COMPOSITION MAGNUS INTEGRATORS

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The Goal

To consider the Magnus series expansion for numerically solving the non-linear ODE

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \qquad \mathbf{x}(0) = \mathbf{x}_0 \in \mathbb{R}^d$$

The Magnus expansion and other geometric numerical integrators have been successfully used to solve the following eqs. separately

$$\frac{d\mathbf{x}}{dt} = A(t)\mathbf{x} \qquad\qquad \frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x})$$

Different versions of the ME have proved highly efficient in a number of problems:

- Quantum Mechanics
- Highly oscillatory problems
- Eigenvalue problems
- etc.

Is it possible to use Magnus for the non-autonomous non-linear problem? (Zanna)
Is it possible to combine both of them for numerically solving the problem?

Standard Procedure: to consider $t = x_t$ on the vector-field and to solve the autonomous equation

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}) \quad \Leftrightarrow \quad \frac{d}{dt}\left\{ \begin{array}{c} \mathbf{x} \\ x_t \end{array} \right\} = \left\{ \begin{array}{c} \mathbf{f}(\mathbf{x}, x_t) \\ 1 \end{array} \right\}$$

using an standard algorithm

Problems:

(i) In general, many evaluations of $\mathbf{f}(\mathbf{x},t)$ at different times, $t_1, \ldots, t_s$. The algorithm can be expensive.

(ii) If the t-dependent functions in $\mathbf{f}(\mathbf{x},t)$ and the $\mathbf{x}$-dependent functions in $\mathbf{f}(\mathbf{x},t)$ evolve at different time-scales $\Rightarrow$ it seems convenient to treat them differently.

(iii) Some times, the structure of the vector-field $\mathbf{f}(\mathbf{x},t)$ is simpler than the structure of $\mathbf{F}(\mathbf{y})$, allowing to use more efficient algorithms

Solution? To use explicit or implicit RK methods with Gaussian or Lobatto quadrature points. This solves (i) but not (ii) and (iii)

Expected Advantages on using Magnus

(i) Efficient treatment of the explicit time-dependent functions on the vector-field $\mathbf{f}(\mathbf{x},t)$ in the following cases:

* $\text{cost}(\mathbf{f}(\mathbf{x},t_1)+\mathbf{f}(\mathbf{x},t_2)) \gg \text{cost}(\mathbf{f}(\mathbf{x_1},t)+\mathbf{f}(\mathbf{x_2},t))$

i.e. $\dot{x} = f_0(t) + f_1(t)x + f_2(t)x^2 + f_3(t)x^3$

Given $t_1, \ldots, t_s$ with $t_i = t_0 + c_i h$, and c_i the quadrature points at order n $\Rightarrow$ with $\mathbf{f}(\mathbf{x},t_1), \ldots, \mathbf{f}(\mathbf{x},t_s)$ allows methods of order n

(ii) The t-dependent functions in $\mathbf{f}(\mathbf{x},t)$ and the $\mathbf{x}$-dependent functions in $\mathbf{f}(\mathbf{x},t)$ are treated separately.

(iii) It is of particular interest for those problems where efficient integrators for the autonomous vector-field $\mathbf{f}(\mathbf{x},\tau)$ are known (with τ a constant).

(iv) The geometric properties are preserved.

Magnus expansion for linear systems

$$\frac{d\mathbf{x}}{dt} = A(t)\mathbf{x} \quad \Rightarrow \quad \mathbf{x}(h) = e^{\Omega(h)}\mathbf{x}_0,$$

where $\Omega = \sum_{k=1}^{\infty} \Omega_k$ with

$$\begin{aligned}
\Omega_1 &= \int_0^h A(t)dt \\
\Omega_2 &= \frac{1}{2}\int_0^h dt_1 \int_0^{t_1} dt_2 [A_{t_1}, A_{t_2}] \\
\Omega_3 &= \frac{1}{6}\int_0^h dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \Big\{ [A_{t_1}, A_{t_2}, A_{t_3}] + [A_{t_3}, A_{t_2}, A_{t_1}] \Big\} \\
\Omega_4 &= \frac{1}{12}\int_0^h dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4 \Big\{ [A_{t_1}, A_{t_4}, A_{t_3}, A_{t_2}] \\
&\quad +[A_{t_2}, A_{t_3}, A_{t_4}, A_{t_1}] + [A_{t_1}, A_{t_2}, A_{t_3}, A_{t_4}] - [A_{t_4}, A_{t_3}, A_{t_2}, A_{t_1}] \Big\} \\
&\vdots
\end{aligned}$$

where $A_{t_i} \equiv A(t_i)$, $[A_1, A_2, A_3] \equiv [A_1, [A_2, A_3]]$, etc.

