EXPLICIT MAGNUS EXPANSIONS FOR NONLINEAR EQUATIONS

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...joint work with

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Outline of the talk

1. Introduction: Magnus for linear equations

2. Magnus expansion for nonlinear problems
   a) General case
   b) Isospectral flows

3. Numerical integrators
   a) New methods
   b) Special methods for (QL)IF
   c) Numerical example

4. Application to highly oscillatory problems
1 Magnus for linear equations

Let us consider a linear matrix ODE evolving in a Lie group $\mathcal{G}$

\[ Y' = A(t)Y, \quad Y(t_0) = Y_0 \in \mathcal{G} \]  

(0)

with $A : [t_0, \infty[ \times \mathcal{G} \rightarrow \mathfrak{g}$ smooth enough.

$\mathfrak{g}$: Lie algebra associated with $\mathcal{G}$

Examples of $\mathcal{G}$: $\text{SL}(n)$, $\text{O}(n)$, $\text{SU}(n)$, $\text{Sp}(n)$, $\text{SO}(n)$, ...

$Y(t) \in \text{Lie group } \mathcal{G}$ if $A(t) \in \text{Lie algebra } \mathfrak{g}$
Magnus procedure: For the equation

\[ Y' = A(t)Y, \quad Y(t_0) = I, \]

*W. Magnus* (1954) proposed

\[ Y(t) = e^{\Omega(t)}, \quad \Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t) \]  \hspace{1cm} (1)
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\[ Y(t) = e^{\Omega(t)}, \quad \Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t) \quad (1) \]

with \(\log(Y(t))\) satisfying

\[ \Omega' = d \exp_{\Omega}^{-1} A(t) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}_{\Omega}^k A(t), \quad \Omega(t_0) = 0, \quad (2) \]
Here

\[ \text{ad}^0_{\Omega} A = A \]

\[ \text{ad}^k_{\Omega} A = [\Omega, \text{ad}^{k-1}_{\Omega} A] \]

\[ [\Omega, A] \equiv \Omega A - A\Omega \]

and \( B_k \) are Bernoulli numbers.
1 Magnus for linear equations (IV)

First terms in the expansion \( A_i \equiv A(t_i) \):

\[
\Omega_1(t) = \int_{t_0}^{t} A(t_1) dt_1
\]

\[
\Omega_2(t) = \frac{1}{2} \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 [A_1, A_2]
\]

\[
\Omega_3(t) = \frac{1}{6} \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 ([A_1, [A_2, A_3]] + [A_3, [A_2, A_1]])
\]

\[ e^{\Omega(t)} \in \mathcal{G} \text{ even if the series } \Omega \text{ is truncated} \]
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$e^{\Omega(t)} \in G$ even if the series $\Omega$ is truncated

* Expansion widely used in Quantum Mechanics, NMR spectroscopy, infrared divergences in QED, control theory,...
Magnus for linear equations (V)

Magnus as a numerical integration method
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Several early attempts:

- Chang–Light (1969)
- De Vries (1985)
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Systematic procedure: Iserles & Nørsett, 1997

* Numerical schemes based on Magnus up to order 8 have been constructed involving the minimum number of commutators in terms of quadratures and/or univariate integrals.

* Efficient in applications (QM, astrophysics, wave propagation in nonhomogeneous media, spectroscopy,...)
2 Magnus for nonlinear problems

\[ Y' = A(t, Y)Y, \quad Y(0) = Y_0 \in \mathcal{G}, \]

With \( Y(t) = e^{\Omega(t)}Y_0 \), then

\[ \Omega' = \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}^k_{\Omega} \left( A(t, e^{\Omega}Y_0) \right), \quad \Omega(0) = O. \]

With Picard's iteration, we get the formal solution

\[ \Omega^{[0]}(t) \equiv O \]

\[ \Omega^{[m+1]}(t) = \int_{0}^{t} \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}^k_{\Omega^{[m]}(s)}A(s, e^{\Omega^{[m]}(s)}Y_0)ds, \quad m = 0, 1, \ldots \]
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We have to truncate appropriately the series.
2.1 General case

Typically $\Omega^{[k]}(t)$ only reproduces the solution $\Omega(t)$ up to certain order $O(t^m)$.

$\Rightarrow$ the (infinite) power series of $\Omega^{[k]}(t)$ and $\Omega^{[k+1]}(t)$ differ in terms $O(t^{m+p})$.

