An Algorithm for Computing Coefficients of Words in Expressions Involving Exponentials and Its Application to the Construction of Exponential Integrators

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Derivation and implementation of the algorithm

Non-commutative symbols, words

- $\mathcal{A}$ ... "alphabet" = set of non-commutative symbols, e.g.,

  $$\mathcal{A} = \{\mathtt{A}, \mathtt{B}\} \text{ or } \mathcal{A} = \{\mathtt{A}_1, \mathtt{A}_2, \dots\}$$

  In Maple:

  ```
  > Physics[Setup](noncommutativeprefix = {A, B});
  ```

- Word = product of non-commutative symbols
  $\mathcal{A}^*$ ... set of all words over alphabet $\mathcal{A}$, e.g.,

  $$\mathrm{Id}, \mathtt{A}, \mathtt{AB}, \mathtt{BA}, \mathtt{BBB} \in \{\mathtt{A}, \mathtt{B}\}^*$$

  Id ... empty word

Expressions involving exponentials

- Example:

$$X = \mathrm{e}^{\frac{1}{2}\mathtt{B}}\mathrm{e}^{\mathtt{A}}\mathrm{e}^{\frac{1}{2}\mathtt{B}} - \mathrm{e}^{\mathtt{A}+\mathtt{B}}$$

  (relevance of this example will be discussed later)
  Exponential function defined by its formal power series

$$\mathrm{e}^{Y} = \exp(Y) = \sum_{n=0}^{\infty} \frac{1}{n!} Y^n$$

- Formal expansion into a series of words:

$$X = \sum_{w \in \mathcal{A}^*} c_w w$$

  $X \in \mathbb{C}\langle\langle\mathcal{A}\rangle\rangle$ ... algebra of formal power series in the non-commutative variables $\in \mathcal{A}$

- How calculate coefficients $c_w = \mathrm{coeff}(w, X)$, $w \in \mathcal{A}^*$?

A family of homomorphisms

- For each word $w = w_1 \cdots w_{\ell(w)} \in \mathcal{A}^*$ of length $\ell(w)$ define map
$$\varphi_w : \mathbb{C}\langle\langle\mathcal{A}\rangle\rangle \to \mathbb{C}^{(\ell(w)+1)\times(\ell(w)+1)}$$
by
$$\varphi_w(X)_{i,j} = \begin{cases} \mathrm{coeff}(w_{i:j-1}, X), & \text{if } i < j, \\ \mathrm{coeff}(\mathrm{Id}, X), & \text{if } i = j, \\ 0, & \text{if } i > j \end{cases}$$
Here, $w_{i:j-1} = w_i w_{i+1} \cdots w_{j-1}$ = subword of w of length $j-i$, starting at position i and ending at position $j-1$
- φ_w is *algebra homomorphism*:
$$\varphi_w(\alpha X + \beta Y) = \alpha\varphi_w(X) + \beta\varphi_w(Y), \quad X, Y \in \mathbb{C}\langle\langle\mathcal{A}\rangle\rangle,\ \alpha, \beta \in \mathbb{C}$$
$$\varphi_w(X \cdot Y) = \varphi_w(X) \cdot \varphi_w(Y), \quad X, Y \in \mathbb{C}\langle\langle\mathcal{A}\rangle\rangle$$
- Furthermore, if $\mathrm{coeff}(\mathrm{Id}, X) = 0$, then
$$\varphi_w(\exp X) = \exp \varphi_w(X)$$
Here, $\varphi_w(X)$ ... strictly upper triangular $\Rightarrow$ nilpotent $\Rightarrow$ Its exponential exactly computable in a finite number of steps

A family of homomorphisms, example

$$\varphi_{\mathtt{AAB}}(\mathrm{e}^{\frac{1}{2}\mathtt{B}}\,\mathrm{e}^{\mathtt{A}}\,\mathrm{e}^{\frac{1}{2}\mathtt{B}}) = \exp\left(\tfrac{1}{2}\varphi_{\mathtt{AAB}}(\mathtt{B})\right)\cdot\exp\left(\varphi_{\mathtt{AAB}}(\mathtt{A})\right)\cdot\exp\left(\tfrac{1}{2}\varphi_{\mathtt{AAB}}(\mathtt{B})\right)$$

$$= \exp\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \end{pmatrix}\cdot\exp\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\cdot\exp\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}\cdot\begin{pmatrix} 1 & 1 & \frac{1}{2} & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\cdot\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 1 & \frac{1}{2} & \frac{1}{4} \\ 0 & 1 & 1 & \frac{1}{2} \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} c_{\mathrm{Id}} & c_{\mathtt{A}} & c_{\mathtt{AA}} & c_{\mathtt{AAB}} \\ 0 & c_{\mathrm{Id}} & c_{\mathtt{A}} & c_{\mathtt{AB}} \\ 0 & 0 & c_{\mathrm{Id}} & c_{\mathtt{B}} \\ 0 & 0 & 0 & c_{\mathrm{Id}} \end{pmatrix}$$