This expansion is of great interest. However, for building efficient integrators it is convenient to write the truncated Magnus series in a more appropriate way

To take profit of the time-symmetry, let us consider the Taylor expansion of $A(t)$ around $t_{1/2} = t_0 + h/2$,

$$A(t) = \sum_{i=0}^{\infty} a_i \left(t - t_{1/2}\right)^i, \qquad a_i = \frac{1}{i!} \frac{d^i A(t)}{dt^i}\Big|_{t=t_{1/2}}$$

then, taking $b_i \equiv a_{i-1} h^i$, $i = 1, 2, 3$

$$\begin{aligned}
\Omega &= b_1 - \frac{1}{12}[b_1, b_2] + \mathcal{O}(h^5) \\
\Omega &= b_1 + \frac{1}{12} b_3 - \frac{1}{12}[b_1, b_2] + \frac{1}{240}[b_2, b_3] \\
&\quad + \frac{1}{360}[b_1, [b_1, b_3]] - \frac{1}{240}[b_2, [b_1, b_2]] \\
&\quad + \frac{1}{720}[b_1, [b_1, [b_1, b_2]]] + \mathcal{O}(h^7)
\end{aligned}$$

$\{b_1, b_2, b_3\}$ generators of a graded free Lie algebra with grades $1, 2, 3$ (Munthe-Kaas & Owren).
$[b_i, b_j, b_k] \equiv [b_i, [b_j, b_k]]$, of order $\mathcal{O}(h^{i+j+k})$.

It is easier to work with.
The time-symmetry is clear

In practice, it seems convenient to consider

$$A_1 = A(t_1), \ \ldots \ , A_s = A(t_s)$$

at some quadrature points with

$$A^{(0)} = \sum_{j=1}^{s} \beta_j A_j = \int_0^h A(t)dt + \mathcal{O}(h^{n+1}),$$

Then $\exists$ constants $\beta_j^{(i)}$ such that

$$A^{(i)} = \sum_{j=1}^{s} \beta_j^{(i)} A_j = \frac{1}{h^i} \int_0^h \left(t - \frac{h}{2}\right)^i A(t)dt + \mathcal{O}(h^{n+1}),$$

$i = 0, 1, 2$ (Iserles & Nørsett; B, Casas & Ros)

Up to order 6: $e^{\Omega^{[n]}} = e^{\Omega} + O(h^{n+1})$

$$\Omega^{[2]} = A^{(0)}$$

$$\Omega^{[4]} = A^{(0)} + [A^{(1)}, A^{(0)}]$$

$Q = [A^{(1)}, \frac{3}{2}A^{(0)} - 6A^{(2)}]$

$$\Omega^{[6]} = A^{(0)} + Q + [A^{(0)}, [A^{(0)}, \frac{1}{2}A^{(2)} - \frac{1}{60}Q]] + \frac{3}{5}[A^{(1)}, Q]$$

This is valid for any n-th order quadrature. We can also use different quadrature formulas for each component, $A_{i,j}(t)$.

Examples: Gaussian Quadratures

Fourth order Consider $A_i = A(c_i h),\ \ i = 1,2$ with $c_{1,2} = \frac{1}{2} \mp \frac{\sqrt{3}}{6}$. Then

$$\begin{aligned}
A^{(0)} &= \frac{h}{2}(A_1 + A_2) \approx \int_0^h \mathbf{A}(t)dt \\
A^{(1)} &= \frac{\sqrt{3}h}{12}(A_2 - A_1) \approx \frac{1}{h}\int_0^h \left(t - \frac{h}{2}\right)\mathbf{A}(t)dt
\end{aligned}$$