$\Rightarrow$ discard in $\Omega^{[k]}(t)$ all terms of order greater than $O(t^m)$. 
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Careful analysis of each term in the expansion
Let us proceed:
2.1 General case (II)

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\[ \Omega^0 = O \text{ implies } (\Omega^1)' = A(t, Y_0) \text{ and } \]

\[ \Omega^1(t) = \int_0^t A(s, Y_0) ds = \Omega(t) + O(t^2). \]
Let us proceed:

\[ \Omega^{[0]} = O \] implies \((\Omega^{[1]})' = A(t, Y_0)\) and

\[ \Omega^{[1]}(t) = \int_0^t A(s, Y_0) ds = \Omega(t) + O(t^2). \]

Since

\[ A(s, e^{\Omega^{[1]}(s)}Y_0) = A(0, Y_0) + O(s) \]

then

\[ -\frac{1}{2} \int_0^t [\Omega^{[1]}(s), A(s, e^{\Omega^{[1]}(s)}Y_0)] \, ds = O(t^3). \]
2.1 General case (III)

When this term in $\Omega^{[2]}(t)$ is included and $\Omega^{[3]}$ is computed, then $\Omega^{[3]}$ reproduces correctly $\Omega^{[2]}$ up to $O(t^2)$. Therefore we truncate at $k = 0$:

$$\Omega^{[2]}(t) = \int_0^t A(s, e^{\Omega^{[1]}(s)}Y_0)\,ds.$$
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$$\Omega^{[2]}(t) = \int_0^t A(s, e^{\Omega^{[1]}(s)}Y_0)ds.$$

In general,

$$\Omega^{[1]}(t) = \int_0^t A(s, Y_0)ds \quad (3)$$

$$\Omega^{[m]}(t) = \sum_{k=0}^{m-2} \frac{B_k}{k!} \int_0^t \text{ad}^k_{\Omega^{[m-1]}(s)}A(s, e^{\Omega^{[m-1]}(s)Y_0}) ds, \quad m \geq 2$$

and take the approximation $\Omega(t) \approx \Omega^{[m]}(t)$. 
This is what we call
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Explicit Magnus expansion for the nonlinear equation $Y' = A(t, Y)Y$. 
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**Explicit Magnus expansion for the nonlinear equation** \( Y' = A(t, Y)Y \).

* Explicit approximation (in terms of multiple integrals of nested commutators)

* \( \Omega[m](t) \in g \) for all \( m \geq 1 \)

* \( \Omega[m](t) \) reproduces exactly the sum of the first \( m \) terms in \( \Omega \) for the linear equation \( Y' = A(t)Y \)
2.1 General case (V)

Order of approximation
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Order of approximation

**Theorem 2.1.** Let $\Omega(t)$ be the exact solution of the initial value problem

$$Y' = A(t, Y)Y, \quad Y(0) = Y_0 \in \mathcal{G},$$

and $\Omega^{[m]}(t)$ the iterate given by scheme (3). Then it is true that

$$\Omega(t) - \Omega^{[m]}(t) = O(t^{m+1}).$$

In other words, $Y^{[m]}(t) = e^{\Omega^{[m]}(t)}Y_0$ is an approximation correct up to order $O(t^{m+1})$. 
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Proof by induction
2.2 Magnus for isospectral flows

Procedure easily adapted to

\[ Y' = [A(Y), Y], \quad Y(0) = Y_0 \in \text{Sym}(n). \] (4)
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\[ Y' = [A(Y), Y], \quad Y(0) = Y_0 \in \text{Sym}(n). \] (4)

Features:

* Solution \( Y(t) \in \text{Sym}(n) \) for all \( t \geq 0 \).

* Eigenvalues of \( Y(t) \) are independent of time (isospectral flow)

* Applications: molecular dynamics, linear algebra,...
2.2 Magnus for isospectral flows (II)

* There exists $Q(t) \in SO(n)$ such that

$$Y(t) = Q(t)Y_0Q^T(t) \implies Q' = A(t, QY_0Q^T) Q, \quad Q(0) = I$$ (5)
2.2 Magnus for isospectral flows (II)

* There exists \( Q(t) \in \text{SO}(n) \) such that

\[
Y(t) = Q(t)Y_0Q^T(t) \quad \Rightarrow \quad Q' = A(t, QY_0Q^T)Q, \quad Q(0) = I \quad (5)
\]

