Multi-product operator splitting as a general method of solving autonomous and non-autonomous equations

Siu A. Chin and Jürgen Geiser

1 Department of Physics, Texas A&M University, College Station, TX 77843, U.S.A.
Tel.: +1-979-845-4190
Fax: +1-979-845-2590
chin@physics.tamu.edu

2 Department of Mathematics, Humboldt-Universität zu Berlin, Unter den Linden 6, D-10099 Berlin, Germany
Tel.: +49-30-2093-5451
Fax: +49-30-2093-5859
geiser@mathematik.hu-berlin.de

Abstract. Prior to the recent development of symplectic integrators, the time-stepping operator $e^{\Delta t(A+B)}$ was routinely decomposed into a sum of products of $e^{\Delta tA}$ and $e^{\Delta tB}$ in the study of hyperbolic partial differential equations. In the context of solving Hamiltonian dynamics, we show that such a decomposition give rise to both even and odd order Runge-Kutta and Nyström integrators. By use of Suzuki’s forward-time derivative operator to enforce the time-ordered exponential, we show that the same decomposition can be used to solve non-autonomous equations. In particular, odd order algorithms are derived on the basis of a highly non-trivial time-asymmetric kernel. Such an operator approach provides a general and unified basis for understanding structure non-preserving algorithms and is especially useful in deriving very high-order algorithms via analytical extrapolations. In this work, algorithms up to the 100th order are tested by integrating the ground state wave function of the hydrogen atom. For such a singular Coulomb problem, the multi-product expansion showed uniform convergence and is free of poles usually associated with structure-preserving methods. Other examples are also discussed.

Keyword General exponential splitting, non-autonomous equations, Runge-Kutta-Nyström integrators, operator extrapolation methods.
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1 Introduction

In the course of devising numerical algorithms for solving the prototype linear hyperbolic equation
\[ \partial_t u = Au_x + Bu_y, \quad u(0) = u_0, \]  
where \( A \) and \( B \) are non-commuting matrices, Strang\([34]\) proposed two second-order algorithms corresponding to approximating  
\[ T(h) = e^{h(A+B)} \]  
either as  
\[ S(h) = \frac{1}{2} \left( e^{hA}e^{hB} + e^{hB}e^{hA} \right) \]  
or as  
\[ S_{AB}(h) = e^{(h/2)B}e^{hA}e^{(h/2)B}. \]  
Following up on Strang’s work, Burstein and Mirin\([8]\) suggested that Strang’s approximations can be generalized to higher orders in the form of a multi-product expansion (MPE),  
\[ e^{h(A+B)} = \sum_k c_k \prod_i e^{a_{ki}hA}e^{b_{ki}hB} \]  
and gave two third-order approximations  
\[ D(h) = \frac{4}{3} \left( S_{AB}(h) + S_{BA}(h) \right) - \frac{1}{3} S(h) \]  
and  
\[ B_{AB}(h) = \frac{9}{8} e^{(h/3)A}e^{(2h/3)B}e^{(2h/3)A}e^{(h/3)B} - \frac{1}{8} e^{hA}e^{hB}. \]  
They credited J. Dunn for finding the decomposition \( D(h) \) and noted that the weights \( c_k \) are no longer positive beyond second order. Thus the stability of the entire algorithm can no longer be inferred from the stability of each component product.

Since (3), (4), (6) and (7) are approximations for the exponential of two general operators, they can be applied to problems unrelated to solving hyperbolic partial differential equations. For example, the evolution of any dynamical variable \( u(q,p) \) (including \( q \) and \( p \) themselves) is given by the Poisson bracket,  
\[ \partial_t u(q,p) = \left( \frac{\partial u}{\partial q} \cdot \frac{\partial H}{\partial p} - \frac{\partial u}{\partial p} \cdot \frac{\partial H}{\partial q} \right) = (A + B) u(q,p). \]  
For a separable Hamiltonian,  
\[ H(p,q) = \frac{p^2}{2m} + V(q), \]  
\( A \) and \( B \) are Lie operators, or vector fields  
\[ A = v \cdot \frac{\partial}{\partial q}, \quad B = a(q) \cdot \frac{\partial}{\partial v} \]
where we have abbreviated $v = p/m$ and $a(q) = -\nabla V(q)/m$. The exponential operators $e^{hA}$ and $e^{hB}$ are then just shift operators, with $S(h)$ giving the second-order Runge-Kutta integrator

$$q = q_0 + hv_0 + \frac{1}{2}h^2a(q_0) \equiv q_1$$  \hspace{1cm} (11)

$$v = v_0 + \frac{h}{2} \left[ a(q_0) + a(q_0 + hv_0) \right]$$  \hspace{1cm} (12)

and $S_{AB}(h)$, the symplectic Verlet or leap-frog algorithm

$$q = q_1$$  \hspace{1cm} (13)

$$v = v_0 + \frac{h}{2} \left[ a(q_0) + a(q) \right].$$  \hspace{1cm} (14)

More interestingly, Dunn’s decomposition $D(h)$ gives

$$q = q_0 + hv_0 + \frac{h^2}{6} \left[ a(q_0) + 2a(q_0 + \frac{h}{2}v_0) \right]$$  \hspace{1cm} (15)

$$v = v_0 + \frac{h}{6} \left[ a(q_0) + 4a(q_0 + \frac{h}{2}v_0) + 2a(q_1) - a(q_1 - \frac{h}{2}^2a(q_0)) \right].$$  \hspace{1cm} (16)

Since

$$2a(q_1) - a(q_1 - \frac{1}{2}h^2a(q_0)) = a\left(q_1 + \frac{1}{2}h^2a(q_0)\right) + O(h^4),$$  \hspace{1cm} (17)

it remains correct to third order to write

$$v = v_0 + \frac{h}{6} \left[ a(q_0) + 4a(q_0 + \frac{h}{2}v_0) + 2a(q_1) - a(q_0 + hv_0 + h^2a(q_0)) \right].$$  \hspace{1cm} (18)

One recognizes that (15) and (18) as _precisely_ Kutta’s third order algorithm[25] for solving a second-order differential equation. Burstein and Mirin’s approximation $B_{AB}(h)$ directly gives, without any change,

$$q = q_0 + hv_0 + \frac{h^2}{4} \left[ a(q_0) + a(q_{2/3}) \right]$$  \hspace{1cm} (19)

$$v = v_0 + \frac{h}{4} \left[ a(q_0) + 3a(q_{2/3}) \right],$$  \hspace{1cm} (20)

with

$$q_{2/3} \equiv q_0 + \frac{2}{3}hv_0 + \frac{2}{9}h^2a(q_0),$$  \hspace{1cm} (21)

which is Nyström’s third order algorithm requiring only two force-evaluations[2, 31]. Since Burstein and Mirin’s approximation is not symmetric, $B_{BA}(h)$ produces a different algorithm

$$q = q_0 + hv_0 + \frac{h^2}{2}a_{1/3}$$  \hspace{1cm} (22)

$$v = v_0 + \frac{h}{4} \left[ 3a_{1/3} + \frac{3}{2}a(q_0 + hv_0 + \frac{4}{9}h^2a_{1/3}) - \frac{1}{2} a(q_0 + hv_0) \right].$$  \hspace{1cm} (23)
where $a_{1/3} = a(q_0 + hv_0/3)$. Again, since

$$\frac{3}{2}a(q_0 + hv_0 + \frac{4}{9}h^2a_{1/3}) - \frac{1}{2}a(q_0 + hv_0 + \frac{2}{3}h^2a_{1/3}) = a(q_0 + hv_0 + \frac{2}{3}h^2a_{1/3}) + O(h^4), \quad (24)$$

(23) can be rewritten as

$$v = v_0 + \frac{h}{4}[3a_{1/3} + a(q_0 + hv_0 + \frac{2}{3}h^2a_{1/3})]. \quad (25)$$

Eqs. (22) and (25) is a new third order algorithm with two force-evaluations but without evaluating the force at the starting position. More recently, Ref. [13] has shown that Nyström’s four-order algorithm [2] with three force-evaluations and Albrecht’s six-order algorithm [1] with five-force evaluations can all be derived from operator expansions of the form (5).