Sixth order Consider $A_i = A(c_i h),\ \ i = 1,2,3$ with $c_{1,3} = \frac{1}{2} \mp \frac{\sqrt{3}}{20}, c_2 = 1/2$. Then

$$\begin{aligned}
A^{(0)} &= \frac{h}{18}(5A_1 + 8A_2 + 5A_3) \approx \int_0^h \mathbf{A}(t)dt \\
A^{(1)} &= \frac{\sqrt{15}h}{36}(A_3 - A_1) \approx \frac{1}{h}\int_0^h \left(t - \frac{h}{2}\right)\mathbf{A}(t)dt \\
A^{(2)} &= \frac{h}{24}(A_1 + A_3) \approx \frac{1}{h}\int_0^h \left(t - \frac{h}{2}\right)^2 \mathbf{A}(t)dt
\end{aligned}$$

This is equivalent to:

1. Consider the equation: $\mathbf{x}' = \mathbf{f}(\mathbf{x},t) = A(t)\mathbf{x}$

2. Frozen the $\mathbf{x}$ coordinates of the vector-field, $\mathbf{f}(\mathbf{x},t)$

3. Take the Magnus time-average $\Rightarrow$ $\mathbf{f}^{\Omega}(\mathbf{x}) = \Omega(h)\mathbf{x}$ (autonomous vector-field)

4. Consider the equation: $\mathbf{y}' = \mathbf{f}^{\Omega}(\mathbf{y}) = \Omega(h)\mathbf{y}$

5. Evaluate the 1-flow: $\mathbf{y}(1) = e^{\Omega} \simeq \mathbf{x}(h)$

Question: Is it possible to follow these steps in a simple way for the non-linear problem?
Answer: YES, but only for the steps 1 to 4. In general, due to the complexity of $\mathbf{f}^{\Omega}$, step 5 requires the evaluation of a very complicated map
Solution: To approximate the complicate map by a composition of simpler maps
$\Rightarrow$ Composition Magnus Integrators

Non-linear autonomous system

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) \qquad (1)$$

with solution $\mathbf{x}(t) = \Phi_{\mathbf{f}}^{t}(\mathbf{x}_0)$. Let us consider the Lie operador

$$L_{\mathbf{f}} = \sum_{i=1}^{n} f_i \frac{\partial}{\partial x_i}.$$

Eq. (1) can be written as

$$\dot{\mathbf{x}} = L_{\mathbf{f}(\mathbf{x})}\mathbf{x} \quad \Rightarrow \quad \frac{d}{dt}\Phi_{\mathbf{f}}^{t}(\mathbf{x}_0) = L_{\mathbf{f}}\Phi_{\mathbf{f}}^{t}(\mathbf{x}_0)$$

and in terms of the evolution operator

$$\boxed{\frac{d}{dt}\Phi_{\mathbf{f}}^{t} = \Phi_{\mathbf{f}}^{t} L_{\mathbf{f}(\mathbf{x_0})}}$$

We have rewritten eq. (1) as a (infinite dimensional) linear eq. with formal solution: $\Phi_{\mathbf{f}}^{t} = \exp(tL_{\mathbf{f}})$

Sol. dif. eq. $\quad \equiv \quad$ Lie Transformation

$$\boxed{\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) \quad \Leftrightarrow \quad \mathbf{x}(t) = \exp(tL_{\mathbf{f}(\mathbf{y})})(\mathbf{y})\Big|_{\mathbf{y}=\mathbf{x}_0}}$$

Non-autonomous System

$$\boxed{\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x},t)}$$

with solution $\mathbf{x}(t) = \Phi_{\mathbf{f}}^t(\mathbf{x}_0)$. The evolution operator satisfy the eq.

$$\boxed{\frac{d}{dt}\Phi_{\mathbf{f}}^t = \Phi_{\mathbf{f}}^t L_{\mathbf{f}(\mathbf{x_0},t)}}$$

It is possible to make use of the Magnus expansion and to write the solution as

$$\Phi_{\mathbf{f}}^t = \exp(L_{\mathbf{f}^{\Omega}(\mathbf{x_0},t)}), \quad \text{with} \quad \mathbf{f}^{\Omega} = \sum_i \mathbf{f}_i^{\Omega}$$

where

$$\begin{aligned} \mathbf{f}_1^{\Omega}(\mathbf{x}_0,t) &= \int_0^t \mathbf{f}(\mathbf{x}_0,s)ds \\ \mathbf{f}_2^{\Omega}(\mathbf{x}_0,t) &= -\frac{1}{2}\int_0^t ds_1 \int_0^{s_1} ds_2 (\mathbf{f}(\mathbf{x}_0,s_1),\mathbf{f}(\mathbf{x}_0,s_2)) \end{aligned}$$

being $\mathbf{h} = (\mathbf{f},\mathbf{g})$ the Lie bracket

$$h_i = (\mathbf{f},\mathbf{g})_i = L_{\mathbf{f}}g_i - L_{\mathbf{g}}f_i = \sum_{j=1}^n \left(f_j \frac{\partial g_i}{\partial x_j} - g_j \frac{\partial f_i}{\partial x_j} \right)$$

