EXPLICIT MAGNUS EXPANSIONS FOR NONLINEAR EQUATIONS

Fernando Casas

Universitat Jaume I, Castellón, Spain

Fernando.Casas@mat.uji.es

Santander, 4th July 2004

...joint work with

Arieh Iserles

University of Cambridge

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 $\mathcal{G}$

$$\boxed{Y' = A(t)Y, \qquad Y(t_0) = Y_0 \in \mathcal{G}} \tag{0}$$

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

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

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

$$\boxed{Y(t) \in \text{Lie group } \mathcal{G} \text{ if } A(t) \in \text{Lie algebra } \mathfrak{g}}$$

1 Magnus for linear equations (II)

Magnus procedure: For the equation

$$Y' = A(t)Y, \qquad Y(t_0) = I,$$

$*$ **W. Magnus** (1954) proposed

$$Y(t) = \mathrm{e}^{\Omega(t)}, \qquad \Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t) \tag{1}$$

1 Magnus for linear equations (II)

Magnus procedure: For the equation

$$Y' = A(t)Y, \qquad Y(t_0) = I,$$

$*$ **W. Magnus** (1954) proposed

$$Y(t) = e^{\Omega(t)}, \qquad \Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t) \tag{1}$$

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

$$\Omega' = d\exp_{\Omega}^{-1} A(t) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k} A(t), \qquad \Omega(t_0) = 0, \tag{2}$$

1 Magnus for linear equations (III)

Here

$$
\begin{aligned}
\mathrm{ad}_{\Omega}^{0} A &= A \\
\mathrm{ad}_{\Omega}^{k} A &= [\Omega, \mathrm{ad}_{\Omega}^{k-1} A]
\end{aligned}
$$

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

and B_k are Bernoulli numbers.

1 Magnus for linear equations (IV)

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

$$
\begin{aligned}
\Omega_1(t) &= \int_{t_0}^{t} A(t_1)dt_1 \\
\Omega_2(t) &= \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 [A_1, A_2] \\
\Omega_3(t) &= \frac{1}{6}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 ([A_1,[A_2,A_3]] + [A_3,[A_2,A_1]])
\end{aligned}
$$

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

1 Magnus for linear equations (IV)

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

$$\begin{aligned}
\Omega_1(t) &= \int_{t_0}^{t} A(t_1)dt_1 \\
\Omega_2(t) &= \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 [A_1, A_2] \\
\Omega_3(t) &= \frac{1}{6}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 ([A_1,[A_2,A_3]] + [A_3,[A_2,A_1]])
\end{aligned}$$

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

* Expansion widely used in Quantum Mechanics, NMR spectroscopy, infrared divergences in QED, control theory,...

1 Magnus for linear equations (V)

Magnus as a numerical integration method

1 Magnus for linear equations (V)

Magnus as a numerical integration method

Several early attempts:

- Chang–Light (1969)
- De Vries (1985)

1 Magnus for linear equations (V)

Magnus as a numerical integration method

Several early attempts:

- Chang–Light (1969)
- De Vries (1985)

Systematic procedure: Iserles & Nørsett, 1997

1 Magnus for linear equations (V)

Magnus as a numerical integration method

Several early attempts:

- Chang–Light (1969)
- De Vries (1985)

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.

1 Magnus for linear equations (V)

Magnus as a numerical integration method

Several early attempts:

- Chang–Light (1969)
- De Vries (1985)

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

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

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

$$\Omega' = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k} \left(A(t, \mathrm{e}^{\Omega} Y_0) \right), \qquad \Omega(0) = O.$$

With Picard's iteration, we get the formal solution

$$\begin{aligned} \Omega^{[0]}(t) &\equiv O \\ \Omega^{[m+1]}(t) &= \int_0^t \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega^{[m]}(s)}^{k} A(s, \mathrm{e}^{\Omega^{[m]}(s)} Y_0) ds, \qquad m = 0, 1, \ldots \end{aligned}$$

2 Magnus for nonlinear problems

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

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

$$\Omega' = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k}\left(A(t, \mathrm{e}^{\Omega}Y_0)\right), \qquad \Omega(0) = O.$$

With Picard's iteration, we get the formal solution

$$\begin{aligned} \Omega^{[0]}(t) &\equiv O \\ \Omega^{[m+1]}(t) &= \int_0^t \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega^{[m]}(s)}^{k} A(s, \mathrm{e}^{\Omega^{[m]}(s)}Y_0)ds, \qquad m = 0, 1, \ldots \end{aligned}$$

We have to <u>truncate appropriately the series</u>

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 $O(t^m)$.

