EFFICIENT COMPUTATION OF THE MATRIX EXPONENTIAL USING PADÉ APPROXIMATION

Yung-Ya Lin and Lian-Pin Hwang*

Department of Chemistry, National Taiwan University, Taipei, Taiwan and Institute of
Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, Republic of China

Abstract—A modified Padé approximation has been proposed to calculate the matrix exponential involved in the numerical solution of linear evolution equations. If the exponential matrix has a band structure, a factorization method may then be conveniently used to reduce computation flops. Numerical solutions of the heat-conduction equation and time-dependent Schrödinger equation are given as numerical examples to illustrate the feasibility. An increase in efficiency and accuracy over conventional methods is obtained.

1. INTRODUCTION

Mathematical models of many chemical and physical problems involve systems of homogeneous linear evolution equations of the form,

$$x'(t) = Kx(t), \quad x(0) = x_0 \tag{1}$$

where $x(t)$ is an n-dimensional vector and the square matrix, K, may be time-dependent. Equation (1) arises frequently in the solution of parabolic partial differential equations discretized in spatial variables such as in the study of time–correlation function for spin relaxation (Hwang & Freed, 1975; Hwang, 1984) and diffusion-controlled reaction rates in liquids (Hwang, 1982).

The motivation for this work results from our efforts to efficiently solve a huge system of equations (1) which describe the magnetization attenuation in NMR pulsed gradient spin echo experiments. The solution of equation (1) can be numerically evaluated by a recursive method,

$$x(t + \Delta t) = \exp(K \Delta t)x(t) = \exp(A)x(t) \tag{2}$$

where $A \equiv K \Delta t$ and time-dependence of K may be incorporated piecewise.

A fundamental step in solving equation (2) is the evaluation of $\exp(A)$. Many methods have been used to compute $\exp(A)$, such as matrix eigenvalues (Kirchner, 1967), approximation theory (Saff, 1971), differential equations (Ehle & Lawson, 1975), matrix characteristic polynomial (Kolodner, 1975), the arithmetic–geometric-mean method (Stickel, 1985), elimination method (Walz, 1988), and polynomial approximation (Tal-Ezer, 1989). Numerous algorithms for computing $\exp(A)$ have been proposed, but most of them are of dubious numerical quality, as

pointed out in the famous survey article by Moler and Van Loan (1978). In practice, consideration of computational accuracy and efficiency indicates that some of the methods are preferable to others, but that none are completely satisfactory when the following attributes are also concerned: generality, reliability, stability, storage requirements, ease of use, and simplicity. The choice will depend upon the details of implementation and upon the particular problem being solved. In this paper, we propose a method based on a modification of the Padé approximation which allows the formulation of a fast and accurate algorithm for the computation of $\exp(A)$. If A has band structure, a pronounced reduction in the amount of computation can be achieved by factorization.

2. PRINCIPLES

Padé approximations have played an important role in the development of applied mathematics, and they are still widely used in many fields (Baker & Graves-Morris, 1981). The series expansion of an appropriate Padé approximation of a function agrees on as many terms as possible with its formal power series in ascending order, i.e. up to the sum of the degrees of the numerator and denominator. The numerator and the denominator of a Padé approximant are then exclusively determined by this condition. The (p, q) Padé approximation to $\exp(A)$ is defined by:

$$R_{pq}(A) = \frac{N_{pq}(A)}{D_{pq}(A)}, \tag{3}$$

where

$$N_{pq}(A) = \sum_{j=0}^{p} \frac{(p + q - j)! \, p!}{(p + q)! \, j! \, (p - j)!} A^j \tag{4}$$

---

* Author for correspondence.

285

and

$$D_{pq}(A) = \sum_{j=0}^{q} \frac{(p+q-j)!q!}{(p+q)!j!(q-j)!}(-A)^j, \qquad (5)$$

where the eigenvalues of A are presumed to be negative. Zakian (1970) and Wragg and Davies (1975) have considered the various representations of these rational approximations (e.g. partial fraction or continued fraction) as well as the choice of p and q to obtain sufficient accuracy.

It should be noted that the Padé approximants are normally useful only near the origin (i.e. the norm of A, $\|A\| \ll 1$), as the following identity reveals (Moler & Van Loan, 1989):

$$\exp(A) = R_{pq}(A) + \frac{(-1)^q}{(p+q)!}[A^{p+q+1}/D_{pq}(A)]$$

$$\times \int_0^1 u^p(1-u)^q \exp[A(1-u)]\,du. \quad (6)$$

However, this restriction can be overcome with the help of the identity $\exp(A) = \exp[(A/l)^l]$. A is scaled by l^{-1} such that $R_{pq}(A/l)$ is a suitable approximation to $\exp(A/l)$. If l is a power of two, the computation may be efficiently performed by repeated squaring. The errors can then be kept negligibly small even though the Padé approximants are not near the origin. There are several reasons why the diagonal approximants $(p = q)$ are preferred over the off diagonal approximants $(p \neq q)$. Let n be the order of the matrix A. For the case of $p < q$, it is found that about qn^3 flops are required to evaluate $R_{pq}(A)$ which is of the order $p + q$. Furthermore, the same amount of computation is needed to compute $R_{qq}(A)$ which is of the order $2q$ $(2q > p + q)$. A similar argument can be applied to the superdiagonal approximants $(p > q)$. To illustrate our scheme with a minimum of detail we will focus on the diagonal case, but the theory, with minor modification, is also applicable to non-diagonal cases.