Similar calculations involving $\varphi_w(\mathrm{e}^{\frac{1}{2}\mathtt{B}}\,\mathrm{e}^{\mathtt{A}}\,\mathrm{e}^{\frac{1}{2}\mathtt{B}})$ for $w \in \{\mathtt{AAA}, \mathtt{AAB}, \mathtt{ABA}, \mathtt{BAA}, \mathtt{ABB}, \mathtt{BAB}, \mathtt{BBA}, \mathtt{BBB}\}$ yield

$$\mathrm{e}^{\frac{1}{2}\mathtt{B}}\,\mathrm{e}^{\mathtt{A}}\,\mathrm{e}^{\frac{1}{2}\mathtt{B}} = \mathrm{Id} + \mathtt{A} + \mathtt{B} + \tfrac{1}{2}\mathtt{AA} + \tfrac{1}{2}\mathtt{AB} + \tfrac{1}{2}\mathtt{BA} + \tfrac{1}{2}\mathtt{BB}$$
$$+ \tfrac{1}{6}\mathtt{AAA} + \tfrac{1}{4}\mathtt{AAB} + \tfrac{1}{4}\mathtt{BAA} + \tfrac{1}{8}\mathtt{ABB} + \tfrac{1}{4}\mathtt{BAB} + \tfrac{1}{8}\mathtt{BBA} + \tfrac{1}{6}\mathtt{BBB} + \dots,$$

where dots represent terms involving words of length > 3

A family of homomorphisms, example

Similarly, calculations like

$$\begin{aligned}\varphi_{\mathtt{AAB}}(\mathrm{e}^{\mathtt{A}+\mathtt{B}}) &= \exp\left(\varphi_{\mathtt{AAB}}(\mathtt{A}) + \varphi_{\mathtt{AAB}}(\mathtt{B})\right) \\ &= \exp\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 1 & \frac{1}{2} & \frac{1}{6} \\ 0 & 1 & 1 & \frac{1}{2} \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}\end{aligned}$$

lead to

$$\begin{aligned}\mathrm{e}^{\mathtt{A}+\mathtt{B}} &= \mathrm{Id} + \mathtt{A} + \mathtt{B} + \tfrac{1}{2}\mathtt{AA} + \tfrac{1}{2}\mathtt{AB} + \tfrac{1}{2}\mathtt{BA} + \tfrac{1}{2}\mathtt{BB} \\ &\quad + \tfrac{1}{6}\mathtt{AAA} + \tfrac{1}{6}\mathtt{AAB} + \tfrac{1}{6}\mathtt{ABA} + \tfrac{1}{6}\mathtt{BAA} + \tfrac{1}{6}\mathtt{ABB} + \tfrac{1}{6}\mathtt{BAB} + \tfrac{1}{6}\mathtt{BBA} + \tfrac{1}{6}\mathtt{BBB} + \dots\end{aligned}$$

and thus

$$\begin{aligned}&\mathrm{e}^{\frac{1}{2}\mathtt{B}}\,\mathrm{e}^{\mathtt{A}}\,\mathrm{e}^{\frac{1}{2}\mathtt{B}} - \mathrm{e}^{\mathtt{A}+\mathtt{B}} \\ &\qquad = \tfrac{1}{12}\mathtt{AAB} - \tfrac{1}{6}\mathtt{ABA} + \tfrac{1}{12}\mathtt{BAA} - \tfrac{1}{24}\mathtt{ABB} + \tfrac{1}{12}\mathtt{BAB} - \tfrac{1}{24}\mathtt{BBA} + \dots \\ &\qquad = \tfrac{1}{12}[\mathtt{A},[\mathtt{A},\mathtt{B}]] - \tfrac{1}{24}[[\mathtt{A},\mathtt{B}],\mathtt{B}] + \dots\end{aligned}$$

