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Lecture: Multi-product operator splitting as a method of solving differential equations

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Outline of the talk (Adjoint work with S.Chin [Chin, Geiser, accepted May 2010 (IMA J.Num.Anal.)]

0) Introduction to Multi-product Expansion methods
1) Theory and Analysis
2) Generalization
3) Numerical Results

Introduction

In our differential equations we deal with general operators:

$$\partial_t u = Au + Bu, \ u(0) = u_0, \tag{1}$$

where A, B are non-commuting operators.
For example we could consider a hyperbolic equations of the form

$$\partial_t u = \tilde{A} u_x + \tilde{B} u_y, \ u(x, y, 0) = u_0(x, y), \tag{2}$$

where $\tilde{A}$, $\tilde{B}$ are non-commuting matrices or also in the spatial discretised form, where we assume to apply characteristics methods.

Further we can also think about a dynamical system:

$$\partial_t u(\mathbf{q},\mathbf{p}) = \Big(\frac{\partial u}{\partial \mathbf{q}} \cdot \frac{\partial H}{\partial \mathbf{p}} - \frac{\partial u}{\partial \mathbf{p}} \cdot \frac{\partial H}{\partial \mathbf{q}}\Big) = (A+B)u(\mathbf{q},\mathbf{p}). \quad (3)$$

For a separable Hamiltonian,

$$H(\mathbf{p},\mathbf{q}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}), \quad (4)$$

A and B are Lie operators, or vector fields

$$A = \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{q}} \qquad B = \mathbf{a}(\mathbf{q}) \cdot \frac{\partial}{\partial \mathbf{v}} \quad (5)$$

where we have abbreviated $\mathbf{v} = \mathbf{p}/m$ and $\mathbf{a}(\mathbf{q}) = -\nabla V(\mathbf{q})/m$.

To solve the problems, we deal with the time-stepping operator

$$\exp h(A+B) \tag{6}$$

which we assume to decompose in the following schemes:
1.) Single product splitting is given as:

$$\mathrm{e}^{h(A+B)} = \prod_i \mathrm{e}^{a_i hA} \mathrm{e}^{b_i hB}, \tag{7}$$

and symplectic integrators can be derived of this schemes,
2.) Multi-product expansion (MPE),

$$\mathrm{e}^{h(A+B)} = \sum_k c_k \prod_i \mathrm{e}^{a_{ki} hA} \mathrm{e}^{b_{ki} hB} \tag{8}$$

which will be the basis of general Nyström integrators and extrapolation scheme of given time-integrators.

Motivation

Single product splitting:

- 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.
- Beyond the second-order requires exponentially growing number of operators
- Problems with unavoidable negative coefficients and cannot be applied to time-irreversible or semi-group problems (modifications are done in complex coefficients, but are also hardly to apply, see analytical semigroups)

Multi product splitting:

- Advantage is a faster algorithms, e.g.
  Symplectic algorithms of orders 4, 6, 8 and 10, required a minimum of 3, 7, 15 and 31 force-evaluations
  MPE algorithms of orders 4, 6, 8, 10, only require 3, 5, 10, 15 force evaluations
- MPE has a advantage in many practical calculations where long term accuracy and structure preserving is not an issue (fast computation of large time intervals).
- Advantages are in long term evaluation, where structure preserving problems are not so important.

Introduction to Multi-product expansion

The multi-product decomposition (8) is obviously more complicated than the single product splitting (7).
We concentrate on lower order kernels for our multi-product expansion (e.g. first or second order).
But such a product is easy to construct, because every left-right symmetric single product *is* second-order. Let $\mathcal{T}_S(h)$ be such a product with $\sum_i a_{ki} = 1$ and $\sum_i b_{ki} = 1$, then $\mathcal{T}_S(h)$ is time-symmetric by construction,

$$\mathcal{T}_S(-h)\mathcal{T}_S(h) = 1, \tag{9}$$

implying that it has only odd powers of h

$$\mathcal{T}_S(h) = \exp(h(A + B) + h^3 E_3 + h^5 E_5 + \cdots) \tag{10}$$

and therefore correct to second-order.

(The error terms E_i are nested commutators of A and B depending on the specific form of $\mathcal{T}_S$.) This immediately suggests that the kth power of $\mathcal{T}_S$ at step size h/k must have the form

$$\mathcal{T}_S^k(h/k) = \exp(h(A+B) + k^{-2}h^3E_3 + k^{-4}h^5E_5 + \cdots), \quad (11)$$

and can serve as a basis for the multi-production expansion (8).