Just as symplectic integrators [30, 19] can be derived from a single product splitting,

$$e^{h(A+B)} = \prod_i e^{a_i hA} e^{b_i hB}, \quad (26)$$

these examples clearly show that the multi-product splitting (5) is the fundamental basis for deriving non-symplectic, Nyström type algorithms. (These are not fully Runge-Kutta algorithms, because the operator $B$ in (10) would not be a simple shift operator if $a(q)$ becomes dependent on $v$. On the other hand, Nyström type algorithms are all that are necessary for the study of most Hamiltonian systems.) As illustrated above, one goal of this work is to show that all traditional results on Nyström integrators can be much more simply derived and understood on the basis of multi-product splitting. In fact, we have the following theorem

**Theorem 1.** Every decomposition of $e^{h(A+B)}$ in the form of

$$\sum_k c_k \prod_i e^{a_{ki} hA} e^{b_{ki} hB} = e^{h(A+B)} + O(h^{n+1}), \quad (27)$$

where $A$ and $B$ are non-commuting operators, with real coefficients $\{c_k, a_{ki}, b_{ki}\}$ and finite indices $k$ and $i$, produces a $n$th-order Nyström integrator.

(Note that the order $n$ of the integrator is defined with respect to the error in approximating the operator $(A+B)$ and therefore the error in the time-stepping operator is one order higher.) The resulting integrator, however, may not be optimal. As illustrated above, at low orders, some force evaluations can be combined without affecting the order of the integrator. However, such a force consolidation is increasingly unlikely at higher orders. This theorem produces, both the traditional Nyström integrators where the force is always evaluated initially, and non-FASL (First as Last) integrators where the force is never evaluated initially, as in (22) and (25).

The advantage of a single product splitting is that the resulting algorithms are structure-preserving, such as being symplectic, unitary, or remain within
the group manifold. However, single product splittings beyond the second-order requires exponentially growing number of operators with unavoidable negative coefficients[33, 35] and cannot be applied to time-irreversible or semi-group problems. Even for time-reversible systems where negative time steps are not a problem, the exponential growth on the number of force evaluations renders high order symplectic integrators difficult to derived and expensive to use. For example, it has been found empirically that symplectic algorithms of orders 4, 6, 8 and 10, required a minimum of 3, 7, 15 and 31 force-evaluations respectively[13]. Here, we show that analytically extrapolated algorithms of odd orders 3, 5, 7, 9 only requires 2, 4, 7, 11 force-evaluations and algorithms of even orders 4, 6, 8, 10, only require 3, 5, 10, 15 force evaluations. Thus at the tenth order, an extrapolated MPE integrator, only requires half the computational effort of a symplectic integrator. Or, for 28 force-evaluations, one can use a 14th order MPE integrator instead. This is a great advantage in many practical calculations where long term accuracy and structure preserving is not an issue. The advantage is greater still beyond the tenth order, where no symplectic integrators and very few RKN algorithms are known. Here, we demonstrated the working of MPE algorithms up to the 100th order.

By use of Suzuki[36] method of implementing the time-ordered exponential, this work shows that the multi-product expansion (27) can be easily adopted to solve the non-autonomous equation

\[ \partial_t Y(t) = A(t)Y(t), \quad Y(0) = Y_0. \]  

In even-order cases, this method reproduces Gragg’s[21] classical result in just a few lines. In odd-order cases, this method demonstrates a highly non-trivial extrapolation of a time-asymmetric kernel, which has never been anticipated before. Finally, we show that the multi-product expansion (27) converges uniformly, in contrast to structure-preserving methods, such as the Magnus expansion, which generally has a finite radius of convergence. The convergence of (27) is verified in various analytical and numerical examples, up to the 100th order.

The paper is outlined as follows: In Section 2, we derive key results of MPE, including the extrapolation of odd-order algorithms. In Section 3, we show how Suzuki’s method can be used to transcribe any splitting scheme for solving non-autonomous equations. In Section 4, we present an error and convergence analysis of the multi-product splitting based on extrapolation. Numerical examples and comparison to the Magnus expansion are given in Section 5. In Section 6, we briefly summarize our results.

2 Multi-product decomposition

The multi-product decomposition (5) is obviously more complicated than the single product splitting (26). Fortunately, nineteen years after Burstein and Mirin, Sheng[33] proved their observation that beyond second-order, \( a_{ki}, b_{ki} \) and \( c_k \) cannot all be positive. This negative result, surprisingly, can be used to completely determine \( a_{ki}, b_{ki} \) and \( c_k \) to all orders. This is because for general applications,
including solving time-irreversible problems, one must have \( a_{ki} \) and \( b_{ki} \) positive. Therefore every single product in (5) can at most be second-order[33,35]. But such a product is easy to construct, because every left-right symmetric single product \( \text{is second-order}. \) Let \( T_S(h) \) be such a product with \( \sum_i a_{ki} = 1 \) and \( \sum_i b_{ki} = 1 \), then \( T_S(h) \) is time-symmetric by construction,

\[
T_S(-h)T_S(h) = 1,
\]

implying that it has only odd powers of \( h \)

\[
T_S(h) = \exp(h(A + B) + h^3E_3 + h^5E_5 + \cdots)
\]

and therefore correct to second-order. (The error terms \( E_i \) are nested commutators of \( A \) and \( B \) depending on the specific form of \( T_S \).) This immediately suggests that the \( k \)th power of \( T_S \) at step size \( h/k \) must have the form

\[
T_S^k(h/k) = \exp(h(A + B) + k^{-2}h^3E_3 + k^{-4}h^5E_5 + \cdots),
\]

and can serve as a basis for the multi-production expansion (5). The simplest such symmetric product is

\[
T_2(h) = S_{AB}(h) \quad \text{or} \quad T_2(h) = S_{BA}(h).
\]

If one naively assumes that

\[
T_2(h) = e^{h(A+B) + Ch^3 + Dh^4 + \cdots},
\]

then a Richardson extrapolation would only give

\[
\frac{1}{k^2 - 1} [k^2T_2^k(h/k) - T_2(h)] = e^{h(A+B)} + O(h^4),
\]

a third-order[32] algorithm. However, because the error structure of \( T_2^k(h/k) \) is actually given by (31), one has

\[
T_2^k(h/k) = e^{h(A+B)} + k^{-2}h^3E_3 + \frac{1}{2}k^{-2}h^4[(A + B)E_3 + E_3(A + B)] + O(h^5),
\]

and both the third and fourth order errors can be eliminated simultaneously, yielding a fourth-order algorithm. Similarly, the leading \( 2n + 1 \) and \( 2n + 2 \) order errors are multiplied by \( k^{-2n} \) and can be eliminated at the same time. Thus for a given set of \( n \) whole numbers \( \{k_i\} \) one can have a \( 2n \)th-order approximation

\[
e^{h(A+B)} = \sum_{i=1}^{n} c_i T_2^{k_i}(\frac{h}{k_i}) + O(h^{2n+1}),
\]

provided that \( c_i \) satisfy the simple Vandermonde equation:

\[
\begin{pmatrix}
    1/k_1^{-2} & 1/k_2^{-2} & 1/k_3^{-2} & \cdots & 1/k_n^{-2} \\
    1/k_1^{-4} & 1/k_2^{-4} & 1/k_3^{-4} & \cdots & 1/k_n^{-4} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    1/k_1^{-2(n-1)} & 1/k_2^{-2(n-1)} & 1/k_3^{-2(n-1)} & \cdots & 1/k_n^{-2(n-1)}
\end{pmatrix}
\begin{pmatrix}
    c_1 \\
    c_2 \\
    \vdots \\
    c_n
\end{pmatrix} =
\begin{pmatrix}
    1 \\
    0 \\
    \vdots \\
    0
\end{pmatrix}
\]
Surprisingly, this equation has closed form solutions\[13\] for all $n$

$$c_i = \prod_{j=1 \neq i}^{n} \frac{k_i^2}{k_i^2 - k_j^2}.$$ (38)

