

## Rational Approximations to Matrix Exponential for Systems of Stiff Differential Equations

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### ABSTRACT

The set of  $N$  equations,

$$\dot{X}(t) = AX(t), \quad X(0) = X_0,$$

where  $X(t)$  is an  $N$ -vector and  $A$  is a constant  $N \times N$  matrix, may be solved by a recursive method,

$$X(t + T) = \exp(AT)X(t).$$

We discuss rational function approximations for the matrix exponential,  $\exp(AT)$ . Calahan has suggested using the Padé  $(N, N)$  approximant, but when the eigenvalues of  $A$  are widely spaced in magnitude, the Padé  $(N, N)$  approximant is inaccurate unless  $T$  is very small.

A new family of rational approximations to the matrix exponential is presented; the best member of the family to use depends upon the distribution of eigenvalues of  $A$ . Contour plots of the absolute square error and of the phase error are given for several approximations.

A numerical solution of the heat equation, discretized in space, is given as a numerical example.

We propose to solve the set of equations

$$\dot{X}(t) = AX(t), \quad X(0) = X_0, \tag{1}$$

where  $X(t)$  is an  $N$ -vector and  $A$  is a constant  $N \times N$  matrix, using the recursive method

$$X(t + T) = \exp(AT)X(t), \tag{2}$$

with a "rational fraction" approximation for the matrix exponential  $\exp(AT)$ . Although we consider only the linear, time-independent homogeneous case, (1), our results are immediately applicable to the general linear case,

$$\dot{X}(t) = A(t)X(t) + B(t). \tag{3}$$

Generalization to

$$\dot{X}(t) = F[X(t), t] \quad (4)$$

can be made by the methods described by Sandberg and Shichman [1] and by Liniger and Willoughby [2].

Systems of equations such as (1) arise frequently in two areas: in the solution of state-equations in circuit analysis [3] and in the solution of parabolic partial differential equations discretized in the space variable [4].

We restrict our consideration to systems for which all eigenvalues of  $A$  have nonpositive real parts; this includes, but is not limited to, all passive systems. Rational fraction approximations to  $\exp(AT)$  can be numerically stable for arbitrarily large step sizes  $T$ , as shown by Calahan [3] and Varga [4, 5].

For purposes of discussion, suppose that  $A$  has been diagonalized by a similarity transformation; then the rational approximation to  $\exp(AT)$  is also diagonal,

$$X_n(t + T) = \exp(\lambda_n T) X_n(t), \quad (5)$$

where  $\lambda_n$  is the  $n$ -th eigenvalue of  $A$ . Thus the same functional form which is to approximate  $\exp(AT)$  must approximate well *each* of the  $\exp(\lambda_n T)$  for the form to be useful. The distribution of the  $\lambda_n$  in the complex plane is of primary importance in choosing the approximation to be used, especially if large step size  $T$  is desired.

The general rational function of type  $(p, q)$  is

$$R_{pq}(y) = \frac{\sum_{n=0}^p b_n y^n}{\sum_{n=0}^q a_n y^n}. \quad (6)$$

There are  $(p + q + 1)$  independent parameters, since a common factor may be divided out of the  $a$ 's and  $b$ 's. To avoid a pole in  $R_{pq}(y)$  at  $y = 0$ ,  $a_0$  must be nonzero; we shall set  $a_0 = 1$ . The remaining  $(p + q + 1)$  coefficients must be chosen to give an accurate, stable approximation to  $\exp(y)$ . If they are chosen so that the Maclaurin expansion of  $R_{pq}(y)$  agrees with the Maclaurin expansion of  $\exp(y)$  to as many terms as possible ( $p + q + 1$  terms), the result is the Padé  $(p, q)$  approximant to  $\exp(y)$ ,  $P_{pq}(y)$ . The matrix analog of  $P_{pq}(y)$ , used to approximate  $\exp(AT)$  in Eq. (2), results in a numerically stable integration method if  $p \leq q$  and the eigenvalues of  $A$  have nonpositive real parts [3, 5]. For a given maximum power  $N$  of  $y$  in the rational function, the Padé  $(N, N)$  approximant,  $P_{NN}(y)$ , agrees with the Maclaurin expansion of  $\exp(y)$  to the largest possible number of terms, and so has been recommended by Calahan [3]. [We consider rational function approximations with given  $N$ , since these all require about the same amount of computation to evaluate  $\exp(AT)$ .]

However,  $P_{NN}(y)$  approaches  $(-1)^N$  for large  $|y|$ , instead of the true value of zero for any  $y$  with negative real part.