Even-order MPE

The simplest such symmetric product is

$$\mathcal{T}_2(h) = S_{AB}(h) \quad \text{or} \quad \mathcal{T}_2(h) = S_{BA}(h), \tag{12}$$

where

$$S_{AB}(h) = \mathrm{e}^{(h/2)B}\mathrm{e}^{hA}\mathrm{e}^{(h/2)B}. \tag{13}$$

is a second order scheme and commuting A and Bwe have the same with S_{BA}.

Only a simple Richardson Extrapolation can only reach one order more, see:
If one naively assumes that

$$\mathcal{T}_2(h) = \mathrm{e}^{h(A+B)} + Ch^3 + Dh^4 + \cdots , \tag{14}$$

then a Richardson extrapolation would only give

$$\frac{1}{k^2 - 1}\left[k^2 \mathcal{T}_2^k(h/k) - \mathcal{T}_2(h)\right] = \mathrm{e}^{h(A+B)} + O(h^4), \tag{15}$$

a third-order algorithm.

However, because the error structure of $\mathcal{T}_2(h/k)$ is actually given by (11), one has

$$\mathcal{T}_2^k(h/k) = \mathrm{e}^{h(A+B)} + k^{-2} h^3 E_3 + \frac{1}{2} k^{-2} h^4 [(A+B)E_3 + E_3(A+B)] + O(h^5), \quad (16)$$

and *both* the third and fourth order errors can be eliminated (one can skip the higher order terms by an extrapolation).

We can derive 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

$$e^{h(A+B)} = \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}\left(\frac{h}{k_i}\right) + O(h^{2n+1}). \qquad (17)$$

We can derive the following c_i satisfy the simple Vandermonde equation:

$$\begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ k_1^{-2} & k_2^{-2} & k_3^{-2} & \dots & k_n^{-2} \\ k_1^{-4} & k_2^{-4} & k_3^{-4} & \dots & k_n^{-4} \\ \dots & \dots & \dots & \dots & \dots \\ k_1^{-2(n-1)} & k_2^{-2(n-1)} & k_3^{-2(n-1)} & \dots & k_n^{-2(n-1)} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \dots \\ c_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \dots \\ 0 \end{pmatrix} \quad (18)$$

This equation has closed form solutions [see Chin2008] for all n

$$c_i = \prod_{j=1(\neq i)}^{n} \frac{k_i^2}{k_i^2 - k_j^2}. \tag{19}$$

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 $\mathcal{T}_2(h)$. For orders four to ten, one has explicitly:

$$\mathcal{T}_4(h) = -\frac{1}{3}\mathcal{T}_2(h) + \frac{4}{3}\mathcal{T}_2^2\left(\frac{h}{2}\right) \tag{20}$$

$$\mathcal{T}_6(h) = \frac{1}{24}\mathcal{T}_2(h) - \frac{16}{15}\mathcal{T}_2^2\left(\frac{h}{2}\right) + \frac{81}{40}\mathcal{T}_2^3\left(\frac{h}{3}\right) \tag{21}$$

$$\mathcal{T}_8(h) = -\frac{1}{360}\mathcal{T}_2(h) + \frac{16}{45}\mathcal{T}_2^2\left(\frac{h}{2}\right) - \frac{729}{280}\mathcal{T}_2^3\left(\frac{h}{3}\right) + \frac{1024}{315}\mathcal{T}_2^4\left(\frac{h}{4}\right) \tag{22}$$

Remark

In [Chin2008] is is shown that $\mathcal{T}_4(h)$ *reproduces Nyström's fourth-order algorithm with three force-evaluations and* $\mathcal{T}_6(h)$ *yielded a new sixth-order Nyström type algorithm with five force-evaluations.*

Remark

The idea of extrapolating symplectic algorithms has been previously considered by Blanes, Casas and Ros in 1999 and Chan and Murua in 2000.
They studied the case of extrapolating an $2n$*-order symplectic integrator, but did not obtain analytical forms for their expansion coefficients.*
By the way they extrapolating a $2n$*-order symplectic integrator will preserve the symplectic character of the algorithm to order* $4n+1$*, (e.g.* 2*nd order kernel, preserves to* 5*th order extrapolation schemes).*

Odd-order MPE

For the odd-order MPE we can derive arbitrary *odd-order* Nyström algorithms.
First we have to apply a h^2-order basis, given as:

$$\mathcal{U}_n(h) = \mathrm{e}^{\frac{h}{2n-1}A}(\mathrm{e}^{\frac{2h}{2n-1}B}\mathrm{e}^{\frac{2h}{2n-1}A})^{n-1}\mathrm{e}^{\frac{h}{2n-1}B} \quad (23)$$

has the remarkable property that it *effectively* behaves as if

$$\begin{aligned}\mathcal{U}_n(h) \quad &= \exp[h(A+B) + x^{-2}(h^2 F_2 + h^3 F_3) \\ &+x^{-4}(h^4 F_4 + h^5 F_5) + \cdots] \end{aligned} \quad (24)$$

where $x = (2n-1)$.