The formal solution at $t = h$ is given by

$$\mathbf{x}(h) \;=\; \exp(L_{\mathbf{f}^{\Omega}(\mathbf{y},h)})(\mathbf{y})\Big|_{\mathbf{y}=\mathbf{x}_0},$$

the 1-flow solution of the autonomous DE

$$\dot{\mathbf{x}} = \mathbf{f}^{\Omega}(\mathbf{x}, h), \qquad \mathbf{x}(0) = \mathbf{x}_0$$

$$\mathbf{f}^{(i)} = \sum_{j=1}^{s} \beta_j^{(i)} \mathbf{f}_j = \frac{1}{h^i} \int_0^h \left(t - \frac{h}{2}\right)^i \mathbf{f}(\mathbf{x}, t)dt + \mathcal{O}(h^{n+1}),$$

$i = 0, 1, 2$

Up to order 6: $\exp\left(L_{\mathbf{f}^{\Omega[n]}}\right) = \exp\left(L_{\mathbf{f}^{\Omega}}\right) + O(h^{n+1})$

$$\mathbf{f}^{\Omega[2]} \;=\; \mathbf{f}^{(0)}$$

$$\mathbf{f}^{\Omega[4]} \;=\; \mathbf{f}^{(0)} - (\mathbf{f}^{(1)}, \mathbf{f}^{(0)})$$

$Q = -(\mathbf{f}^{(1)}, \frac{3}{2}\mathbf{f}^{(0)} - 6\mathbf{f}^{(2)})$

$$\mathbf{f}^{\Omega[6]} \;=\; \mathbf{f}^{(0)} + Q + (\mathbf{f}^{(0)}, (\mathbf{f}^{(0)}, \frac{1}{2}\mathbf{f}^{(2)} - \frac{1}{60}Q)) + \frac{3}{5}(\mathbf{f}^{(1)}, Q)$$

The vector-field containing Lie brackets are, in general, very complicate and their maps are computationally expensive.

Solution: To approximate this map by a composition of simpler maps

This is closely related to the commutator-free methods (Celledoni & Owren)

Which simpler maps can be used?

A map is the 1-flow solution of a differential equation.

Which differential equations can be exactly or efficiently computed?

This dependes on the particular problem.

Given the quadrature points, $t_1, \ldots, t_s$, we consider the following cases:

(i) Suppose the autonomous equation can be efficiently solved up to $t = h$

$$\dot{\mathbf{x}} = \alpha_1 \mathbf{f}(\mathbf{x}, t_1) + \cdots + \alpha_s \mathbf{f}(\mathbf{x}, t_s)$$

i.e. suppose it is easy to approximate the map

$$\mathbf{x}(h) = \exp\left(h\alpha_1 L_{\mathbf{f}(\mathbf{x},t_1)} + \cdots + h\alpha_s L_{\mathbf{f}(\mathbf{x},t_s)}\right)(\mathbf{x}_0)$$

(ii) Given $\mathbf{f} = \mathbf{f}_A + \mathbf{f}_B$, suppose we can solve

$$\begin{aligned} \dot{\mathbf{x}} &= \alpha_1 \mathbf{f}_A(\mathbf{x}, t_1) + \cdots + \alpha_s \mathbf{f}_A(\mathbf{x}, t_s) \\ \dot{\mathbf{x}} &= \beta_1 \mathbf{f}_B(\mathbf{x}, t_1) + \cdots + \beta_s \mathbf{f}_B(\mathbf{x}, t_s) \end{aligned}$$

i.e. suppose we can approximate the maps

$$\begin{aligned} \mathbf{x}(h) &= \exp\left(h\alpha_1 L_{\mathbf{f}_A(\mathbf{x},t_1)} + \cdots + h\alpha_s L_{\mathbf{f}_A(\mathbf{x},t_s)}\right)(\mathbf{x}_0) \\ \mathbf{x}(h) &= \exp\left(h\beta_1 L_{\mathbf{f}_B(\mathbf{x},t_1)} + \cdots + h\beta_s L_{\mathbf{f}_B(\mathbf{x},t_s)}\right)(\mathbf{x}_0) \end{aligned}$$

