, an efficient computational procedure is outlined for the Chebyshev method.

INTRODUCTION

A procedure for using Chebyshev rational approximations to e^{-x} in $[0, \infty)$ was introduced in [1] for numerically solving linear parabolic equations. This method was extended in a more recent paper by Cody, Meinardus, and Varga [2]. An important feature of this Chebyshev rational method is that good numerical approximations to solutions of linear parabolic problems can be obtained in a *single* time step, as opposed to several time steps required for the conventional methods (i.e., the explicit and backward implicit methods [3] and the Crank–Nicolson implicit method [3, 4]). The purpose of this paper is to present some numerical results which compare "Chebyshev finite difference" approximations and the Crank–Nicolson implicit approximations to problems involving linear parabolic equations in one space variable. Two types of problems are examined. One problem involves homogeneous boundary conditions and time-independent source (sink) terms, while the other has homogeneous boundary conditions and piecewise-constant in time source terms. In addition to presenting numerical results, computationally efficient means of applying the Chebyshev rational methods are discussed.

Test Problems

The comparison of the Chebyshev rational and the Crank-Nicolson methods is based on numerical solutions for the following problem:

$$\frac{1}{\eta}\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial u}{\partial x}\right) + \sum_{j=1}^{k} \gamma_j(t)\,\delta(x - \bar{x}_j), \qquad 0 < x < L, \quad t > 0 \tag{1}$$

subject to the homogeneous boundary conditions

$$u(0, t) = u(L, t) = 0 \qquad \text{for all} \quad t > 0, \tag{2}$$

and the homogeneous initial condition

$$u(x, 0) = u_0 = 0, \qquad 0 \leqslant x \leqslant L, \tag{3}$$

where $\alpha(x)$[1] and η are assumed to be positive constants, $\delta(x - \bar{x}_j)$ is the Dirac delta function (with the $\bar{x}_j$ chosen to correspond with mesh points) used to represent source and sink terms, and $\gamma_j(t)$ is a constant in the first test problem for all $t \geqslant 0$, and a positive piecewise-constant in the second test problem with

$$\gamma_j(t) \equiv bq_j^{\,n} \qquad \text{for} \quad t_{n-1} < t \leqslant t_n\,, \qquad n = 1, 2, \ldots, \tag{4}$$

where

$$0 \equiv t_0 < t_1 < \cdots \tag{5}$$

is a partition of the nonnegative real axis. Two source terms ($q = 10$) located at $\bar{x}_1 = L/4$, $\bar{x}_3 = 3L/4$ and a sink ($q = -10$) at $\bar{x}_2 = L/2$ are used in the first problem. For the second class of problems, the source-sink data are given in Tables 4 and 5. The class of physical problems which effectively reduces to Eqs. (1)–(3) is extensive, and includes problems associated with fluid flow in porous media [5], heat transfer [6] and mass transfer [7].

[1] The problems considered here treat α as a constant, but the numerical methods studied can also treat the case where $\alpha(x)$ is a positive continuous or a piecewise continuous function of x in $0 \leqslant x \leqslant L$.

The two test problems outlined above actually describe the flow of a slightly compressible homogeneous fluid in a porous medium [5]. The specific values and engineering units of the different variables used in these problems are defined in the nomenclature.

Semidiscrete and Fully Discrete Approximations

Let Π_{N+1} be a partition of the interval [0, L], $\Pi_{N+1}: 0 = x_0 < x_1 < \cdots < x_{N+1} = L$, such that each source or sink term in Eq. (1) coincides with one of the grid points x_i. Spatial difference equations are derived by replacing the differential equation at each mesh point with an appropriate semidiscrete [3] finite difference equation. If the standard three-point, difference approximation [3, p. 175] of the spatial derivatives in (1) is used, then the *semidiscrete* approximation $\hat{u}(x_i, t) \equiv \hat{u}_i(t)$ satisfies the following ordinary matrix differential equation:

$$B(d\bar{u}/dt) = -A\bar{u} + \bar{g}(t), \quad t > 0, \tag{6}$$

where

$$\bar{u}(0) = \bar{u}_0 \equiv 0, \tag{7}$$

and $\bar{u}(t) = (\hat{u}_1(t), \hat{u}_2(t),..., \hat{u}_{N-1}(t), \hat{u}_N(t))^T$. The matrix B is a positive real diagonal $N \times N$ matrix with diagonal elements $b_{ii} = 1/\eta$, and A is a real symmetric tridiagonal positive definitive $N \times N$ matrix. The vector $\bar{g}(t)$ represents the point source terms in Eq. (1).

