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A Note on Asymptotic Splitting and its Applications

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Abstract—Explicit forms of the remainder terms of the asymptotic splitting formulae associated with the first order splitting, Strange's splitting, and the parallel splitting are derived. Using the identities obtained, we establish the global error estimates for the asymptotic splitting formulae. Both the theoretical investigation and numerical experiments indicate that it is a more efficient and accurate way to use the asymptotic splitting than the conventional splitting formulae.

Keywords—Asymptotic splitting, Exponential splitting, Global error estimate, Order of accuracy.

1. INTRODUCTION

Various kinds of splitting methods are used nowadays to achieve simplicity and efficiency in scientific computations. Many of them, however, can be viewed as special cases of the exponential splitting. For instance, by introducing suitable approximations, the weakly nonlinear n-dimensional convection-diffusion problem

$$u_t = \sum_{i=1}^{n} \left(a_i^2 u_{x_i x_i} - b_i u u_{x_i}\right) - cu, \qquad x \in \Omega, \quad t_0 < t \le T, \tag{1.1}$$

$$u = \phi, \qquad x \in \partial\Omega, \quad t_0 < t \le T, \tag{1.2}$$

$$u = u_0, \qquad x \in \Omega, \quad t = t_0, \tag{1.3}$$

where a_i, b_i, c, u_0, $1 \le i \le n$ are functions of x, ϕ is a function of x, t, $x = (x_1, x_2, \dots, x_n)$, and Ω is the open spatial domain considered, can be discretized into a system of ordinary differential equations

$$v_t = \sum_{i=1}^{n} A_i v, \qquad t_0 < t \le T, \tag{1.4}$$

$$v = v_0, \quad t = t_0, \tag{1.5}$$

where the matrices $A_i = A_i(t, v)$, $1 \le i \le n$, do not, in general, commute. In the case when the coefficient matrices A_i, $i = 1, 2, \dots, n$, are independent of t and v, system (1.4)–(1.5) can be integrated to yield

$$v = P v_0, \tag{1.6}$$

where $P = P(t) = \exp\{t \sum_{i=1}^{n} A_i\}$ and v_0 is the initial vector given by (1.5). Hence, solving (1.1)–(1.3) numerically is equivalent to seek for a suitable approximation to the matrix exponential

Typeset by $\mathcal{A}_\mathcal{M}\mathcal{S}$-TEX operator P and it is not difficult to see that a first-order splitting

$$S_1(A_1, A_2, \dots, A_n; t) = \prod_{i=1}^{n} e^{tA_i}, \tag{1.7}$$

together with different rational approximations to the matrix exponentials e^{tA_i}, $i = 1, 2, \dots, n$, offers a wide class of the known splitting schemes [1].

Much effort has been put during recent years for the implementation of the splitting approximation of P in the extended form

$$S(t) = \sum_{k=1}^{K} \gamma_k \prod_{i=1}^{m(k)} e^{\alpha_{i,k} t A_{r(i,k)}}, \tag{1.8}$$

where $1 \le r(i,k) \le n$. One of the earliest approaches can be found in the investigation of Trotter [2,3], in which products of matrix exponentials play a crucial role in the approximants. Later, Strang [4] introduced a second-order accurate sequential splitting, and in 1970, Burstein and Mirin [5] proposed higher order splitting formulae for solving fluid equations. However, Sheng in 1989 [6] and later in 1991 Suzuki [7] proved that such a higher-order splitting with positive coefficients γ, α does not exist.

Apart from (1.7), widely used conventional splittings are Strang's splitting

$$S_2(A_1, A_2, \dots, A_n; t) = \prod_{i=1}^{n-1} e^{(t/2)A_i} \times e^{tA_n} \times \prod_{i=1}^{n-1} e^{(t/2)A_{n-i}} \tag{1.9}$$

and the parallel splitting

$$S_3(A_1, A_2, \dots, A_n; t) = \frac{1}{2}\left(S_1(A_1, A_2, \dots, A_n; t) + S_1(A_n, A_{n-1}, \dots, A_1; t)\right) \tag{1.10}$$

(c.f. [4,8–11]).

Matrix exponential operators associated with splittings have important physical and scientific meanings in practical applications. Interested readers are referred to [7,12–16] and references therein.

In this paper, we investigate properties of the generalized asymptotic splitting [1,4]

$$\Phi_{k,m}(t) = \left(\prod_{i=1}^{m} S_{r(i)}\left(\frac{t}{mk}\right)\right)^{k}, \qquad m, k \in \mathbb{N}^+, \quad t > 0, \tag{1.11}$$

where $S_{r(i)}$, $1 \le r(i) \le N$, $1 \le i \le m$, are conventional exponential splitting formulae of the form (1.8) and $\mathbb{N}^+$ is the set of positive integers.

The plan of this paper is as follows: In Section 2, we shall give the definition of order of accuracy and establish several important identities for the first-order splitting, Strang's splitting, and the parallel splitting. In Section 3, global error analysis will be studied for the asymptotic splitting. In particular, we shall investigate cases in which the most often used conventional splittings are involved. Numerical experiments will be given. It is found that, when the index number k is chosen to be sufficiently large, the asymptotic splittings can offer better numerical solutions than the conventional splitting methods. Finally in Section 4, we shall provide several remarks about our investigations. Here, a perturbation problem is also considered. The spectral norm $\|\cdot\|$, commutator of two matrices, $[A, B] = AB - BA$, and the logarithmic norm $\mu(A) = \max\{\lambda \mid \lambda$ an eigenvalue of $(A + A^*)/2\}$ are used throughout our discussion.

2. SPLITTING IDENTITIES

Let $T(t)$ be an approximation of the matrix exponential operator $P(t) = \exp\{\sum_{i=1}^{n} tA_i\}$.

DEFINITION 2.1. *We say that the approximation T is accurate to order ρ if*

$$\|T - P\| = O\left(t^{\rho+1}\right), \qquad t > 0.$$

LEMMA 2.1. *Let $S_1(t), S_2(t), \dots, S_N(t)$ be conventional exponential splitting approximants to P with the order of accuracy $\rho_1, \rho_2, \dots, \rho_N$, respectively. If $\mu(A_i) \le 0$, $1 \le i \le N$, then the order of accuracy of the product formula*

$$T_m(t) = \prod_{j=1}^{m} S_{r(j)}\left(\frac{t}{m}\right), \qquad 1 \le r(j) \le N, \quad 1 \le j \le m, \tag{2.1}$$

is at least ρ, $\rho \ge \min\{\rho_1, \rho_2, \dots, \rho_N\}$.