The natural sequence $\{k_i\} = \{1, 2, 3 \ldots n\}$ produces a $2n$th-order algorithm with the minimum $n(n + 1)/2$ evaluations of $T_2(h)$. For orders four to ten, one has explicitly:

$$T_4(h) = -\frac{1}{3} T_2(h) + \frac{4}{3} T_2^2 \left( \frac{h}{2} \right)$$ (39)

$$T_6(h) = \frac{1}{24} T_2(h) - \frac{16}{15} T_2^2 \left( \frac{h}{2} \right) + \frac{81}{40} T_2^3 \left( \frac{h}{3} \right)$$ (40)

$$T_8(h) = -\frac{1}{360} T_2(h) + \frac{16}{45} T_2^2 \left( \frac{h}{2} \right) - \frac{729}{280} T_2^3 \left( \frac{h}{3} \right) + \frac{1024}{315} T_2^4 \left( \frac{h}{4} \right)$$ (41)

$$T_{10}(h) = \frac{1}{8640} T_2(h) - \frac{64}{945} T_2^2 \left( \frac{h}{2} \right) + \frac{6561}{4480} T_2^3 \left( \frac{h}{3} \right) - \frac{16384}{2835} T_2^4 \left( \frac{h}{4} \right) + \frac{390625}{72576} T_2^5 \left( \frac{h}{5} \right) \ldots$$ (42)

As shown in Ref.\[13\], $T_4(h)$ reproduces Nyström’s fourth-order algorithm with three force-evaluations and $T_6(h)$ yielded a new sixth-order Nyström type algorithm with five force-evaluations.

**Remark 1.** It is easy to show that the Verlet algorithm (13) and (14) corresponding to $S_{AB}(h)$ produces the same trajectory as Stömer’s second order scheme

$$q_1 - 2q_0 + q_{-1} = h^2 a(q_0).$$ (43)

However, it is extremely difficult to deduce from (43) that the underlying error structure is basically (30) and allows for a $h^2$-extrapolation. This is the great achievement of Gragg\[21\]. Nevertheless, the power of the present operator approach is that we can reproduce his results in a few lines. The error structure here, (30), is a simple consequence of the symmetric character of the product, and allows us to bypass Gragg’s lengthy proof on the asymptotic errors of (43). Moreover, this $h^2$-extrapolation can be applied to any $T_S(h)$, not necessarily restricted to (43). For example, the use of $S_{BA}(h)$ produces an entirely different sequence of extrapolations\[13\], distinct from that based on (43).

**Remark 2.** In the original work of Gragg, the use of (43) as the basis for his extrapolation is a matter of default; it is a well-known second-order solution. Here, in extrapolating operators, the use of $S_{AB}(h)$ or $S_{BA}(h)$ is for the specific purpose that they can be applied to time-irreversible problems. While all positive time steps algorithms are possible in the fourth-order\[37, 10\] by including the operator $[B, [A, B]]$, MPE is currently the only way of producing sixth and
higher-order algorithms in solving the imaginary time Schrödinger equation\cite{14} and in doing Path-Integral Monte Carlo simulations\cite{41}. The fact that MPE is no longer norm preserving nor even strictly positive, does not affect the higher order convergences in these applications. These non-structure preserving elements are within the error noise of the algorithm. MPE is less useful in solving the real time Schrödinger equation where, unitarity is of critical importance.

Remark 3. The explicit coefficient $c_i$ coincide with the diagonal elements of the Richardson-Aitken-Neville extrapolation\cite{24} table. This is not surprising, since they are coefficients of extrapolation. As shown in \cite{13}, $c_i = L_i(0)$, where $L_i(x)$ are the Lagrange interpolating polynomials with interpolation points $x_i = k_i^{-2}$. What is novel here is that $c_i$ is known analytically and a simple routine calling it repeatedly to execute $\mathcal{T}_2(h)$ will generate an arbitrary even order algorithm without any table construction. The resulting algorithm is extremely portable and compact and can serve as a benchmark by which all integrators of the same order can be compared. In Ref.\cite{13}, the only algorithm that have outperformed MPE is Dormand and Prince's\cite{15} 12th-order integrator as given in Ref.\cite{7}.

Having the explicit solutions $c_i$ now suggests new ways of solving old problems. Suppose one wishes to integrate the system to time $t$. One may begin by using a second-order algorithm and iterate it $m$ time at time step $h = t/m$,

$$\mathcal{T}_{2,m}(h) = \mathcal{T}_{2}(t/m).$$

(44)

Every position on the trajectory will then be correct to second order in $h$. However, if one were only interested in the final position at time $t$, then one can correct this final position to fourth order by simply computing one more $\mathcal{T}_2(t)$ and modify (44) via

$$\mathcal{T}_{4,m}(h) = \frac{m^2}{m^2 - 12} \mathcal{T}_{2,m}^m(t/m) - \frac{1^2}{m^2 - 12} \mathcal{T}_2(t),$$

(45)

or correct it to sixth-order via

$$\mathcal{T}_{6,m}(h) = \frac{m^4 \mathcal{T}_2^m(t/m)}{(m^2 - 1^2)(m^2 - 2^2) + \frac{2^4 \mathcal{T}_2^2(t/2)}{2^2 - 1^2}(2^2 - m^2) + \frac{1^4 \mathcal{T}_2(t)}{1^2 - 2^2}(1^2 - m^2)}$$

(46)

and so on, to any even order. The expansion coefficients are given by $\{k_i\}$ equal to $\{m, 1\}$, $\{m, 2, 1\}$, $\{m, 3, 2, 1\}$ etc. This is similar to the idea of process algorithms\cite{3}, but much, much simpler. The processor for correcting (44) beyond the fourth-order can be quite complex if the entire algorithm were to remain symplectic. Here, for Nyström integrators, the extrapolation coefficient is known to all even orders. Alternatively, one can view the above as correcting every $m$th step of the basic algorithm $\mathcal{T}_{2}(t/m)$ over a short time interval of $t$. Thus knowing $c_i$ allows great flexibility is designing algorithms that run the gamut from being correct to arbitrary high order at every time-step, every other time-step, every third time-step, etc., to only at the final time step. With MPE, one can easily produce versatile adaptive algorithms by varying both the time step size $h$ and the order of the algorithm.
Remark 4. Since MPE is an extrapolation, it is expected to be more prone to round-off errors. Thus if $n$ is too large in (45), the second term may be too small and the correction is lost to round-off errors. However, as seen in (17) and (24), the required substractions are sometime well-defined and the the round-off errors are within the error noise of the algorithm. As will be shown in Section 5, the round-off errors are sometime less severe than expected.

Remark 5. The idea of extrapolating symplectic algorithms has been considered by previously by Blanes, Casas and Ros[6] and Chan and Murua[9]. They studied the case of extrapolating an $2n$-order symplectic integrator. They did not obtain analytical forms for their expansion coefficients but noted that extrapolating a $2n$-order symplectic integrator will preserve the symplectic character of the algorithm to order $4n + 1$. While this is more general, such an extrapolation cannot be applied to time-irreversible systems for $n > 1$.

Finally, we note that

$$e^{h(A+B)} = \lim_{n \to \infty} \sum_{i=1}^{n} c_i T_i^{k_i} \left( \frac{h}{k_i} \right).$$

(47)

In principle, for any countable sets of $\{k_i\}$, we have achieved an exact decomposition, with known coefficients. This is in contrast to the structure-preserving, but impractical Zassenhaus formula.