The semidiscrete approximation to $u(x, t)$ in Eq. (6) can be placed in a fully discrete form suitable for numerical solution by applying either the Crank–Nicolson method or the Chebyshev rational method. Because a detailed description of the Crank–Nicolson method can be found in [1, 3], it will not be discussed further.

Assuming that vector $\bar{g}$ is *time-independent*, the solution $\bar{u}(t)$ of (6)–(7) can be expressed as

$$\bar{u}(t) = A^{-1}\bar{g} + \exp(-tB^{-1}A)\{\bar{u}_0 - A^{-1}\bar{g}\} \tag{8}$$

for all $t \geqslant 0$. For any fixed nonnegative integers m and n with $0 \leqslant m \leqslant n^2$, let $\hat{r}_{m,n}(x) \equiv \hat{p}_m(x)/\hat{q}_n(x)$ denote the (m, n)-th Chebyshev rational approximation to e^{-x} in $[0, \infty)$, where $\hat{p}_m(x)$ and $\hat{q}_n(x)$ are polynomials with real coefficients of degree m and n, respectively. For additional details, see Ref. [2]. The Chebyshev rational method provides an approximation to $\bar{u}(t)$ by formally replacing the matrix exponential in (8) with the rational approximation

$$(\hat{q}_n(tB^{-1}A))^{-1}. \quad (\hat{p}_m(tB^{-1}A)).$$

[2] In this work, m is chosen equal to n, since there is little to be gained computationally by choosing m less than n (see Ref. [2]).

In this manner, the (m, n)-th Chebyshev approximation $\bar{u}_{m,n}(t)$ of $\bar{u}(t)$ is defined, in analogy with (8), for all $t \geqslant 0$ as

$$\bar{u}_{m,n}(t) = A^{-1}\bar{g} + (\hat{q}_n(tB^{-1}A))^{-1}(\hat{p}_m(tB^{-1}A))\{\bar{u}_0 - A^{-1}\bar{g}\}, \tag{9}$$

or equivalently, as

$$(\hat{q}_n(tB^{-1}A))\,\bar{u}_{m,n}(t) = \hat{q}_n(tB^{-1}A)(A^{-1}\bar{g}) + \hat{p}_m(tB^{-1}A)\{\bar{u}_0 - A^{-1}\bar{g}\} \tag{10}$$

for all $t \geqslant 0$.

It should be noted that in solving (10), the matrix A should *not* be inverted. Rather, the steady-state equation $A\bar{w} = \bar{g}$ is first solved for $\bar{w}$. Then, Eq. (10) can be replaced by

$$(\hat{q}_n(tB^{-1}A))^{-1}\,\bar{u}_{m,n}(t) = \hat{q}_n(tB^{-1}A)\,\bar{w} + \hat{p}_m(tB^{-1}A)\{\bar{u}_0 - \bar{w}\}. \tag{11}$$

The fundamental theorem of algebra permits factorization of $\hat{q}_n(x)$ and $\hat{p}_m(x)$ into products of linear and quadratic polynomials with real coefficients, hence the linear system in (11) can be replaced by

$$\left[\prod_{i=1}^{m_q} V_i(tB^{-1}A)\right]\bar{u}_{m,n}(t) = \left[\prod_{i=1}^{m_p} W_i(tB^{-1}A)\right]\{\bar{u}_0 - A^{-1}\bar{g}\} + \left\{\prod_{i=1}^{m_q} V_i(tB^{-1}A)\right\} A^{-1}\bar{g}, \tag{12}$$

where V_i and W_i are matrix polynomials of degree one or two. Setting the right hand side of (12) equal to $\bar{X}_0$, the solution $\bar{u}_{m,m}(t)$ can be obtained by solving successively the following m_q sets of linear equations for $\bar{X}_i$:

$$V_i(tB^{-1}A)\,\bar{X}_i = \bar{X}_{i-1}, \qquad i = 1, 2, \ldots, m_q. \tag{13}$$

Finally $\bar{X}_{m_q} = \bar{u}_{m,n}(t)$. This factorization procedure is computationally more attractive than simply utilizing a Gaussian elimination method to solve (11). To implement the numerical application of the Chebyshev rational method, we give the factorizations of $\hat{p}_m(x)$ and $\hat{q}_n(x)$ (for the case $m = n$) for $2 \leqslant n \leqslant 6$ in Table 6.

The technique of factorization presented in (12) and (13) is equivalent to solving m_q linear systems, each system being either tridiagonal (V_i is a linear factor) or five-diagonal (V_i is a quadratic factor). The power of this factorization technique is that it permits the possible use of high order approximations in the Chebyshev rational method while it keeps the computational problem at each step [cf. (13)] relatively simple. For example, if the (6, 6)-th Chebyshev rational approximation is used, $\hat{q}_6(tB^{-1}A)$ can be factored into the product of three quadratic matrix polynomials. Solving (11) for any value of time "t" then becomes a matter of solving three linear five-diagonal systems of equations.