PROOF. It is observed that

$$\begin{aligned}
P(t) - \prod_{j=1}^{m} S_{r(j)}\left(\frac{t}{m}\right) &= \exp\left\{t\sum_{i=1}^{N} A_i\right\} - \exp\left\{\frac{(m-1)t}{m}\sum_{i=1}^{N} A_i\right\} S_{r(m)}\left(\frac{t}{m}\right) \\
&\quad + \exp\left\{\frac{(m-1)t}{m}\sum_{i=1}^{N} A_i\right\} S_{r(m)}\left(\frac{t}{m}\right) \\
&\quad - \exp\left\{\frac{(m-2)t}{m}\sum_{i=1}^{N} A_i\right\} S_{r(m-1)}\left(\frac{t}{m}\right) \\
&\quad \times S_{r(m)}\left(\frac{t}{m}\right) + \exp\left\{\frac{(m-2)t}{m}\sum_{i=1}^{N} A_i\right\} S_{r(m-1)}\left(\frac{t}{m}\right) S_{r(m)}\left(\frac{t}{m}\right) \\
&\quad - \exp\left\{\frac{(m-3)t}{m}\sum_{i=1}^{N} A_i\right\} S_{r(m-2)}\left(\frac{t}{m}\right) S_{r(m-1)}\left(\frac{t}{m}\right) S_{r(m)}\left(\frac{t}{m}\right) \\
&\quad + \cdots + \cdots \\
&\quad + \exp\left\{\frac{t}{m}\sum_{i=1}^{N} A_i\right\} S_{r(2)}\left(\frac{t}{m}\right) S_{r(3)}\left(\frac{t}{m}\right) \cdots S_{r(4)}\left(\frac{t}{m}\right) \\
&\quad - \prod_{j=1}^{m} S_{r(j)}\left(\frac{t}{m}\right) \\
&= \exp\left\{\frac{(m-1)t}{m}\sum_{i=1}^{N} A_i\right\} \left(e^{(t/m)\sum_{i=1}^{N} A_i} - S_{r(m)}\left(\frac{t}{m}\right)\right) \\
&\quad + \exp\left\{\frac{(m-2)t}{m}\sum_{i=1}^{N} A_i\right\} \left(e^{(t/m)\sum_{i=1}^{N} A_i} - S_{r(m-1)}\left(\frac{t}{m}\right)\right) S_{r(m)}\left(\frac{t}{m}\right) \\
&\quad + \cdots + \cdots \\
&\quad + \left(e^{(t/m)\sum_{i=1}^{N} A_i} - S_{r(1)}\left(\frac{t}{m}\right)\right) - \prod_{j=2}^{m} S_{r(j)}\left(\frac{t}{m}\right).
\end{aligned}$$

Thus, we have

$$\left\|\exp\left\{t\sum_{i=1}^{N} A_i\right\} - \prod_{j=1}^{m} S_{r(j)}\left(\frac{t}{m}\right)\right\| \le \sum_{i=1}^{m} c_i t^{\rho_i+1} = ct^{\rho+1},$$

where $\rho = \min_{1\le i\le m}\{\rho_i\}$ and this completes the proof. ∎

We note that, in fact, the order of accuracy of the above product formula may be higher than the order of any of the conventional splittings S_i, $i = 1, 2, \dots, N$, used in the product. One of the examples is that if we choose first-order splittings $S_1(t) = e^{tA_1}e^{tA_2}$ and $S_2(t) = e^{tA_2}e^{tA_1}$, then

$$S_1\left(\frac{t}{2}\right) S_2\left(\frac{t}{2}\right) = e^{(t/2)A_1}e^{tA_2}e^{(t/2)A_1}$$

is Strang's splitting which is clearly second-order, while the product

$$S_1\left(\frac{t}{2}\right) S_1\left(\frac{t}{2}\right)$$

remains as a first-order splitting.

THEOREM 2.1. *Let $S_1(t), S_2(t), \dots, S_N(t)$ be conventional exponential splitting approximants to P with the order of accuracy $\rho_1, \rho_2, \dots, \rho_N$, respectively. If $\mu(A_i) \le 0$, $1 \le i \le N$, then the order of accuracy of the asymptotic splitting $\Phi_{k,m}(t)$ is at least ρ, where $\rho \ge \min\{\rho_1, \rho_2, \dots, \rho_N\}$.*

PROOF. Let $T_m(t) = \prod_{j=1}^m S_{r(j)}(t/m)$ and $A_0 = O$ be the null matrix. We have

$$\begin{aligned}\Phi_{k,m}(t) - P(t) &= \left(T_m\left(\frac{t}{k}\right)\right)^k - \exp\left\{t\sum_{i=1}^n A_i\right\}\\ &= \sum_{j=0}^{k-1}\left(e^{(t/k)\sum_{i=1}^n A_i}\right)^j \left(e^{(t/k)\sum_{i=1}^n A_i} - T_m\left(\frac{t}{k}\right)\right)\left(T_m\left(\frac{t}{k}\right)\right)^{k-j-1}.\end{aligned}$$

Hence, it turns out that the order of the asymptotic splitting should be at least the same as the product formula $T_m(t)$ and this proves the theorem. ∎

To further discuss the properties of the asymptotic splitting, we need to establish some useful identities.

LEMMA 2.2. *Let $A_1, A_2, \dots, A_n$ be square matrices which do not commute. Then,*

$$\begin{aligned}\exp\left\{t\sum_{i=1}^n A_i\right\} &= S_1(A_1, A_2, \dots, A_n; t)\\ &\quad + \sum_{i=1}^{n-1}\prod_{j=1}^{i} e^{tA_{j-1}}\int_0^t e^{(t-\tau)\sum_{k=i}^n A_k}\left[A_i, e^{\tau\sum_{k=i+1}^n A_i}\right]e^{\tau A_i}\,d\tau \qquad (2.2)\\ &= S_1(A_1, A_2, \dots, A_n; t)\\ &\quad + \sum_{i=1}^{n-1}\prod_{j=1}^{i} e^{tA_{j-1}}\int_0^t\int_0^\tau e^{(t-\tau)\sum_{k=i}^n A_k}e^{(\tau-s)\sum_{k=i+1}^n A_k}\left[A_i, \sum_{k=i+1}^n A_k\right]\\ &\quad \times e^{s\sum_{k=i+1}^n A_k}e^{\tau A_i}\,ds\,d\tau, \qquad (2.3)\end{aligned}$$

where $A_0 = O$ is the null matrix and S_1 is defined in (1.7).