We consider as an example  $P_{22}(y)$ ,

$$P_{22}(y) = \frac{1 + \frac{1}{2}y + \frac{1}{12}y^2}{1 - \frac{1}{2}y + \frac{1}{12}y^2}, \quad (7)$$

whose Maclaurin expansion agrees with that of  $e^y$  to five terms. Figure 1 is a contour plot of the squared error,

$$|e^y - P_{22}(y)|^2, \quad (8)$$

for  $-10 \leq \text{Real}(y) \leq 0$  and  $0 \leq \text{Imag}(y) \leq 4.5$ . The plot is symmetric about the  $\text{Real}(y)$  axis. (Note the change in the horizontal scale at  $-5$ .) For small

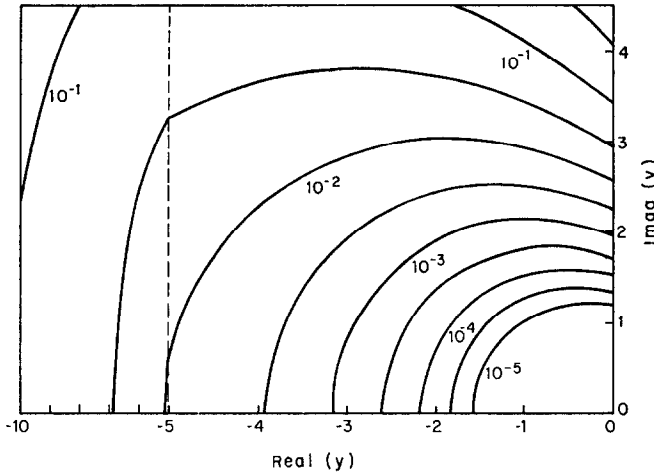


FIG. 1. Contour plot of  $|e^y - P_{22}(y)|^2$ . Note change in horizontal scale at  $\text{Real}(y) = -5$ .

$|y|$ ,  $P_{22}(y)$  is an excellent approximation to  $e^y$ , but the approximation is much poorer for large  $|y|$ . The use of

$$[I - \frac{1}{2}(AT) + \frac{1}{12}(AT)^2]^{-1}[I + \frac{1}{2}(AT) + \frac{1}{12}(AT)^2] \quad (9)$$

in place of  $\exp(AT)$  in (2) results in a stable numerical integration method for any  $T \geq 0$ , but for accuracy  $T$  must be chosen so the  $y_n = \lambda_n T$  lie in the region of the complex  $y$  plane where  $P_{22}(y)$  is a good approximation to  $e^y$ , i.e., small  $|y|$ . Since stiff differential equations are characterized by widely-varying  $\lambda$ 's, and  $T$  must be chosen so that  $|\lambda_{\max} T|$  is small, use of the Padé (2, 2) approximant necessitates the use of a small step size  $T$ .

For a rational function  $R_{pq}(y)$  to go to zero for large  $y$ , it is necessary that  $p < q$ . This suggests the use, for a given maximum power  $N$  of  $y$ , of the Padé approximant  $P_{N-1,N}(y)$  to  $e^y$ . As an example, we consider  $P_{12}(y)$ ,

$$P_{12}(y) = \frac{1 + \frac{1}{3}y}{1 - \frac{2}{3}y + \frac{1}{6}y^2}, \tag{10}$$

whose Maclaurin expansion agrees with that of  $e^y$  to four terms. Figure 2 is a contour plot of the squared error,  $|e^y - P_{12}(y)|^2$ , similar to Fig. 1.  $P_{12}(y)$  is an

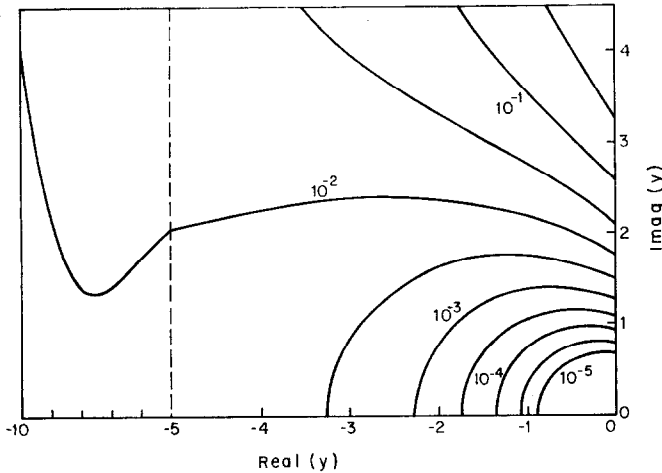


FIG. 2. Contour plot of  $|e^y - P_{12}(y)|^2$ . Note change in horizontal scale at  $\text{Real}(y) = -5$ .