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 $O(t^m)$.

Careful analysis of each term in the expansion

2.1 General case (II)

Let us proceed:

2.1 General case (II)

Let us proceed:

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

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

2.1 General case (II)

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 $k = 0$:

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

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 $k=0$:

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

In general,

$$\begin{aligned} \Omega^{[1]}(t) &= \int_0^t A(s, Y_0) ds \qquad (3) \\ \Omega^{[m]}(t) &= \sum_{k=0}^{m-2} \frac{B_k}{k!} \int_0^t \mathrm{ad}^k_{\Omega^{[m-1]}(s)} A(s, \mathrm{e}^{\Omega^{[m-1]}(s)} Y_0)) ds, \qquad m \geq 2 \end{aligned}$$

and take the approximation $\Omega(t) \approx \Omega^{[m]}(t)$.

2.1 General case (IV)

This is what we call

2.1 General case (IV)

This is what we call

Explicit Magnus expansion for the nonlinear equation $Y' = A(t,Y)Y$.

2.1 General case (IV)

This is what we call

Explicit Magnus expansion for the nonlinear equation $Y' = A(t, Y)Y$.

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

* $\Omega^{[m]}(t) \in \mathfrak{g}$ for all $m \geq 1$

* $\Omega^{[m]}(t)$ reproduces exactly the sum of the first m terms in Ω for the linear equation $Y' = A(t)Y$

2.1 General case (V)

Order of approximation

2.1 General case (V)

Order of approximation

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

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

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

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

In other words, $Y^{[m]}(t) = \mathrm{e}^{\Omega^{[m]}(t)}Y_0$ is an approximation correct up to order $\mathcal{O}(t^{m+1})$.

Order of approximation

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

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

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, $Y^{[m]}(t) = \mathrm{e}^{\Omega^{[m]}(t)} Y_0$ is an approximation correct up to order $O(t^{m+1})$.

Proof by induction

2.2 Magnus for isospectral flows

Procedure easily adapted to

$$Y' = [A(Y), Y], \qquad Y(0) = Y_0 \in \mathrm{Sym}(n). \tag{4}$$

2.2 Magnus for isospectral flows

Procedure easily adapted to

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

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 $Q(t) \in \mathrm{SO}(n)$ such that

$$Y(t) = Q(t)Y_0Q^T(t) \quad \Rightarrow \quad Q' = A(t, QY_0Q^T)\,Q, \qquad Q(0) = I \tag{5}$$

2.2 Magnus for isospectral flows (II)

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

$$Y(t) = Q(t) Y_0 Q^T(t) \quad \Rightarrow \quad Q' = A(t, QY_0Q^T)\,Q, \qquad Q(0) = I \tag{5}$$

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

$$Y(t) = \mathrm{e}^{\Omega(t)} Y_0\, \mathrm{e}^{-\Omega(t)}, \qquad t \geq 0, \qquad \Omega(t) \in \mathfrak{so}(n), \tag{6}$$

so that

$$\Omega' = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k} \left(A(\mathrm{e}^{\Omega} Y_0 \mathrm{e}^{-\Omega}) \right), \qquad \Omega(0) = O. \tag{7}$$

2.2 Magnus for isospectral flows (III)

Now, Picard's iteration + truncation of the series at $k = m - 2$ + truncation of $e^{\Omega} Y_0 e^{-\Omega} = e^{\mathrm{ad}_\Omega} Y_0$ gives

$$
\begin{aligned}
\Omega^{[1]}(t) &= \int_0^t A(Y_0)ds \\
\Theta_{m-1}(t) &= \sum_{l=0}^{m-1} \frac{1}{l!} \mathrm{ad}^l_{\Omega^{[m-1]}(t)} Y_0 \qquad (8) \\
\Omega^{[m]}(t) &= \sum_{k=0}^{m-2} \frac{B_k}{k!} \int_0^t \mathrm{ad}^k_{\Omega^{[m-1]}(s)} A(\Theta_{m-1}(s))ds, \qquad m \geq 2
\end{aligned}
$$