For a general time-dependent source term, the solution $u(t)$ of (6)–(7) is given by

$$\bar{u}(t) = \exp(-tB^{-1}A)\,\bar{u}(0) + \exp(-tB^{-1}A)\int_0^t \exp(\lambda B^{-1}A) \times B^{-1}\bar{g}(\lambda)\,d\lambda \qquad \text{for all} \quad t > 0. \tag{14}$$

If the vector $\bar{g}(t)$ is piecewise-constant as a function of $t \geqslant 0$, the interval $[0, +\infty)$ can be partitioned as $0 = t_0 < t_1 < t_2 < t_3 < \cdots$, so that $\bar{g}(t) \equiv \bar{g}_n$ for all $t_{n-1} \leqslant t < t_n$. In this case, it follows from (14) that

$$\bar{u}(t_{n+1}) = \exp(-(t_{n+1} - t_n)\,B^{-1}A)\{\bar{u}(t_n) - A^{-1}\bar{g}_{n+1}\} + A^{-1}\bar{g}_{n+1}. \tag{15}$$

In analogy with the transition from Eq. (8) to Eq. (9), the matrix

$$\exp(-(t_{n+1} - t_n)\,B^{-1}A)$$

in (15) is approximated by the matrix

$$\hat{r}_{m,n}((t_{n+1} - t_n)\,B^{-1}A) = (\hat{q}_n((t_{n+1} - t_n)\,B^{-1}A))^{-1}\,(\hat{p}_m((t_{n+1} - t_n)\,B^{-1}A))$$

to define the (m, n)-th Chebyshev rational approximation $\bar{u}_{m,n}(t_{n+1})$ to $\bar{u}(t_{n+1})$. Thus,

$$\bar{u}_{m,n}(t_{n+1}) = \hat{r}_{m,n}((t_{n+1} - t_n)\,B^{-1}A)\{\bar{u}_{m,n}(t_n) - A^{-1}\bar{g}_{n+1}\} + A^{-1}\bar{g}_{n+1}, \quad n = 0, 1, 2,..., \tag{16}$$

where $\bar{u}_{m,n}(t_0) \equiv \bar{u}_0$ and $\bar{g}_n = b(0, 0,..., 0, q_1{}^n/\Delta x, 0,..., 0, q_k{}^n/\Delta x, 0,..., 0)^T$.

Numerical Results

As mentioned earlier, both test problems utilized the standard, three-point, finite difference approximation to discretize the spatial derivative term in (1). A uniform partition Π_{N+1}, of size $\Delta x = L/N + 1$ is used for both problems. Comparison of the Crank–Nicolson and the Chebyshev rational methods is based on numerical solutions to the first problem in which the source term is time-independent. The exact solution to (1)–(3) (see [6]), at two different time levels, is presented in Fig. 1. Tables I and II present error data on the two methods of solution for various time levels. It sould be noted that results presented in Table II for the Chebyshev rational method are obtained in a single step for each time level reported. The measure of accuracy used is the discrete L_∞ norm

$$\| \hat{w}(\cdot, t) - u(\cdot, t)\|_{L_\infty} \equiv \max_{1\leqslant i\leqslant N} | \hat{w}(x_i, t) - u(x_i, t)|, \tag{17}$$

where $\hat{w}(x, t)$ is either the Crank–Nicolson approximation or the Chebyshev rational approximation of $u(x, t)$. The error behavior in Table I is similar to that