Same idea is used as in the even order case and we skip the $2n$ and $2n+1$ order errors.
In this case (25) can be extrapolated as

$$e^{h(A+B)} = \sum_{i=1}^{n} \tilde{c}_i \mathcal{U}_i(h) + O(h^{2n}), \qquad (25)$$

where $\tilde{c}_i$ satisfies the same Vandermonde equation (18), with the same solution (19), 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:

$$\mathcal{T}_3(h) = -\frac{1}{8}\mathcal{U}_1(h) + \frac{9}{8}\mathcal{U}_2(h) \tag{26}$$

$$\mathcal{T}_5(h) = \frac{1}{192}\mathcal{U}_1(h) - \frac{81}{128}\mathcal{U}_2(h) + \frac{625}{384}\mathcal{U}_3(h) \tag{27}$$

$$\mathcal{T}_7(h) = -\frac{1}{9216}\mathcal{U}_1(h) + \frac{729}{5120}\mathcal{U}_2(h) - \frac{15625}{9216}\mathcal{U}_3(h) + \frac{117649}{46080}\mathcal{U}_4(h) \tag{28}$$

$$\begin{aligned}\mathcal{T}_9(h) &= \frac{1}{737280}\mathcal{U}_1(h) - \frac{729}{40960}\mathcal{U}_2(h) + \frac{390625}{516096}\mathcal{U}_3(h) \\ &\quad - \frac{5764801}{1474560}\mathcal{U}_4(h) + \frac{4782969}{1146880}\mathcal{U}_5(h).\end{aligned} \tag{29}$$

Errors and convergence of the Multi-product expansion

The analysis is based on a general framework for unbounded operators, here we discuss with respect to bounded operators, see [Hansen and Ostermann 2008].

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

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

$$||\mathcal{T}_2(h)|| = ||\exp(\frac{1}{2}hD)\exp(hA(t))\exp(\frac{1}{2}hD)|| \leq \exp(c\omega h), \quad (30)$$

with c only depend on the coefficients of the method and ω is a positive number, see the work of convergence analysis on this splitting by Janke and Lubich in 2000.

We can then derive the following convergence results for the multi-product expansion.

Theorem

For the numerical solution of (1), we consider the MPE algorithm (17) of order $2n$. *Further we assume the error estimate in equation (30), then we have the following convergence result:*

$$|| \left(S^m - \exp(mh(A(t) + D))\right) u_0|| \leq C \; O(h^{2n+1}), mh \leq t_{end}, \tag{31}$$

where $S = \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i})$ *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:

$$\left(S^m - \exp(mh(A(t) + D))\right) u_0 =$$
$$\sum_{\nu=0}^{m-1} S^{m-\nu-1}(S - \exp(h(A(t) + D))) \exp(\nu h(A(t) + D)) u_0,$$

where $S = \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i})$ □

We apply the error estimate in (30) to obtain the stability requirement:

$$|| \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i})|| \leq \exp(c\omega h). \tag{32}$$

Assuming the consistency of

$$|| \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i}) - \exp(h(A+D))|| \leq C O(h^{2n+1}), \tag{33}$$

we have the following error bound:

$$|| \left(S^m - \exp(mh(A(t)+D))\right) u_0|| \leq C O(h^{2n+1}), mh \leq t_{end}. \tag{34}$$

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

Theorem

For the numerical solution of (1), we have the following consistency:

$$|| \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i}) - \exp(h(A+D))|| \leq CO(h^{2n+1}). \quad (35)$$

Proof.

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

$$\sum_{k=1}^{n} c_k \mathcal{T}_2^k(\frac{h}{k}) = \sum_{k=1}^{n} c_k \Big(\exp((A+D)h) \tag{36}$$

$$-(k^{-2} h^3 E_3 + k^{-4} h^5 E_5 + \ldots)\Big) , \tag{37}$$

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

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

where the coefficients are given in (19).

Lemma

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

Proof.

We use our assumption $||A(t)||$ is to be bounded in the interval $0 < t < t_{end}$.
So we can find $||A(t)|| < C$ for $0 < t < t_{end}$, 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. □

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

Lemma

We will assume that for sufficiently small h, the Burstein and Mirin's decomposition is bounded as follow:

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

with c only dependent on the coefficients of the method and ω is a positive number.