PROOF. We start with $n = 2$ and for convenience let $A_1 = A$, $A_2 = B$. Consider the matrix exponential function

$$E_1(t) = e^{t(A+B)} - e^{tA}e^{tB}.$$

Differentiating both sides of the above equation, we get

$$E_1'(t) = (A+B)E_1(t) + \left[B, e^{tA}\right]e^{tB}.$$

Solving the above equation, we obtain

$$E_1(t) = \int_0^t e^{(t-\tau)(A+B)}\left[B, e^{\tau A}\right]e^{\tau B}\,d\tau. \qquad (2.4)$$

Further, we have

$$\frac{d}{d\tau}\left[B,e^{\tau A}\right] = A\left[B,e^{\tau A}\right] + \left[B,e^{\tau A}\right]e^{\tau A}.$$

Thus, it follows that

$$\left[B,e^{\tau A}\right] = \int_0^\tau e^{(\tau-s)A}[B,A]e^{sA}\,ds. \tag{2.5}$$

On the other hand, it is observed that

$$\begin{aligned}
\exp\left\{t\sum_{i=1}^n A_i\right\} - \prod_{i=1}^n e^{tA_i} &= \left(e^{t\sum_{i=1}^n A_i} - e^{tA_i}e^{t\sum_{i=2}^n A_i}\right)\\
&\quad + \left(e^{tA_1}e^{t\sum_{i=2}^n A_i} - e^{tA_1}e^{tA_2}e^{t\sum_{i=3}^n A_i}\right)\\
&\quad + \left(e^{tA_1}e^{tA_2}e^{t\sum_{i=3}^n A_i} - e^{tA_1}e^{tA_2}e^{tA_3}e^{t\sum_{i=4}^n A_i}\right)\\
&\quad + \cdots + \cdots\\
&\quad + \left(e^{tA_1}e^{tA_2}\cdots e^{tA_{n-2}}e^{t(A_{n-1}+A_n)} - e^{tA_1}e^{tA_2}\cdots e^{tA_n}\right)\\
&= \sum_{i=1}^{n-1}\prod_{j=1}^{i} e^{tA_{j-1}}\left(e^{t\sum_{k=i}^n A_k} - e^{tA_i}e^{t\sum_{k=i+1}^n A_k}\right).
\end{aligned} \tag{2.6}$$

Now substituting (2.4) into (2.6) with $A = A_i$, $B = \sum_{k=i+1}^n A_k$, $i = 1,2,\dots,n-1$, respectively, we obtain immediately (2.2). The identity (2.3) is a direct consequence of an application of (2.5) in (2.6). ∎

LEMMA 2.3. *Let $A_1, A_2, \dots, A_n$ be square matrices which do not commute. Then*

$$\begin{aligned}
\exp\left\{t\sum_{i=1}^n A_i\right\} &= S_2\left(A_1,A_2,\dots,A_n;t\right) + \sum_{i=1}^{n-2}\prod_{j=1}^{i} e^{(t/2)A_{j-1}}\\
&\quad\times\int_0^t e^{(t/2)A_i}\left[\frac{1}{2}A_i + \sum_{k=i+1}^n A_k, e^{\tau\sum_{k=i+1}^n A_k}e^{(\tau/2)A_i}\right]\\
&\quad\times e^{(t-\tau)\sum_{k=i}^n A_k}\,d\tau\prod_{j=i}^n e^{(t/2)A_{n-j}}
\end{aligned} \tag{2.7}$$

$$\begin{aligned}
&= S_2\left(A_1,A_2,\dots,A_n;t\right)\\
&\quad + \frac{1}{2}\sum_{i=1}^{n-2}\prod_{j=1}^{i} e^{(t/2)A_{j-1}}\int_0^t\int_0^\tau e^{(t/2)A_i}e^{(\tau-s)\left((1/2)A_i+\sum_{k=i+1}^n A_k\right)}\\
&\quad\times\left[\frac{1}{2}A_i + \sum_{k=i+1}^n A_k, \left[e^{s\sum_{k=i+1}^n A_k}, A_i\right]e^{(s/2)A_i}\right]\\
&\quad\times e^{(t-\tau)\sum_{k=i}^n A_k}\,ds\,d\tau\prod_{j=1}^n e^{(t/2)A_{n-i}},
\end{aligned} \tag{2.8}$$

where $A_0 = O$ is the null matrix and S_2 is defined in (1.9).

PROOF. The proof is similar to that of Lemma 2.2. We again start with $n = 2$ and let $A_1 = A$, $A_2 = B$. It is easy to see that

$$e^{(t/2)A}e^{tB}e^{(t/2)A}e^{-t(A+B)} = I + \int_0^t e^{(\tau/2)A}\left[\frac{1}{2}A + B, e^{\tau B}e^{(\tau/2)A}\right]e^{-\tau(A+B)}\,d\tau. \tag{2.9}$$

Now let us consider the commutator

$$F(\tau) = \left[\frac{1}{2}A + B, e^{\tau B}e^{(\tau/2)A}\right]. \tag{2.10}$$

Differentiating the both sides of (2.10), we find that

$$
\begin{aligned}
F'(\tau) = \left(\frac{1}{2}A + B\right) F(\tau) + \left(\frac{1}{2}A + B\right) \left[e^{\tau B}, \frac{1}{2}A\right] e^{(\tau/2)A} \\
- \left[\frac{1}{2}A, e^{\tau B}\right] e^{(\tau/2)A} \left(\frac{1}{2}A + B\right),
\end{aligned}
\tag{2.11}
$$

and this leads to the equality

$$
F(\tau) = \frac{1}{2} \int_0^{\tau} e^{(\tau-s)((1/2)A+B)} \left[\frac{1}{2}A + B, \left[e^{sB}, A\right] e^{(s/2)A}\right] ds.
$$

Substituting the above into (2.9) and then multiplying the both sides of the equation obtained by $e^{t(A+B)}$, we immediately obtain the integral equation

$$
\begin{aligned}
&e^{(t/2)A} e^{tB} e^{(t/2)A} - e^{t(A+B)} \\
&\quad = \frac{1}{2} \int_0^t \int_0^{\tau} e^{(\tau/2)A} e^{(\tau-s)((1/2)A+B)} \left[\frac{1}{2}A + B, \left[e^{sB}, A\right] e^{(s/2)A}\right] e^{(t-\tau)(A+B)}\, ds\, d\tau.
\end{aligned}
\tag{2.12}
$$

On the other hand, we have

$$
\begin{aligned}
e^{t\sum_{i=1}^{n} A_i} = \prod_{i=1}^{n-1} e^{(t/2)A_i} e^{tA_n} \prod_{i=1}^{n-1} e^{(t/2)A_{n-i}} + \sum_{i=1}^{n-2} \prod_{j=1}^{i} e^{(t/2)A_{j-1}} \\
\times \left(e^{(t/2)A_i} e^{t\sum_{k=i+1}^{n} A_k} e^{(t/2)A_i} - e^{t\sum_{k=i}^{n} A_k}\right) \prod_{j=1}^{i} e^{(t/2)A_{i-j}}.
\end{aligned}
\tag{2.13}
$$

Now replacing A by A_i and B by $\sum_{k=i+1}^{n} A_k$ in (2.9)–(2.12), $i = 1, 2, \dots, n$, respectively, and substituting (2.9) into (2.13), we find (2.7). Further, by means of the relation (2.12), we readily obtain (2.8) and this completes the proof. ∎

EXAMPLE 2.1. Let

$$
\begin{aligned}
\Phi_{k,2}(t) &= \left(S_1\left(A_1, A_2, \dots, A_n; \frac{t}{2k}\right) S_1\left(A_1, A_2, \dots, A_n; \frac{t}{2k}\right)\right)^k, \qquad k \in \mathbb{N}^+, \\
\tilde{\Phi}_{k,2}(t) &= \left(S_1\left(A_1, A_2, \dots, A_n; \frac{t}{2k}\right) S_1\left(A_n, A_{n-1}, \dots, A_1; \frac{t}{2k}\right)\right)^k, \qquad k \in \mathbb{N}^+.
\end{aligned}
$$