2.2 Magnus for isospectral flows (IV)

* $\Omega(t) = \Omega^{[m]}(t) + O(t^{m+1})$
* $\Omega^{[m]}(t) \in \mathfrak{so}(n)$ for all $m \geq 1$ and $t \geq 0$

2.2 Magnus for isospectral flows (IV)

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

* $\Omega^{[m]}(t) \in \mathfrak{so}(n)$ 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)

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

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

$\Rightarrow$ 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

$$A_{k,l}(Y) = \begin{cases} Y_{k+1,l} - Y_{k,l-1}, & 1 \le k < l \le n, \\ 0, & 1 \le k = l \le n, \\ Y_{k-1,l} - Y_{k,l+1}, & 1 \le l < k \le n. \end{cases}$$

2.2 Magnus for isospectral flows (VI)

In that case the iterative scheme gives

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

with

$$\begin{aligned} \omega_1 &= A(Y_0) \\ 2\,\omega_2 &= A(\mathrm{ad}_{\omega_1} Y_0) \end{aligned}$$

2.2 Magnus for isospectral flows (VII)

$$
\begin{aligned}
l\,\omega_l \quad = \quad & \sum_{j=1}^{l-1} \frac{1}{j!} \sum_{\substack{k_1+\cdots+k_j=l-1 \\ k_1\geq 1,\ldots,k_j\geq 1}} A(\mathrm{ad}_{\omega_{k_1}} \cdots \mathrm{ad}_{\omega_{k_j}} Y_0) \\
& + \sum_{j=1}^{l-1} \frac{B_j}{j!} \sum_{\substack{k_1+\cdots+k_j=l-1 \\ k_1\geq 1,\ldots,k_j\geq 1}} \mathrm{ad}_{\omega_{k_1}} \cdots \mathrm{ad}_{\omega_{k_j}} A(Y_0) \\
& + \sum_{j=2}^{l-1} \left(\sum_{s=1}^{j-1} \frac{B_s}{s!} \sum_{\substack{k_1+\cdots+k_s=j-1 \\ k_1\geq 1,\ldots,k_s\geq 1}} \mathrm{ad}_{\omega_{k_1}} \cdots \mathrm{ad}_{\omega_{k_s}} \right) \\
& \quad \left(\sum_{p=1}^{l-j} \frac{1}{p!} \sum_{\substack{k_1+\cdots+k_p=l-j \\ k_1\geq 1,\ldots,k_p\geq 1}} A(\mathrm{ad}_{\omega_{k_1}} \cdots \mathrm{ad}_{\omega_{k_p}} Y_0) \right) \qquad l \geq 3
\end{aligned}
$$

2.2 Magnus for isospectral flows (VIII)

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

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

$$t_c = \frac{\xi}{\mu K \|Y_0\|} \qquad (9)$$

and

$$\xi = \int_0^{2\pi} \frac{\mathrm{e}^{-x}}{2 + \frac{x}{2}(1 - \cot\frac{x}{2})} dx \simeq 0{,}688776\ldots$$

2.2 Magnus for isospectral flows (IX)

Example:

2.2 Magnus for isospectral flows (IX)

Example:

Double bracket flow

$$Y' = [[Y,N],Y], \qquad Y(0) = Y_0 \in \mathrm{Sym}(n) \tag{10}$$

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

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

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

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

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

For instance, with the trapezoidal rule,

$$\Omega^{[2]}(h) = \frac{h}{2}\left(A(0, Y_0) + A(h, e^{\Omega^{[1]}(h)} Y_0)\right) + O(h^3). \tag{13}$$

3.1 New methods (II)

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

$$
\begin{aligned}
v_1 &\equiv \frac{h}{2}\left(A(0,Y_0) + A(h, \mathrm{e}^{hA(0,Y_0)}Y_0)\right) = \Omega^{[2]}(h) + O(h^3) \\
Y_1 &= \mathrm{e}^{v_1}Y_0, \qquad (14)
\end{aligned}
$$

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

$$
\begin{array}{c|cc}
0 & & \\
1 & 1 & \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