It is known that the series expansion of the (q, q) diagonal Padé approximant agrees with that of the exponential function to order $2q$. For example, the exponential of a matrix is defined by:

$$\exp(A) \equiv \sum_{i=0}^{\infty} \frac{A^i}{i!}$$

$$= I + A + \frac{A^2}{2} + \frac{A^3}{6} + \frac{A^4}{24} + \frac{A^5}{120} + \frac{A^6}{720}$$

$$+ \frac{A^7}{5040} + \frac{A^8}{40320} + \frac{A^9}{362880} + O(A^{10}), \quad (7)$$

and the series expansion of the (3,3) diagonal Padé approximant is

$$R_{33}(A) = \frac{I + A/2 + A^2/10 + A^3/120}{I - A/2 + A^2/10 - A^3/120}$$

$$= I + A + \frac{A^2}{2} + \frac{A^3}{6} + \frac{A^4}{24} + \frac{A^5}{120} + \frac{A^6}{720}$$

$$+ \frac{A^7}{4800} + \frac{A^8}{28800} + \frac{7A^9}{864000} + O(A^{10}). \quad (8)$$

To increase the accuracy to the next higher order, we define the modified diagonal Padé approximation as

$$\tilde{R}_{qq}(A) \equiv R_{qq}(A) + \frac{cA^{2q+1}}{D_{qq}(A)^2}$$

$$= \frac{N_{qq}(A)}{D_{qq}(A)} + \frac{cA^{2q+1}}{D_{qq}(A)^2}. \quad (9)$$

The coefficient c may be determined by comparing the A^{2q+1} term in the series expansion of equation (9) with equation (7). The interesting result is that the accuracy is in fact increased up to the order $2q + 2$. A brief derivation is as follows. After some algebraic manipulation from equation (6) one may obtain the coefficients A^{2q+1} and A^{2q+2} in the series expansion of R_{qq}:

$$R_{qq}(A) = \sum_{i=0}^{2q} \frac{A^i}{i!} + \frac{1}{(2q+1)!}$$

$$\times \left[1 - \frac{(-1)^q(q!)^2}{(2q)!}\right]A^{2q+1} + \frac{1}{(2q+1)!}$$

$$\times \left[\frac{1}{(2q+2)} - \frac{(-1)^q(q!)^2}{(2q)!}\right]A^{2q+2}$$

$$+ O(A^{2q+3}). \quad (10)$$

Now, since the expansion of the added term, $cA^{2q+1}/D_{qq}(A)^2$, is

$$\frac{cA^{2q+1}}{D_{qq}(A)^2} = cA^{2q+1} + cA^{2q+2} + O(A^{2q+3}), \quad (11)$$

we conclude that the modified (q, q) diagonal Padé approximation has an order of $2q + 2$ if we choose

$$c = \frac{(-1)^q(q!)^2}{(2q+1)!(2q)!}. \quad (12)$$

For example, the series expansion of $\tilde{R}_{33}(A)$ with undetermined coefficient c is

$$I + A + \frac{A^2}{2} + \frac{A^3}{6} + \frac{A^4}{24} + \frac{A^5}{120} + \frac{A^6}{720}$$

$$+ \left(\frac{1}{4800} + c\right)A^7 + \left(\frac{1}{28800} + c\right)A^8$$

$$+ \left(\frac{7}{864000} + \frac{11}{20}c\right)A^9 + O(A^{10}). \quad (13)$$

Comparing with equation (7), $c = -1/100800$ and $\tilde{R}_{33}(A)$ has an order of 8.