The proof follows by rewriting equation (38) as a product of the Strang and the A-B splitting schemes:

Proof.

Equation (38) can be rewritten as:

$$
\begin{aligned}
& \mathrm{e}^{\frac{h}{2n-1}A(t)}\left(\mathrm{e}^{\frac{2h}{2n-1}D}\mathrm{e}^{\frac{2h}{2n-1}A(t)}\right)^{n-1}\mathrm{e}^{\frac{h}{2n-1}D} \qquad (38) \\
= \; & \left(\mathrm{e}^{\frac{h}{2n-1}A(t)}\mathrm{e}^{\frac{2h}{2n-1}D}\mathrm{e}^{\frac{h}{2n-1}A(t)}\right)^{n-1}\mathrm{e}^{\frac{h}{2n-1}A(t)}\mathrm{e}^{\frac{h}{2n-1}D}, \; \forall t \geq 0,
\end{aligned}
$$

The error bound and underlying convergence analysis for both the Strang and the A-B splitting have been previously studied by Jahnke and Lubich [Jahnke, Lubich 2000]. □

We assume the following derivation of the higher order MPE:

Assumption

We assume the following higher order decomposition,

$$\mathrm{e}^{h(A+D)} = \sum_{i=1}^{n} \tilde{c}_i \, \mathcal{U}_i(h) + O(h^{2n}), \tag{39}$$

where $\tilde{c}_i$ are derived based on the Vandermonde equation (18) with $\{k_i\}$ being a set of odd whole numbers.

We can then derive the following convergence results for the multi-product expansion.

Theorem

For the numerical solution of (1), we consider the Assumption 3 of order $2n-1$ *and we apply Lemma 4, then we have a convergence result given as:*

$$|| \left(S^m - \exp(mh(A(t) + D)) \right) u_0 || \leq CO(h^{2n}), mh \leq t_{end}, \quad (40)$$

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

Proof.

We apply the same proof ideas as for the even case.

Theorem

For the numerical solution of (1), we have the following consistency:

$$|| \sum_{i=1}^{n} \tilde{c}_i \, \mathcal{U}_i(h) - \exp(h(A + D))|| \leq CO(h^{2n}). \qquad (41)$$

Proof.

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

□

Remark

The same proof idea can be used to generalize the higher order schemes.

Generalization

In the generalization, we discuss the construction with respect to higher order kernel functions. The expansion coefficients c_i are determined by a specially simple Vandermonde equation, where the generalization can be done by a modification in the coefficients.

a.) Generalization to even kernels:
Here we can construct extrapolations with the kernels: $\mathcal{T}_2, \mathcal{T}_4, \mathcal{T}_6$ etc., i.e. $m = 0, 1, 2, \ldots$

Lemma

The closed form of the coefficients for the extrapolation is given as
with closed form solutions

$$c_i = \frac{k_i^{2m}}{\sum_{j=1}^n k_j^2} \prod_{j=1(\neq i)}^{n} \frac{k_i^2}{k_i^2 - k_j^2}, \tag{42}$$

and error coefficient,

$$e_{2m+2n+1} = (-1)^{n-1} \frac{k_i^{2m}}{\sum_{j=1}^{n} k_j^2} \prod_{i=1}^{n} \frac{1}{k_i^2} \tag{43}$$

Here we have closed forms (42) and (46) and are the keys to the multi-product expansion and its error analysis.

Proof.

The proof is done with the Vandermonde equation:

$$\begin{pmatrix} 1 & 1 & 1 \ldots & 1 & \\ k_1^{-2m-2} & k_2^{-2m-2} & k_2^{-2m-2} & \ldots & k_n^{-2m-2} \\ k_1^{-2m-4} & k_2^{-2m-4} & k_2^{-2m-4} & \ldots & k_n^{-2m-4} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ k_1^{-2m-2n} & k_2^{-2m-2n} & k_2^{-2m-2n} & \ldots & k_n^{-2m-2n} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \ldots \\ c_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \ldots \\ 0 \end{pmatrix} \quad (44)$$

Complete induction with the assumption of equation (42) is followed.

We start with n=1, n=2, n=3.