3.1 New methods (III)

* Not all the explicit RKMK methods can be recovered in this way

3.1 New methods (III)

* Not all the explicit RKMK methods can be recovered in this way

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

3.1 New methods (III)

* Not all the explicit RKMK methods can be recovered in this way

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

Order 3. In addition,

$$\Omega^{[3]}(t) = \int_0^t \left(A_2(s) - \frac{1}{2}[\Omega^{[2]}(s), A_2(s)] \right) ds, \qquad (15)$$

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

3.1 New methods (IV)

With Simpson,

$$
\begin{aligned}
\Omega^{[3]}(h) \quad = \quad & \frac{h}{6}\left(A(0,Y_0)+4A_2(h/2)+A_2(h)\right) \\
& -\frac{h}{3}[\Omega^{[2]}(h/2),A_2(h/2)]-\frac{h}{12}[\Omega^{[2]}(h),A_2(h)]+O(h^4).
\end{aligned}
$$

$\Omega^{[1]}$: Euler

$\Omega^{[2]}(h)$: midpoint rule, and

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

$\Rightarrow$ Algorithm:

3.1 New methods (V)

$$
\begin{aligned}
u_1 &= 0 \\
k_1 &= hA(0, Y_0) \\
u_2 &= \frac{1}{2} k_1 \\
k_2 &= hA(h/2, e^{u_2} Y_0) \\
u_3 &= \frac{1}{4}(k_1 + k_2) \\
k_3 &= hA(h/2, e^{u_3} Y_0) \\
u_4 &= k_2 \\
k_4 &= hA(h, e^{u_4} Y_0) \\
v_3 &= \frac{1}{6}(k_1 + 4k_3 + k_4) - \frac{1}{3}[u_3, k_3] - \frac{1}{12}[u_4, k_4] \\
Y_1 &= e^{v_3} Y_0
\end{aligned}
\tag{16}
$$

3.1 New methods (VI)

Resembles closely the RKMK scheme based on the Butcher tableau

$$
\begin{array}{c|ccc}
0 & & & \\
\frac{1}{2} & \frac{1}{2} & & \\
1 & -1 & 2 & \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
\tag{17}
$$

3.1 New methods (VI)

Resembles closely the RKMK scheme based on the Butcher tableau

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \tag{17}$$

3.1 New methods (VII)

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

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

and this allows to discard terms.

3.1 New methods (VII)

With

$$
\begin{aligned}
Q_1 &= k_1 = O(h) \\
Q_2 &= k_2 - k_1 = O(h^2) \\
Q_3 &= k_3 - k_2 = O(h^3) \\
Q_4 &= k_4 - 2k_2 + k_1 = O(h^3)
\end{aligned} \tag{18}
$$

one has in the previous algorithm

$$
\begin{aligned}
u_1 &= 0 \\
u_2 &= \frac{1}{2} Q_1 \\
u_3 &= \frac{1}{2} Q_1 + \frac{1}{4} Q_2 \\
u_4 &= Q_1 + Q_2 \\
v_3 &= Q_1 + Q_2 + \frac{2}{3} Q_3 + \frac{1}{6} Q_4 - \frac{1}{6} [Q_1, Q_2]
\end{aligned}
\tag{19}
$$

3.1 New methods (VIII)

one has in the previous algorithm

$$
\begin{aligned}
u_1 &= 0 \\
u_2 &= \frac{1}{2} Q_1 \\
u_3 &= \frac{1}{2} Q_1 + \frac{1}{4} Q_2 \\
u_4 &= Q_1 + Q_2 \\
v_3 &= Q_1 + Q_2 + \frac{2}{3} Q_3 + \frac{1}{6} Q_4 - \frac{1}{6} [Q_1, Q_2]
\end{aligned}
\tag{19}
$$

$\Rightarrow$ 4 A evaluations, 1 commutator, 3 matrix exponentials

3.2 Computational cost

Order	Method	A evaluations	Commutators	Exponentials
2	RKMK	2	0	2
	Magnus	2	0	2
3	RKMK	3	1	3
	Magnus	4	1	4
4	RKMK	4	2	4
	Magnus	6	2	6

3.2 Computational cost (II)

* More computational effort per time step than RKMK of the same order (one has to compute lower order approximations to Ω at the internal stages)