Problem to solve

$$\begin{aligned}
\exp(\Omega) &= \exp\left(b_1 - \frac{1}{12}[b_1, b_2]\right) + \mathcal{O}(h^5) \\
&= \prod_{i=1}^{m} \exp\left(\alpha_{i,1} b_1 + \alpha_{i,2} b_2\right) + \mathcal{O}(h^5) \\
\exp(\Omega) &= \exp\left(b_1 + \frac{1}{12} b_3 - \frac{1}{12}[b_1, b_2] + \frac{1}{240}[b_2, b_3] \right. \\
&\quad + \frac{1}{360}[b_1,[b_1,b_3]] - \frac{1}{240}[b_2,[b_1,b_2]] \\
&\quad \left. + \frac{1}{720}[b_1,[b_1,[b_1,b_2]]]\right) + \mathcal{O}(h^7) \\
&= \prod_{i=1}^{m} \exp\left(\alpha_{i,1} b_1 + \alpha_{i,2} b_2 + \alpha_{i,3} b_3\right) + \mathcal{O}(h^7)
\end{aligned}$$

The coefficients $\alpha_{i,j}$ have to solve a system of non-linear equations.

Time-symmetry. It can be preserved with

$$\begin{aligned}
\alpha_{m+1-i,1} &= \alpha_{i,1} \\
\alpha_{m+1-i,2} &= -\alpha_{i,2} \\
\alpha_{m+1-i,3} &= \alpha_{i,3}
\end{aligned}$$

Order Conditions

Given the time-symmetric composition

$$e^{\alpha_{1,1}b_1+\alpha_{1,2}b_2+\alpha_{1,3}b_3}\ e^{\alpha_{2,1}b_1+\alpha_{2,2}b_2+\alpha_{2,3}b_3}\ \ldots$$
$$\ldots e^{\alpha_{2,1}b_1-\alpha_{2,2}b_2+\alpha_{2,3}b_3}\ e^{\alpha_{1,1}b_1-\alpha_{1,2}b_2+\alpha_{1,3}b_3}$$

and a general (time-symmetric) element

$$\begin{aligned} C(\beta^{(k)}) &= \beta_1^{(k)}b_1 + \beta_2^{(k)}b_3 + \beta_3^{(k)}[1,2] + \beta_4^{(k)}[2,3] \\ &+ \beta_5^{(k)}[1,1,3] + \beta_6^{(k)}[2,1,2] + \beta_7^{(k)}[1,1,1,2] \end{aligned}$$

the order conditions can be easily obtained from the recursive relation

$$e^{xb_1+yb_2+zb_3}\ e^{C(\beta^{(k)})}\ e^{xb_1-yb_2+zb_3} = e^{C(\beta^{(k+1)}(x,y,z))}$$

Next, we must solve the equations

$$\begin{aligned} &(\beta_1^{(m)},\beta_2^{(m)},\beta_3^{(m)},\beta_4^{(m)},\beta_5^{(m)},\beta_6^{(m)},\beta_7^{(m)}) \\ = &\left(1,\ \frac{1}{12},\ -\frac{1}{12},\ \frac{1}{240},\frac{1}{360},\ -\frac{1}{240},\ \frac{1}{720}\right) \end{aligned}$$

Finally, we write the solution in terms of $A^{(0)}, A^{(1)}, A^{(2)}$

Example: Fourth-order composition methods
(B & Moan)

Linear problem

$$
\begin{aligned}
e^{\mathbf{\Omega}} &\simeq \exp\left(b_1 + \frac{1}{12}[b_2, b_1]\right) \\
&\simeq \exp\left(A^{(0)} + [A^{(1)}, A^{(0)}]\right) \\
&\simeq \exp\left(\frac{1}{2}A^{(0)} + 2A^{(1)}\right) \ \exp\left(\frac{1}{2}A^{(0)} - 2A^{(1)}\right) \\
&\simeq \exp\left(A^{(1)}\right) \ \exp\left(A^{(0)}\right) \ \exp\left(-A^{(1)}\right)
\end{aligned}
$$