The induction step with $n \rightarrow n+1$, with the assumption of equation (42).

b.) Generalization to odd and prime number kernels:

Here we can construct extrapolations with the kernels: $\mathcal{T}_2, \mathcal{T}_3, \mathcal{T}_5$ etc., i.e. $m = 0, 1, 2, \ldots$

Lemma

The closed form of the coefficients for the extrapolation is given as
with closed form solutions

$$c_i = \frac{k_i^{a\,m}}{\sum_{j=1}^n k_j^a} \prod_{j=1(\neq i)}^n \frac{k_i^a}{k_i^a - k_j^a} \tag{45}$$

and error coefficient,

$$e_{a\,m+a\,n+1} = (-1)^{n-1} \frac{k_i^{a\,m}}{\sum_{j=1}^{n} k_j^a} \prod_{i=1}^{n} \frac{1}{k_i^a} \tag{46}$$

Here we have closed forms (45) and (46) and are the keys to the multi-product expansion and its error analysis.

Proof.

The proof is also done with the Vandermonde equation:

$$\begin{pmatrix} 1 & 1 & 1 \ldots & 1 & \\ k_1^{-am-a} & k_2^{-am-a} & k_2^{-am-a} & \ldots & k_n^{-am-a} \\ k_1^{-am-2a} & k_2^{-am-2a} & k_2^{-am-2a} & \ldots & k_n^{-am-2a} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ k_1^{-am-an} & k_2^{-am-an} & k_2^{-am-an} & \ldots & k_n^{-am-an} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \ldots \\ c_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \ldots \\ 0 \end{pmatrix} \tag{47}$$

Complete induction with the assumption of equation (45) is followed.

We start with n=1, n=2, n=3.

The induction step with $n \to n+1$, with the assumption of equation (45).

The higher order extrapolation allows to start with more accurate Kernels. The higher accuracy starts in a higher order form.

Example

A 8th order algorithm from an even 4th order kernel function is given as:

$$c_1 = \frac{k_1^6}{(k_1^2 - k_2^2)(k_1^2 - k_3^2)(k_1^2 + k_2^2 + k_3^2)} \tag{48}$$

$$c_2 = \frac{k_2^6}{(k_2^2 - k_1^2)(k_2^2 - k_3^2)(k_1^2 + k_2^2 + k_3^2)} \tag{49}$$

$$c_3 = \frac{k_3^6}{(k_3^2 - k_1^2)(k_3^2 - k_2^2)(k_1^2 + k_2^2 + k_3^2)} \tag{50}$$

Multiproduct expansion as generator for Nyström algorithms (Application to Hamiltonian problems)

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

Every decomposition of $\mathrm{e}^{h(A+B)}$ *in the form of*

$$\sum_k c_k \prod_i \mathrm{e}^{a_{ki}hA}\mathrm{e}^{b_{ki}hB} = \mathrm{e}^{h(A+B)} + O(h^{n+1}), \tag{51}$$

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 nth-order Nyström integrator.*

The splitting $\mathcal{T}_3(h)$ 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 with four force-evaluations:

$$\begin{aligned} \mathbf{q} &= \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{192}\Big[23\mathbf{a}_0 + 75\mathbf{a}_{2/5} - 27\mathbf{a}_{2/3} \\ &\quad +25\mathbf{a}_{4/5}\Big] \qquad (52) \\ \mathbf{v} &= \mathbf{v}_0 + \frac{h}{192}\Big[23\mathbf{a}_0 + 125\mathbf{a}_{2/5} - 81\mathbf{a}_{2/3} + 125\mathbf{a}_{4/5}\Big], \qquad (53) \end{aligned}$$

Further we have given $\mathbf{a}_{i/k} = \mathbf{a}(\mathbf{q}_{i/k})$ with

$$\begin{aligned}
\mathbf{q}_{2/5} &= \mathbf{q}_0 + \frac{2}{5} h \mathbf{v}_0 + \frac{2}{25} h^2 \mathbf{a}_0 \\
\mathbf{q}_{2/3} &= \mathbf{q}_0 + \frac{2}{3} h \mathbf{v}_0 + \frac{2}{9} h^2 \mathbf{a}_0 \\
\mathbf{q}_{4/5} &= \mathbf{q}_0 + \frac{4}{5} h \mathbf{v}_0 + \frac{4}{25} h^2 (\mathbf{a}_0 + \mathbf{a}_{2/5})
\end{aligned} \tag{54}$$

Analytical and numerical verifications

In this section, we discuss the application of both the even and odd order MPE algorithms.

Remark

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.