excellent approximation to  $e^y$  for small  $|y|$ . For large negative  $\text{Real}(y)$ , the error is again small, although the relative error is large. If the matrix analog of  $P_{12}(y)$  is used to approximate  $\exp(AT)$ , modes with large negative eigenvalues will die out, but not as rapidly as does the correct solution. For  $\text{Real}(y)$  less than about  $-60$ , the squared error is again less than  $10^{-3}$ , but between  $-60$  and about  $-2.3$  the error is larger. This indicates that  $P_{12}(y)$  would be useful for stiff differential equations, (1), such that some eigenvalues are small in absolute value, and that the remaining eigenvalues have large negative real parts. Then the step size  $T$  may be chosen so that both the large and small eigenvalues have  $y = \lambda T$  in the region where the error in  $P_{12}(y)$  is less than the desired amount. For squared errors of  $10^{-2}$  (or larger), the eigenvalues need not be widely separated, since the area in the  $y$  plane where the squared error is less than  $10^{-2}$  is one contiguous region, rather than two widely-separated regions. Having one contiguous region of satisfactory error is superior to having two separated regions because less need be known about the eigenvalues of  $A$  in order to choose  $T$  properly.

However,  $P_{12}(y)$  has one contiguous region of satisfactory error only for squared error greater than  $9.6 \times 10^{-3}$ , the maximum squared error along the negative real  $y$  axis. Other rational approximations of type (1, 2) to  $e^y$  exist which have less accuracy near the origin, but improved accuracy farther from the origin. We consider a rational approximation of type (1, 2) and match the first three terms of the Maclaurin expansion of  $e^y$ . This results in a rational approximation with one undetermined coefficient. We let  $a_2 = \beta$  and express the result as

$$R_{12}(y; \beta) = \frac{1 + (\frac{1}{2} - \beta)y}{1 - (\frac{1}{2} + \beta)y + \beta y^2}. \quad (11)$$

The roots of the denominator are in the right hand half of the  $y$ -plane for  $\beta \geq 0$ ; in addition,  $R_{12}(y; \beta)$  is less than or equal to 1 in absolute value for purely imaginary  $y$  if  $\beta \geq 0$ . Using Calahan's [3] criteria, we see that the use of  $R_{12}(y; \beta)$  for  $\beta \geq 0$  results in a stable method for any step size  $T$ , if the eigenvalues of  $A$  all have nonpositive real parts. Three of the Padé approximants are special cases of  $R_{12}(y; \beta)$ : the "degenerate" case,  $P_{11}(y) = R_{12}(y; 0)$ ;  $P_{12}(y) = R_{12}(y; \frac{1}{6})$ ; and  $P_{02}(y) = R_{12}(y; \frac{1}{2})$ .

For many physical applications giving rise to systems of stiff differential equations, the large-magnitude eigenvalues lie near the negative real axis. For this type of system, we may choose  $\beta$  so that the error in  $R_{12}(y; \beta)$  is small for negative real  $y$ . The  $\beta$  for which the maximum error along the negative real  $y$  axis is least is  $\beta = 0.306$ ; Fig. 3 is a contour plot of the squared error of  $R_{12}(y; 0.306)$ . The

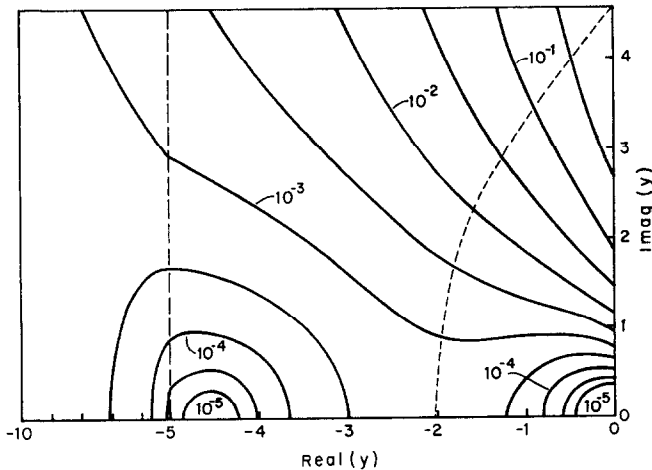


FIG. 3. Contour plot of  $|e^y - R_{12}(y; 0.306)|^2$ . Note change in horizontal scale at  $\text{Real}(y) = -5$ .  $P_{12}(y)$  is more accurate than  $R_{12}(y; 0.306)$  to the right of the dashed line starting near  $\text{Real}(y) = -2$ .

error is higher than that in  $P_{12}(y)$  to the right of the dashed line, and less to the left. For squared errors larger than  $5.9 \times 10^{-4}$ ,  $R_{12}(y; 0.306)$  has one contiguous region of satisfactory error. This value is the smallest possible for  $R_{12}(y; \beta)$ , with any choice of  $\beta$ . Note that, for  $\text{Imag}(y) < 0.45 \text{ Real}(y)$ , the squared error is less than  $10^{-3}$  for any  $y$  in the left half-plane; for  $\text{Imag}(y) < 0.75$ , the squared error is also less than  $10^{-3}$ . [A mode with  $\text{Real}(\lambda) = 0$  is purely oscillatory; then  $\text{Imag}(y) = \text{Imag}(\lambda T) = 0.75$  corresponds to taking time steps of approximately  $.75/2\pi \approx 1/8$  of a period.]