The advantage of the modified (q, q) diagonal Padé approximation is that it gives a more accurate result but requires only slightly more calculation. This may
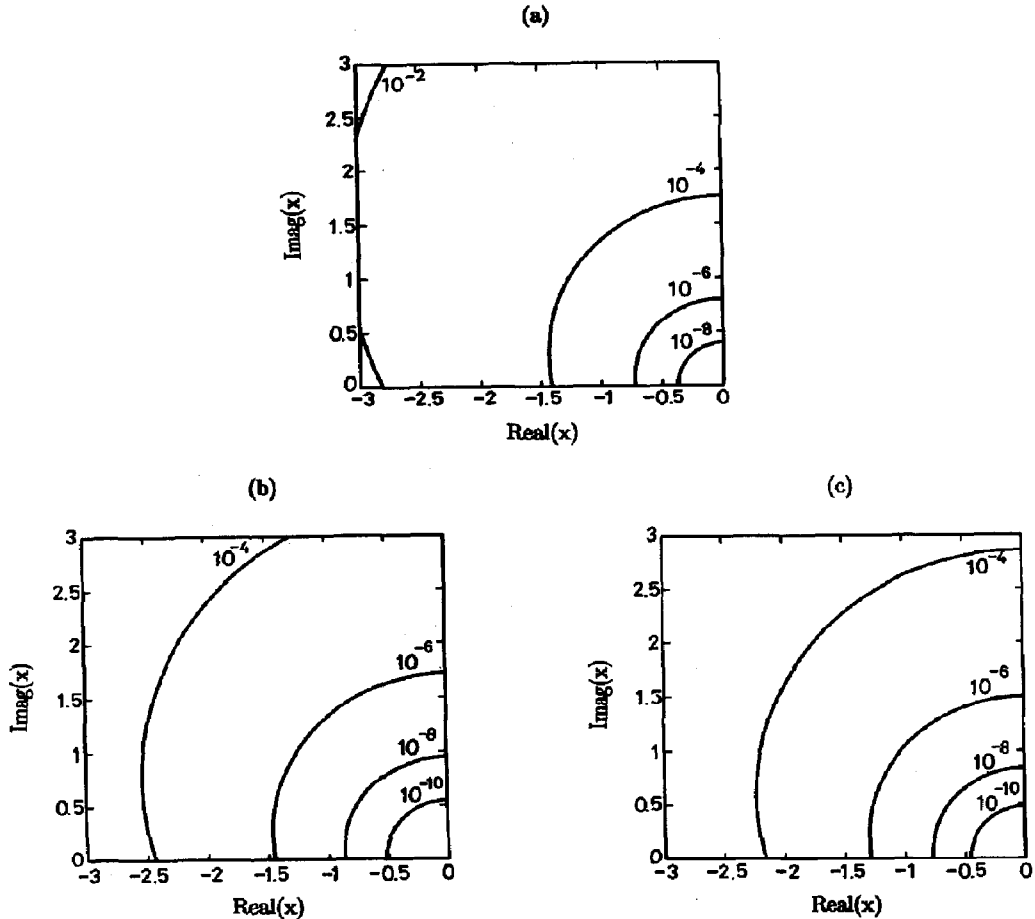
(a)

(b)   **(c)**

Fig. 1. Contour plots of the absolute errors of $|\exp(x) - R_{qq}(x)|$: (a) $|\exp(x) - R_{33}(x)|$; (b) $|\exp(x) - R_{44}(x)|$; (c) $|\exp(x) - \tilde{R}_{33}(x)|$. These plots are symmetric about the real(x) axis. The absolute errors are cited in the figure for every curve.

be understood by the following example using the (q, q) diagonal Padé approximation,

$$\mathbf{x}(t + \Delta t) = \exp(\mathbf{A})\mathbf{x}(t) \cong R_{qq}(\mathbf{A})\mathbf{x}(t)$$

$$= \frac{N_{qq}(\mathbf{A})\mathbf{x}(t)}{D_{qq}(\mathbf{A})}, \qquad (14)$$

which is equivalent to solving

$$D_{qq}(\mathbf{A})\mathbf{x}(t + \Delta t) = N_{qq}(\mathbf{A})\mathbf{x}(t). \qquad (15)$$

The numerical evaluation of equation (15) may be performed by the following steps:
(a) Form the product $\mathbf{b} \equiv N_{qq}(\mathbf{A})\mathbf{x}(t)$;
(b) Form the matrix $D_{qq}(\mathbf{A})$;
(c) Perform the LU-factorization of $D_{qq}(\mathbf{A})$ ($\equiv \mathbf{LU}$), where $\mathbf{L}$ is a lower triangular matrix, and $\mathbf{U}$ is an upper triangular matrix (Moler & Van Loan, 1989);
(d) If we let $\mathbf{z} = \mathbf{Ux}$, then from equation (15) we have $\mathbf{Lz} = \mathbf{b}$ which can be solved by forward substitution since $\mathbf{L}$ is lower triangular;

(e) Once we have obtained $\mathbf{z}$, the solution, $\mathbf{x}$, can then be obtained by solving $\mathbf{Ux} = \mathbf{z}$. Since $\mathbf{U}$ is upper triangular this step requires back substitution.

Note that, while in general steps (b) and (c) entail $O(n^3)$ operations, steps (a), (d), and (e) require $O(n^2)$ operations. Moreover, suppose we are solving $\mathbf{x}(t + \Delta t) = \tilde{R}_{qq}(\mathbf{A})\mathbf{x}(t)$, which can be expressed by the following identity:

$$\mathbf{x}(t + \Delta t) = \tilde{R}_{qq}(\mathbf{A})\mathbf{x}(t)$$

$$= R_{qq}(\mathbf{A})\mathbf{x}(t) + \frac{c\mathbf{A}^{2q+1}\mathbf{x}(t)}{D_{qq}(\mathbf{A})^2}. \qquad (16)$$