3.2 Computational cost (II)

* More computational effort per time step than RKMK of the same order (one has to compute lower order approximations to Ω at the internal stages)

* local extrapolation for controlling the step size at each iteration

3.2 Computational cost (II)

* More computational effort per time step than RKMK of the same order (one has to compute lower order approximations to Ω at the internal stages)

* local extrapolation for controlling the step size at each iteration

* even a variable order technique could be incorporated into the algorithm

3.2 Computational cost (II)

* More computational effort per time step than RKMK of the same order (one has to compute lower order approximations to Ω at the internal stages)

* local extrapolation for controlling the step size at each iteration

* even a variable order technique could be incorporated into the algorithm

* it allows the use of specially adapted quadrature rules (e.g. for highly oscillatory problems)

3.2 Computational cost (II)

* More computational effort per time step than RKMK of the same order (one has to compute lower order approximations to Ω at the internal stages)

* local extrapolation for controlling the step size at each iteration

* even a variable order technique could be incorporated into the algorithm

* it allows the use of specially adapted quadrature rules (e.g. for highly oscillatory problems)

* 'Hybrid' schemes: exactly computed integrals + quadratures

3.3 Methods for quasilinear IF

Explicit solution for Magnus can be used to construct especially adapted numerical integrators requiring <u>much less</u> computational effort. Up to order 4

$$
\begin{aligned}
\omega_1 &= A(Y_0) \\
2\,\omega_2 &= A(\mathrm{ad}_{\omega_1} Y_0) \\
3\omega_3 &= A\left(\mathrm{ad}_{\omega_2} Y_0 + \frac{1}{2}\mathrm{ad}_{\omega_1}^2 Y_0\right) - \frac{1}{2}\mathrm{ad}_{\omega_1}\omega_2 \\
4\omega_4 &= A\left(\mathrm{ad}_{\omega_3} Y_0 + \frac{1}{2}\mathrm{ad}_{\omega_1}\mathrm{ad}_{\omega_2} Y_0 + \frac{1}{2}\mathrm{ad}_{\omega_2}\mathrm{ad}_{\omega_1} Y_0 + \frac{1}{6}\mathrm{ad}_{\omega_1}^3 Y_0\right) \\
&\quad -\mathrm{ad}_{\omega_1}\omega_3 - \frac{1}{6}\mathrm{ad}_{\omega_1}^2\omega_2,
\end{aligned}
$$

3.3 Methods for quasilinear IF (II)

This can be grouped as

$$
\begin{aligned}
\theta_1 &= Y_0 \\
\omega_1 &= A(\theta_1) \\
d_1 &= [\omega_1, Y_0] \\
\theta_2 &= d_1 \\
\omega_2 &= \frac{1}{2}A(\theta_2); \quad \longrightarrow \quad \Omega^{[2]}(h) = \omega_1 h + \omega_2 h^2 \\
d_2 &= [\omega_2, Y_0]; \qquad d_3 = [\omega_1, d_1]; \qquad d_4 = [\omega_1, \omega_2] \\
\theta_3 &= d_2 + \frac{1}{2}d_3
\end{aligned}
\tag{20}
$$

3.3 Methods for quasilinear IF (III)

$$
\begin{aligned}
\omega_3 &= \frac{1}{3}A(\theta_3) - \frac{1}{6}d_4 \quad \longrightarrow \quad \Omega^{[3]}(h) = \Omega^{[2]}(h) + \omega_3 h^3 \\
d_5 &= [\omega_3 - d_4/2, Y_0]; \qquad d_6 = [\omega_1, d_2 + d_3/6]; \\
d_7 &= \frac{1}{3}[\omega_1, A(\theta_3)]; \quad \theta_4 = d_5 + d_6 \\
\omega_4 &= \frac{1}{4}(A(\theta_4) - d_7) \\
\Omega^{[4]}(h) &= \sum_{i=1}^{4} \omega_i h^i
\end{aligned}
$$