Another possibility: \( Q(t) = \exp(\Omega(t)) \),

\[
Y(t) = e^{\Omega(t)}Y_0 e^{-\Omega(t)}, \quad t \geq 0, \quad \Omega(t) \in \mathfrak{so}(n), \quad (6)
\]

so that

\[
\Omega' = \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}_\Omega^k \left( A(e^{\Omega}Y_0e^{-\Omega}) \right), \quad \Omega(0) = O. \quad (7)
\]
Now, Picard’s iteration + truncation of the series at $k = m - 2 +$ truncation of $e^{\Omega}Y_0e^{-\Omega} = e^{\text{ad}\Omega}Y_0$ gives

$$\begin{align*}
\Omega^{[1]}(t) &= \int_0^t A(Y_0)ds \\
\Theta_{m-1}(t) &= \sum_{l=0}^{m-1} \frac{1}{l!} \text{ad}^l \Omega^{[m-1]}(t) Y_0 \\
\Omega^{[m]}(t) &= \sum_{k=0}^{m-2} \frac{B_k}{k!} \int_0^t \text{ad}^k \Omega^{[m-1]}(s) A(\Theta_{m-1}(s))ds, \quad m \geq 2
\end{align*}$$
2.2 Magnus for isospectral flows (IV)

* \( \Omega(t) = \Omega^m(t) + O(t^{m+1}) \)

* \( \Omega^m(t) \in \mathfrak{s}\mathfrak{o}(n) \) for all \( m \geq 1 \) and \( t \geq 0 \)
2.2 Magnus for isospectral flows (IV)

* $\Omega(t) = \Omega^m(t) + O(t^{m+1})$

* $\Omega^m(t) \in \mathfrak{s}\mathfrak{o}(n)$ for all $m \geq 1$ and $t \geq 0$

$\Rightarrow$ the procedure preserves the isospectrality of the flow
2.2 Magnus for isospectral flows (IV)

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

* \( \Omega^{[m]}(t) \in \mathfrak{s\&o}(n) \) for all \( m \geq 1 \) and \( t \geq 0 \)

\[ \implies \text{the procedure preserves the isospectrality of the flow} \]

**Important case:**

**quasilinear isospectral flows,**

when \( A \) is a linear function in the entries of \( Y \), i.e.,

\[ A(\alpha_1 Y_1 + \alpha_2 Y_2) = \alpha_1 A(Y_1) + \alpha_2 A(Y_2). \]
2.2 Magnus for isospectral flows (V)

Examples:

* double-bracket flow,

* periodic Toda lattice,

* certain classes of Lie–Poisson flows,

* Toeplitz annihilator

\[ A_{k,l}(Y) = \begin{cases} 
Y_{k+1,l} - Y_{k,l-1}, & 1 \leq k < l \leq n, \\
0, & 1 \leq k = l \leq n, \\
Y_{k-1,l} - Y_{k,l+1}, & 1 \leq l < k \leq n.
\]
In that case the iterative scheme gives

$$\Omega^{[m]}(t) = \sum_{l=1}^{m} t^l \omega_l,$$

with

$$\omega_1 = A(Y_0)$$
$$2\omega_2 = A(\text{ad}_{\omega_1} Y_0)$$
\[ l \omega_l = \sum_{j=1}^{l-1} \frac{1}{j!} \sum_{k_1 + \cdots + k_j = l-1 \atop k_1 \geq 1, \ldots, k_j \geq 1} A(\text{ad} \omega_{k_1} \cdots \text{ad} \omega_{k_j} Y_0) \]

\[ + \sum_{j=1}^{l-1} \frac{B_j}{j!} \sum_{k_1 + \cdots + k_j = l-1 \atop k_1 \geq 1, \ldots, k_j \geq 1} \text{ad} \omega_{k_1} \cdots \text{ad} \omega_{k_j} A(Y_0) \]

\[ + \sum_{j=2}^{l-1} \left( \sum_{s=1}^{j-1} \frac{B_s}{s!} \sum_{k_1 + \cdots + k_s = j-1 \atop k_1 \geq 1, \ldots, k_s \geq 1} \text{ad} \omega_{k_1} \cdots \text{ad} \omega_{k_s} \right) \]

\[ \left( \sum_{p=1}^{l-j} \frac{1}{p!} \sum_{k_1 + \cdots + k_p = l-j \atop k_1 \geq 1, \ldots, k_p \geq 1} A(\text{ad} \omega_{k_1} \cdots \text{ad} \omega_{k_p} Y_0) \right) \quad l \geq 3 \]
2.2 Magnus for isospectral flows (VIII)