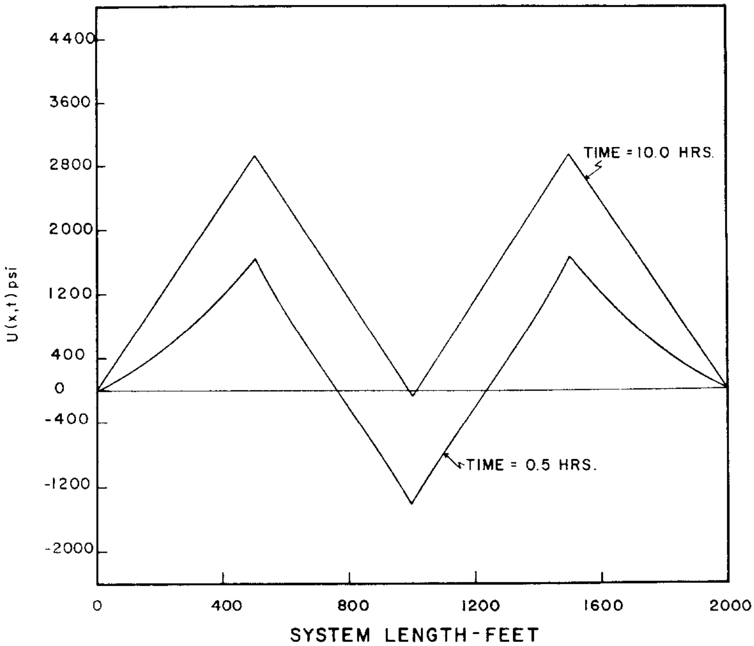

FIG. 1. Exact Solution to Eqs. (1)-(3).

TABLE I

L_∞ Error for Crank–Nicolson-CDA Method[a]

Cumulative time (hr)	(Time-Independent Source Case) Time step size (hr)					
	Δt = Cum. time	$\Delta t = 0.5$	$\Delta t = 0.25$	$\Delta t = 0.1$	$\Delta t = 0.05$	$\Delta t = 0.005$
0.5	547.5	547.5	168.4	43.8	2.9	3.3
1.0	912.8	266.2	120.4	12.5	1.6	1.4
2.0	1283.9	193.0	69.4	2.2	2.0	2.0
3.0	1414.0	151.8	43.5	1.5	1.9	1.9
4.0	1443.5	127.6	28.8	1.6	1.7	1.7
5.0	1514.7	108.9	19.6	1.5	1.6	1.6
6.0	1611.5	93.7	13.6	1.5	1.5	1.5
7.0	1699.0	81.2	9.5	1.4	1.4	1.4
8.0	1778.7	70.8	6.6	1.3	1.4	1.4
9.0	1851.1	62.3	4.5	1.3	1.3	1.3
10.0	2687.3	55.0	3.0	1.3	1.3	1.3

[a] $\Delta x = L/40$ and CDA refers to central finite difference approximation to the spatial derivatives.

TABLE II

L_∞ Error for (n, n)-th Chebyshev Rational-CDA Method
(Time-Independent Source Case)

Cumulative time (hr)	Order of Chebyshev rational method[a]				
	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
1.0	210.1	17.3	1.7	1.4	1.4
2.0	100.1	11.6	3.5	2.0	2.0
3.0	44.1	17.4	1.8	2.0	1.9
4.0	127.3	12.7	1.9	1.8	1.7
5.0	180.6	8.6	2.3	1.5	1.6
6.0	211.5	14.0	1.8	1.3	1.6
7.0	226.8	16.6	1.2	1.3	1.4
8.0	231.7	16.6	1.7	1.3	1.4
9.0	230.0	14.9	1.9	1.4	1.3
10.0	224.4	12.1	1.9	1.5	1.3

[a] $\Delta X = L/40$ and each solution was obtained in one time step. CDA refers to the central finite difference approximation to the spatial derivatives.

in Table II. That is, the error approaches a constant for each time level as the time increment decreases in the Crank–Nicolson method or as the order (m, n) of the Chebyshev rational method increases. This asymptotic error is the space truncation error resulting from the finite difference approximation to the spatial derivative term in (1).

The data presented in Tables I and II indicate that, for the same accuracy criterion, several time steps are required for the Crank–Nicolson method, as opposed to a single time step for the Chebyshev rational method. However, it is obvious that the ability to use large time steps and still retain accuracy with the Chebyshev rational method is obtained at the expense of added computations. Thus an equitable comparison must account for the computations associated with each method. To this end, Table III presents the number of equivalent multiplications as a function of the number N of internal spatial mesh points for the two methods of approximation. The data pertaining to the Chebyshev rational method in Table III represents operational counts made for the linear systems in Eq. (13). The term "equivalent multiplication" means that each algebraic operation (i.e., division, addition, subtraction) is expressed as a multiplication operation by employing the appropriate computer execution times (based on the IBM 360-85 computer execution times) for each type operation.

Figures 2 and 3 were obtained from the data presented in Tables I–III. These figures present the ratio of the number of operations (directly proportional to the

TABLE III

Operational Count for Crank–Nicolson and Chebyshev Rational Methods[a]

Solution method	Total number of equivalent multiplications
Crank–Nicolson	$1/2\,(11N - 3) + \tau(11N - 3)$[b]
(1, 1)-Chebyshev	$33N - 9$
(2, 2)-Chebyshev	$1/2\,(113N - 59)$
(3, 3)-Chebyshev	$77N - 34$
(4, 4)-Chebyshev	$1/2\,(199N - 109)$
(5, 5)-Chebyshev	$(120N - 59)$
(6, 6)-Chebyshev	$1/2\,(287N - 159)$

[a] Both methods employ the standard three point centered finite difference approximation to the spatial derivative of Eq. (1).