It follows that

$$
\begin{aligned}
\Phi_{k,2}(t) &= \exp\left\{t \sum_{i=1}^{n} A_i\right\} - \sum_{j=0}^{2k-1} \left(e^{(t/2k)\sum_{i=1}^{n} A_i}\right)^j \left(\sum_{i=1}^{n-1} \prod_{\ell=1}^{i} e^{tA_{\ell-1}}\right. \\
&\quad \times \left. \int_0^t \int_0^{\tau} e^{(t-\tau)\sum_{p=i}^{n} A_p} e^{(\tau-s)\sum_{q=i+1}^{n} A_q} \left[A_i, \sum_{p=i+1}^{n} A_p\right] e^{s\sum_{q=i+1}^{n} A_q} e^{\tau A_i}\, ds\, d\tau\right) \\
&\quad \times \left(S_1\left(A_1, A_2, \dots, A_n; \frac{t}{2k}\right)\right)^{2k-j-1};
\end{aligned}
\tag{2.14}
$$

$$
\begin{aligned}
\tilde{\Phi}_{k,2}(t) &= \exp\left\{t \sum_{i=1}^{n} A_i\right\} - \frac{1}{2} \sum_{j=0}^{2k-1} \left(e^{(t/2k)\sum_{i=1}^{n} A_i}\right)^j \left(\sum_{i=1}^{n-2} \prod_{\ell=1}^{i} e^{(t/2)A_{\ell-1}}\right. \\
&\quad \times \int_0^t \int_0^{\tau} e^{(t/2k)A_i} e^{(\tau-s)\left((1/2k)A_i + \sum_{p=i+1}^{n} A_p\right)}
\end{aligned}
$$

$$\times \left[\frac{1}{2} A_i + \sum_{q=i+1}^{n} A_q, \left[e^{s \sum_{p=i+1}^{n} A_p}, A_i \right] e^{(s/2)A_i} \right]$$
$$\times e^{(t-\tau)\sum_{q=i}^{n} A_q} \, ds \, d\tau \prod_{p=1}^{n} e^{(t/2k)A_{n-i}} \Bigg) \left(S_2 \left(A_1, A_2, \dots, A_n; \frac{t}{2k} \right) \right)^{2k-j-1}. \tag{2.15}$$

By the same token, we may prove an identity for the general sequential exponential splittings. Indeed, we have the following theorem.

THEOREM 2.2. *Let $A_1, A_2, \dots, A_n$ be square matrices which do not commute. Then*

$$\left(\prod_{i=1}^{m} S_{r(i)} \left(\frac{t}{km} \right) \right)^k = \exp\left\{ t \sum_{i=1}^{n} A_i \right\} + \sum_{j=0}^{k-1} \left(e^{(t/k)\sum_{i=1}^{n} A_i} \right)^j$$
$$\times \left(e^{(t/k)\sum_{i=1}^{n} A_i} - \prod_{i=1}^{m} S_{r(i)} \left(\frac{t}{km} \right) \right) \left(\prod_{i=1}^{m} S_{r(i)} \left(\frac{t}{km} \right) \right)^{k-j-1}, \tag{2.16}$$

where $S_{r(i)}$, $1 \le r(i) \le N$, $1 \le i \le m$, are conventional splitting formulae.

3. GLOBAL ERROR ESTIMATES

By means of the established identities in the previous section, we may obtain interesting global error inequalities for asymptotic exponential splitting formulae. We state this in the following lemma.

LEMMA 3.1. *Let $A_1, A_2, \dots, A_n$ be square matrices which do not commute and $t \ge 0$. Then*

$$\left\| \left(\prod_{i=1}^{m} S_{r(i)} \left(\frac{t}{km} \right) \right)^k - P(t) \right\| \le C \left\| \exp\left\{ \frac{t}{k} \sum_{i=1}^{n} A_i \right\} - \prod_{i=1}^{m} S_{r(i)} \left(\frac{t}{km} \right) \right\|, \tag{3.1}$$

where

$$C = \sum_{j=0}^{k-1} \left\| \exp\left\{ \frac{tj}{k} \sum_{i=1}^{n} A_i \right\} \left(\prod_{i=1}^{m} S_{r(i)} \left(\frac{t}{km} \right) \right)^{k-j-1} \right\|.$$

EXAMPLE 3.1. Consider the following asymptotic splitting formulae

$$T_1(t) = \left(S_1 \left(A_1, A_2; \frac{t}{4} \right) S_1 \left(A_1, A_2; \frac{t}{4} \right) \right)^2;$$
$$T_2(t) = \left(S_1 \left(A_1, A_2; \frac{t}{4} \right) S_1 \left(A_2, A_1; \frac{t}{4} \right) \right)^2;$$
$$T_3(t) = \left(S_2 \left(A_1, A_2; \frac{t}{4} \right) S_2 \left(A_1, A_2; \frac{t}{4} \right) \right)^2;$$
$$T_4(t) = \left(S_2 \left(A_1, A_2; \frac{t}{4} \right) S_2 \left(A_2, A_1; \frac{t}{4} \right) \right)^2.$$

The error bounds given by (3.1) together with the actual errors are plotted in Figures 1 and 2, respectively. A_1, A_2 are 10×10 real matrices which are randomly chosen with $\mu(A_i) < 0$, $i = 1, 2$. The estimated error bounds are plotted with circle symbols. The graphics indicates that the bounds are accurate to use for the splitting formulae, especially when $t > 1$.