The above derivation of even-order algorithms, is at most an elaboration on Gragg’s seminal work. Below, we will derive arbitrary odd-order Nyström algorithms which have not been anticipated in any classical study. Since

$$T_1(h) = e^{h A} e^{h B} = \exp[h(A + B) + h^2 F_2 + h^3 F_3 + h^4 F_4 + \cdots],$$

(48)

contain errors of all orders ($\{F_i\}$ are nested commutators of the usual Baker-Campbell-Hausdorff formula), extrapolations based on $T_i^k(h/k)$ will not yield a $h^2$-order scheme. However, there is a $h^2$-order basis hidden in Burstein and Mirin’s original decomposition (7). The following basis for $n = 1, 2, 3 \ldots$

$$U_n(h) = e^{\frac{h}{2n} A} (e^{\frac{h}{2n} B} e^{\frac{h}{2n} A})^{n-1} e^{\frac{h}{2n} B}$$

(49)

has the remarkable property that it effectively behaves as if

$$U_n(h) = \exp[h(A + B) + x^{-2}(h^2 F_2 + h^3 F_3) + x^{-4}(h^4 F_4 + h^5 F_5) + \cdots] \tag{50}$$

where $x = (2n - 1)$. (By effectively we mean that $U_n(h)$ actually has the form

$$U_n(h) = \exp[h(A + B) + x^{-2}(h^2 F_2 + h^3 F_3)$$

$$+(x^{-2} - x^{-4}) h^4 F'_2 + x^{-4}(h^4 F_4 + h^5 F_5) + \cdots] \tag{51}$$

where $F'_2$ are additional commutators not present in (48). However, this is essentially (50) with altered $F_i$ but without changing the crucial power pattern of
force-evaluations: produces, without any tinkering, Nyström's fifth-order integrators\(^2\) with four
(38), but with \(\{k_i\}\) consists of only odd whole numbers. The first few odd order decompositions corresponding to \(\{k_i\}\) being \(\{1, 3\}, \{1, 3, 5\}, \{1, 3, 5, 7\}\) and \(\{1, 3, 5, 7, 9\}\) are:

\[
\mathcal{T}_3(h) = -\frac{1}{8} u_1(h) + \frac{9}{8} u_2(h)
\]

\[
\mathcal{T}_5(h) = \frac{1}{192} u_1(h) - \frac{81}{128} u_2(h) + \frac{625}{384} u_3(h)
\]

\[
\mathcal{T}_7(h) = -\frac{1}{9216} u_1(h) + \frac{729}{5120} u_2(h) - \frac{15625}{9216} u_3(h) + \frac{117649}{46080} u_4(h)
\]

\[
\mathcal{T}_9(h) = \frac{1}{737280} u_1(h) - \frac{729}{40960} u_2(h) + \frac{390625}{516096} u_3(h) - \frac{5764801}{1146880} u_4(h)
\]

The splitting \(\mathcal{T}_5(h)\) explains the original form of Burstein and Mirin’s decomposition and Nyström’s third-order algorithm. The splitting \(\mathcal{T}_5(h)\) again produces, without any tinkering, Nyström’s fifth-order integrators\(^2\) with four force-evaluations:

\[
q = q_0 + h v_0 + \frac{h^2}{192} \left[ 23 a_0 + 75 a_{2/5} - 27 a_{2/3} + 25 a_{4/5} \right]
\]

\[
v = v_0 + \frac{h}{192} \left[ 23 a_0 + 125 a_{2/5} - 81 a_{2/3} + 125 a_{4/5} \right]
\]

where we have denoted \(a_{i/k} = a(q_{i/k})\) with

\[
q_{2/5} = q_0 + \frac{2}{5} h v_0 + \frac{2}{25} h^2 a_0
\]

\[
q_{4/5} = q_0 + \frac{4}{5} h v_0 + \frac{4}{25} h^2 (a_0 + a_{2/5})
\]

and where \(q_{2/3}\) has been given earlier in (21). (Interchange of \(A \leftrightarrow B\) in \(\mathcal{T}_5(h)\)
will also yield a fifth-order algorithm, but since the final force-evaluations can only be combined as in (24) to order \(O(h^4)\), such a force consolidation cannot be used for a fifth-order algorithm. The algorithm will then require six force-evaluations, which is undesirable. We shall therefore ignore this alternative case from now on.) With three more force-evaluations at

\[
q_{2/7} = q_0 + \frac{2}{7} h v_0 + \frac{2}{49} h^2 a_0
\]

\[
q_{4/7} = q_0 + \frac{4}{7} h v_0 + \frac{4}{49} h^2 (a_0 + a_{2/7})
\]

\[
q_{6/7} = q_0 + \frac{6}{7} h v_0 + \frac{2}{49} h^2 (3 a_0 + 4 a_{2/7} + 2 a_{4/7})
\]
$T_{7}(h)$ produces the following seventh-order algorithm with seven force-evaluations, which has never been derived before,

$$
q = q_0 + h v_0 + \frac{h^2}{23040} \left[ 1682a_0 + 729a_{2/3} - 3125(3a_{2/5} + a_{4/5}) + 2401(5a_{2/7} + 3a_{4/7} + a_{6/7}) \right], \quad (61)
$$

$$
v = v_0 + \frac{h}{23040} \left[ 1682a_0 + 2167a_{2/3} - 15625(a_{2/5} + a_{4/5}) + 16807(a_{2/7} + a_{4/7} + a_{6/7}) \right]. \quad (62)
$$

These analytical derivations are of course unnecessary in practical applications. As in the even-order case, both the coefficients $c_k$ and the algorithm corresponding to $U_n(h)$ can be called repeatedly to generate any odd-order integrators. Since each $U_n(h)$ requires $n$ force evaluation, but have the initial force in common, each $(2n-1)$ order algorithm requires $\frac{1}{2}n(n-1)+1$ force-evaluations. Thus for odd-orders 3, 5, 7, 9, the number of force-evaluation required are 2, 4, 7, 11. As alluded to earlier, for even-order 4, 6, 8, 10, the number of force-evaluation required are 3, 5, 10, 15. These sequences of extrapolated algorithms therefore provide a natural explanation for the order barrier in Nyström algorithms. For order $p < 7$, the number of force-evaluation can be $p - 1$, but for $p > 7$, the number of force-evaluation must be greater than $p$.

**Remark 6.** In general we have the following order notation for the even and odd algorithms:

- The order of the even algorithm is $2n$, its decomposition error is $2n + 1$.
- The order of the odd algorithm is $2n - 1$, its decomposition error is $2n$.

### 3 Solving non-autonomous equations

The solution to the non-autonomous equation (28) can be formally written as

$$
Y(t + h) = T \left( \exp \int_{t}^{t+h} A(s)ds \right) Y(t), \quad (63)
$$

aside from the conventional expansion

$$
T \left( \exp \int_{t}^{t+h} A(s)ds \right) = 1 + \int_{t}^{t+h} A(s_1)ds_1 + \int_{t}^{t+h} ds_1 \int_{s_1}^{s_2} ds_2 A(s_1)A(s_2) + \cdots, \quad (64)
$$

the time-ordered exponential can also be interpreted more intuitively as

$$
T \left( \exp \int_{t}^{t+h} A(s)ds \right) = \lim_{n \to \infty} T \left( e^{\frac{h}{n} \sum_{i=1}^{n} A(t+i\frac{h}{n})} \right), \quad (65)
$$

$$
= \lim_{n \to \infty} e^{\frac{h}{n}A(t+\frac{h}{n})} \cdots e^{\frac{h}{n}A(t+2\frac{h}{n})} e^{\frac{h}{n}A(t+h)}. \quad (66)
$$
The time-ordering is trivially accomplished in going from (65) to (66). To enforce latter, Suzuki[36] introduces the forward time derivative operator, also called super-operator:

$$D = \frac{\partial}{\partial t}$$

such that for any two time-dependent functions $F(t)$ and $G(t)$,

$$F(t)e^{hD}G(t) = F(t + h)G(t).$$

If $F(t) = 1$, we have

$$e^{hD}G(t) = e^{hD}G(t) = G(t).$$

Trotter’s formula then gives

$$\exp[h(A(t) + D)] = \lim_{n \to \infty} \left( e^{\frac{h}{n}A(t)} e^{\frac{h}{n}D} \right)^n,$$