[b] N is the total number of internal (spatial) mesh points and τ is the total number of time steps for the Crank–Nicolson method.

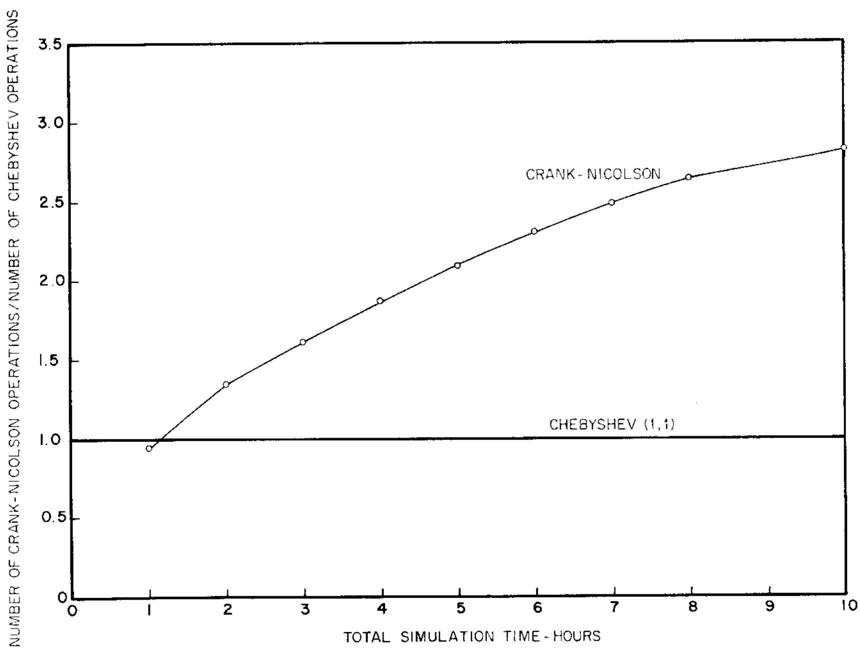

FIG. 2. Comparison of Number of Operations—Crank-Nicolson Method vs. Chebyshev Rational Method (L_∞ Norm = 231.7 psi).

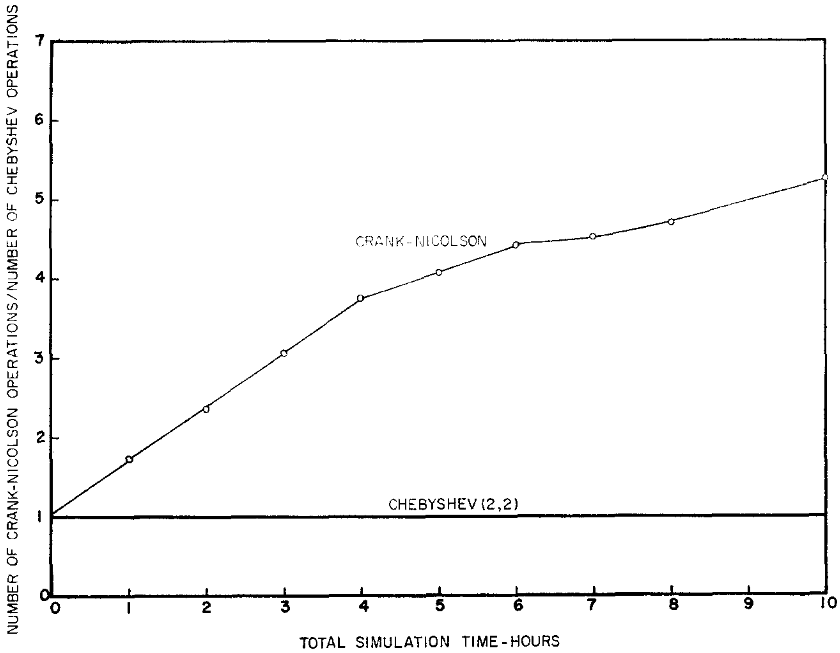

Fig. 3. Comparison of Number of Operations—Crank-Nicolson Method vs. Chebyshev Method (L_∞ Norm = 17.4 psi).