Domain of convergence when $m \to \infty$: 
Domain of convergence when $m \to \infty$:

Norm in $\mathfrak{so}(n)$ and $\mu > 0$ satisfying $\|[X, Y]\| \leq \mu \|X\| \|Y\|$ and suppose that $A$ is such that $\|A(Y)\| \leq K\|Y\|$ for a certain constant $K$. Then

$$
\sum_{l=1}^{\infty} t^l \|\omega_l\|
$$

converges for $0 \leq t < t_c$, where

$$
t_c = \frac{\xi}{\mu K \|Y_0\|}
$$

and

$$
\xi = \int_0^{2\pi} \frac{e^{-x}}{2 + \frac{x}{2} \left(1 - \cot \frac{x}{2}\right)} \, dx \simeq 0.688776\ldots
$$
2.2 Magnus for isospectral flows (IX)

Example:
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Example:

Double bracket flow

\[ Y' = [[Y, N], Y], \quad Y(0) = Y_0 \in \text{Sym}(n) \] \hspace{1cm} (10)

\( N \) is a constant matrix in \( \text{Sym}(n) \)

Quasilinear flow with \( A(Y) \equiv [Y, N] \)

Then \( \|A(Y)\| \leq K\|Y\| \) with \( K = \mu \|N\| \) and one recovers results previously obtained (including convergence).
3 Numerical integrators

Issues in the construction of integration methods:
3 Numerical integrators

Issues in the construction of integration methods:

- Integrals replaced by numerical quadratures
- Reduce the computational complexity of the procedure
  (commutators and matrix exponentials)

Let us analyse methods of order 2 and 3
3.1 New methods

**Order 2**

\[
\Omega^{[1]}(t) = \int_0^t A(s, Y_0) \, ds \tag{11}
\]

\[
\Omega^{[2]}(t) = \int_0^t A(s, e^{\Omega^{[1]}(s)} Y_0) \, ds. \tag{12}
\]

If (11) can be exactly computed, then we have to replace the integral (12) with a quadrature rule of order 2.
3.1 New methods

Order 2

\[ \Omega^{[1]}(t) = \int_0^t A(s, Y_0) \, ds \]  

(11)

\[ \Omega^{[2]}(t) = \int_0^t A(s, e^{\Omega^{[1]}(s)} Y_0) \, ds. \]  

(12)

If (11) can be exactly computed, then we have to replace the integral (12) with a quadrature rule of order 2.

For instance, with the trapezoidal rule,

\[ \Omega^{[2]}(h) = \frac{h}{2} \left( A(0, Y_0) + A(h, e^{\Omega^{[1]}(h)} Y_0) \right) + O(h^3). \]  

(13)
If only a first order approximation is used, \( \Omega^{[1]}(h) = hA(0, Y_0) + O(h^2) \), a new method results:

\[
\begin{align*}
\nu_1 & \equiv \frac{h}{2} \left( A(0, Y_0) + A(h, e^{hA(0, Y_0)}Y_0) \right) = \Omega^{[2]}(h) + O(h^3) \\
Y_1 &= e^{\nu_1}Y_0, \tag{14}
\end{align*}
\]

a Runge–Kutta–Munthe-Kaas (RKMK) method with Butcher tableau

\[
\begin{array}{c|cc}
 & 0 & 1 \\
0 & \frac{1}{2} & 1 \\
\hline
1 & \frac{1}{2} & \frac{1}{2}
\end{array}
\]
* Not all the explicit RKMK methods can be recovered in this way
3.1 New methods (III)

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* RKMK methods always require to discretise $\Omega^{[1]}$ with a first-order quadrature, something not necessary for schemes based on Magnus.
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Order 3. In addition,

$$\Omega^{[3]}(t) = \int_0^t \left( A_2(s) - \frac{1}{2} [\Omega^{[2]}(s), A_2(s)] \right) ds,$$

where $A_2(s) \equiv A(s, e^{\Omega^{[2]}(s)}Y_0)$. 
3.1 New methods (IV)

With Simpson,

\[
\Omega^3(h) = \frac{h}{6} (A(0, Y_0) + 4A_2(h/2) + A_2(h)) \\
- \frac{h}{3} [\Omega^2(h/2), A_2(h/2)] - \frac{h}{12} [\Omega^2(h), A_2(h)] + O(h^4).
\]