Here, terms of length < 3 cancel, terms of length 3 can be written as Lie polynomial

Maple implementation

$\mathrm{coeff}(w, X)$ is the entry of $\varphi_w(X)$ in the upper right corner:

$$\mathrm{coeff}(w, X) = \varphi_w(X)_{1,\ell(w)+1}$$

Implement Maple function `phiv` which computes

$$\texttt{phiv}(w, X, v) = \varphi_w(X) \cdot v \text{ for vector } v \in \mathbb{C}^{\ell(w)+1}$$

without explicitly generating the matrix $\varphi_w(X)$. Then

$$\mathrm{coeff}(w, X) = \text{first component of } \texttt{phiv}(w, X, (0, \dots, 0, 1)^T)$$

`phiv` recursively traverses expression tree representing expression X
Evaluation branches out depending on whether current node represents

- a non-commutative symbol (the atomic case which terminates the recursion)
- a sum of subexpressions
- a product of subexpressions
- a power of a subexpression
- a commutator of subexpressions, or
- an exponential of a subexpression

Maple implementation

```
> phiv := proc (w, X, v)
    local i, v1, v2, f, zero;
    if type(X, name) and type(X, noncommutative) then
        return [seq(`if`(op(i,w)=X, v[i+1], 0),
                i=1..nops(w)), 0]
    elif type(X, `+`) then
        return add(phiv(w, op(i, X), v), i=1..nops(X))
    elif type(X, `*`) then
        v1 := v; zero := [0$nops(w)+1];
        for i from nops(X) to 1 by -1 do
            v1 := phiv(w, op(i, X), v1);
            if v1=zero then return zero end if;
        end do;
        return v1
    elif type(X, anything^integer) then
        v1 := v; zero := [0$nops(w)+1];
        for i from 1 to op(2, X) do
            v1 := phiv(w, op(1, X), v1);
            if v1=zero then return zero end if;
        end do;
        return v1
    elif (type(X, function) and
          op(0, X) = Physics[Commutator]) then
        return phiv(w, op(1, X), phiv(w, op(2, X), v))
             - phiv(w, op(2, X), phiv(w, op(1, X), v))
    elif type(X, exp(anything)) then
        v1 := v; v2 := v; zero := [0$nops(w)+1]; f := 1;
        for i from 1 to nops(w) do
            f := f*i; v1 := phiv(w, op(X), v1);
            if v1=zero then return v2 end if;
            v2 := v2 + v1/f;
        end do;
        return v2
    end if;
    return [seq(X*x, x=v)]
  end proc:
```

```
> wcoeff := proc (w, X)
    return phiv(w, X, [0$nops(w), 1])[1]
  end proc:
```

Derivation of order conditions for the construction of exponential integrators

Exponential integrators

- Example: evolution equation of the form

$$\partial_t u(t) = Au(t) + Bu(t)$$

We already obtained

$$\mathrm{e}^{\frac{1}{2}\mathtt{B}}\,\mathrm{e}^{\mathtt{A}}\,\mathrm{e}^{\frac{1}{2}\mathtt{B}} - \mathrm{e}^{\mathtt{A}+\mathtt{B}} = \tfrac{1}{12}[\mathtt{A},[\mathtt{A},\mathtt{B}]] - \tfrac{1}{24}[[\mathtt{A},\mathtt{B}],\mathtt{B}] + \dots$$

Substitute $\mathtt{A} \simeq \tau A = O(\tau)$, $\mathtt{B} \simeq \tau B = O(\tau)$ $\rightsquigarrow$

$$\mathrm{e}^{\frac{1}{2}\tau B}\,\mathrm{e}^{\tau A}\,\mathrm{e}^{\frac{1}{2}\tau B} = \mathrm{e}^{\tau(A+B)} + O(\tau^3)$$

$\rightsquigarrow$ 2nd order Strang splitting; τ … *step-size*

- More generally, consider expressions of the form

$$X = \mathrm{e}^{\Phi_J}\cdots\mathrm{e}^{\Phi_1} - \mathrm{e}^{\Omega}$$

$\Phi_1, \dots, \Phi_J$, and Ω … linear combinations of non-commutative symbols $\in \mathcal{A}$ and commutators thereof (=Lie polynomials)
$\mathrm{e}^{\Phi_J}\cdots\mathrm{e}^{\Phi_1}$ … exponential integrator
e^{Ω} … exact local solution operator
X … local error