We recognize that the first term is a conventional (q, q) Padé approximant and can be solved by the above steps. The LU-factorization of $D_{qq}(\mathbf{A})$, which has already been computed, together with additional computation of matrix-vector products and back-substitutions may then be used to evaluate the second term. Since the matrix-vector products
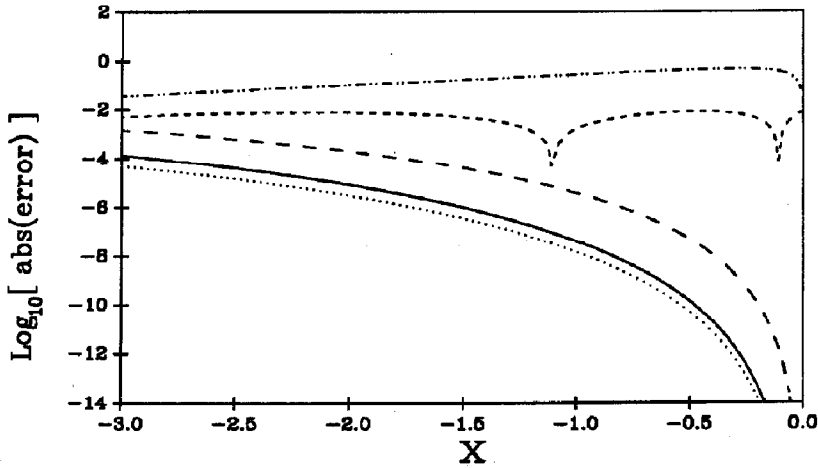
Fig. 2. Comparison of accuracy of some rational approximations to exp(x). $--$ Padé (3,3); $\cdots$ Padé (4,4); —— modified Padé (3,3); —$\cdot\cdot$— Chebyshev rational approximant; and $---$ geometric convergent sequence.

and back-substitutions require only $O(n^2)$ operations respectively, the additional amount of computation required for the modified diagonal Padé approximation is about an order smaller than that already incurred in computing the diagonal Padé approximation.

Contour plots of the absolute errors of $|\exp(x) - R_{33}(x)|$, $|\exp(x) - R_{44}(x)|$, and $|\exp(x) - \tilde{R}_{33}(x)|$ for $-3 \leqslant \text{Real}(x) \leqslant 0$ and $0 \leqslant \text{Imag}(x) \leqslant 3$ are given in Fig. 1. For small $|x|$, the errors of all these three approximants are acceptable. However, the errors become pronounced for large $|x|$. As expected, $R_{44}(A)$ is the best of all the approximants and about 100 times more accurate than $R_{33}(A)$. $\tilde{R}_{33}(A)$ gives similar accuracy to $R_{44}(A)$.

Padé approximation is also compared with other rational approximations to exponential function, such as the Chebyshev rational approximation (Cody et al., 1969) and geometric convergent sequence (Saff et al., 1976), in Fig. 2 for x ranging from 0 to -3. These models all have approximately the same cut-off order ($\cong$ sixth order). It is obvious that for small $|x|$ the Padé approximants are the most accurate. Among the three Padé approximants, the results of their respective accuracies are similar to the conclusions drawn for Fig. 1.

In many applications involving linear systems, the equations as given in equation (1) may be rearranged so that the coefficient matrix $\mathbf{K}$ forms a banded structure. It often occurs when the finite difference method is used to solve partial differential equations. Substantial reductions in computation time can be achieved when solving banded systems because the triangular factors in LU are also banded. Moreover, we can further reduce the operations needed to compute the modified diagonal Padé approximation by using the factorization method,

$$N_{qq}(\mathbf{A}) = \prod_{j=1}^{q} (\mathbf{I} + k_j \mathbf{A}) \qquad (17)$$

where all k_j are distinct, nonzero, either real or in complex conjugate pairs (Staff & Varga, 1975). Because $D_{qq}(\mathbf{A}) = N_{qq}(-\mathbf{A})$ for the diagonal Padé approximation, we can write the (q, q) diagonal Padé approximant $R_{qq}(\mathbf{A})$ in complex factorized form,

$$R_{qq}(\mathbf{A}) = \frac{N_{qq}(\mathbf{A})}{D_{qq}(\mathbf{A})} = \prod_{j=1}^{q} \frac{(\mathbf{I} + k_j \mathbf{A})}{(\mathbf{I} - k_j^* \mathbf{A})} \qquad (18)$$

where k_j^* is the complex conjugate of k_j. For example,

$$R_{33}(\mathbf{A}) = \frac{\mathbf{I} + \mathbf{A}/2 + \mathbf{A}^2/10 + \mathbf{A}^3/120}{\mathbf{I} - \mathbf{A}/2 + \mathbf{A}^2/10 - \mathbf{A}^3/120}$$

$$\cong \left[\frac{\mathbf{I} + 0.2153\mathbf{A}}{\mathbf{I} - 0.2153\mathbf{A}} \right]$$

$$\times \left[\frac{\mathbf{I} + (0.1423 + 0.1358i)\mathbf{A}}{\mathbf{I} - (0.1423 - 0.1358i)\mathbf{A}} \right]$$

$$\times \left[\frac{\mathbf{I} + (0.1423 - 0.1358i)\mathbf{A}}{\mathbf{I} - (0.1423 + 0.1358i)\mathbf{A}} \right]. \qquad (19)$$