\(\Omega^1\): Euler

\(\Omega^2\): midpoint rule, and

\[
\Omega^2\left(\frac{h}{2}\right) = \frac{h}{4} \left( A(0, Y_0) + \frac{h}{4} A\left(\frac{h}{2}, e^{\frac{h}{2}A(0, Y_0)}Y_0\right) \right) + O(h^3)
\]

⇒ Algorithm:
3.1 New methods (V)

\[ u_1 = 0 \]
\[ k_1 = hA(0, Y_0) \]
\[ u_2 = \frac{1}{2} k_1 \]
\[ k_2 = hA(h/2, e^{u_2 Y_0}) \]
\[ u_3 = \frac{1}{4} (k_1 + k_2) \]
\[ k_3 = hA(h/2, e^{u_3 Y_0}) \]
\[ u_4 = k_2 \]
\[ k_4 = hA(h, e^{u_4 Y_0}) \]
\[ v_3 = \frac{1}{6} (k_1 + 4k_3 + k_4) - \frac{1}{3} [u_3, k_3] - \frac{1}{12} [u_4, k_4] \]
\[ Y_1 = e^{v_3 Y_0} \]
3.1 New methods (VI)

Resembles closely the RKMK scheme based on the Butcher tableau

\[
\begin{array}{c|ccc}
0 & & \\
\frac{1}{2} & \frac{1}{2} & \\
1 & -1 & 2 \\
\hline \\
\frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\
\end{array}
\]
3.1 New methods (VI)

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\[
\begin{array}{c|ccc}
0 & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & -1 & 2 \\
1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\
\end{array}
\]

(17)
Technique developed by Munthe-Kaas & Owren (1999) to reduce the number of commutators: transformed variables

\[ Q_i = \sum_{j=1}^{i} V_{ij} k_j = O(h^{q_i}), \]

where \( V_{ij} \) are chosen in such a way that \( q_i \) are as large as possible. Then

\[ [Q_i, [Q_{i_2}, \ldots, [Q_{i_{m-1}}, Q_{i_m}] \ldots]] = O(h^{q_{i_1} + \ldots + q_{i_m}}) \]

and this allows to discard terms.
3.1 New methods (VII)

With

\[ Q_1 = k_1 = O(h) \]
\[ Q_2 = k_2 - k_1 = O(h^2) \]
\[ Q_3 = k_3 - k_2 = O(h^3) \]
\[ Q_4 = k_4 - 2k_2 + k_1 = O(h^3) \]
3.1 New methods (VIII)

one has in the previous algorithm

\[ \begin{align*}
    u_1 &= 0 \\
    u_2 &= \frac{1}{2}Q_1 \\
    u_3 &= \frac{1}{2}Q_1 + \frac{1}{4}Q_2 \\
    u_4 &= Q_1 + Q_2 \\
    v_3 &= Q_1 + Q_2 + \frac{2}{3}Q_3 + \frac{1}{6}Q_4 - \frac{1}{6}[Q_1, Q_2]
\end{align*} \]
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\[ u_1 = 0 \]
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\[ u_3 = \frac{1}{2} Q_1 + \frac{1}{4} Q_2 \]
\[ u_4 = Q_1 + Q_2 \]
\[ v_3 = Q_1 + Q_2 + \frac{2}{3} Q_3 + \frac{1}{6} Q_4 - \frac{1}{6} [Q_1, Q_2] \]

\[ \Rightarrow 4 \text{ A evaluations, 1 commutator, 3 matrix exponentials} \]
### 3.2 Computational cost

<table>
<thead>
<tr>
<th>Order</th>
<th>Method</th>
<th>$A$ evaluations</th>
<th>Commutators</th>
<th>Exponentials</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>RKMK</td>
<td>2</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td></td>
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<tr>
<td></td>
<td>Magnus</td>
<td>6</td>
<td>2</td>
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</tr>
</tbody>
</table>
3.2 Computational cost (II)