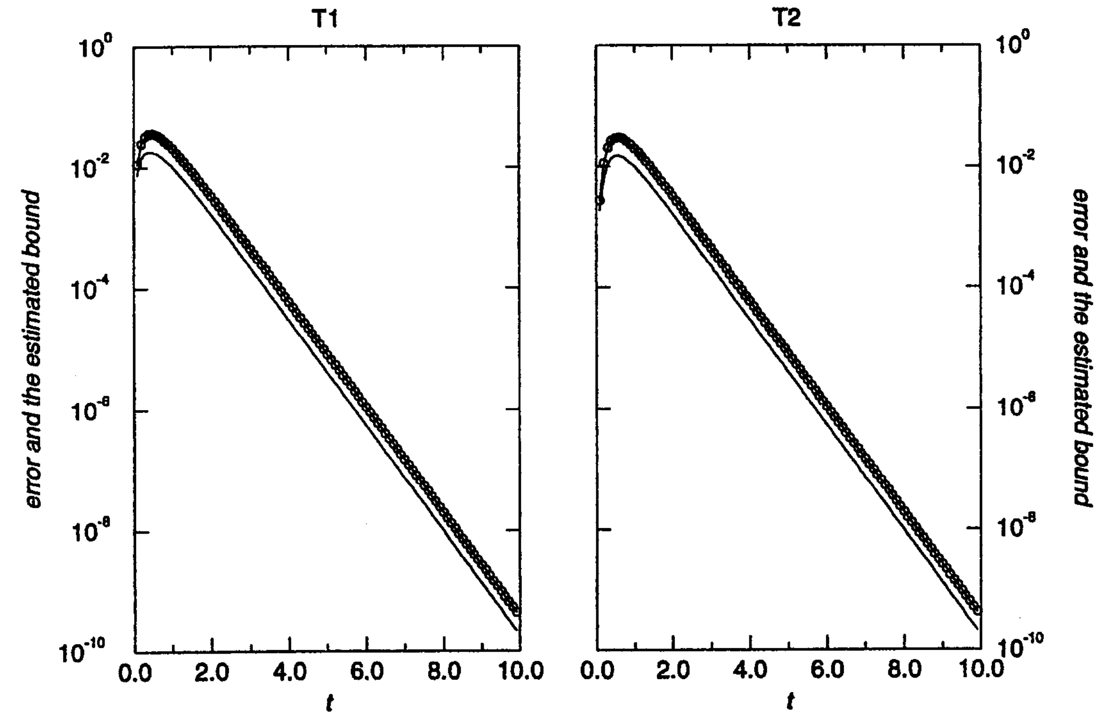

Figure 1. Error and error bound for T_1 and T_2.

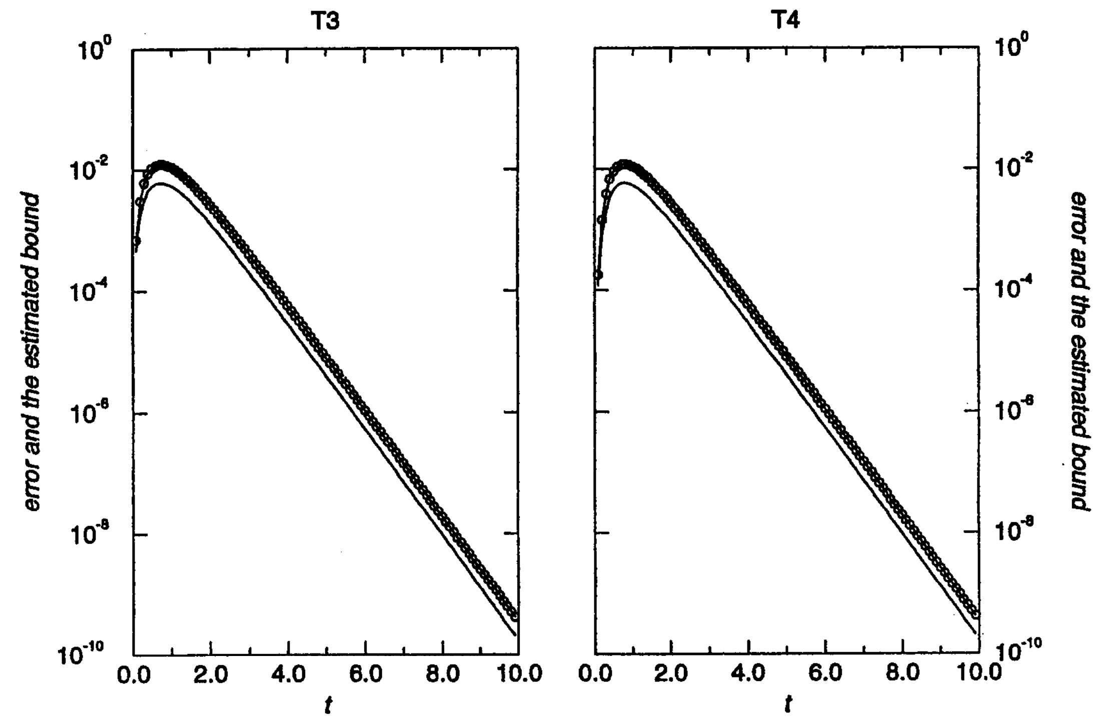

Figure 2. Error and error bound for T_3 and T_4.

THEOREM 3.1. *Let $A_1, A_2, \dots, A_n$ be square matrices which do not commute. If $\mu(A_1 + A_2 + \cdots + A_n) \le 0$ and*

$$\left\| \prod_{i=1}^{m} S_{r(i)}(t) \right\| \le 1,$$

then

$$\lim_{k\to\infty}\left(\prod_{i=1}^{m} S_{r(i)}\left(\frac{t}{km}\right)\right)^{k} = \exp\left\{t\sum_{i=1}^{n} A_i\right\}. \tag{3.2}$$

PROOF. We note that

$$\left\|\exp\left\{t\sum_{i=1}^{n} A_i\right\}\right\| \le \exp\left\{t\mu\left(\sum_{i=1}^{n} A_i\right)\right\} \le 1,$$

and hence, the theorem is clear from Lemma 3.1. ∎

In fact, (3.2) can be viewed as a generalized version of Trotter's formula [3].

EXAMPLE 3.2. We consider the matrix exponential function

$$P(t) = \exp\{t(A+B)\}$$

and the corresponding asymptotic splitting approximations

$$\Phi_1(t) = \left(T_1\left(\frac{t}{2k}\right)T_2\left(\frac{t}{2k}\right)\right)^k, \quad \Phi_2(t) = \left(T_3\left(\frac{t}{2k}\right)T_4\left(\frac{t}{2k}\right)\right)^k,$$

where $A, B \in \mathbb{R}^{10\times 10}$ are randomly generated, but satisfy constraints $\mu(A), \mu(B) < 0$. We compute the error $\|P - \Phi_i\|$, $i = 1, 2$, $t = 0.2$ and plot the error, together with the estimated error bound in Figures 3 and 4. We also list values of the error and error bound in Table 1.

Table 1. Errors and error bounds for $P - \Phi_i$, $i = 1, 2$.

k	$\|e_{\Phi_1}\|$	error bound for Φ_1	$\|e_{\Phi_2}\|$	error bound for Φ_2
2	7.6695e−04	1.3729e−03	2.5428e−05	4.5722e−05
10	3.1777e−04	1.0868e−03	1.9558e−06	6.6950e−06
20	1.7031e−04	6.4414e−04	5.2567e−07	1.9929e−06
30	1.1605e−04	4.5436e−04	2.3903e−07	9.3851e−07
40	8.7981e−05	3.5051e−04	1.3596e−07	5.4338e−07
50	7.0835e−05	2.8519e−04	8.7596e−08	3.5384e−07
60	5.9279e−05	2.4035e−04	6.1098e−08	2.4857e−07
70	5.0963e−05	2.0768e−04	4.5029e−08	1.8413e−07
80	4.4693e−05	1.8282e−04	3.4556e−08	1.4185e−07
90	3.9796e−05	1.6327e−04	2.7353e−08	1.1262e−07
100	3.5866e−05	1.4749e−04	2.2188e−08	9.1573e−08

These examples show that the use of asymptotic splitting formulae may efficiently increase the accuracy in computations. Though the use of the formula T_1 or T_3 can be viewed as repeatedly using splitting formulae with fractional time steps, the use of T_2 and T_4 is in fact no longer the same case. In particular, T_2 increases the order of accuracy by paying little extra in computational costs. This may also explain why, in order to achieve better numerical results, one should always alternate the order of calculating directions in each time step when using splitting methods such as the ADI and LOD methods.