The solution procedure is then to unfold the products of equation (18) pair by pair. Each substep of a given time step is of the form

$$(\mathbf{I} - k_1^* \mathbf{A})\mathbf{x}^{(1)} = (\mathbf{I} + k_1 \mathbf{A})\mathbf{x}^{(0)}$$
$$(\mathbf{I} - k_2^* \mathbf{A})\mathbf{x}^{(2)} = (\mathbf{I} + k_2 \mathbf{A})\mathbf{x}^{(1)}$$
$$(\mathbf{I} - k_3^* \mathbf{A})\mathbf{x}^{(3)} = (\mathbf{I} + k_3 \mathbf{A})\mathbf{x}^{(2)}$$
$$\vdots$$
$$(\mathbf{I} - k_q^* \mathbf{A})\mathbf{x}^{(q)} = (\mathbf{I} + k_q \mathbf{A})\mathbf{x}^{(q-1)} \qquad (20)$$

where $\mathbf{x}^{(0)} = \mathbf{x}(t)$ and $\mathbf{x}(t + \Delta t) = \mathbf{x}^{(q)}$.

If $\mathbf{A}$ is a band matrix, the factorization method is superior to direct evaluation of equation (15). The key point is that $D_{qq}(\mathbf{A})$ will generally lose its band structure and become a nearly full matrix for even moderately large q. Suppose $\mathbf{A}$ is a band matrix with $m_u = m_l = m \ll n$ where m_u is the upper bandwidth,
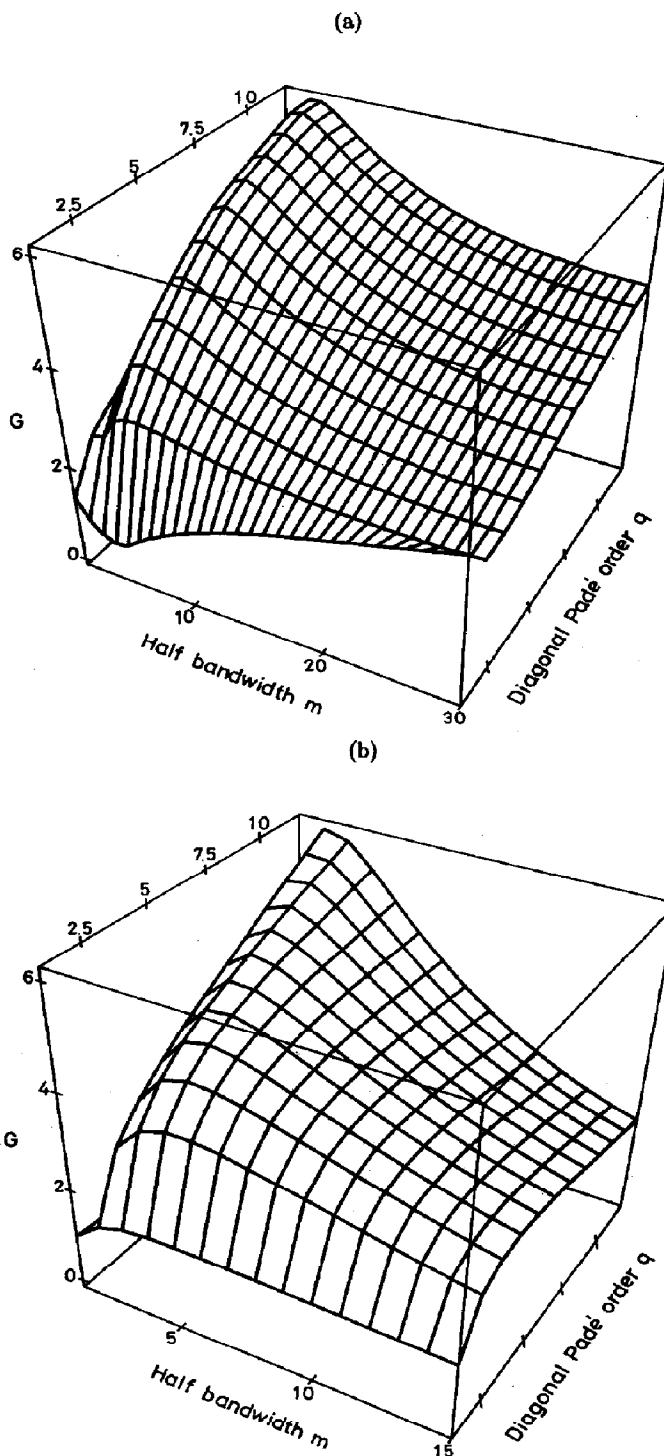
(a)

(b)

Fig. 3. G factor for factorization method with $n = 60$: (a) real factorization method; (b) complex factorization method.