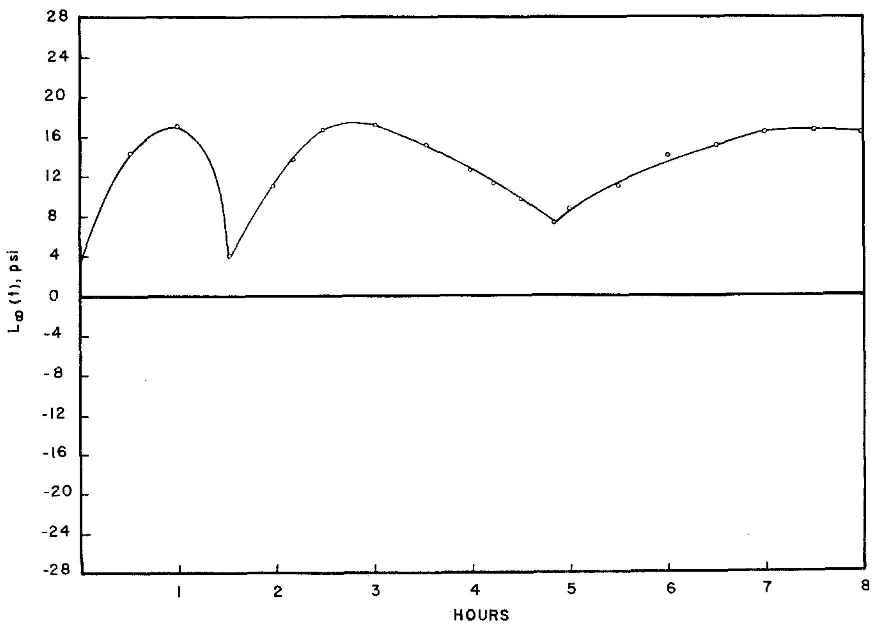

Fig. 4. Discrete L_∞ Norm Behavior for (2,2) Chebyshev Rational Method.

ratio of computer time) for the Crank–Nicolson and Chebyshev rational methods versus simulation time for a *fixed* error. [$\| \hat{w}(\cdot, t) - u(\cdot, t) \|_{L_\infty} = 231.7$ in Fig. 2 and $\| w(\cdot, t) - u(\cdot, t) \|_{L_\infty} = 17.4$ in Fig. 3]. In each of these figures, the error corresponds to the maximum error incurred at any time level using the indicated Chebyshev rational method. The actual error behavior for the Chebyshev rational method for the time period represented in Fig. 3 is presented in Fig. 4. Employing the discrete L_∞ norm to construct Figs. 2 and 3 places the Chebyshev rational method at a slight disadvantage but facilitates the comparison of the two methods. The data in these two figures clearly illustrate the superiority of the Chebyshev approach for generating solutions for a fixed accuracy range for any time step sufficiently large (see Remarks Section). The computational advantage of the Chebyshev rational method clearly increases as the time from the initial condition lengthens. For example (using Fig. 3), the Crank–Nicolson method would require approximately 1.75 times as much computer time as the (2, 2) Chebyshev rational method at one hour but 5.0 times as much computer time at nine hours.

Final numerical results presented in Tables IV and V and in Figs. 5 and 6

TABLE IV

Data for Single Time-Dependent Source Problem
[$k = 1$ in Eq. (1) and Eq. (16)]

n	t_n (hr)	q_1^n
1	1	5
2	2	−3
3	3	4
4	4	−3
5	5	0
6	6	2

$\Delta x = 2000/100$ ft.
$\bar{x}_1 = 1000$ ft.

illustrate that the Chebyshev rational method can be used in the "time-step" fashion indicated by Eq. (16) to give useful numerical approximations to certain linear problems involving piecewise-constant in time source terms or boundary conditions.

Remarks

The data presented here, although limited in scope, indicate that the Chebyshev rational method originally outlined in [1] and later extended by Cody, Meinardus

TABLE V

Data for Multi Time-Dependent Source Problem
[($k = 3$ in Eq. (1) and Eq. (16)]

n	t_n (hours)	q_1^n	q_2^n	q_3^n
1	360	1	−1	1
2	720	2	−2	2
3	1080	3	−3	3
4	1440	4	−4	4

$\Delta x = 2000/100$ ft.
$\bar{x}_1 = 500$ ft.
$\bar{x}_2 = 1000$ ft.
$\bar{x}_3 = 1500$ ft.