Numerical Experiments

Example 1: Benchmark 10×10 ODE system (Starting kernel)
We deal in the first with an ODE and separate the complex operator in two simpler operators.
We deal with the 10×10 ODE system:

$$\partial_t u_1 = -\lambda_{1,1}(t) u_1 + \lambda_{2,1}(t) u_2 + \cdots + \lambda_{10,1}(t) u_{10}, \quad (55)$$

$$\partial_t u_2 = \lambda_{1,2}(t) u_1 - \lambda_{2,2}(t) u_2 + \cdots + \lambda_{10,2}(t) u_{10} \;, \quad (56)$$

$$\vdots \quad (57)$$

$$\partial_t u_{10} = \lambda_{1,10}(t) u_1 + \lambda_{2,10}(t) u_2 + \cdots - \lambda_{10,10}(t) u_{10} \;, \quad (58)$$

$$u_1(0) = u_{1,0}, \ldots, \; u_{10}(0) = u_{10,0} \text{ (initial conditions)} \;, \quad (59)$$

where $\lambda_{1,1}(t), \ldots, \lambda_{10,10}(t)$ are the decay factors and $u_{1,0}, \ldots, u_{10,0} \in \mathbb{R}^+$. We have the time-interval $t \in [0, T]$.

We rewrite the equation (55) in operator notation, we concentrate us to the following equations :

$$\partial_t u = A(t)u + B(t)u \,, \tag{60}$$

where $u_1(0) = u_{10} = 1.0$, $u_2(0) = u_{20} = 1.0$ are the initial conditions, where we have $\lambda_1(t) = t$ and $\lambda_2(t) = t^2$.
and our spitted operators are

$$A = \begin{pmatrix} -\lambda_{1,1}(t) & \dots & \lambda_{10,1}(t) \\ \lambda_{1,5}(t) & \dots & \lambda_{10,5}(t) \\ 0 & \dots & 0 \end{pmatrix} \,,\; B = \begin{pmatrix} 0 & 0 & \\ \lambda_{1,6}(t) & \dots & \lambda_{10,6}(t) \\ \lambda_{1,10}(t) & \dots & -\lambda_{10,10}(t) \end{pmatrix} \tag{61}$$

The parameters are given as:

$$\lambda_{1,1}(t) = 0.09\lambda_1(t), \lambda_{2,1}(t) = 0.01\lambda_2(t), \ldots, \lambda_{10,1}(t) = 0.01\lambda_2(t)$$

$$\vdots$$

$$\lambda_{1,10}(t) = 0.01\lambda_2(t), \ldots \lambda_{9,10}(t) = 0.01\lambda_2(t), \ldots, \lambda_{10,10}(t) = 0.09\lambda$$

The higher order schemes with method with a fourth order kernel is presented in Figure 1. We see the same bahaviour as for lower ODE systems. With higher order schemes, we can really accelerate the convergence rates to machine precision, which is about 10^{-13}. Accelarations are obtained with second order method.

We tested at least to 4th order kernel for the MPE method. Often higher order kernels are delicate to compute and fail in accuracy (Optimal are first and second order kernels).

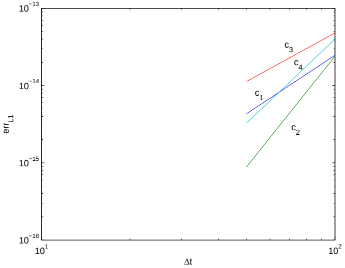

Figure: Numerical errors of the starting kernels (1st (A-B kernel), 2nd (Strang kernel), 3rd (Strang + Richardson), 4th ([Chin 2008]), x-axis: time, y-axis: max-error (we reach also accuracy of the computer).

Example 2: 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 [moan 2008] of

$$A(t) = \begin{pmatrix} 2 & t \\ 0 & -1 \end{pmatrix}. \tag{62}$$

The exact solution to (1) with $Y(0) = I$ is

$$Y(t) = \begin{pmatrix} e^{2t} & f(t) \\ 0 & e^{-t} \end{pmatrix}, \tag{63}$$

with

$$f(t) = \frac{1}{9} \mathrm{e}^{-t} (\mathrm{e}^{3t} - 1 - 3t) \quad (64)$$

$$= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} \quad (65)$$

$$+ \frac{31 t^8}{40320} + \frac{t^9}{6720} + \frac{13 t^{10}}{403200} + \frac{13 t^{11}}{178200} \quad (66)$$

For the Magnus expansion, one has the series

$$\Omega(t) = \begin{pmatrix} 2t & g(t) \\ 0 & -t \end{pmatrix}, \tag{67}$$

with, up to the 10th order,

$$g(t) = \frac{1}{2}t^2 - \frac{1}{4}t^3 + \frac{3}{80}t^5 - \frac{9}{1120}t^7 + \frac{81}{44800}t^9 + \cdots \tag{68}$$

$$\rightarrow \frac{t(\mathrm{e}^{3t} - 1 - 3t)}{3(\mathrm{e}^{3t} - 1)}. \tag{69}$$