and m_1 the lower bandwidth. Let μ be the flops required to execute the FORTRAN statement, $Y(I) = Y(I) + T \times X(I)$. There are two major advantages in using factorization over direct computation in equation (15). First, in computing equation (20), the flops needed to invert A q times using the factorization method is about $q(2nm^2 + 3nm)\mu$, while those required to invert $D_{qq}(A)$ is about $(n^3/3 + n^2)\mu$. Thus
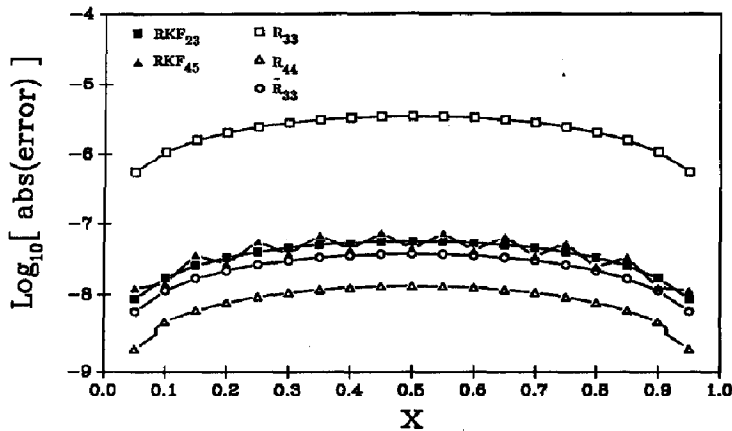
Fig. 4. Comparison of accuracy in solving heat-conduction equation (21) using several different methods
as cited in the figure with $M = 20$ and single time step for $t = 0.1$ s.

factorization is much more efficient when $n \gg m$. Secondly, the extra computation of explicit formation of $N_{qq}(A)$, $D_{qq}(A)$, and $N_{qq}(A)x(t)$ is avoided. We call the above approach the complex factorization method because it generally involves complex arithmetic. When the initial values of x and A are real, the use of complex arithmetic is not economical. Since the complex coefficients occur in conjugate pairs, it is possible to rearrange the terms of equation (18) into a product with real quadratic and/or real linear factors. We may call it the real factorization method. This real factorization method should be superior for real problems, while being only slightly more difficult to implement.

To describe the efficiency of computation enhanced by the factorization method, we define $G \equiv \alpha/\beta$, where α and β are the flops required to solve equation (15) using diagonal Padé approximations without and with the factorization method, respectively. We consider the matrix band structure for selecting appropriate algorithms and subroutines at every stage of the computation to minimize both α and β. The G factor for different diagonal Padé order q and half bandwidth m ($= m_u = m_l$) using the real and complex factorization method is given in Fig. 3. It is clear that G nears optimal when $m < 5$. This is normally the case in general chemical and physical problems.

3. NUMERICAL TESTS AND RESULTS

To illustrate the gain in efficiency and accuracy obtained over conventional methods using the modified diagonal Padé approximation and factorization method, numerical solutions of the 1-D heat-conduction equation and time-dependent Schrödinger equation are given. A similar algorithm may be extended to higher dimensions.

Example 1: Heat-conduction equation

Now consider solving the normalized 1-D heat-conduction equation,

$$\frac{\partial u(x, t)}{\partial t} = \frac{\partial^2 u(x, t)}{\partial x^2}, \quad 0 < x < 1, \quad t > 0, \quad (21)$$

subject to the boundary conditions

$$u(0, t) = u(1, t) = 0 \quad \text{for all } t > 0, \quad (22)$$

and the initial condition

$$u(x, 0) = \sin(\pi x) \quad \text{for } 0 < x < 1. \quad (23)$$

We discretize the spatial variable, dividing $(0, 1)$ into M equal intervals $\Delta x = 1/M$, and let $U_j(t) = u(j \Delta x, t)$. We use the three-point central-difference approximation for the second derivative,

$$\frac{\partial^2 u(j \Delta x, t)}{\partial x^2} \cong \frac{U_{j+1}(t) - 2U_j(t) + U_{j-1}(t)}{(\Delta x)^2}. \quad (24)$$

Then, since $U_0(t) = U_M(t) = 0$, equation (21) is in the form of equation (1) with $n = M - 1$. The matrix A is tridiagonal, with diagonal elements $-2/(\Delta x)^2$ and sub- and super-diagonal elements $1/(\Delta x)^2$.

Example 2: Time-dependent Schrödinger equation

We concentrate here upon 1-D quantum-mechanical scattering (reflection–transmission) phenomena as described by the time-dependent Schrödinger equation. Basically, it is a parabolic partial differential equation for the evolution of complex wave function ψ. Although this equation can be solved accurately in many ways, there is still great interest in developing simpler and more accurate algorithms (Galbraith *et al.*, 1984). For the scattering of a wave packet by a 1-D potential $V(x)$, the equation has the form,