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* ‘Hybrid’ schemes: exactly computed integrals + quadratures
Explicit solution for Magnus can be used to construct especially adapted numerical integrators requiring much less computational effort. Up to order 4

\[
\begin{align*}
\omega_1 &= A(Y_0) \\
2\omega_2 &= A(\text{ad}_{\omega_1} Y_0) \\
3\omega_3 &= A \left( \text{ad}_{\omega_2} Y_0 + \frac{1}{2} \text{ad}_{\omega_1}^2 Y_0 \right) - \frac{1}{2} \text{ad}_{\omega_1} \omega_2 \\
4\omega_4 &= A \left( \text{ad}_{\omega_3} Y_0 + \frac{1}{2} \text{ad}_{\omega_1} \text{ad}_{\omega_2} Y_0 + \frac{1}{2} \text{ad}_{\omega_2} \text{ad}_{\omega_1} Y_0 + \frac{1}{6} \text{ad}_{\omega_1}^3 Y_0 \right) \\
&\quad - \text{ad}_{\omega_1} \omega_3 - \frac{1}{6} \text{ad}_{\omega_1}^2 \omega_2,
\end{align*}
\]
This can be grouped as

\[
\begin{align*}
\theta_1 &= Y_0 \\
\omega_1 &= A(\theta_1) \\
d_1 &= [\omega_1, Y_0] \\
\theta_2 &= d_1 \\
\omega_2 &= \frac{1}{2} A(\theta_2); \quad \rightarrow \quad \Omega^{[2]}(h) = \omega_1 h + \omega_2 h^2 \\
d_2 &= [\omega_2, Y_0]; \quad d_3 = [\omega_1, d_1]; \quad d_4 = [\omega_1, \omega_2] \\
\theta_3 &= d_2 + \frac{1}{2} d_3
\end{align*}
\]
3.3 Methods for quasilinear IF (III)

\[
\omega_3 = \frac{1}{3} A(\theta_3) - \frac{1}{6} d_4 \quad \Rightarrow \quad \Omega^3(h) = \Omega^2(h) + \omega_3 h^3
\]

\[
d_5 = \left[ \omega_3 - d_4/2, Y_0 \right]; \quad d_6 = \left[ \omega_1, d_2 + d_3/6 \right];
\]

\[
d_7 = \frac{1}{3} \left[ \omega_1, A(\theta_3) \right]; \quad \theta_4 = d_5 + d_6
\]

\[
\omega_4 = \frac{1}{4} \left( A(\theta_4) - d_7 \right)
\]

\[
\Omega^4(h) = \sum_{i=1}^{4} \omega_i h^i
\]
3.3 Methods for quasilinear IF (III)

\[ \omega_3 = \frac{1}{3} A(\theta_3) - \frac{1}{6} d_4 \quad \rightarrow \quad \Omega^3(h) = \Omega^2(h) + \omega_3 h^3 \]

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\[ d_7 = \frac{1}{3} [\omega_1, A(\theta_3)]; \quad \theta_4 = d_5 + d_6 \]

\[ \omega_4 = \frac{1}{4} (A(\theta_4) - d_7) \]

\[ \Omega^4(h) = \sum_{i=1}^{4} \omega_i h^i \]

Finally

\[ Y(t_k + h) = e^{\Omega^m(h)} Y(t_k) e^{-\Omega^m(h)} \]
### 3.3 Methods for quasilinear IF (IV)

#### Computational cost

<table>
<thead>
<tr>
<th>Order</th>
<th>Method</th>
<th>A evaluations</th>
<th>Commutators</th>
<th>Exponentials</th>
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<tr>
<td></td>
<td>Magnus-QL</td>
<td>5</td>
<td>15</td>
<td>1</td>
</tr>
</tbody>
</table>
3.3 Methods for quasilinear IF (V)

* $m$th-order Magnus method only requires $m$ evaluations of the matrix $A$
3.3 Methods for quasilinear IF (V)

* $m$th-order Magnus method only requires $m$ evaluations of the matrix $A$

* new methods more efficient than the RKMK class of algorithms, even with a fixed step size implementation.
### 3.4 Numerical example

**Periodic Toda lattice**

Hamiltonian system (3 particles) with

$$H(q, p) = \frac{1}{2}(p_1^2 + p_2^2 + p_3^2) + e^{-(q_2-q_1)} + e^{-(q_3-q_2)} + e^{-(q_1-q_3)} - 3.$$  