4. SPLITTINGS IN THE PRESENCE OF SMALL PARAMETERS

To complete our discussion, we consider a special case in which small parameters, such as in singular perturbation problems, are involved. Let

$$P_\epsilon(t) = \exp\{t(A+\epsilon B)\}, \qquad t, \epsilon > 0. \tag{4.1}$$

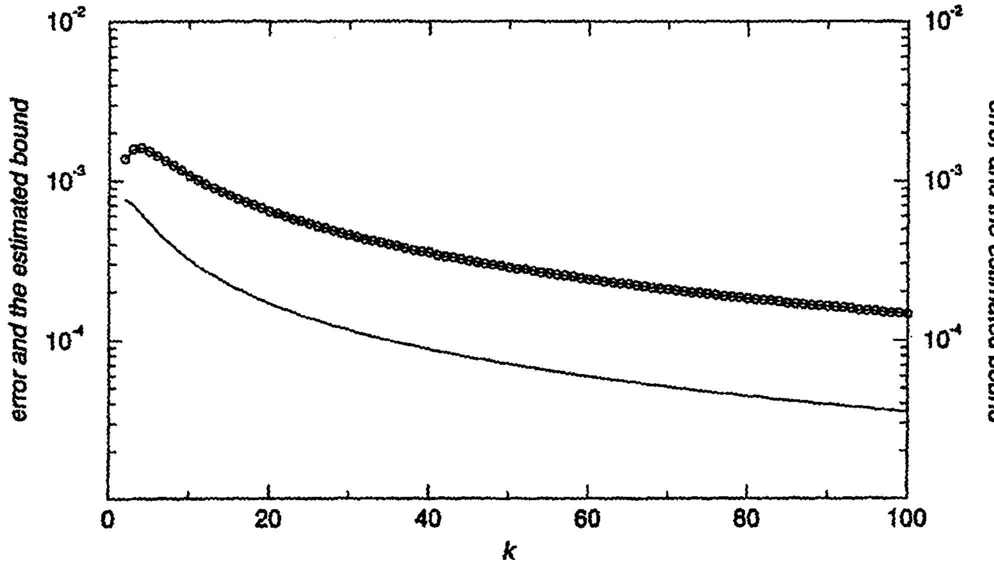

Figure 3. Error and error bound for $P - \Phi_1$.

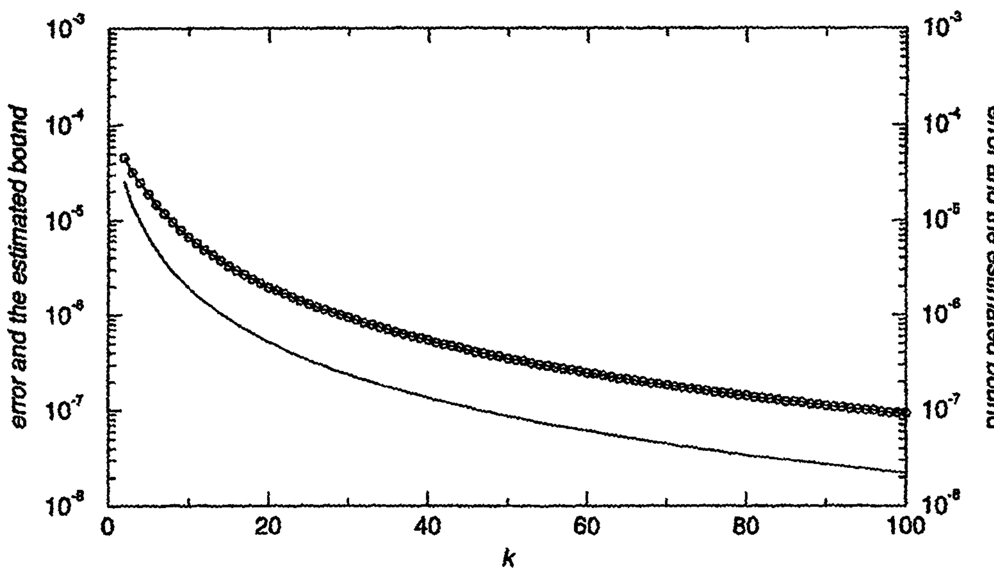

Figure 4. Error and error bound for $P - \Phi_2$.

The matrix exponential P_ϵ appears frequently in perturbation theory, astronomical research and fluid dynamics [1,7,16–18]. Though we consider the convergence of a splitting operator when $\epsilon > 0$ is fixed, in practice ϵ is so important that we cannot avoid taking it into account [14]. Thus, we have to estimate the accuracy of the splitting approximation both in t and ϵ. To emphasize that our main concern is still the splitting in respect to t, we prefer the following definition rather than McLachlan's.

DEFINITION 4.1. *We say that the splitting method S_ϵ is of order $(p; q_p, q_{p+1}, \dots)$, if*

$$S_\epsilon(t) - P_\epsilon(t) = \sum_{k=p}^{\infty} a_k t^{k+1} \epsilon^{q_k}, \qquad t, \epsilon > 0. \tag{4.2}$$

Note that we should not expect $q_j > q_i$, $j > i$, neither $\min_{k \geq p} q_k > 1$ since in the expansion of such a splitting S_ϵ, there are infinite number of terms of each order in ϵ while finite number of terms of each order in t.

THEOREM 4.1. *The first-order, Strang's and the parallel splittings are of order* $(1;1,1,\dots)$, $(2;1,1,\dots)$ *and* $(2;1,1,\dots)$, *respectively.*

PROOF. This result can be easily proved by using the standard local and global error analyses (see [11]). ∎

Obviously, it is sensible to demand the quantity $\min_{i\ge p}(i+q_i)$ to be as large as possible.

DEFINITION 4.2. *We say that the splitting method* S_ϵ *is of approximate order* ρ, *if* $\rho = \min_{i\ge p}(i+q_i)$ *such that*

$$\|S_\epsilon(t) - P_\epsilon(t)\| = O\left(t^{p+i-1}\epsilon^{q_i}\right), \qquad t,\epsilon > 0. \tag{4.3}$$

The following order 4 examples are due to [14].

EXAMPLE 4.1. It is not difficult to show that

$$e^{(3-\sqrt{3}/6)tA}e^{(t\epsilon/2)B}e^{(t/\sqrt{3})A}e^{(t\epsilon/2)B}e^{(3-\sqrt{3}/6)tA} = e^{t(A+\epsilon B)} + c_1t^3\epsilon^2 + O\left(t^4\epsilon\right), \qquad t,\epsilon>0,$$
$$e^{(t/6)A}e^{(t\epsilon/2)B}e^{(2t/3)A}e^{(t\epsilon/2)B}e^{(t/6)A} = e^{t(A+\epsilon B)} + c_2t^3\epsilon^2 + O\left(t^4\epsilon\right), \qquad t,\epsilon>0,$$

where c_1, c_2 are functions of A and B.