$$\lim_{n \to \infty} e^{\frac{h}{n}A(t)} e^{\frac{h}{n}D} \cdots e^{\frac{h}{n}A(t + \frac{h}{n})} e^{\frac{h}{n}A(t + \frac{h}{n})},$$

where property (69) has been applied repeatedly and accumulatively. Comparing (66) with (70) yields Suzuki’s decomposition of the time-ordered exponential[36]

$$\mathcal{T} \left( \exp \int_t^{t+h} A(s) ds \right) = \exp[h(A(t) + D)].$$

Thus time-ordering can be achieve by splitting an additional operator $D$. This is extremely useful and transforms any existing splitting algorithms into integrators of non-autonomous equations. For example, one has the following symmetric splitting

$$\mathcal{T}_2(h) = e^{\frac{h}{2}hD} e^{\frac{h}{2}A(t)} e^{\frac{h}{2}D} = e^{hA(t + \frac{h}{2})},$$

which is the second-order mid-point approximation. Every occurrence of the operator $e^{\frac{h}{2}hD}$, from right to left, updates the current time $t$ to $t + d_i h$. If $t$ is the time at the start of the algorithm, then after the first occurrence of $e^{\frac{h}{2}hD}$, time is $t + \frac{h}{2}$. After the second $e^{\frac{h}{2}hD}$, time is $t + h$. Thus the leftmost $e^{\frac{h}{2}hD}$ is not without effect, it correctly updates the time for the next iteration. Thus the iterations of $\mathcal{T}_2(h)$ implicitly imply

$$\mathcal{T}_2^2 \left( h/2 \right) = e^{\frac{h}{4}hA(t + \frac{h}{2})} e^{\frac{h}{4}hA(t + \frac{h}{2})} e\frac{h}{4}hA(t + \frac{h}{2}),$$

$$\mathcal{T}_2^3 (h/3) = e^{\frac{h}{8}hA(t + \frac{h}{3})} e\frac{h}{8}hA(t + \frac{h}{3}) e\frac{h}{8}hA(t + \frac{h}{3}).$$

For the odd-order basis, we have

$$\mathcal{U}_1(h) = e^{hD} e^{hA(t)} = e^{hA(t)}$$

$$\mathcal{U}_2(h) = e^{\frac{h}{2}hD} e^{\frac{h}{2}hA(t)} e^{\frac{h}{2}hD} e^{\frac{h}{2}A(t)} = e^{\frac{h}{2}hA(t + \frac{h}{2})} e^{\frac{h}{2}hA(t)}$$

$$\mathcal{U}_3(h) = e^{\frac{h}{4}hA(t + \frac{h}{4})} e^{\frac{h}{4}hA(t + \frac{h}{4})} e^{\frac{h}{4}hA(t + \frac{h}{4})} e^{\frac{h}{4}hA(t + \frac{h}{4})}$$

$$\cdots$$

(73)
Remark 7. The recent work by Wiebe et al.\cite{38} suggests that Suzuki’s decomposition \eqref{eq:71} only holds if $A(t)$ is sufficiently smooth. In cases where the derivatives of $A(t)$ cease to exist, high-order integrators based on \eqref{eq:71} maybe degraded to lower orders.

For $A(t) = T + V(t)$, since $[D, T] = 0$, the second-order algorithm can be obtained as

\[
\mathcal{T}_2(h) = e^{\frac{1}{2}h(T + D)} e^{hV(t)} e^{\frac{1}{2}h(T + D)} = e^{\frac{1}{2}hT} e^{\frac{1}{2}hD} e^{hD} e^{hV(t)} e^{\frac{1}{2}hD} e^{\frac{1}{2}hT} = e^{\frac{1}{2}hT} e^{hV(t + h/2)} e^{\frac{1}{2}hT}.
\]  \hfill (75)

For odd order algorithms, we now have the following sequence of basis product

\[
\mathcal{U}_1(h) = e^{hT} e^{hV(t)}
\]
\[
\mathcal{U}_2(h) = e^{\frac{1}{2}hT} e^{\frac{1}{2}hV(t + \frac{h}{2})} e^{\frac{1}{2}hT} e^{\frac{1}{2}hV(t)}
\]
\[
\mathcal{U}_3(h) = e^{\frac{1}{4}hT} e^{\frac{1}{4}hV(t + \frac{h}{4})} e^{\frac{1}{4}hT} e^{\frac{1}{4}hV(t + \frac{h}{4})} e^{\frac{1}{4}hT} e^{\frac{1}{4}hV(t + \frac{h}{4})} e^{\frac{1}{4}hT} e^{\frac{1}{4}hV(t)}
\]
\[
\ldots
\]  \hfill (76)

While any power of $\mathcal{T}_2(h)$ is time-symmetric, each $\mathcal{U}_n(h)$ is time asymmetric,

\[
\mathcal{U}_n(-h) \neq \mathcal{U}_n(h).
\]  \hfill (77)

4 Errors and convergence of the Multi-product expansion

While extrapolation methods are well-known in the study of differential equations, there is a virtually no work done in the context of operators. Here, we extend the method of extrapolation to the decomposition of two operators, which is the basis of the MPE method. Working at the operator, rather than at the solution level, allows the extrapolation method be widely applied to many time-dependent equations. In particular, we will use the constructive details in\cite{13} to prove convergence results for the multi-product expansion. While this work is restricted to exponential splitting, our proof of convergence based on the general framework of \cite{22}.

4.1 Analysis of the even-order kernel $\mathcal{T}_2$

We will assume that at sufficient small $h$, the Strang splitting is bounded as follow:

\[
||\mathcal{T}_2(h)|| = ||\exp(\frac{1}{2}hD) \exp(hA(t)) \exp(\frac{1}{2}hD)|| \leq \exp(\omega h),
\]  \hfill (78)

with $c$ only depend on the coefficients of the method, see the work of convergence analysis on this splitting by Janke and Lubich \cite{27}. We can then derive the following convergence results for the multi-product expansion.
Theorem 2. For the numerical solution of (28), we consider the MPE algorithm (36) of order $2n$. Further we assume the error estimate in equation (78), then we have the following convergence result:

$$ \| (S^m - \exp(mh(A(t) + D))) u_0 \| \leq CO(h^{2n+1}), \quad mh \leq t_{\text{end}}, \quad (79) $$

where $S = \sum_{i=1}^{n} c_i T_2^{k_i} \left( \frac{h}{k_i} \right)$ and $C$ is to be chosen uniformly on bounded time intervals and independent of $m$ and $h$ for sufficient small $h$.

Proof. We apply the telescopic identity and obtain:

$$ (S^m - \exp(mh(A(t) + D))) u_0 = \sum_{\nu=0}^{m-1} (S - \exp(h(A(t) + D))) \exp(\nu h(A(t) + D)) u_0. \quad (80) $$

where $S = \sum_{i=1}^{n} c_i T_2^{k_i} \left( \frac{h}{k_i} \right)$

We apply the error estimate in (78) to obtain the stability requirement:

$$ \| \sum_{i=1}^{n} c_i T_2^{k_i} \left( \frac{h}{k_i} \right) \| \leq \exp(c\omega h). \quad (82) $$

Assuming the consistency of

$$ \| \sum_{i=1}^{n} c_i T_2^{k_i} \left( \frac{h}{k_i} \right) - \exp(h(A + D)) \| \leq CO(h^{2n+1}) \quad (83) $$

we have the following error bound:

$$ \| (S^m - \exp(mh(A(t) + D))) u_0 \| \leq CO(h^{2n+1}), \quad mh \leq t_{\text{end}}, \quad (84) $$

The consistency of the error bound is derived in the following theorem.