New variables $\alpha_j$, $\beta_j$ obtained by

$$\alpha_j = \frac{1}{2} e^{-(q_{j+1} - q_j)/2}$$

$$\beta_j = \frac{1}{2} p_j$$

$(q_4 \equiv q_1)$. 
Then the equations of motion are

\[ Y' = [A(Y), Y] \]

with

\[
Y = \begin{pmatrix}
\beta_1 & \alpha_1 & \alpha_3 \\
\alpha_1 & \beta_2 & \alpha_2 \\
\alpha_3 & \alpha_2 & \beta_3
\end{pmatrix},
\]

\[
A(Y) = \begin{pmatrix}
0 & -\alpha_1 & \alpha_3 \\
\alpha_1 & 0 & -\alpha_2 \\
-\alpha_3 & \alpha_2 & 0
\end{pmatrix},
\]

(21)
3.4 Numerical example (III)

* We compare the 4th order algorithm with RK4 and RKMK based on

\[
\begin{array}{cccc}
0 & & & \\
\frac{1}{2} & 1 & & \\
\frac{1}{2} & 0 & \frac{1}{2} & \\
1 & 0 & 0 & 1 \\
\hline
\frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
\] (22)

Interval: \( t \in [0, 3000] \) with constant step size \( h \)

Initial condition \( q_0 = (0, 0, 0), p_0 = (1, 1, 0) \)
3.4 Numerical example (IV)

Error: Frobenius norm of the difference between the approximate and the exact solution matrices at $t_f$

⇒ Figure:

Error vs. CPU time
3.4 Numerical example (V)
3.4 Numerical example (VI)

* Preservation of the isospectral character of the flow.

Exact eigenvalues:

\[
\lambda_1 = \frac{1 + \sqrt{3}}{2}, \quad \lambda_2 = 0, \quad \lambda_3 = \frac{1 - \sqrt{3}}{2}
\]

⇒ Figure:

Difference in eigenvalues at \( t_f = 3000 \) obtained with RK4 and the special method for QL isospectral flows
3.4 Numerical example (VII)

The diagram shows a graph with the x-axis labeled "step size" and the y-axis labeled "eigenv. error." The graph plots several curves that represent the behavior of the eigenvalue error as the step size changes. The curves are labeled with different markers and line styles, indicating various methods or conditions being compared. The range of the step size is from -2.6 to 0, and the range of the eigenvalue error is from -16 to 0.
The procedure can be adapted to cope with highly oscillatory problems in a natural way as follows:
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Suppose we have

\[ y' = A(t, y)y, \quad y(0) = y_0 \in \mathbb{R}^d \]

whose solution oscillates rapidly.
The procedure can be adapted to cope with highly oscillatory problems in a natural way as follows:

Suppose we have

\[ y' = A(t, y)y, \quad y(0) = y_0 \in \mathbb{R}^d \]

whose solution oscillates rapidly.

* From \( y_n \approx y(t_n) \), to obtain \( y_{n+1} \) we introduce

\[ y(t_n + x) = e^{xA(t_n,y_n)}z(x). \]
Then
\[ z' = B(x)z, \quad z(0) = y_0 \]  

(23)

with
\[ B(x) = e^{-xA(t_n,y_n)} \left[ A(t_n + x, e^{xA(t_n,y_n)} z(x)) - A(t_n, y_n) \right] e^{xA(t_n,y_n)} \]

and \( B(0) = O \).
Then

\[
    z' = B(x)z, \quad z(0) = y_0
\]

(23)

with

\[
    B(x) = e^{-xA(t_n,y_n)} \left[ A(t_n + x, e^{xA(t_n,y_n)}z(x)) - A(t_n, y_n) \right] e^{xA(t_n,y_n)}
\]

and \( B(0) = O \).

Now (23) can be solved by nonlinear Magnus.
Several possibilities:

* Use the same quadrature rules as in the ‘standard’ Magnus (Euler, trapezoidal, Simpson,...)

or
4 Highly oscillatory problems (III)

Several possibilities:

* Use the same quadrature rules as in the ‘standard’ Magnus (Euler, trapezoidal, Simpson,...)

or

* special quadrature methods for highly oscillatory integrands (Filon-type quadrature rules)
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* Use the same quadrature rules as in the ‘standard’ Magnus (Euler, trapezoidal, Simpson,...)

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* special quadrature methods for highly oscillatory integrands (Filon-type quadrature rules)

⇒ preliminary but very promising results

Work in progress
5 Some conclusions

* Generalization of Magnus for nonlinear problems
* Explicit integrators
* Possibility of constructing high order schemes
* Flexible tool: several quadratures, exact integrals
* For specific problems it provides more efficient schemes
The End

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