Grading of words and homogeneous Lie elements, free graded Lie algebra

- Symbols $\in \mathcal{A}$ represent objects depending on parameter τ
  Choose grading function on $\mathcal{A}$

$$\mathrm{grade}(a) \in \{1, 2, \dots\}, \quad a \in \mathcal{A}$$

  such that it reflects order of magnitude of represented objects:

$$a \simeq O(\tau^{\mathrm{grade}(a)}), \quad a \in \mathcal{A}$$

- Extension to words:

$$\mathrm{grade}(w) = \sum_{j=1}^{\ell(w)} \mathrm{grade}(w_j), \quad w = w_1 \dots w_{\ell(w)} \in \mathcal{A}^*$$

- Lie element is called *homogeneous Lie element of grade q* if it can be expanded into linear combination of words of grade q
  $\rightsquigarrow$ free graded Lie algebra generated by $\mathcal{A}$:

$$[\mathbb{C}\langle\mathcal{A}\rangle] = \bigoplus_{q=1}^{\infty} \mathfrak{g}_q, \ \mathfrak{g}_q = \{\text{homogeneous Lie elements of grade } q\}$$

Leading error term

- **Theorem:** $\Phi_1, \ldots, \Phi_J, \Omega$ ... Lie polynomials in variables $\mathcal{A}$
  Expansion into series of words:

$$\mathrm{e}^{\Phi_J} \cdots \mathrm{e}^{\Phi_1} - \mathrm{e}^{\Omega} = \sum_{w \in \mathcal{A}^*} c_w w = \Theta + R$$

  $q_{\min}$ ... minimal q such that $\exists$ terms $c_w w, c_w \neq 0$ of grade q
  Θ contains terms of minimal grade $q_{\min}$
  R contains terms of grade $> q_{\min}$
  Then: Θ representing the *leading error term* is a *homogeneous Lie element of grade* $q_{\min}$

- $\mathrm{e}^{\Phi_J} \cdots \mathrm{e}^{\Phi_1}$ *self-adjoint* (symmetric) if for

$$\Phi_j = \sum_k X_{j,k}, \;\; X_{j,k} \in \mathfrak{g}_k : \quad \Phi_{J-j+1} = \sum_k (-1)^{k+1} X_{j,k}$$

  Conforms with the usual definition of an self-adjoint exponential integrator

  Lemma: $\mathrm{e}^{\Phi_J} \cdots \mathrm{e}^{\Phi_1}$ and e^{Ω} self-adjoint $\Rightarrow$ $q_{\min}$ odd

Leading error term (representation in a basis)

- Representation of homogeneous Lie element of grade q in a basis $\mathcal{B}_q$ of $\mathfrak{g}_q$:

$$\Theta = \sum_{b\in\mathcal{B}_q} c_b\, b$$

  How compute coefficients c_b ?

- $\mathcal{W}_q$ ... set of words of grade q such that matrix

$$T_q = (\mathrm{coeff}(w,b))_{w\in\mathcal{W}_q, b\in\mathcal{B}_q}$$

  is invertible

- From $c_w = \mathrm{coeff}(w,\Theta) = \sum_{b\in\mathcal{B}_q} c_b\, \mathrm{coeff}(w,b)$ for $w\in\mathcal{W}_q$ it follows

$$(c_w)_{w\in\mathcal{W}_q} = T_q\cdot (c_b)_{b\in\mathcal{B}_q}$$

  and thus

$$(c_b)_{b\in\mathcal{B}_q} = T_q^{-1}\cdot (c_w)_{w\in\mathcal{W}_q}$$

- Suitable choices for $\mathcal{W}_q$, $\mathcal{B}_q$: *Lyndon words* of grade q and corresponding *Lyndon basis*