However, there is still the question of whether we can construct explicitly even higher order splittings in approximations for which $\min_{i\ge p} q_i \ge 2$. A standard suggestion from the theoretical study is to use variants on the Baker-Cambell-Hausdorf formula or the Zassenhaus formula [1]. But this seems to be too difficult to implement in practice.

The above discussion can be extended to multi-parameter cases. Further, our results can be extended to more general Banach space operators $A_1, A_2, \dots, A_n$ without major difficulties.

EXAMPLE 4.2. Consider the numerical solution of the singularly perturbed convection-diffusion equation

$$u_t = \left(\frac{1}{x^2+y^2+1} + \sin(x)\sin(y)\right)u_{xx} + \epsilon u_{yy} - \frac{1}{2}u_x - \frac{x^2+y^2}{3}u_y - u, \tag{4.4}$$
$$0<x,y<1, \quad t>0, \quad \epsilon>0,$$

together with the initial and boundary conditions

$$u(0,y,t)=0, \qquad u(1,y,t)=0, \qquad 0<y<1, \qquad t>0, \tag{4.5}$$
$$u_y(x,0,t)=0, \qquad u(x,1,t)=0, \qquad 0<x<1, \qquad t>0; \tag{4.6}$$
$$u(x,y,0)=\cos(\pi x)\sin(\pi y), \qquad 0\le x,y\le 1. \tag{4.7}$$

We adopt the semi-discretized Il'in's scheme ([19], also see [20])

$$\begin{aligned} u'_{i,j}(t) = {} & \frac{1/(x_i^2+y_j^2)+\sin(x_i)\sin(y_j)}{h^2}\left(u_{i+1,j}(t) - 2u_{i,j}(t) + u_{i-1,j}(t)\right) \\ & + \gamma_{i,j}\frac{1}{h^2}\left(u_{i,j+1}(t) - 2u_{i,j}(t) + u_{i,j-1}(t)\right) - \frac{1}{4h}\left(u_{i+1,j}(t) - u_{i-1,j}(t)\right) \\ & - \frac{(x_i^2+y_j^2)}{6h}\left(u_{i,j+1}(t) - u_{i,j-1}(t)\right) - u_{i,j}(t), \qquad 1\le i,j\le m-1, \quad t>0; \end{aligned} \tag{4.8}$$
$$u_{0,j}(t)=0, \qquad u_{m,j}(t)=0, \qquad 0<j<m, \qquad t>0, \tag{4.9}$$
$$u_{i,0}(t)=u_{i,2}(t), \qquad u_{i,m}(t)=0, \qquad 0<i<m, \qquad t>0, \tag{4.10}$$
$$u_{i,j}(0)=\cos(\pi x_i)\sin(\pi y_j), \qquad 0\le i,j\le m, \tag{4.11}$$

where $u_{i,j}(t) = u(x_i,y_j,t)$ and the fitting factor

$$\gamma_{i,j} = \frac{h}{6}\,\mathrm{cth}\left(\frac{(x_i^2+y_j^2)h}{6\epsilon}\right), \tag{4.12}$$

for $x_i = ih$, $y_j = jh$, $0 \le i, j \le m$, $x_m = y_m = 1$. It is easy to show that for any fixed ϵ, we have

$$|\gamma - \epsilon| \le Ch^2\epsilon^{-1},$$

where $C > 0$ is a constant. We employ formulae S_1, S_2, T_1, T_2, T_3 and T_4 in the computation and then compare the numerical solutions with the result of (4.8)–(4.11) solving by the standard method without splitting. For this the time step, $\tau = 0.1$ is used. The value of ϵ is taken to be 0.005 and $h = 0.1$.

Figure 5 and Table 2 show the case when asymptotic splitting formulae T_1, T_2, T_3 and T_4 are used to compute the numerical solution of the problem, respectively. From the top to the bottom, the curves stand for errors of the numerical solutions when S_1, T_1, S_2, T_2, T_3 and T_4 are used, respectively. It is observed that though being first-order accuracy, T_1 is better than S_1, and the same happens for T_2 and S_2. This is due to the fact that we are actually using finer steps in the computation. The numerical solutions using asymptotic splittings T_3, T_4 are much better than that of conventional splittings S_1, S_2, however. In particular, by adopting T_4, the numerical error drops to about 1/10 from that of second-order conventional splitting S_2. Therefore, asymptotic splitting formulae are worth being considered in practical computations, even in computations in which singularities such as singular perturbation and quenching are involved.

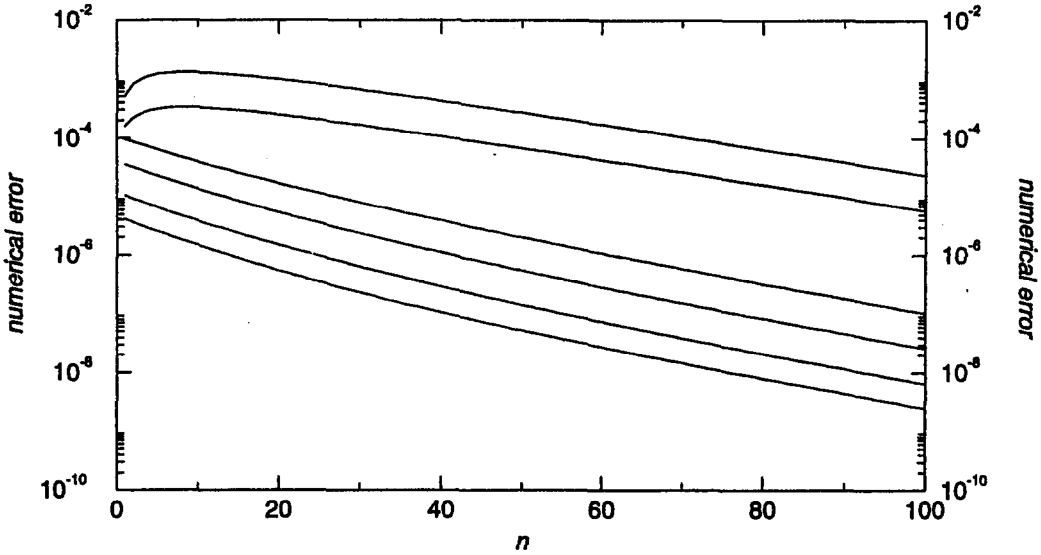

Figure 5. Errors of the numerical solutions using S_1, S_2, T_1, T_2, T_3 and T_4.