Figures 4-6 are contour plots of the phase error [the phase of  $\exp(y)$  is  $\text{Imag}(y)$ ],

$$\text{Imag}(y) - \text{Phase}[R_{pq}(y)] \tag{12}$$

for the three rational fractions considered, for

$$-5 \leq \text{Real}(y) \leq 0 \quad \text{and} \quad 0 \leq \text{Imag}(y) \leq 4.5.$$

Since the phase error can be no larger than  $\pi$ , and no less than  $-\pi$ , each plot has a "branch cut." These branch cuts start at the zeros of the numerator. The Padé (2, 2) approximation has two branch cuts, starting at  $y = -3 \pm i\sqrt{3}$ ; the Padé (1, 2) branch cut runs from  $y = -3$  along the real axis to  $-\infty$ ; and the  $R_{12}(y; 0.306)$  branch cut runs from  $y = -5.16$  along the real axis to  $-\infty$ .

Thus for large negative  $\text{Real}(y)$ ,  $P_{12}$  and  $R_{12}(y; \beta)$  have large phase errors, but small magnitude errors. The time evolution of rapidly-decaying components of  $X(t)$  will not be calculated exactly, but these components *will* decay.

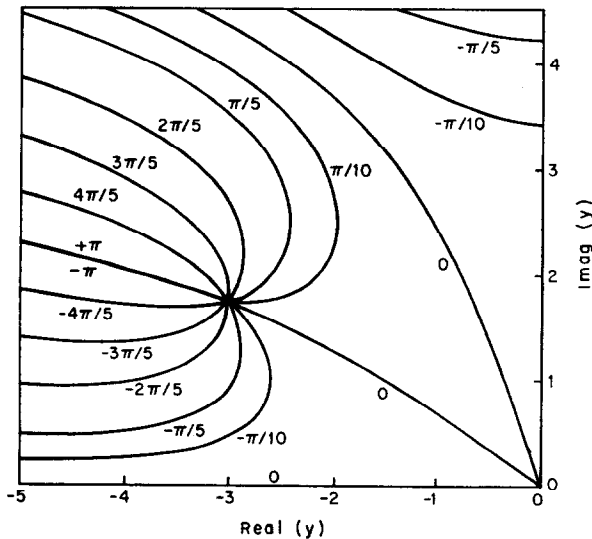


FIG. 4. Contour plot of phase error,  $\text{Imag}(y) - \text{Phase}[P_{22}(y)]$ .

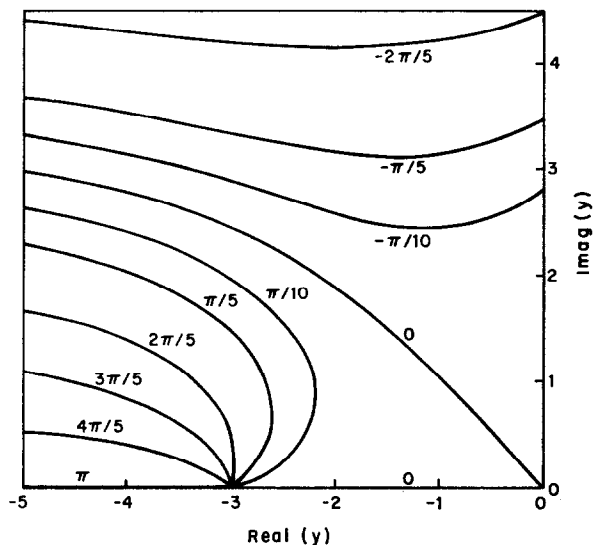


FIG. 5. Contour plot of phase error,  $\text{Imag}(y) - \text{Phase}[P_{13}(y)]$ .