3.3 Methods for quasilinear IF (III)

$$
\begin{aligned}
\omega_3 &= \frac{1}{3} A(\theta_3) - \frac{1}{6} d_4 \quad \longrightarrow \quad \Omega^{[3]}(h) = \Omega^{[2]}(h) + \omega_3 h^3 \\
d_5 &= [\omega_3 - d_4/2, Y_0]; \qquad d_6 = [\omega_1, d_2 + d_3/6]; \\
d_7 &= \frac{1}{3}[\omega_1, A(\theta_3)]; \quad \theta_4 = d_5 + d_6 \\
\omega_4 &= \frac{1}{4}(A(\theta_4) - d_7) \\
\Omega^{[4]}(h) &= \sum_{i=1}^{4} \omega_i h^i
\end{aligned}
$$

Finally

$$
Y(t_k + h) = \mathrm{e}^{\Omega^{[m]}(h)} Y(t_k) \, \mathrm{e}^{-\Omega^{[m]}(h)}
$$

3.3 Methods for quasilinear IF (IV)

Computational cost

Order	Method	A evaluations	Commutators	Exponentials
2	RKMK	2	0	2
	Magnus-QL	2	1	1
3	RKMK	3	1	3
	Magnus-QL	3	4	1
4	RKMK	4	2	4
	Magnus-QL	4	7	1
5	RKMK	7	6	6
	Magnus-QL	5	15	1

3.3 Methods for quasilinear IF (V)

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

3.3 Methods for quasilinear IF (V)

* mth-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

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

New variables α_j, β_j obtained by

$$\begin{aligned} \alpha_j &= \tfrac{1}{2}\,\mathrm{e}^{-(q_{j+1}-q_j)/2} \\ \beta_j &= \tfrac{1}{2}\,p_j \end{aligned} \qquad j = 1,2,3$$

$(q_4 \equiv q_1)$.

3.4 Numerical example (II)

Then the equations of motion are

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

with

$$Y = \begin{pmatrix} \beta_1 & \alpha_1 & \alpha_3 \\ \alpha_1 & \beta_2 & \alpha_2 \\ \alpha_3 & \alpha_2 & \beta_3 \end{pmatrix}, \qquad A(Y) = \begin{pmatrix} 0 & -\alpha_1 & \alpha_3 \\ \alpha_1 & 0 & -\alpha_2 \\ -\alpha_3 & \alpha_2 & 0 \end{pmatrix}, \tag{21}$$

3.4 Numerical example (III)

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

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ \frac{1}{2} & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \end{array} \qquad (22)$$