Table 2. Errors of the numerical solutions using S_1, S_2, T_1, T_2, T_3 and T_4.

n	$\|e_{S_1}\|$	$\|e_{S_2}\|$	$\|e_{T_1}\|$	$\|e_{T_2}\|$	$\|e_{T_3}\|$	$\|e_{T_4}\|$
1	5.2438e−4	9.4456e−5	1.5626e−4	3.5661e−5	1.0376e−5	4.1300e−6
10	1.2989e−3	3.9487e−5	3.3052e−4	1.3548e−5	3.8390e−6	1.4619e−6
20	9.8217e−4	1.6923e−5	2.4761e−4	5.3687e−6	1.4815e−6	5.4336e−7
30	6.5482e−4	7.8823e−6	1.6451e−4	2.3459e−6	6.3198e−7	2.2778e−7
40	4.2309e−4	3.8918e−6	1.0610e−4	1.1014e−6	2.9077e−7	1.0543e−7
50	2.6930e−4	2.0084e−6	6.7457e−5	5.4685e−7	1.4205e−7	5.2379e−8
60	1.6923e−4	1.0716e−6	4.2362e−5	2.8371e−7	7.2792e−8	2.7273e−8
70	1.0503e−4	5.8552e−7	2.6279e−5	1.5208e−7	3.8678e−8	1.4643e−8
80	6.4414e−5	3.2496e−7	1.6111e−5	8.3366e−8	2.1079e−8	8.0222e−9
90	3.9071e−5	1.8207e−7	9.7702e−6	4.6349e−8	1.1675e−8	4.4542e−9
100	2.3462e−5	1.0253e−7	5.8659e−6	2.5978e−8	6.5288e−9	2.4945e−9

In Figure 6 and Table 3, we demonstrate that for asymptotic splitting

$$T(k,t) = \left(S_2\left(A,B;\frac{t}{2k}\right)S_2\left(B,A;\frac{t}{2k}\right)\right)^k,$$

the numerical error tends to zero exponentially when $k \to \infty$. This confirms our Theorem 3.1. The numerical solutions are taken at $t = 2$.

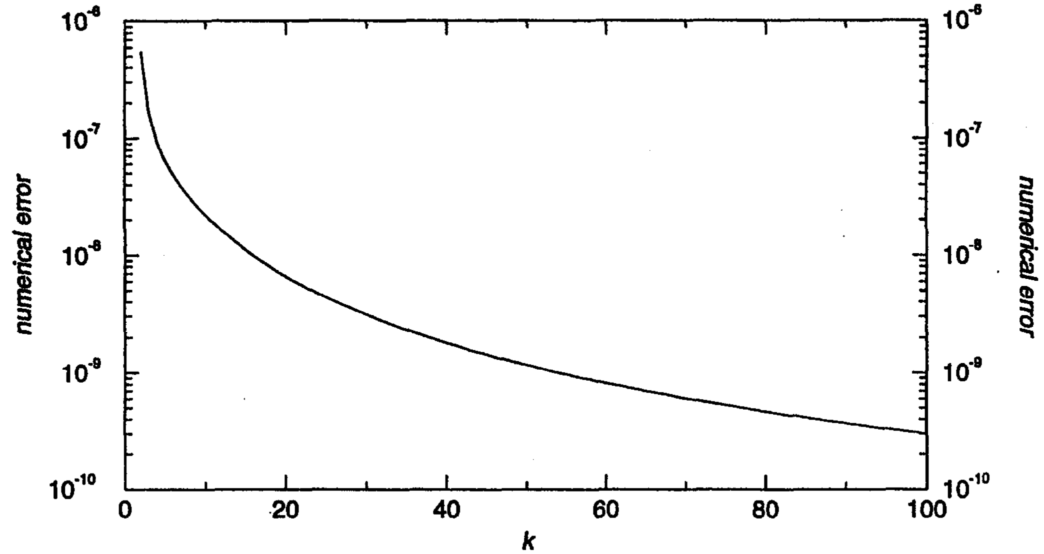

Figure 6. Errors of the numerical solutions using $T(k,t)$.

Table 3. Errors of the numerical solution using $T(k,t)$.

k	$\|e_T\|$
2	5.4336e−07
10	2.2265e−08
20	6.6250e−09
30	3.1122e−09
40	1.7987e−09
50	1.1698e−09
60	8.2099e−10
70	6.0775e−10
80	4.6790e−10
90	3.7134e−10
100	3.0182e−10

REFERENCES

1. Q. Sheng, Solving partial differential equations by exponential splitting, Ph.D. Thesis, DAMTP, Univ. Cambridge, Cambridge, (1989).
2. H.F. Trotter, Approximation of semi-groups of operators, *Pacific J. Math* **8**, 887–919 (1958).
3. H.F. Trotter, On the product of semi-groups of operators, *Proc. Amer. Math. Soc.* **10**, 545–551 (1959).
4. G. Strang, On the construction and comparison of difference schemes, *SIAM J. Numer. Anal.* **5**, 507–517 (1968).
5. S.Z. Burstein and A.A. Mirin, Third order difference methods for hyperbolic equations, *J. Comp. Phys.* **5**, 547–571 (1970).
6. Q. Sheng, Solving linear partial differential equations by exponential splitting, *IMA J. Numer. Anal.* **9**, 199–212 (1989).

7. M. Suzuki, General theory of fractal path integrals with applications to many-body theories and statistical physics, *J. Math. Phys.* **32**, 400–407 (1991).
8. D. Goldman and T.J. Kaper, N^{th}-order operator splitting schemes and nonreversible systems, Research Report 93-16, Center for Fluid Mechanics Turbulence and Computation, U.S.A., (1993).
9. A. Iserles and Q. Sheng, Implementation of splitting methods, Research Report 87/NA8, DAMTP, Univ. Cambridge, Cambridge, (1987).
10. R.J. LeVeque and J. Oliger, Numerical methods based on additive splittings for hyperbolic partial differential equations, *Math. Comp.* **40**, 469–497 (1983).
11. Q. Sheng, Global error estimates for exponential splitting, *IMA J. Numer. Anal.* **14**, 27–56 (1993).
12. D.S. Berstein, Problem: Commuting matrix exponentials, *SIAM Review* **30**, 123 (1988).
13. T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, (1966).
14. R.I. McLachlan, Composition methods in the presence of small parameters, Research Report 94-1, Forschungsinstitut für Mathematik, Zürich, (1994).
15. M. Suzuki, Fractal path integrals with applications to quantum many-body systems, *Physica A* **191**, 501–515 (1992).
16. J. Wisdom and M. Holman, Symplectic maps for the N-body problem, *Astron. J.* **104**, 1528–1538 (1991).
17. R.J. LeVeque and H.C. Yee, A study of numerical methods for hyperbolic conservation laws with stiff source terms, *J. Comp. Phy.* **86**, 187–210 (1990).
18. R.E. O'Malley, Jr., *Singular Perturbation Methods for Ordinary Differential Equations*, Springer-Verlag, (1991).
19. A.M. Il'in, *Matching of Asymptotic Expansions of Solutions of Boundary Value Problems*, Amer. Math. Soc., (1992).
20. Q. Sheng, Uniformly convergent difference method for convection-diffusion singular perturbation problems in curved boundary regions, *Appl. Math. Mech.* **3**, 269–278 (1986).