Lyndon words and Lyndon bases

$\mathcal{W}_q$ and $\mathcal{B}_q$ for $\mathcal{A} = \{\mathtt{A}, \mathtt{B}\}$ and $\mathrm{grade}(\mathtt{A}) = \mathrm{grade}(\mathtt{B}) = 1$:

q	Lyndon words $\mathcal{W}_q$	Lyndon basis $\mathcal{B}_q$
1	A, B	A, B
2	AB	$[\mathtt{A}, \mathtt{B}]$
3	AAB, ABB	$[\mathtt{A}, [\mathtt{A}, \mathtt{B}]]$, $[[\mathtt{A}, \mathtt{B}], \mathtt{B}]$
4	AAAB, AABB, ABBB	$[\mathtt{A}, [\mathtt{A}, [\mathtt{A}, \mathtt{B}]]]$, $[\mathtt{A}, [[\mathtt{A}, \mathtt{B}], \mathtt{B}]]$, $[[[\mathtt{A}, \mathtt{B}], \mathtt{B}], \mathtt{B}]$
5	AAAAB, AAABB, AABAB, AABBB, ABABB, ABBBB	$[\mathtt{A}, [\mathtt{A}, [\mathtt{A}, [\mathtt{A}, \mathtt{B}]]]]$, $[\mathtt{A}, [\mathtt{A}, [[\mathtt{A}, \mathtt{B}], \mathtt{B}]]]$, $[[\mathtt{A}, [\mathtt{A}, \mathtt{B}]], [\mathtt{A}, \mathtt{B}]]$, $[\mathtt{A}, [[[\mathtt{A}, \mathtt{B}], \mathtt{B}], \mathtt{B}]]$, $[[\mathtt{A}, \mathtt{B}], [[\mathtt{A}, \mathtt{B}], \mathtt{B}]]$, $[[[[\mathtt{A}, \mathtt{B}], \mathtt{B}], \mathtt{B}], \mathtt{B}]$

$\mathcal{W}_q$ and $\mathcal{B}_q$ for $\mathcal{A} = \{\mathtt{A}_1, \ldots, \mathtt{A}_q\}$ and $\mathrm{grade}(\mathtt{A}_k) = k$:

q	Lyndon words $\mathcal{W}_q$	Lyndon basis $\mathcal{B}_q$
1	$\mathtt{A}_1$	$\mathtt{A}_1$
2	$\mathtt{A}_2$	$\mathtt{A}_2$
3	$\mathtt{A}_1\mathtt{A}_2$, $\mathtt{A}_3$	$[\mathtt{A}_1, \mathtt{A}_2]$, $\mathtt{A}_3$
4	$\mathtt{A}_1\mathtt{A}_1\mathtt{A}_2$, $\mathtt{A}_1\mathtt{A}_3$, $\mathtt{A}_4$	$[\mathtt{A}_1, [\mathtt{A}_1, \mathtt{A}_2]]$, $[\mathtt{A}_1, \mathtt{A}_3]$, $\mathtt{A}_4$
5	$\mathtt{A}_1\mathtt{A}_1\mathtt{A}_1\mathtt{A}_2$, $\mathtt{A}_1\mathtt{A}_1\mathtt{A}_3$, $\mathtt{A}_1\mathtt{A}_2\mathtt{A}_2$, $\mathtt{A}_1\mathtt{A}_4$, $\mathtt{A}_2\mathtt{A}_3$, $\mathtt{A}_5$	$[\mathtt{A}_1, [\mathtt{A}_1, [\mathtt{A}_1, \mathtt{A}_2]]]$, $[\mathtt{A}_1, [\mathtt{A}_1, \mathtt{A}_3]]$, $[[\mathtt{A}_1, \mathtt{A}_2], \mathtt{A}_2]$, $[\mathtt{A}_1, \mathtt{A}_4]$, $[\mathtt{A}_2, \mathtt{A}_3]$, $\mathtt{A}_5$

Order conditions

- **Theorem:** If for Lie elements $\Phi_1, \dots, \Phi_J, \Omega$ the *order conditions*

$$\operatorname{coeff}(w, \mathrm{e}^{\Phi_J} \cdots \mathrm{e}^{\Phi_1} - \mathrm{e}^{\Omega}) = 0, \quad w \in \bigcup_{q=1}^{p} \mathcal{W}_q$$

  are satisfied for all *Lyndon words* of grade $q \leq p$, then these equations are satisfied for *all words* $w \in \mathcal{A}^*$ of grade $\leq p$
- For $\mathrm{e}^{\Phi_J} \cdots \mathrm{e}^{\Phi_1}$ and e^{Ω} self-adjoint the Theorem holds already if the order conditions are satisfied only for all Lyndon words of *odd* grade $q \leq p$, and we may assume p is odd
- Recall: symbols $\in \mathcal{A}$ represent objects depending on small parameter τ such that

$$a \simeq O(\tau^{\mathrm{grade}(a)}), \quad a \in \mathcal{A}$$

  The conclusion of the Theorem states that

$$\mathrm{e}^{\Phi_J} \cdots \mathrm{e}^{\Phi_1} - \mathrm{e}^{\Omega} = O(\tau^{p+1})$$

  i.e., $\mathrm{e}^{\Phi_J} \cdots \mathrm{e}^{\Phi_1}$ is an approximation of e^{Ω} of order $p+1$