Theorem 3. For the numerical solution of (28), we have the following consistency:

$$ \| \sum_{i=1}^{n} c_i T_2^{k_i} \left( \frac{h}{k_i} \right) - \exp(h(A + D)) \| \leq CO(h^{2n+1}). \quad (85) $$

Proof. Based on the derivation of the coefficients via the Vandermonde equation the product is bounded and we have:

$$ \sum_{k=1}^{n} c_k T_2^{k} \left( \frac{h}{k} \right) = \sum_{k=1}^{n} c_k \left( \exp((A + D)h) - (k^{-2}h^3E_3 + k^{-4}h^5E_5 + \ldots) \right), \quad (86) $$

$$ = \sum_{k=1}^{n} c_k \left( \exp((A + D)h) - \sum_{i=1}^{n} k^{-2i}h^{2i+1}E_{2i+1} \right), \quad (87) $$

$$ = \left( \exp((A + D)h) - \sum_{k=1}^{n} c_k \sum_{i=1}^{n} k^{-2i}h^{2i+1}E_{2i+1} \right), \quad (87) $$

$$ = O(h^{2n+1}), \quad (87) $$
where the coefficients are given in (38).

**Lemma 1.** We assume $||A(t)||$ to be bounded in the interval $t \in (0, t_{\text{end}})$. Then $\mathcal{T}_2$ is non-singular for sufficiently small $h$.

**Proof.** We use our assumption $||A(t)||$ is to be bounded in the interval $0 < t < t_{\text{end}}$. So we can find $||A(t)|| < C$ for $0 < t < t_{\text{end}}$, where $C \in \mathbb{R}^+$ a bound of operator $A(t)$ independent of $t$.

Therefore $\mathcal{T}_2$ is always non-singular for sufficiently small $h$.

**Remark 8.** Based on these results the kernel $\mathcal{T}_2$ is also uniform convergent.

The same argument can be used by applying to MPE formula, while all operators are convergent, the sum of all is also bounded and convergent, see [16] and [18].

**Remark 9.** For higher kernels, e.g. 4th order, there exists also error bounds so that uniform convergent results can be derived, see e.g. [20]. Such kernels can also be used to the MPE method to achieve higher order accuracy with uniform convergent series. But as we noted earlier, these cannot be applied to time-irreversible problems.

### 4.2 Analysis of the odd-order kernel $\mathcal{U}_n$

**Lemma 2.** We will assume that for sufficiently small $h$, the Burstein and Mirin’s decomposition is bounded as follow:

$$||\mathcal{U}_n(h)|| = ||e^{\frac{h}{2n}A(t)}(e^{\frac{h}{2n}D}e^{\frac{h}{2n}A(t)})^{n-1}e^{\frac{h}{2n}D}|| \leq \exp(c\omega h), \forall t \geq 0, (88)$$

with $c$ only dependent on the coefficients of the method.

The proof follows by rewriting equation (88) as a product of the Strang and the A-B splitting schemes:

**Proof.** Equation (88) can be rewritten as:

$$e^{\frac{h}{2n}A(t)}(e^{\frac{h}{2n}D}e^{\frac{h}{2n}A(t)})^{n-1}e^{\frac{h}{2n}D} (89)$$

The error bound and underlying convergence analysis for both the Strang and the A-B splitting have been previously studied by Janke and Lubich [27].

We assume the following derivation of the higher order MPE:

**Assumption 1** We assume the following higher order decomposition,

$$e^{h(A+D)} = \sum_{i=1}^{n} \hat{c}_i \mathcal{U}_i(h) + O(h^{2n}). (90)$$

where $\hat{c}_i$ are derived based on the Vandermonde equation (37) with $\{k_i\}$ being a set of odd whole numbers.
We can then derive the following convergence results for the multi-product expansion.

**Theorem 4.** For the numerical solution of (28), we consider the Assumption 1 of order $2n-1$ and we apply Lemma 2, then we have a convergence result given as:

$$|| (S^m - \exp(mh(A + D))) u_0 || \leq CO(h^{2n}), \quad m h \leq t_{\text{end}},$$

with $n = 1, 2, 3, \ldots$, and where $S = \sum_{i=1}^{n} \tilde{c}_i U_i(h)$ and $C$ is to be chosen uniformly on bounded time intervals and independent of $m$ and $h$ for sufficient small $h$.

**Proof.** The same proof ideas can be followed after the proof of Theorem 2.

The consistency of the error bound is derived in the following theorem.

**Theorem 5.** For the numerical solution of (28), we have the following consistency:

$$|| \sum_{i=1}^{n} \tilde{c}_i U_i(h) - \exp(h(A + D)) || \leq CO(h^{2n}).$$

**Proof.** The same proof ideas can be followed after the proof of Theorem 3.

**Remark 10.** The same proof idea can be used to generalise the higher order schemes.

## 5 Analytical and numerical verifications

In this section, we seek to verify and assess the convergence of both the even and odd order MPE algorithms. For a single product splitting, there are no known splittings that are exact in the limit of large number of operators. Even in the case of the Zassenhaus formula, it is non-trivial to compute the higher order products, not to mention evaluating them. For this purpose, we turn to the much studied Magnus expansion, where the exact limit can be computed in simple cases.

The Magnus expansion[5] solves (28) in the form

$$Y(t) = \exp(\Omega(t))Y(0), \quad \Omega(t) = \sum_{n=1}^{\infty} \Omega_n(t)$$

where the first few terms are

$$\Omega_1(t) = \int_0^t dt_1 A_1$$

$$\Omega_2(t) = \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [A_1, A_2]$$

$$\Omega_3(t) = \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([A_1, [A_2, A_3] + [[A_1, A_2], A_3])$$

$$\ldots.$$
with \( A_n \equiv A(t_n) \). In practice, it is more useful to define the \( n \)th order Magnus operator

\[
\Omega^{[n]}(t) = \Omega(t) + O(t^{n+1})
\]

(95)
such that

\[
Y(t) = \exp[\Omega^{[n]}(t)] Y(0) + O(t^{n+1}).
\]

(96)

Thus the second-order Magnus operator is

\[
\Omega^{[2]}(t) = \int_0^t dt_1 A(t_1)
\]

\[
= tA \left( \frac{1}{2} t \right) + O(t^3)
\]

(97)

and a fourth-order Magnus operator[5] is

\[
\Omega^{[4]}(t) = \frac{1}{2} t(A_1 + A_2) - c_3 t^2 [A_1, A_2]
\]

(98)

where \( A_1 = A(c_1 t), A_2 = A(c_2 t) \) and

\[
c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, \quad c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6}, \quad c_3 = \frac{\sqrt{3}}{12}.
\]

(99)

For the ubiquitous case of

\[
A(t) = T + V(t),
\]

(100)

one has

\[
e^{\Omega^{[2]}(t)} = e^{[T + V(t/2)]}
\]

\[
= e^{\frac{1}{2} tT} e^{\frac{1}{2} tV(t/2)} e^{\frac{1}{2} tT} + O(t^3)
\]

(101)

and

\[
e^{\Omega^{[4]}(t)} = e^{c_3 t(V_2 - V_1)} e^{\left( T + \frac{1}{6} (V_1 + V_2) \right) t} e^{-c_3 t(V_2 - V_1)} + O(t^5)
\]

(102)

where

\[
V_1 = V(c_1 t), \quad V_2 = V(c_2 t).
\]

(103)

The Magnus expansion (96) is automatically structure-preserving because it is a single exponential operator approximation. However, since one must further split \( \Omega^{[n]} \) into computable parts, the expansion is as complex, if not more so, than a single product splitting. In the following, the comparison is not strictly equitable, because the MPE is not structure-preserving. Nevertheless it is useful to know that, perhaps for that reason, MPE can be uniformly convergent.