$$i \frac{\partial \psi}{\partial t} = H\psi \quad (25)$$

where the operator H is defined by,

$$H = -\frac{\partial^2}{\partial x^2} + V(x). \quad (26)$$

Here we have chosen units so that Planck's constant $\hbar = 1$ and the particle mass $m = 1/2$. The initial wave
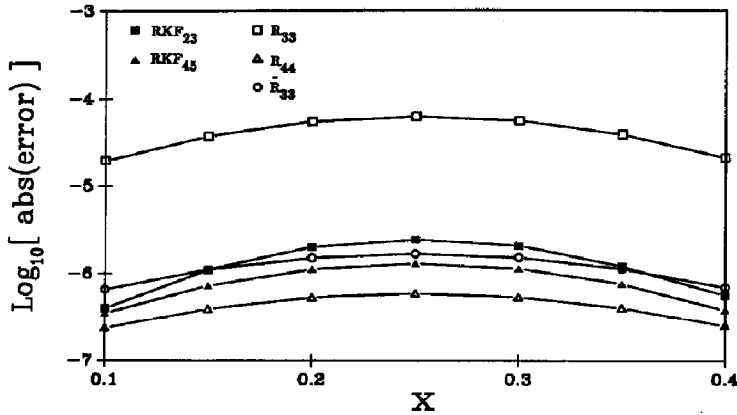
Fig. 5. Comparison of accuracy in solving time-dependent Schrödinger equation (25) using several different methods as cited in the figure with $M = 20$ and single time step for $t = 0.001$ s.

packet $\psi(x, t = 0)$ together with boundary conditions $\psi \to 0$ as $x \to \pm \infty$ is given. Since the underlying physical problem requires that the total probability of finding the particle somewhere remains unity,

$$\int_{-\infty}^{+\infty} |\psi|^2 \, dx = 1. \qquad (27)$$

The formal solution of equation (25) is

$$\psi(x, t) = \exp(-iHt)\psi(x, 0) \qquad (28)$$

which is of the same form as equation (2). On replacing H by its finite difference approximation in x, we have a complex tridiagonal system to solve. For convenience, we represent the initial state of the particle which impinges upon the potential by a Gaussian wave packet. Thus we put

$$\psi(x, 0) = \exp(ik_0 x)\exp[-(x - x_0)^2/2\sigma_0^2]. \qquad (29)$$

We see that this wave packet is centered about $x = x_0$ with a spread in x governed by σ_0. The factor $\exp(ik_0 x)$ makes our initial wave function move to the right with average momentum k_0. We appropriately set the box length $= 1$, $x_0 = 1/4$, $\sigma_0 = 1/35$, and $k_0 = \pi/10$. The potential well is $V(x) = -1/2$ for $29/60 \leqslant x \leqslant 32/60$. Then the finite difference method is applied as in the previous example.

The accuracy of the various methods is compared for solving example 1 in Fig. 4 and for solving example 2 in Fig. 5. The methods used were the Padé (3,3), R_{33}; the Padé (4,4), R_{44}; the modified Padé (3,3), $\tilde{R}_{33}$; the Runge–Kutta–Fehlberg method using 2nd and 3rd order formulas, RKF_{23}; and the Runge–Kutta–Fehlberg method using 4th and 5th order formulas, RKF_{45} (Ehle & Lawson, 1975). The errors in Figs 4 and 5 are with respect to the exact solutions obtained from numerically-calculated eigenvalues and eigenvectors, EIG. In solving the examples using the Runge–Kutta–Fehlberg method, the tolerance in the programs was adjusted to make the errors approximately the same as those obtained
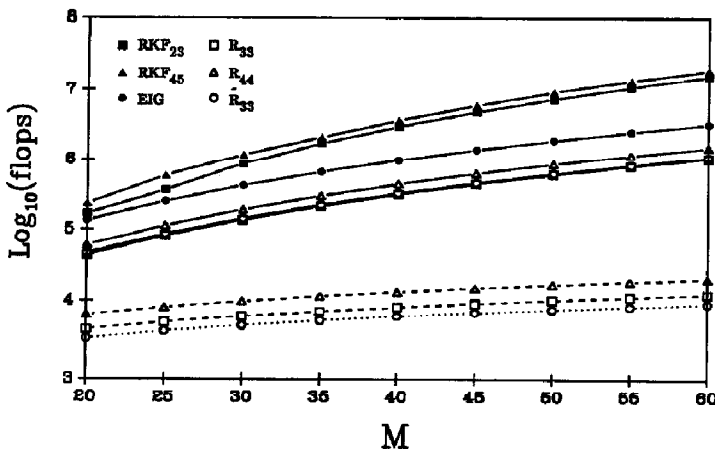

Fig. 6. Comparison of computation flops in solving heat-conduction equation (21) using several different methods as cited in the figure with M varying from 20 to 60 and single time step for $t = 0.1$ s. —— treated as full matrix; – – – treated as band matrix without real factorization method; and $\cdots\cdots$ treated as band matrix with real factorization method.
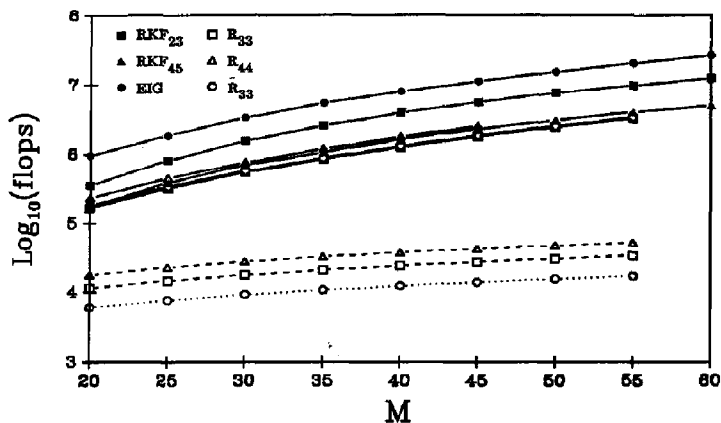
Fig. 7. Comparison of computation flops in solving time-dependent Schrödinger equation using several different methods as cited in the figure with M varying from 20 to 60 and single time step for $t = 0.001$ s. —— treated as full matrix; – – – treated as band matrix without real factorization method; and · · · · treated as band matrix with complex factorization method.