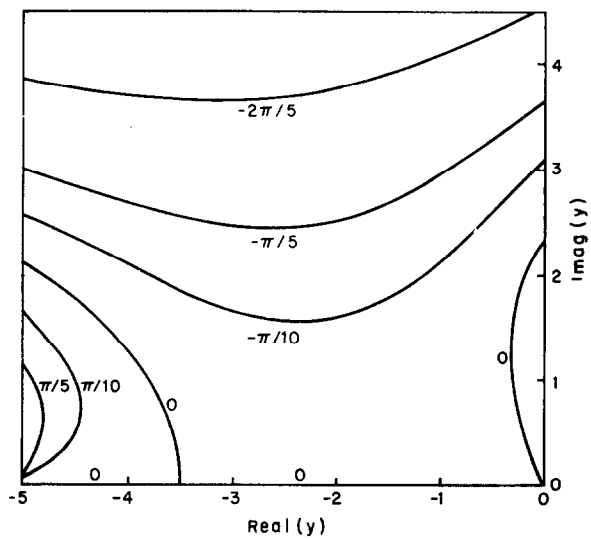


FIG. 6. Contour plot of phase error,  $\text{Imag}(y) - \text{Phase}[R_{1v}(y; 0.306)]$ .

The same techniques may of course be used to construct higher-order approximations. For example,  $R_{23}(y; \gamma)$  may be obtained by a method similar to that used to obtain  $R_{12}(y; \beta)$ :

$$R_{23}(y; \gamma) = \frac{1 + (\frac{1}{2} - 6\gamma)y + (\frac{1}{12} - 2\gamma)y^2}{1 - (\frac{1}{2} + 6\gamma)y + (\frac{1}{12} + 4\gamma)y^2 - \gamma y^3}.$$

$R_{23}(y; \gamma)$  results in a stable numerical integration method for any step size  $T$  if  $\gamma \geq 0$ . Special cases are

$$P_{22}(y) = R_{23}(y; 0); \quad P_{23}(y) = R_{23}(y; \frac{1}{60}); \quad \text{and} \quad P_{13}(y) = R_{23}(y; \frac{1}{24}).$$

For  $R_{23}(y; 0.0939)$ , the maximum squared error along the negative real  $y$  axis is smaller than that for any other  $\gamma$ ; this squared error is  $9.79 \times 10^{-5}$ . Figure 7 is a contour plot of the squared error, and Fig. 8 the phase error, of  $R_{23}(y; 0.0939)$ .

In order to illustrate the properties of these matrix exponential approximations, we consider solving the normalized heat equation,

$$\frac{\partial u(x, t)}{\partial t} = \frac{\partial^2 u(x, t)}{\partial x^2}, \quad \begin{matrix} 0 < x < 1 \\ 0 < t \end{matrix} \quad (14)$$

with boundary conditions  $u(0, t) = u(1, t) = 0$ , and initial conditions  $u(x, 0) = (\sin \pi x)^2$ . We discretize the space variable, dividing  $(0, 1)$  into  $M$  equal intervals

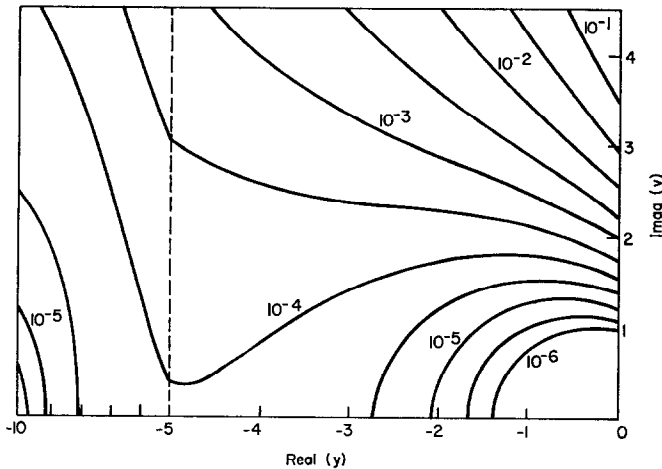


FIG. 7. Contour plot of  $|e^y - R_{23}(y; 0.0939)|^2$ . Note change in horizontal scale at  $\text{Real}(y) = -5$ .



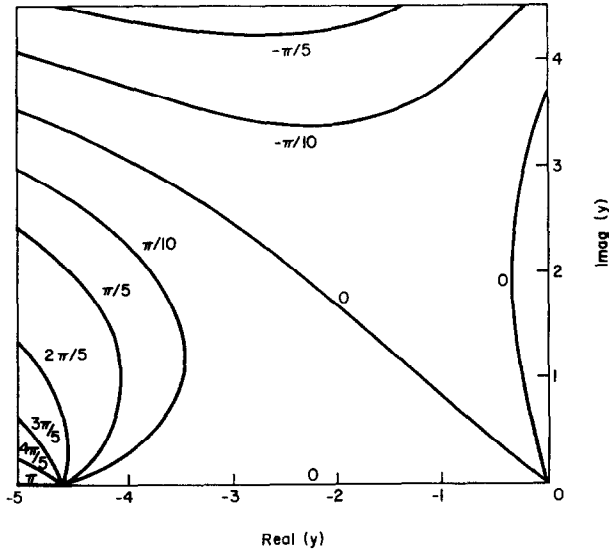


FIG. 8. Contour plot of phase error,  $\text{Imag}(y) - \text{Phase}[R_{22}(y; 0.0939)]$ .