Interval: $t \in [0, 3000]$ with <u>constant step size</u> h

Initial condition $q_0 = (0,0,0)$, $p_0 = (1,1,0)$

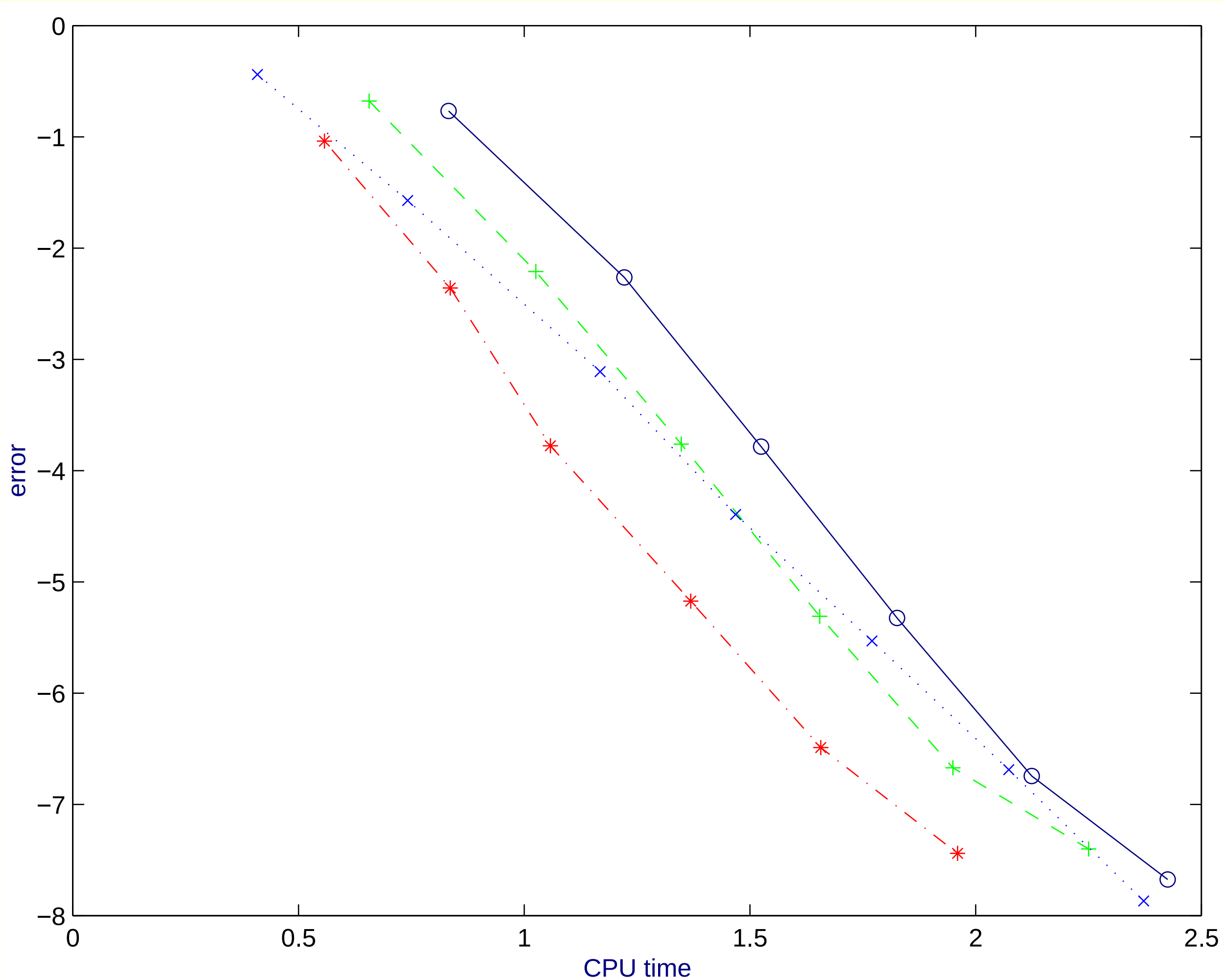
3.4 Numerical example (IV)

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

$\Rightarrow$ Figure:

Error vs. CPU time

3.4 Numerical example (V)



3.4 Numerical example (VI)

* Preservation of the isospectral character of the flow.