Exponentiating (67) yields (63) with

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

$$\rightarrow t\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1)\left(\frac{1}{9t} - \frac{1}{3(\mathrm{e}^{3t} - 1)}\right) \tag{70}$$

The multi-product expansion suffers no such drawbacks. By setting $h = t$ and $t = 0$, we have

$$\mathcal{T}_2(t) = \exp\left[t \begin{pmatrix} 2 & \frac{1}{2}t \\ 0 & -1 \end{pmatrix}\right] = \begin{pmatrix} \mathrm{e}^{2t} & f_2(t) \\ 0 & \mathrm{e}^{-t} \end{pmatrix} \tag{71}$$

with

$$f_2(t) = \frac{1}{6} t\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1). \tag{72}$$

This is identical to first term of the Magnus series (70) and is an entire function of t. Since higher order MPE uses only powers of $\mathcal{T}_2$, higher order MPE approximations are also entire functions of t. Thus up to the 10th order, one finds

$$f_4(t) = t\mathrm{e}^{-t}\left(\frac{\mathrm{e}^{3t}-5}{18}+\frac{2\mathrm{e}^{3t/2}}{9}\right) \tag{73}$$

$$f_6(t) = t\mathrm{e}^{-t}\left(\frac{11\mathrm{e}^{3t}-109}{360}+\frac{9}{40}(\mathrm{e}^{2t}+\mathrm{e}^{t})-\frac{8}{45}\mathrm{e}^{3t/2}\right) \tag{74}$$

$$f_8(t) = t\mathrm{e}^{-t}\left(\frac{151\mathrm{e}^{3t} - 2369}{7560} + \frac{256}{945}(\mathrm{e}^{9t/4} + \mathrm{e}^{3t/4}) - \frac{81}{280}(\mathrm{e}^{2t} + \mathrm{e}^{t}) + \frac{104}{315}\mathrm{e}^{3t/2}\right) \quad (75)$$

$$f_{10}(t) = t\mathrm{e}^{-t}\left(\frac{15619\mathrm{e}^{3t} - 347261}{1088640} + \frac{78125}{217728}(\mathrm{e}^{12t/5} + \mathrm{e}^{9t/5} + \mathrm{e}^{6t/5} + \mathrm{e}^{3t/5}) - \frac{4096}{8505}(\mathrm{e}^{9t/4} + \mathrm{e}^{3t/4}) + \frac{729}{4480}(\mathrm{e}^{2t} + \mathrm{e}^{t}) - \frac{4192}{8505}\mathrm{e}^{3t/2}\right). \quad (76)$$

When expanded, the above yields

$$\begin{aligned} f_2(t) &= \frac{t^2}{2} + \frac{t^3}{4} + \cdots \\ f_4(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{5t^5}{192} + \cdots \\ f_6(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{384} + \cdots \end{aligned} \qquad (77)$$

$$
\begin{aligned}
f_8(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} \\
&\quad + \frac{1307t^9}{8601600} + \cdots \qquad (78) \\
f_{10}(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{t^9}{6720} \\
&\quad + \frac{13t^{10}}{403200} + \frac{13099t^{11}}{232243200} + \cdots \qquad (79)
\end{aligned}
$$

and agree with the exact solution to the claimed order.

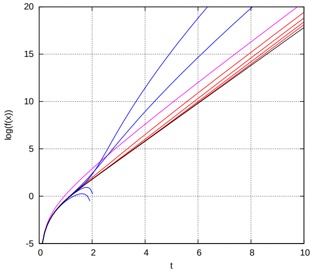

Figure: The black line is the exact result (64). The blue lines are the Magnus fourth to tenth order results (70), which diverge from the exact result beyond $t > 2$. The red lines are the multi-product expansions. The purple line is their common second order result.

Results:
The Magnus series (68) and (70) only converge for $|t| < \frac{2}{3}\pi$ due to the pole at $t = \frac{2}{3}\pi i$.
The MPE series convergences uniform for all t.

Experiment 3: The radial Schödinger equation
We consider the radial Schrödinger equation

$$\frac{\partial^2 u}{\partial r^2} = f(r, E)u(r) \tag{80}$$

where

$$f(r, E) = 2V(r) - 2E + \frac{l(l+1)}{r^2}\ , \tag{81}$$

By relabeling $r \to t$ and $u(r) \to q(t)$, (80) can be viewed as harmonic oscillator with a time dependent spring constant

$$k(t, E) = -f(t, E) \tag{82}$$

and Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}k(t, E)q^2. \quad (83)$$

Thus any eigenfunction of (80) is an exact time-dependent solution of (83). For example, the ground state of the hydrogen atom with $l = 0$, $E = -1/2$ and

$$V(r) = -\frac{1}{r} \quad (84)$$

yields the exact solution

$$q(t) = t \exp(-t) \quad (85)$$

with initial values $q(0) = 0$ and $p(0) = 1$.