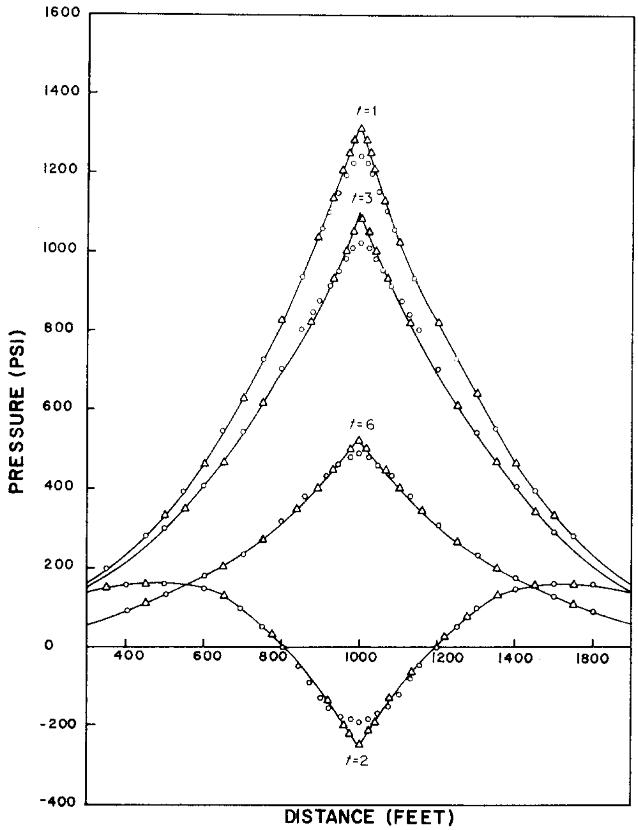

FIG. 5. Numerical Solutions to Eq. (16) Using Table IV Date (Δ — (2,2) Chebyshev Method; ○ — Crank-Nicolson Method ($\Delta t = 0.25$);—Exact Solution).

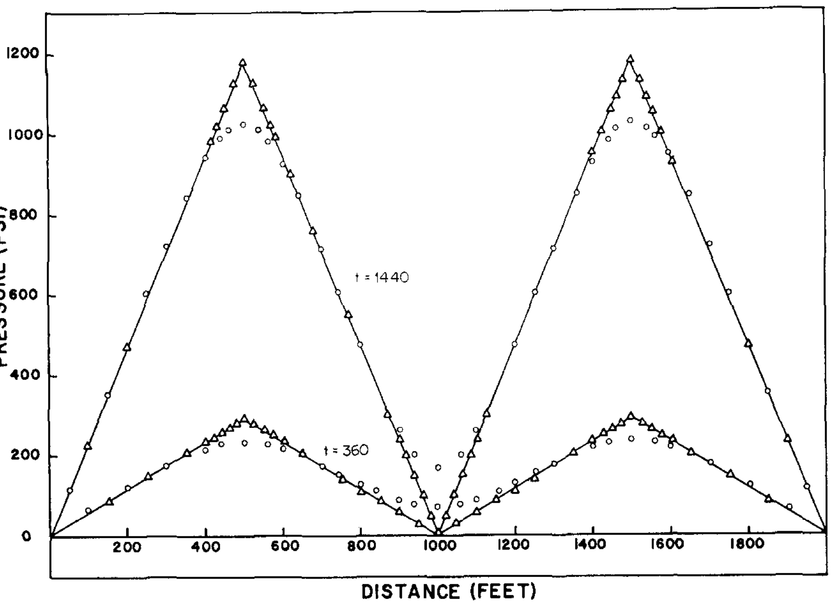

FIG. 6. Numerical Solutions to Eq. (16) Using Table V Data (Δ — (2,2) Chebyshev Method; o — Crank-Nicolson Method ($\Delta t = 15.0$); — Exact Solution).

and Varga [2] is an important new approach to obtaining numerical solutions to certain linear parabolic problems. It has been shown that the Chebyshev rational method can exhibit a significant computational advantage over more conventional approximations, and that it can be applied to a wide range of important problems. These include problems with piecewise-constant in time boundary conditions and/or source terms and problems involving time-independent but spatially dependent coefficients [cf. (1)]. In addition, it is anticipated that the Chebyshev rational method will offer the same advantages in multidimensional problems. In two-dimensional problems, for example, the spatial approximations normally used lead to sparce band matrices and the factorization method of (12) allows one to use block iterative techniques [3]. Finally, it should be pointed out that for very small values of $t > 0$, the Crank–Nicolson method is preferable to the single step Chebyshev rational method (see Fig. 2). This is essentially because the Crank–Nicolson method for linear problems can be viewed as a third-order rational approximation of $\exp(-tB^{-1}A)$ in (8) (cf. [3, p. 266]). The Chebyshev method, on the other hand, is defined from a rational matrix approximation of $\exp(-tB^{-1}A)$ which has maximum error at $t = 0$. This weakness in the Chebyshev rational method can be partially rectified by use of the following modified form of the Chebyshev rational method [8]: Let σ be the smallest positive zero of $\hat{r}_{m,n}(x) - e^{-x}$,