$\Delta x = 1/M$ , and let  $U_n(t) = u(n\Delta x, t)$ . We use the three-point central-difference approximation for the second derivative,

$$\frac{\partial^2 u(n\Delta x, t)}{\partial x^2} \cong \frac{U_{n+1}(t) - 2U_n(t) + U_{n-1}(t)}{(\Delta x)^2}. \quad (15)$$

Then, since  $U_0(t) = U_M(t) = 0$ , (13) is of the form (1) with  $N = M - 1$ . The matrix  $A$  is tridiagonal, with diagonal elements  $-2/(\Delta x)^2$  and sub- and super-diagonal elements  $1/(\Delta x)^2$ . Similar problems have been considered by Varga [4], by Makinson [6], and by Cody, Meinardus, and Varga [8].

Since  $A$  is symmetric, it has only real eigenvalues. The lower magnitude eigenvalues of  $A$  approximate the lower magnitude eigenvalues of the continuous problem,  $-n^2\pi^2$ ,  $n = 0, 1, 2, \dots$ . With  $M = 20$ , the 19 eigenvalues of  $A$  range from about  $-10$  to  $-1600$ . The eigenfunctions of the continuous problem are  $\sin(n\pi x)$ ,  $n = 0, 1, 2, \dots$ ; the initial condition was chosen to include some of the more rapidly-decaying eigenfunctions. Makinson considers this problem with  $u(x, 0) = \sin(\pi x)$ , which is approximately equal to the eigenfunction of the lowest-magnitude eigenvalue. Since the higher eigenfunctions are missing from the solution, this initial condition does not adequately test the method.

For  $M = 20$ , the discretized problem was solved for  $0 \leq t \leq 0.5$ , using time steps of 0.025, 0.05, and 0.1, using several different rational fraction approxi-

mations to  $\exp(AT)$ . These included the Padé (2, 2); the Padé (1, 2);  $R_{12}(\cdot; 0.306)$ ; and the Padé (1, 1),

$$P_{11}(y) = \frac{1 + \frac{1}{2}y}{1 - \frac{1}{2}y}. \tag{16}$$

When  $P_{11}(\cdot)$  is applied to the heat equation, the resulting method is known as the Crank-Nicholson method [7]. In addition, Makinson's formula with  $N = 2$  was tested,

$$e^y \cong \frac{1 - \frac{1}{3}\sqrt{3}y - \frac{1}{3}(1 + \sqrt{3})y^2}{[1 - \frac{1}{2}(1 + \frac{1}{3}\sqrt{3})y]^2}. \tag{17}$$

Since, in  $0 < x < 1$ ,

$$(\sin \pi x)^2 = \frac{8}{\pi} \left\{ \frac{\sin \pi x}{3} - \frac{\sin 3\pi x}{1 \cdot 3 \cdot 5} - \frac{\sin 5\pi x}{3 \cdot 5 \cdot 7} - \dots \right\}, \tag{18}$$

the true solution to the continuous problem (13) is

$$u(x, t) = \frac{-8}{\pi} \sum_{k=0}^{\infty} \frac{\sin(2k + 1) \pi x}{(2k - 1)(2k + 1)(2k + 3)} e^{-(2k+1)^2 \pi^2 t}. \tag{19}$$

For testing the rational function approximations, it is appropriate to compare the approximate solutions to the true solution of the discretized problem. This was computed using numerically-calculated values for the eigenvalues and eigenvectors.

TABLE I  
Numerical and Analytic Solutions  $U_n(0,1)$ ,  $T = 0.1$

$n \Delta x$	Numerical Solutions					Analytic Solution	
	$P_{11}$	$P_{22}$	$P_{12}$	$R_{12}(y; .306)$	Makinson	Discrete	Continuous
.05	.12106	.00833	.05811	.05354	.09618	.04958	.04948
.10	.20040	.04488	.11210	.10506	.16547	.09794	.09774
.15	.24540	.09573	.15968	.15308	.21205	.14389	.14360
.20	.26359	.15153	.19978	.19651	.24027	.18631	.18593
.25	.26256	.20600	.23225	.23452	.25455	.22414	.22369
.30	.24965	.25490	.25743	.26645	.25918	.25646	.25594
.35	.23163	.29536	.27597	.29180	.25811	.28246	.28189
.40	.21427	.32548	.28857	.31018	.25471	.30151	.30089
.45	.20198	.34401	.29586	.32132	.25158	.31313	.31249
.50	.19757	.35026	.29824	.32506	.25035	.31704	.31639

Solutions obtained from (2) using the various rational fraction approximations to  $\exp(AT)$  were compared with the analytic solution of the discretized problem. Table I contains some sample results for  $U_n(0.1)$ , obtained by one time step of size  $T = 0.1$ . It is clear that  $P_{11}$ ,  $P_{22}$ , and Makinson's method, (16), are less accurate than  $P_{12}$  and  $R_{12}(\cdot; 0.306)$  for this particular problem.