### 5.1 The non-singular matrix case

To assess the convergence of the Multi-product expansion with that of the Magnus series, consider the well known example[29] of

\[
A(t) = \begin{pmatrix} 2 & t \\ 0 & -1 \end{pmatrix}
\]

(104)
The exact solution to (28) with $Y(0) = I$ is

$$Y(t) = \begin{pmatrix} e^{2t} & f(t) \\ 0 & e^{-t} \end{pmatrix},$$

with

$$f(t) = \frac{1}{9} e^{-t}(e^{3t} - 1 - 3t) \tag{106}$$

$$= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^7}{80} + \frac{31t^8}{40320} + \frac{t^9}{6720} + \frac{13t^{10}}{403200} + \frac{13t^{11}}{178200} \tag{107}$$

For the Magnus expansion, one has the series

$$\Omega(t) = \begin{pmatrix} 2t & g(t) \\ 0 & -t \end{pmatrix},$$

with, up to the 10th order,

$$g(t) = \frac{1}{2} t^2 - \frac{1}{4} t^3 + \frac{3}{80} t^5 - \frac{9}{1120} t^7 + \frac{81}{44800} t^9 + \cdots \tag{109}$$

$$\rightarrow t(e^{3t} - 1 - 3t) \tag{110}$$

Exponentiating (108) yields (105) with

$$f(t) = te^{-t}(e^{3t} - 1) \left( \frac{1}{6} - \frac{1}{12} t + \frac{1}{80} t^3 - \frac{3}{1120} t^5 + \frac{27}{44800} t^7 + \cdots \right) \tag{111}$$

$$\rightarrow te^{-t}(e^{3t} - 1) \left( \frac{1}{9t} - \frac{1}{3(e^{3t} - 1)} \right) \tag{112}$$

Whereas the exact solution (106) is an entire function of $t$, the Magnus series (109) and (111) only converge for $|t| < \frac{2}{3}\pi$ due to the pole at $t = \frac{2}{3}\pi i$. The Magnus series (111) is plot in Fig.1 as blue lines. The pole at $|t| = \frac{2}{3}\pi \approx 2$ is clearly visible.

For the even order multi-product expansion, from (72), by setting $h = t$ and $t = 0$, we have

$$T_2(t) = \exp \left[ t \begin{pmatrix} 2 & \frac{1}{4}t \\ 0 & -1 \end{pmatrix} \right] = \begin{pmatrix} e^{2t} & f_2(t) \\ 0 & e^{-t} \end{pmatrix} \tag{113}$$

and we compute $T_2^2(t)$ according to (73) as

$$T_2^2(t/2) = \exp \left[ \frac{t}{2} \begin{pmatrix} 2 & \frac{3}{4}t \\ 0 & -1 \end{pmatrix} \right] \begin{pmatrix} e^t & f_2(t/2) \\ 0 & e^{-t/2} \end{pmatrix} \tag{114}$$

with

$$f_2(t) = \frac{1}{6} te^{-t}(e^{3t} - 1). \tag{115}$$
Fig. 1. The black line is the exact result (106). The dotted blue lines are the Magnus fourth to tenth order results (111), which diverge from the exact result beyond \( t > 2 \). The solid red lines are the multi-product expansions. The dashed-purple line is their common second order result.

This is identical to first term of the Magnus series (111) and is an entire function of \( t \). Since higher order MPE uses only powers of \( T^2 \), higher order MPE approximations are also entire functions of \( t \). Thus up to the 10th order, one finds

\[
f_4(t) = te^{-t} \left( \frac{e^{3t} - 5}{18} + \frac{2e^{3t/2}}{9} \right) \tag{116}
\]

\[
f_6(t) = te^{-t} \left( \frac{11e^{3t} - 109}{360} + \frac{9}{40}(e^{2t} + e^t) - \frac{8}{45}e^{3t/2} \right) \tag{117}
\]

\[
f_8(t) = te^{-t} \left( \frac{151e^{3t} - 2369}{7560} + \frac{256}{945}(e^{9t/4} + e^{3t/4}) - \frac{81}{280}(e^{2t} + e^t) + \frac{104}{315}e^{3t/2} \right) \tag{118}
\]

\[
f_{10}(t) = te^{-t} \left( \frac{15619e^{3t} - 347261}{1088640} + \frac{78125}{217728}(e^{12t/5} + e^{9t/5} + e^{6t/5} + e^{3t/5}) \\
- \frac{4096}{8505}(e^{3t/4} + e^{3t/4}) + \frac{729}{4480}(e^{2t} + e^t) - \frac{4192}{8505}e^{3t/2} \right). \tag{119}
\]
These even order approximations are plotted as red lines in Fig.1. The convergence is uniform for all \( t \).

When expanded, the above yields

\[
\begin{align*}
\mathcal{U}_1(t) &= \exp \left[ t \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix} \right] = \begin{pmatrix} e^{2t} & 0 \\ 0 & e^{-t} \end{pmatrix} \\
\mathcal{U}_2(t) &= \exp \left[ \frac{2}{3} t \begin{pmatrix} 2 & \frac{2t}{3} \\ 0 & -1 \end{pmatrix} \right] \exp \left[ \frac{1}{3} t \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix} \right] \\
&= \begin{pmatrix} e^{2t} & \frac{2t}{3}(e^t - e^{-t}) \\ 0 & e^{-t} \end{pmatrix}
\end{align*}
\]

and the MPE (53) to (56) give

\[
\begin{align*}
f_3(t) &= \frac{t^2}{2} + \frac{t^4}{12} + \cdots \\
f_5(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{11t^6}{1000} + \cdots \\
f_7(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{420} + \frac{t^7}{2469600} + \cdots \\
f_9(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{420} + \frac{t^7}{2469600} + \frac{t^8}{49392000} + \cdots \\
f_{10}(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{420} + \frac{t^7}{2469600} + \frac{t^8}{49392000} + \frac{t^9}{49392000} + \cdots
\end{align*}
\]

and agree with the exact solution to the claimed order. Similarly, the m-step extrapolated algorithms \( \mathcal{T}_{2n,m}, \mathcal{T}_{4n,m}, \text{etc.} \), are also correct up to the claimed order.

For odd orders, by again setting \( h = t \) and \( t = 0 \), the basis defined in (74) now reads

\[
\begin{align*}
\mathcal{U}_1(t) &= \exp \left[ t \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix} \right] = \begin{pmatrix} e^{2t} & 0 \\ 0 & e^{-t} \end{pmatrix} \\
\mathcal{U}_2(t) &= \exp \left[ \frac{2}{3} t \begin{pmatrix} 2 & \frac{2t}{3} \\ 0 & -1 \end{pmatrix} \right] \exp \left[ \frac{1}{3} t \begin{pmatrix} 2 & 0 \\ 0 & -1 \end{pmatrix} \right] \\
&= \begin{pmatrix} e^{2t} & \frac{2t}{3}(e^t - e^{-t}) \\ 0 & e^{-t} \end{pmatrix}
\end{align*}
\]

and the MPE (53) to (56) give

\[
\begin{align*}
f_3(t) &= \frac{t^2}{2} + \frac{t^4}{12} + \cdots \\
f_5(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{11t^6}{1000} + \cdots \\
f_7(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{420} + \frac{t^7}{2469600} + \cdots \\
f_9(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{420} + \frac{t^7}{2469600} + \frac{t^8}{49392000} + \cdots \\
f_{10}(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{420} + \frac{t^7}{2469600} + \frac{t^8}{49392000} + \frac{t^9}{49392000} + \cdots
\end{align*}
\]

Results (120) and (122) constitute an analytical verification of the even and odd order MPE (39)-(42) and (53)-(56).