Denoting

$$Y(t) = \left(\begin{array}{c} q(t) \\ p(t) \end{array} \right), \tag{86}$$

the time-dependent oscillator (83) now corresponds to

$$A(t) = \left(\begin{array}{cc} 0 & 1 \\ f(t) & 0 \end{array} \right) = \left(\begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array} \right) + \left(\begin{array}{cc} 0 & 0 \\ f(t) & 0 \end{array} \right) \equiv T + V(t), \tag{87}$$

with

$$f(t) = (1 - \frac{2}{t}). \tag{88}$$

In this case, the second-order midpoint algorithm is

$$\begin{aligned} \mathcal{T}_2(h,t) &= \mathrm{e}^{\frac{1}{2}hT}\mathrm{e}^{hV(t+h/2)}\mathrm{e}^{\frac{1}{2}hT} \\ &= \begin{pmatrix} 1+\frac{1}{2}h^2 f(t+\frac{1}{2}h) & h+\frac{1}{4}h^3 f(t+\frac{1}{2}h) \\ hf(t+\frac{1}{2}h) & 1+\frac{1}{2}h^2 f(t+\frac{1}{2}h), \end{pmatrix} \end{aligned} \tag{89}$$

and for $q(0)=0$ and $p(0)=1$, (setting $t=0$ and $h=t$), correctly gives the second order result,

$$q_2(t) = t + \frac{1}{4}t^3 f(\frac{1}{2}t) = t - t^2 + \frac{1}{4}t^3. \tag{90}$$

Higher order multi-product expansions, using (89), then yield

$$
\begin{aligned}
q_4(t) &= t - t^2 + \frac{7t^3}{18} - \frac{t^4}{9} + \frac{t^5}{96} \\
q_6(t) &= t - t^2 + \frac{211t^3}{450} - \frac{31t^4}{225} + \frac{17t^5}{600} + \cdots \\
q_8(t) &= t - t^2 + \frac{32233t^3}{66150} - \frac{5101t^4}{33075} + \frac{3139t^5}{88200} + \cdots \\
q_{10}(t) &= t - t^2 + \frac{88159t^3}{1786050} - \frac{143177t^4}{893025} + \frac{91753t^5}{2381400} + \cdots
\end{aligned}
$$

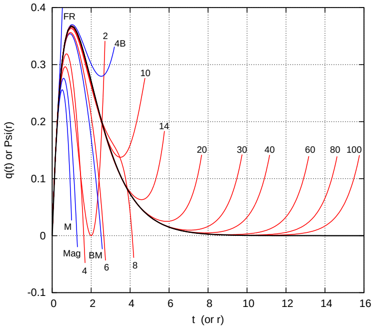

Figure: The uniform convergence of the multi-product expansion in solving for the hydrogen ground state wave function. (Black line: exact ground state wave function, The numbers indicates the order of the MPE. Blue lines: various fourth-order algorithms.

Remarks:
While wel-known higher order splitting method, as FR (Forest-Ruth 1990, 3 force-evaluations), M (McLachlan 1995, 4 force-evaluations), BM (Blanes-Moan 2002, 6 force-evaluations), Mag4 (Magnus integrator, see below, ≈ 2.5 force-evaluations) leaks with the accuracy, MPE series up to the 100th order, matches against the exact solution and 4B [Chin 2006] (a *forward* symplectic algorithm with only ≈ 2 evaluations).

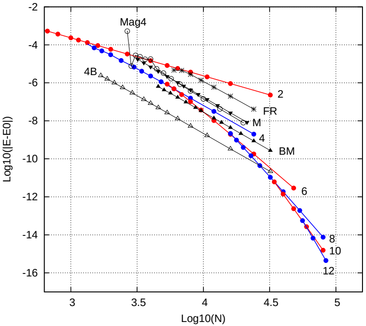

Figure: A precision-effort comparison of various fourth-order algorithms with that of MPE for computing the ground state of a spiked harmonic oscillator. N is the number of force-evaluations.

Conclusions

- Alternative method: MPE of operators together with Suzuki's rule of incorporating the time-ordered exponential for solving differential equations
- MPE method is compared with Magnus expansion with different kernels and found that MPE converges uniformly.
- MPE requires far less operators at higher orders than either the Magnus series or conventional exponential-splitting.

In the future we will focus on applying MPE method for solving nonlinear differential equations and applications to advection-diffusion problems (next adjoint work with S.Chin).