Although  $P_{11}$  and  $P_{22}$  result in numerical methods which are stable for any step size  $T$ , the solutions obtained with large step sizes may be unusable. It is evident from Table I that  $T = 0.1$  is too large a step for  $P_{11}$ ; after another time step of  $T = 0.1$ , the solution is negative at several points.

Figure 9 shows  $U_n(0.1)$  for the data shown in Table I;  $u(x, 0)$  is also shown. The points at  $n\Delta x$  are connected with a smooth line for clarity. Only the region  $0 \leq x \leq .5$  is shown, since  $u$  is symmetric about  $x = .5$ . The true solution to the

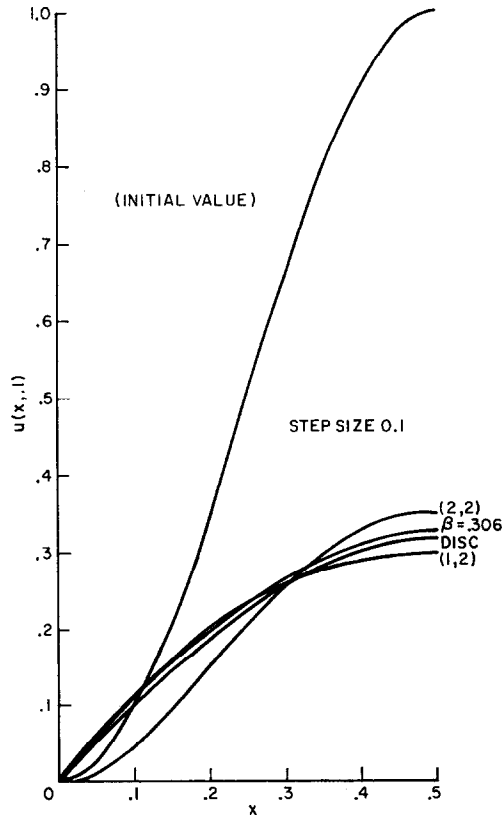


FIG. 9. Initial value of  $u(x, t)$ . Solutions  $U_n(0.1)$  obtained after one time step  $T = 0.1$ . Points at  $n\Delta x$  are connected with a smooth curve. Disc: true solution to discretized problem. (2, 2): Padé (2, 2) approximant. (1, 2): Padé (1, 2) approximant.  $\beta = 0.306$ ;  $R_{12}(\gamma; 0.306)$ .

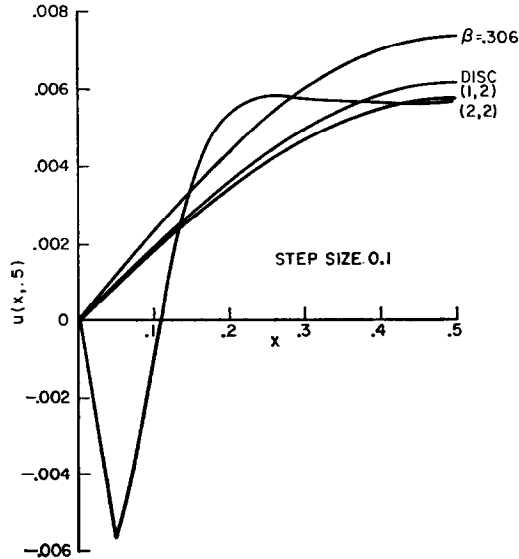


FIG. 10. Solutions  $U_n(0.5)$  obtained after five time steps  $T = 0.1$ . Points at  $n \Delta x$  are connected with a smooth line. Curve labelling as in Fig. 9.

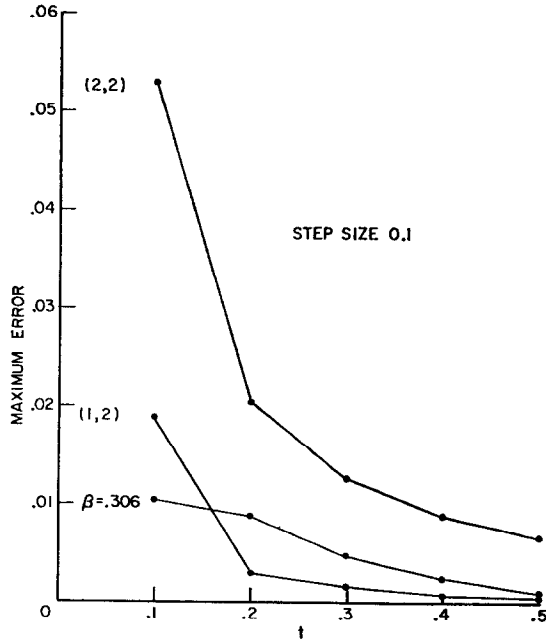


FIG. 11. Absolute value of maximum error in  $U_n(t)$  for three approximate solutions. Time step  $T = 0.1$ . Curve labelling as in Fig. 9.