using the modified (3,3) Padé approximation. The computation flops needed for these methods with M varying from 20 to 60 are compared in Fig. 6 for example 1 and in Fig. 7 for example 2. Since example 1 only involves real arithmetic, we use real factorization instead of complex factorization.

Both Figs 4 and 5 illustrate that the modified Padé (3,3) approximation greatly enhances the accuracy compared with the regular Padé (3,3) by about 100 times. In fact, the modified Padé (3,3) gives almost the same accuracy as Padé (4,4) which is consistent with equations (10) and (11). In general, the modified Padé (q, q) approximation has an order of $2q + 2$. Figures 6 and 7 show that, without the factorization method, the modified Padé (3,3) approximation is only slightly more tedious than the regular Padé (3,3) approximation. But on introducing the factorization method, we can effectively reduce the amount of computation. It is also noted that, for the same accuracy, the Runge–Kutta–Fehlberg method is very computationally expensive in these two examples given above. Both of the numerical tests illustrate the feasibility of our proposed approach in terms of efficiency and accuracy.

4. CONCLUSIONS

The combination of the modified Padé approximation with the factorization method is an efficient means for the evaluation of matrix exponentials. Although we considered only the homogeneous case of equation (1), the method is immediately applicable to the general linear case, $x'(t) = Kx(t) + y(t)$, which commonly occurs in diffusion problems under a time-dependent external field or in the description of the Brownian motion by Langevin equation (Myron, 1986).

The application of the present algorithm to simulate the spin-echo attenuation of the probe signal in intracellular and extracellular diffusion processes

from pulsed field gradient NMR experiments has been successfully carried out in our laboratory. This novel approach greatly reduces the computation time needed and increases the accuracy. We have also used this method to analyze the effect of gradient pulse imperfection due to both coil inductance and eddy current in the pulsed field gradient experiments. This analysis needs hundreds of matrix exponential computations in order to achieve the required precision. Further modification and application shall be reserved for a later occasion.

REFERENCES

Baker G. A. & Graves-Morris P. R. (1981) *Padé Approximants, Part II: Extensions and Applications*. Addison-Wesley, London.
Cody W. J., Meinardus G. & Varga R. S. (1969) *J. Approx. Theory* **2**, 50.
Dongarra J. J., Moler C. B., Bunch J. R. & Steward G. W. (1979) *LINPACK User's Guide*, SIAM, Philadelphia.
Ehle B. L. & Lawson J. D. (1975) *J. Inst. Math. Appl.* **16**, 11.
Galbraith I., Ching Y. S. & Abraham E. (1984) *Am. J. Phys.* **52**, 60.
Hwang L. P. & Freed J. H. (1975) *J. Chem. Phys.* **63**, 4017.
Hwang L. P. (1982) *J. Chem. Phys.* **76**, 4037.
Hwang L. P. (1984) *Mol. Phys.* **51**, 1235.
Kirchner R. B. (1967) *Am. Math. Monthly* **74**, 1200.
Kolodner I. I. (1975). *J. Math. Anal. Appl.* **52**, 514.

Moler C. B. & Van Loan C. F. (1978) *SIAM Review* **20,** 801 (and references therein).

Moler C. B. & Van Loan C. F. (1989) *Matrix Computation,* 2nd edition. The Johns Hopkins University Press, Baltimore, MD.

Myron W. E. (1986) *J. Chem. Soc., Faraday Trans. 2* **82,** 653.

Saff E. B. (1971) *Trans. Am. Math. Soc.* **73,** 2.

Saff E. B. & Varga R. S. (1975) *Numer. Math.* **25,** 1.

Saff E. B., Schonhage A. & Varga R. S. (1976) *Numer. Math.* **25,** 307.

Smith B. T., Boyle J. M., Dongarra J. J., Garbow B. S., Ikebe Y., Klema V. C. & Moler C. B. (1976) *Matrix Eigensystem Routines—EISPACK Guide,* Lecture Notes in Computer Science, Vol. 6, 2nd edition. Springer-Verlag, Berlin.

Stickel E. U. (1985) *Analysis* **5,** 163.

Tal-Ezer H. (1989) *J. Sci. Comput.* **4,** 25.

Varga R. S. (1969) *J. Approx. Theory* **2,** 50.

Walz G. (1988) *J. Comput. Appl. Math.* **21,** 119.

Wragg A. & Davies C. J. (1975) *J. Inst. Math. Appl.* **11,** 369.

Zakian V. (1970) *Electron. Lett.* **6,** 814.