TABLE VI

Chebyshev Rational Polynomial Approximation Factorizations

Factorization coefficient	Order of Chebyshev approximation					
	(1,1)	(2,2)	(3,3)	(4,4)	(5,5)	(6,6)
a_1	−0.066772793	0.007358499138	$-7.99388825706\times10^{-4}$	$0.865209232811\times10^{-4}$	$-0.934560441811\times10^{-5}$	$1.008441269472\times10^{-6}$
b_1	9.249241439	1.1695686212	−1.368858393	−0.7357098172	−2.155410611	4.801192294
b_2		1.74746355744	0.3964389844	13.51715577344	2.881181642	7.18641850936
b_3			5.85093269818	3.096769796	7.82082944459	2.317090362
b_4				3.81793552685	−2.079022748	14.40880197235
b_5					25.30066786786	−3.56399274
b_6						41.57227060363
d_1	−0.5788712011	6.103692212	7.220150954	26.62217967	18.61654038	29.5663415
d_2		38.62055119	13.25692962	221.6465325	47.2605873	76.78257721
d_3			104.7569514	−20.03339944	403.8647075	665.8878371
d_4				101.0766013655	−22.2032242	16.49204758
d_5					128.4332550013	−25.3051307
d_6						171.2210434466

$$\hat{r}_{1,1}(x) = \frac{a_1(x-b_1)}{x-d_1}; \qquad \hat{r}_{2,2}(x) = \frac{a_1(x-d_1)(x-d_2)}{x^2+b_1x+b_2};$$

$$\hat{r}_{3,3}(x) = \frac{a_1(x-d_1)(x^2+d_2x+d_3)}{(x-b_1)(x^2+b_2x+b_3)}; \qquad \hat{r}_{4,4}(x) = \frac{a_1(x_1-d_1)(x_2-d_2)(x^2+d_3x+d_4)}{(x^2+b_1x+b_2)(x^2+b_3x+b_4)}$$

$$\hat{r}_{5,5}(x) = \frac{a_1(x-d_1)(x-d_2)(x-d_3)(x^2+d_4x+d_5)}{(x-b_1)(x^2+b_2x+b_3)(x^2+b_4x+b_5)}; \qquad \hat{r}_{6,6}(x) = \frac{a_1(x_1-d_1)(x-d_2)(x-d_3)(x-d_4)(x^2+d_5x+d_6)}{(x^2+b_1x+b_2)(x^2+b_3x+b_4)(x^2+b_5x+b_6)}$$

where $\hat{r}_{m,n}(x)$ is the "best" (m, n)-th Chebyshev rational approximation of e^{-x} in $[0, \infty)$. Define a new rational approximation $\hat{r}'_{m,n}(x)$ of e^{-x} by

$$\hat{r}'_{m,n}(x) = \hat{p}_m'(x)/\hat{q}_n'(x) \equiv e^{\sigma}\hat{r}_{m,n}(x + \sigma),\ x \in [0, \infty). \tag{18}$$

Clearly, the rational approximation $\hat{r}'_{m,n}(x)$ of e^{-x} has zero error at $x = 0$ and can be used in the obvious manner to define the modified Chebyshev rational method. Finally, it should be noted that replacement of $\hat{q}_n(tB^{-1}A)$ and $\hat{p}_m(tB^{-1}A)$ in Eq. (10) by $\hat{q}_n'(tB^{-1}A)$ and $\hat{p}_m'(tB^{-1}A)$, respectively, allows one to eliminate the direct dependence in this equation on A^{-1}. To see this, note that we can write Eq. (12) as

$$\hat{q}_n'(tB^{-1}A)\,\bar{u}_{m,n}(t) = \hat{p}_m'(tB^{-1}A)\,\bar{u}_0(0) + (\hat{q}_n'(tB^{-1}A) - \hat{p}_m'(tB^{-1}A))\,A^{-1}\bar{g}. \tag{19}$$

But since, by construction, $\hat{r}'_{m,n}(0) = 1$, we evidently have, after normalization, that $\hat{q}_n'(0) = \hat{p}_m'(0) = 1$. Thus, $\hat{q}_n'(x) - \hat{p}_m'(x)$ admits a factor of x, which we write as $\hat{q}_m'(x) - \hat{p}_m'(x) = s(x) \cdot x$, where $s(x)$ is a polynomial of degree at most $n - 1$. This means that the last term in Eq. (19) can be expressed simply as

$$\{s(tB^{-1}A) \cdot tB^{-1}A\}\,A^{-1}\bar{g} = ts(tB^{-1}A)\,B^{-1}\bar{g},$$

so that Eq. (19) loses its dependence on A^{-1} in this case. This procedure of circumventing the problem of computing A^{-1} is particularly important in multidimensional problems.

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