discretized problem and the solutions using  $P_{22}$ ,  $P_{12}$ , and  $R_{12}(\cdot; 0.306)$  are shown. Note that in one time step these methods successfully change the solution by a large amount.  $R_{12}(\cdot; 0.306)$  has the smallest maximum error.

Figure 10 shows the corresponding curves at  $t = 0.5$ , after five time steps  $T = 0.1$ ; now  $P_{12}$  is best and it is evident that  $P_{22}$  has not produced a usable solution. The reason that  $P_{12}$  is now better than  $R_{12}(\cdot; 0.306)$  is that, at  $t = .5$ , the solution is dominated by the eigenfunction (approximately equal to  $\sin \pi x$ ) with the smallest magnitude eigenvalue (approximately equal to  $-\pi^2$ ). For this eigenfunction,  $\lambda T$  is approximately  $-1$ ; from Fig. 3 it may be seen that  $P_{12}$  propagates this eigenfunction more accurately than does  $R_{12}(\cdot; 0.306)$ . The next higher eigenvalue is approximately  $-9\pi^2$ , so  $\lambda T$  is approximately  $-9$ ;  $R_{12}(\cdot; 0.306)$  propagates all but the lowest eigenfunction more accurately than does  $P_{12}$ . After the higher eigenfunctions in the approximate solutions have died out, the solution produced by  $P_{12}$  is superior.

In Fig. 11 is plotted  $\max_n |U_n(t) - u_{\text{disc}}(n \Delta x, t)|$  for  $t = 0.1, 0.2, 0.3, 0.4, 0.5$ , where  $u_{\text{disc}}$  is the true solution to the discretized problem, for three rational approximations to  $\exp(AT)$ . A time step  $T = 0.1$  was used. For clarity, the points are shown connected. After two time steps,  $P_{12}$  is better than  $R_{12}(\cdot; 0.306)$ .

Figure 12 is similar to Fig. 11, except that the time step is  $T = 0.025$ . After four time steps  $P_{22}$  is better than  $R_{12}(\cdot; 0.306)$ ; after twelve time steps,  $P_{22}$  is better than  $P_{12}$ .

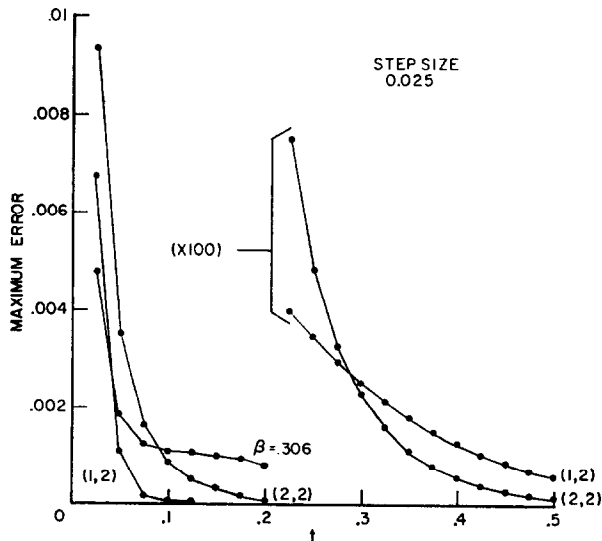


FIG. 12. Absolute value of maximum error in  $U_n(t)$  for three approximate solutions. Time step  $T = 0.025$ . Curve labelling as in Fig. 9. After  $t = 0.225$ , curves are blown up by 100. Error at  $t = 0.5$  for  $R_{12}(\gamma; 0.306)$  is 0.0012.

In the sample problem, after a few time steps  $P_{12}$  was more accurate than  $R_{12}(\cdot; 0.306)$ . In a linear, but nonhomogeneous problem, this would not necessarily be so, since the nonhomogeneous term would in general introduce new components of the higher eigenfunctions into the solution. Similar considerations apply to nonlinear problems.

We have discussed the use of rational function approximations to the exponential of a matrix, and have presented two useful families of approximations. For many stiff differential equations arising from physical problems,  $R_{12}(\cdot; 0.306)$  or  $R_{23}(\cdot; 0.0939)$  should be useful. The numerical example of the solution of the heat equation illustrates the feasibility of a large step size  $T$  with the methods discussed in this paper.

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