Order conditions, example

Wanted: $a, b, c, d \in \mathbb{R}$ such that $\mathrm{e}^{b\mathtt{B}}\mathrm{e}^{a\mathtt{A}}\mathrm{e}^{c\mathtt{B}+d[\mathtt{B},[\mathtt{A},\mathtt{B}]]}\mathrm{e}^{a\mathtt{A}}\mathrm{e}^{b\mathtt{B}}$ is a 5th order approximation of $\mathrm{e}^{\mathtt{A}+\mathtt{B}}$

$\mathcal{A} = \{\mathtt{A}, \mathtt{B}\}$; $\mathtt{A}, \mathtt{B}$ both have grade 1 corresponding to $\mathtt{A}, \mathtt{B} \simeq O(\tau)$

Both expressions self-adjoint $\rightsquigarrow$ Lyndon words of odd length ≤ 4:

$$\mathcal{W} = \mathcal{W}_1 \cup \mathcal{W}_3 = \{\mathtt{A}, \mathtt{B}, \mathtt{AAB}, \mathtt{ABB}\}$$

```
> Physics[Setup](noncommutativeprefix = {A, B}):
> C := Physics[Commutator]:
> X := exp(b*B)*exp(a*A)*exp(c*B+d*C(B, C(A, B)))*
       exp(a*A)*exp(b*B) - exp(A+B):
> W := [[A], [B], [A, A, B], [A, B, B]]:
> eqs := [seq(simplify(wcoeff(w, X)), w in W)];
```

$$eqs := \left[-1 + 2a, -1 + 2b + c, -\frac{1}{6} + 2a^2 b + \frac{1}{2}a^2 c, -\frac{1}{6} + \frac{1}{2}ac^2 + acb + ab^2 - c\right.$$

```
> sol := solve(eqs);
```

$$sol := \left\{a = \frac{1}{2}, b = \frac{1}{6}, c = \frac{2}{3}, d = \frac{1}{72}\right\}$$

Non-trivial application: Construction of 8th order commutator-free Magnus-type integrators involving only 8 exponentials

Magnus-type integrators

Non-autonomous evolution equation:

$$\partial_t u(t) = A(t)u(t), \quad t \geq t_0, \quad u(t_0) = u_0, \quad A(t) \in \mathbb{C}^{d\times d}$$

One step $(t_n, u_n) \mapsto (t_{n+1}, u_{n+1})$ of step-size τ:

$$t_{n+1} = t_n + \tau, \quad u_{n+1} = \mathcal{S}(\tau, t_n)u_n,$$

where $\mathcal{S}(\tau, t_n) \approx \mathcal{E}(\tau, t_n)$ approximates exact local solution operator

$$\mathcal{E}(\tau, t_n) = \mathrm{e}^{\Omega(\tau, t_n)}$$

involving the *Magnus series* $\Omega = \Omega(\tau, t_n)$

Legendre Expansions

Expansion of $A(t_n + t)$ on interval $[t_n, t_n + \tau]$ into a series of shifted Legendre polynomials:

$$A(t_n + t) = A_1 \tilde{P}_0(t) + A_2 \tilde{P}_1(t) + A_3 \tilde{P}_2(t) + \dots, \quad t \in [0, \tau]$$

with

$$\tilde{P}_k(t) = \frac{1}{\tau} P_k\left(\frac{t}{\tau}\right), \quad P_k(x) = (-1)^k \sum_{j=0}^{k} \binom{k}{j} \binom{k+j}{j} (-1)^j x^j$$