### 5.2 The singular matrix case

Consider the radial Schrödinger equation

\[
\frac{\partial^2 u}{\partial r^2} = f(r, E) u(r)
\]

(123)
where
\[ f(r, E) = 2V(r) - 2E + \frac{l(l + 1)}{r^2}. \] (124)

By relabeling \( r \to t \) and \( u(r) \to q(t) \), (123) can be viewed as harmonic oscillator with a time dependent spring constant
\[ k(t, E) = -f(t, E) \] (125)
and Hamiltonian
\[ H = \frac{1}{2}p^2 + \frac{1}{2}k(t, E)q^2. \] (126)

Thus any eigenfunction of (123) is an exact time-dependent solution of (126). For example, the ground state of the hydrogen atom with \( l = 0 \), \( E = -1/2 \) and \( V(r) = -\frac{1}{r} \) yields the exact solution
\[ q(t) = t \exp(-t) \]
\[ = t - t^2 + \frac{t^3}{6} - \frac{t^4}{24} + \frac{t^5}{120} - \frac{t^6}{720} - \frac{t^7}{5040} \cdots, \]
\[ = t - t^2 + \frac{t^3}{2} - 0.1667t^4 + 0.0417t^5 - 0.0083t^6 \cdots \] (128)
with initial values \( q(0) = 0 \) and \( p(0) = 1 \). Denoting
\[ Y(t) = \begin{pmatrix} q(t) \\ p(t) \end{pmatrix}, \] (129)
the time-dependent harmonic oscillator (126) now corresponds to
\[ A(t) = \begin{pmatrix} 0 & 1 \\ f(t) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ f(t) & 0 \end{pmatrix} = T + V(t), \] (130)
with a singular matrix element
\[ f(t) = (1 - \frac{2}{t}). \] (131)

The second-order midpoint algorithm is
\[ T_2(h, t) = e^{\frac{1}{2}hT}e^{hV(t+h/2)}e^{\frac{1}{2}hT} \]
\[ = \left( \begin{array}{cc} 1 + \frac{1}{2}h^2 f(t + \frac{1}{2}h) & h + \frac{1}{2}h^3 f(t + \frac{1}{2}h) \\ hf(t + \frac{1}{2}h) & 1 + \frac{1}{2}h^2 f(t + \frac{1}{2}h) \end{array} \right), \] (132)
and for \( q(0) = 0 \) and \( p(0) = 1 \), (setting \( t = 0 \) and \( h = t \)), correctly gives the second order result,

\[
q_2(t) = t + \frac{1}{4} t^3 f\left(\frac{1}{2} t\right) = t - t^2 + \frac{1}{4} t^3. \tag{133}
\]

The even order multi-product expansions (39)-(42) then yield

\[
q_4(t) = t - t^2 + 0.3889 t^3 - 0.1111 t^4 + 0.0104 t^5 \\
q_6(t) = t - t^2 + 0.4689 t^3 - 0.1378 t^4 + 0.0283 t^5 - 0.0043 t^6 \\
q_8(t) = t - t^2 + 0.4873 t^3 - 0.1542 t^4 + 0.0356 t^5 - 0.0062 t^6 \ldots \\
q_{10}(t) = t - t^2 + 0.4936 t^3 - 0.1603 t^4 + 0.0385 t^5 - 0.0073 t^6 \ldots \tag{134}
\]

where we have converted fractions to decimal forms for easier comparison with the exact solution (128). One sees that MPE no longer matches the Taylor expansion beyond second-order. This is due to the singular nature of the Coulomb potential, which makes the problem a challenge to solve. (If one naively makes a Taylor expansion about \( t = 0 \) starting with \( q(0) = 0 \) and \( p(0) = 1 \), then every term beyond the initial values would either be divergent or undefined.)

Since \( A(t) \) is now singular at \( t = 0 \), the previous proof of uniform convergence no longer holds. Nevertheless, from the exact solution (128), one sees that force (or acceleration)

\[
\lim_{t \to 0} f(t) q(t) = -2 \tag{135}
\]

remains finite. It seems that this is sufficient for uniform convergence as the coefficients of \( t^n \) do approach their correct value with increasing order.

For odd order MPE, while each term \( e^{(h/x)} V(t) \) of the basis product in (76) is singular at \( t = 0 \), but because of (135),

\[
\lim_{t \to 0} e^{(h/x)} V(t) \begin{pmatrix} g(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 - 2h/x \end{pmatrix}. \tag{136}
\]

Interpreting the action of the first operator this way, the basis products of (76) then yield, according to the MPE (53)-(56),

\[
q_3(t) = t - t^2 + \frac{t^3}{2} - 0.1111 t^4 \\
q_5(t) = t - t^2 + \frac{t^3}{2} - 0.1458 t^4 + 0.0333 t^5 - 0.0033 t^6 \\
q_7(t) = t - t^2 + \frac{t^3}{2} - 0.1628 t^4 + 0.0382 t^5 - 0.0067 t^6 \ldots \\
q_9(t) = t - t^2 + \frac{t^3}{2} - 0.1655 t^4 + 0.0406 t^5 - 0.0078 t^6 \ldots \tag{137}
\]

Now \( q_3(t) \) is correct to third order, but higher order algorithms are still downgraded and only approaches the exact solution asymptotically but uniformly.

To see this uniform convergence, we show in Fig.2, how higher order MPE, both even and odd, up to the 100th order, compares with the exact solution. The
Fig. 2. The uniform convergence of the multi-product expansion in solving for the hydrogen ground state wave function. The black line is the exact ground state wave function. The numbers denote the order of the multi-product expansion. The dotted blue lines denote results of various fourth-order algorithms.

calculation is done numerically rather than by evaluating the analytical expressions such as (134) or (137). The order of the MPE algorithms are indicated by numbers. For odd order algorithms, we do not even bother to incorporate (136), but just avoid the singularity by starting the algorithm at $t = 10^{-6}$. Also shown are some well known fourth-order symplectic algorithm FR (Forest-Ruth[19], 3 force-evaluations), M (McLachlan[28], 4 force-evaluations), BM (Blanes-Moan[4], 6 force-evaluations), Mag4 (Magnus integrator, 4 force-evaluations) and 4B[12] (a forward symplectic algorithm with $\approx 2$ evaluations). These symplectic integrators steadily improves from FR, to M, to Mag4, to BM to 4B. Forward algorithm 4B is noteworthy in that it is the only fourth-order algorithm that can go around the wave function maximum at $t = 1$, yielding

$$q_{4B}(t) = t - t^2 + \frac{t^3}{2} - 0.1635t^4 + 0.0397t^5 - 0.0070t^6 + 0.0009t^7 \cdots, \quad (138)$$

with the correct third-order coefficient and comparable higher order coefficients as the exact solution (128). By contrast, the FR algorithm, which is well known to have rather large errors, has the expansion,

$$q_{FR}(t) = t - t^2 - 0.1942t^3 + 3.528t^4 - 2.415t^5 + 0.5742t^6 - 0.0437t^7 \cdots, \quad (139)$$
with terms of the wrong signs beyond $t^2$. The failure of these fourth-order algorithms to converge correctly due to the singular nature of the Coulomb potential is consistent with the findings of Wiebe et al. [38]. However, their finding does not explain why the second-order algorithm can converge correctly and only higher order algorithms fail. A deeper understanding of Suzuki’s method is necessary to resolve this issue.

\[ f(t) = t^2 - 3, \quad (140) \]
and exact ground state solution

\[ q(t) = te^{-t^2/2} = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{t^{11}}{3840} + \cdots, \quad (141) \]

the multi-product expansion has no problem in reproducing the exact solution to the claimed order:

\[ q_6(t) = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{13t^7}{576} + \cdots \]
\[ q_7(t) = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{1082t^9}{385875} + \cdots \]
\[ q_8(t) = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{20803t^9}{7741440} + \cdots \]
\[ q_9(t) = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{341t^{11}}{1224720} + \cdots \]
\[ q_{10}(t) = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{50977t^{11}}{19353600} + \cdots . \quad (142) \]

In this case, the odd order algorithms have the advantage of being correct one order higher.

### 6 Concluding summary and discussions

In this work, we have shown that the most general framework for deriving Nyström type algorithms for solving autonomous and non-autonomous equations is multi-product splitting. By expanding on a suitable basis of operators, the resulting multi-product expansion not only can reproduce conventional extrapolated integrators of even-order but can also yield new odd-order algorithms. By use of Suzuki’s rule of incorporating the time-ordered exponential, any multi-product splitting algorithm can be adopted for solving explicitly time-dependent problems. The analytically know expansion coefficients allow great flexibility in designing adaptive algorithms. Unlike structure-preserving methods, such as the Magnus expansion, which has a finite radius of convergence, our multi-product expansion converges uniformly. Moreover, MPE requires far less operators at higher orders than either the Magnus expansion or conventional single-product splittings. The general order-condition for multi-product splitting is not known and should be developed. In the future we will focus on applying MPE methods for solving nonlinear differential equations and time-irreversible or semi-group problems.

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