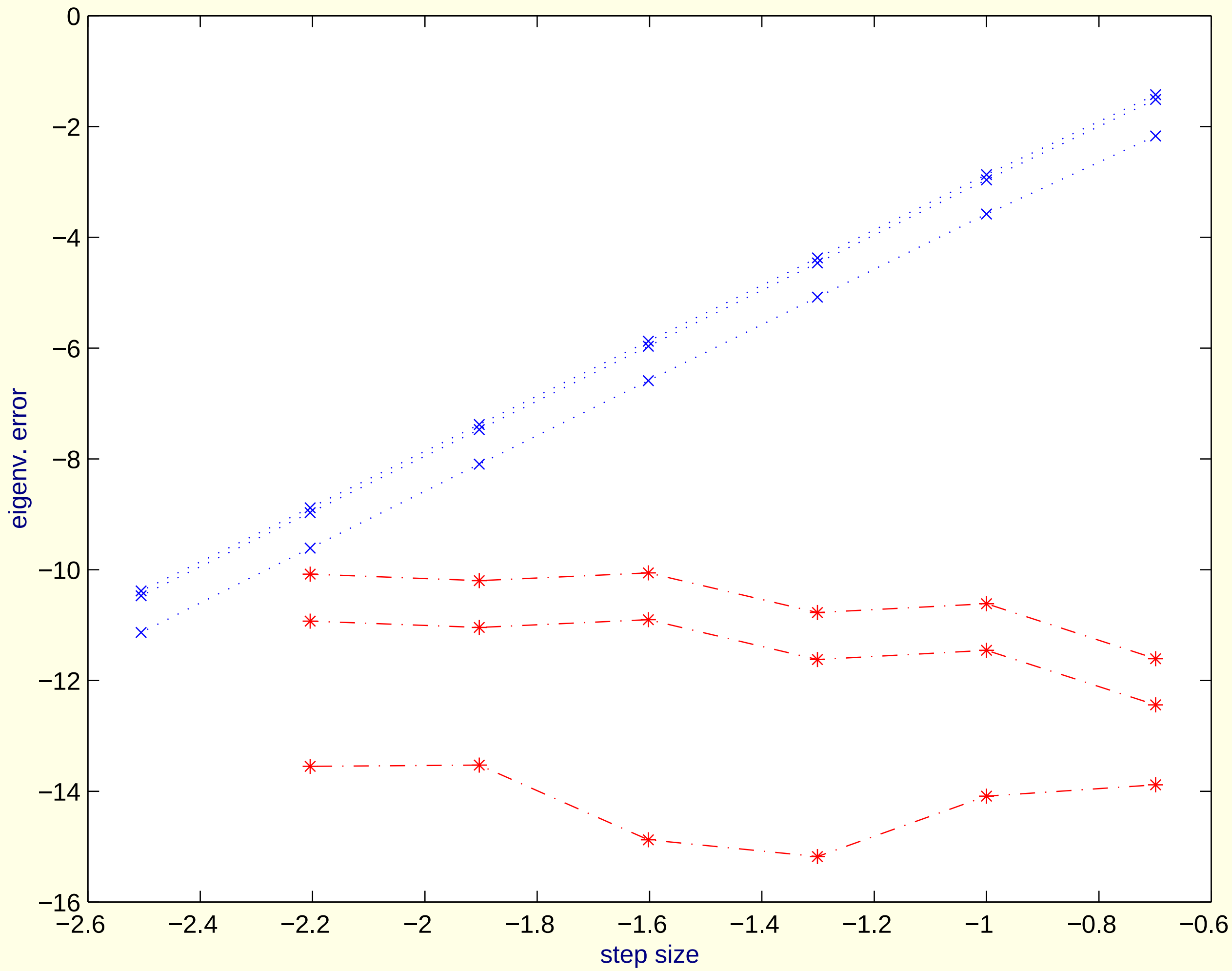
Exact eigenvalues:

$$\lambda_1 = \frac{1+\sqrt{3}}{2}, \qquad \lambda_2 = 0, \qquad \lambda_3 = \frac{1-\sqrt{3}}{2}$$

$\Rightarrow$ Figure:

Difference in eigenvalues at $t_f = 3000$ obtained with RK4 and the special method for QL isospectral flows

3.4 Numerical example (VII)



4 Highly oscillatory problems

The procedure can be adapted to cope with highly oscillatory problems in a natural way as follows:

4 Highly oscillatory problems

The procedure can be adapted to cope with highly oscillatory problems in a natural way as follows:

Suppose we have

$$\mathbf{y}' = A(t, \mathbf{y})\mathbf{y}, \qquad \mathbf{y}(0) = \mathbf{y}_0 \in \mathbb{R}^d$$

whose solution oscillates rapidly.

4 Highly oscillatory problems

The procedure can be adapted to cope with highly oscillatory problems in a natural way as follows:

Suppose we have

$$\mathbf{y}' = A(t,\mathbf{y})\mathbf{y}, \qquad \mathbf{y}(0) = \mathbf{y}_0 \in \mathbb{R}^d$$

whose solution oscillates rapidly.

* From $\mathbf{y}_n \approx \mathbf{y}(t_n)$, to obtain $\mathbf{y}_{n+1}$ we introduce

$$\mathbf{y}(t_n + x) = e^{xA(t_n,\mathbf{y}_n)}\mathbf{z}(x).$$

4 Highly oscillatory problems (II)

Then

$$\mathbf{z}' = B(x)\mathbf{z}, \qquad \mathbf{z}(0) = \mathbf{y}_0 \tag{23}$$

with

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

and $B(0) = O$.

4 Highly oscillatory problems (II)

Then

$$\mathbf{z}' = B(x)\mathbf{z}, \qquad \mathbf{z}(0) = \mathbf{y}_0 \tag{23}$$

with

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

and $B(0) = O$.

Now (23) can be solved by nonlinear Magnus.

4 Highly oscillatory problems (III)

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)

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)

$\Rightarrow$ preliminary but <u>very promising results</u>

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

Fernando Casas

Universitat Jaume I, Castellón, Spain

`Fernando.Casas@mat.uji.es`