Matrix-valued coefficients A_k given by

$$A_k = (2k-1)\tau \int_0^1 P_{k-1}(x) A(t_n + \tau x)\,\mathrm{d}x$$

depend on both t_n and τ and satisfy

$$A_k = O(\tau^k)$$

Magnus series in terms of these coefficients:

$$\begin{aligned}\Omega \;=\; & A_1 - \tfrac{1}{6}[A_1, A_2] + \tfrac{1}{60}[A_1, [A_1, A_3]] - \tfrac{1}{60}[A_2, [A_1, A_2]] \\ & + \tfrac{1}{360}[A_1, [A_1, [A_1, A_2]]] - \tfrac{1}{30}[A_2, A_3] + \dots .\end{aligned}$$

Order conditions for Magnus-type integrators

- Magnus-type integrator: Exponential integrator of the form

$$\mathcal{S}(\tau, t_n) = \mathrm{e}^{\widetilde{\Phi}_J(\tau,t_n)} \dots \mathrm{e}^{\widetilde{\Phi}_1(\tau,t_n)}$$

  $\widetilde{\Phi}_j$ ... linear combinations of (commutators of) $\widetilde{A}_k \approx A_k$
  $\widetilde{A}_k$ obtained by numerical approximation of the integral defining A_k

- $\mathcal{S}(\tau, t_n)$ formally corresponds to

$$S = \mathrm{e}^{\Phi_J} \cdots \mathrm{e}^{\Phi_1}$$

  Φ_j... Lie elements over alphabet $\mathcal{A} = \{\mathtt{A}_1, \mathtt{A}_2, \dots\}$
  with symbols $\mathtt{A}_k$ representing $\widetilde{A}_k \approx A_k$ and

$$\mathrm{grade}(\mathtt{A}_k) = k \text{ conforming to } A_k = O(\tau^k)$$

Order conditions for Magnus-type integrators (continued)

- Order conditions as in the Theorem:

$$\mathrm{coeff}(w, \mathrm{e}^{\Phi_J} \cdots \mathrm{e}^{\Phi_1}) - \mathrm{coeff}(w, \mathrm{e}^{\Omega}) = 0, \quad w \in \bigcup_{q=1}^{p} \mathcal{W}_q$$

  Have to hold for all *Lyndon words* of grade $\leq p$ over the alphabet $\mathcal{A} = \{\mathtt{A}_1, \mathtt{A}_2, \dots\}$ with $\mathrm{grade}(\mathtt{A}_k) = k$
  $\rightsquigarrow$ Magnus-type integrator of (global) order p
  (*local* order $p+1 \Rightarrow$ *global* order p)

- Explicit formula for $\mathrm{coeff}(w, \mathrm{e}^{\Omega})$:

$$\mathrm{coeff}(\mathtt{A}_{d_1} \cdots \mathtt{A}_{d_\ell}, \mathrm{e}^{\Omega}) = \sum_{\substack{(k_1,\dots,k_\ell) \\ 1 \leq k_l \leq d_l}} \prod_{j=1}^{\ell} \frac{(-1)^{d_j+k_j} \binom{d_j-1}{k_j-1} \binom{d_j+k_j-2}{k_j-1}}{\sum_{i=j}^{\ell} k_i}$$

- $\mathrm{coeff}(w, \mathrm{e}^{\Omega}) = 0$ if $\mathrm{grade}(w) \leq p$ and w contains $\mathtt{A}_d$ with $d \geq \frac{p}{2} + 1$ (due to orthogonality of Legendre polynomials)

8th order commutator-free Magnus-type integrator

- Self-adjoint ansatz with 8 exponentials involving $\mathtt{A}_1, \mathtt{A}_2, \mathtt{A}_3, \mathtt{A}_4$:

```
> Physics[Setup](noncommutativeprefix = {A}):
> S := exp(f11*A1-f12*A2+f13*A3-f14*A4)*
       exp(f21*A1-f22*A2+f23*A3-f24*A4)*
       exp(f31*A1-f32*A2+f33*A3-f34*A4)*
       exp(f41*A1-f42*A2+f43*A3-f44*A4)*
       exp(f41*A1+f42*A2+f43*A3+f44*A4)*
       exp(f31*A1+f32*A2+f33*A3+f34*A4)*
       exp(f21*A1+f22*A2+f23*A3+f24*A4)*
       exp(f11*A1+f12*A2+f13*A3+f14*A4):
```

- 22 Lyndon words of odd grade over $\mathcal{A} = \{\mathtt{A}_1, \mathtt{A}_2, \mathtt{A}_3, \mathtt{A}_4\}$
  $\rightsquigarrow$ 22 order conditions for $p = 8$
  BUT: only 16 unknowns `f11`, ..., `f44`

  Remarkable that this over-determined system of polynomial equations has solutions

  Theoretical explanation for this fact available

8th order commutator-free Magnus-type integrator (cont.)

- Order conditions corresponding to Lyndon words involving A_1, A_2:

```
> W12 := [[A1], [A1, A2], [A1, A1, A1, A2], [A1, A2, A2],
          [A1, A1, A1, A1, A1, A2], [A1, A1, A1, A2, A2],
          [A1, A1, A2, A1, A2], [A1, A2, A2, A2]]:
> rhs12 := [1, -1/6, -1/40, 1/60, -1/1008, 1/420, 1/2520, -1
> eqs12 := [seq(expand(wcoeff(w, S)), w in W12)] - rhs12:
```

- Standard Maple function `solve` finds a symbolic representation of the general solution of the system:

```
> vars12 := [f11, f21, f31, f41, f12, f22, f32, f42]:
> sols12 := solve(eqs12, vars12):
```

- All possible values in numerical form (very high precision needed!):

```
> Digits := 200:
> FF := seq(evalf(allvalues(sol)), sol in sols12):
```

  99 solutions altogether, 17 real

  Each parameter set `f11`, `f21`, `f31`, `f41`, `f12`, `f22`, `f32`, `f42` corresponding to any of these solutions can be extended to a full parameter set satisfying the remaining order conditions

8th order commutator-free Magnus-type integrator (cont.)

In

$$S = \prod_{j=8,\dots,1} \exp\Big(\sum_{k=1}^{4} f_{j,k}\mathtt{A}_k\Big)$$

substitute

$$\mathtt{A}_k \simeq (2k-1)\tau \int_0^1 P_{k-1}(x) A(t_n + \tau x)\,\mathrm{d}x$$

by

$$(2k-1)\tau \sum_{l=1}^{K} w_k P_{k-1}(x_l) A(t_n + \tau x_l)$$

with Gaussian quadrature nodes and weights of order 8

$$(x_k) = \left(\tfrac{1}{2} - \sqrt{\tfrac{15+2\sqrt{30}}{140}},\ \tfrac{1}{2} - \sqrt{\tfrac{15-2\sqrt{30}}{140}},\ \tfrac{1}{2} + \sqrt{\tfrac{15-2\sqrt{30}}{140}},\ \tfrac{1}{2} + \sqrt{\tfrac{15+2\sqrt{30}}{140}}\right),$$

$$(w_k) = \left(\tfrac{1}{4} - \tfrac{\sqrt{30}}{72},\ \tfrac{1}{4} + \tfrac{\sqrt{30}}{72},\ \tfrac{1}{4} + \tfrac{\sqrt{30}}{72},\ \tfrac{1}{4} - \tfrac{\sqrt{30}}{72}\right)$$

8th order commutator-free Magnus-type integrator (cont.)

We obtain 8th order commutator-free Magnus-type integrator involving 8 exponentials:

$$\mathcal{S}(t_n, \tau) = \prod_{j=8,\dots,1} \exp\left(\tau \sum_{k=1}^{4} a_{j,k} A(t_n + \tau x_k)\right)$$

with coefficients $a_{j,k}$ given by:

$k=1$	$k=2$	$k=3$	$k=4$
-1.232611007291861933e+0	1.381999278877963415e-1	-3.352921035850962622e-2	6.861942424401394962e-3
1.452637092757343214e+0	-1.632549976033022450e-1	3.986114827352239259e-2	-8.211316003097062961e-3
-1.783965547974815151e-2	-8.850494961553933912e-2	-1.299159096777419811e-2	4.448254906109529464e-3
-2.982838328015747208e-2	4.530735723950198008e-1	-6.781322579940055086e-3	-1.529505464262590422e-3
-1.529505464262590422e-3	-6.781322579940055086e-3	4.530735723950198008e-1	-2.982838328015747208e-2
4.448254906109529464e-3	-1.299159096777419811e-2	-8.850494961553933912e-2	-1.783965547974815151e-2
-8.211316003097062961e-3	3.986114827352239259e-2	-1.632549976033022450e-1	1.452637092757343214e+0
6.861942424401394962e-3	-3.352921035850962622e-2	1.381999278877963415e-1	-1.232611007291861933e+0

https://github.com/HaraldHofstaetter/Expocon.mpl

Thank you for your attention!