Non-linear problem

$$
\begin{aligned}
\exp(L_{\mathbf{f}\Omega}) &\simeq \exp\left(L_{\mathbf{f}^{(0)} - (\mathbf{f}^{(1)}, \mathbf{f}^{(0)})}\right) \\
&\simeq \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)} - 2\mathbf{f}^{(1)}}\right) \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)} + 2\mathbf{f}^{(1)}}\right) \\
&\simeq \exp\left(-L_{\mathbf{f}^{(1)}}\right) \exp\left(L_{\mathbf{f}^{(0)}}\right) \exp\left(L_{\mathbf{f}^{(1)}}\right)
\end{aligned}
$$

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t)$$

$$\mathbf{x}_2(1) = \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)} - 2\mathbf{f}^{(1)}}\right) \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)} + 2\mathbf{f}^{(1)}}\right)(\mathbf{x}_0)$$

$$\begin{aligned} \dot{\mathbf{x}}_1 &= \frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_1) - 2\mathbf{f}^{(1)}(\mathbf{x}_1), & \mathbf{x}_1(0) &= \mathbf{x}_0, \\ \dot{\mathbf{x}}_2 &= \frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_2) + 2\mathbf{f}^{(1)}(\mathbf{x}_2), & \mathbf{x}_2(0) &= \mathbf{x}_1(1) \end{aligned}$$
$$\mathbf{x}_2(1) = \mathbf{x}(h) + O(h^5)$$

$$\mathbf{x}_3(1) = \exp\left(-L_{\mathbf{f}^{(1)}}\right) \exp\left(L_{\mathbf{f}^{(0)}}\right) \exp\left(L_{\mathbf{f}^{(1)}}\right)(\mathbf{x}_0)$$

$$\begin{aligned} \dot{\mathbf{x}}_1 &= -\mathbf{f}^{(1)}(\mathbf{x}_1), & \mathbf{x}_1(0) &= \mathbf{x}_0, \\ \dot{\mathbf{x}}_2 &= \mathbf{f}^{(0)}(\mathbf{x}_2), & \mathbf{x}_2(0) &= \mathbf{x}_1(1), \\ \dot{\mathbf{x}}_3 &= \mathbf{f}^{(1)}(\mathbf{x}_3), & \mathbf{x}_3(0) &= \mathbf{x}_2(1) \end{aligned}$$
$$\mathbf{x}_3(1) = \mathbf{x}(h) + O(h^5)$$

Illustrative Example:

$$\dot{x} = f_0(t) + f_1(t)x + f_2(t)x^2 + f_3(t)x^3$$

Evaluate the constants

$$f_i^{(0)} \simeq \int_0^h f_i(t)dt, \qquad f_i^{(1)} \simeq \frac{1}{h}\int_0^h \left(t - \frac{h}{2}\right) f_i(t)dt,$$

$i = 0, \ldots, 3$ (using a fourth-order quadrature)

$$a_i = \frac{1}{2}f_i^{(0)} - 2f_i^{(1)}, \qquad b_i = \frac{1}{2}f_i^{(0)} + 2f_i^{(1)}$$

Finally, we must solve the autonomous eqs.

$$\begin{aligned} \dot{x}_1 &= a_0 + a_1x_1 + a_2x_1^2 + a_3x_1^3, \qquad x_1(0) = x_0 \\ \dot{x}_2 &= b_0 + b_1x_2 + b_2x_2^2 + b_3x_2^3, \qquad x_2(0) = x_1(1) \end{aligned}$$

Solution from the method

$$x_2(1) = x(h) + O(h^5)$$

Optimization

It is possible to improve the accuracy following different procedures

Suppose the constant part of the vector-field, b_1, is the dominant term, then

$$\Omega = b_1 - \frac{1}{12}[b_1, b_2] + \cdots + c_j[\overbrace{b_1, ..., b_1}^{j\ b_1's}, b_2] + \cdots$$
$$+ \frac{1}{12} b_3 - \frac{1}{80}[b_1, b_4] + \frac{1}{240}[b_2, b_3] + \cdots$$

where the coefficients c_k are given by

$$\sum_{k \geq 0} c_k x^k = \frac{1 - \frac{x}{2} - \frac{x}{e^x - 1}}{x} = g(x).$$

The dominating error term is then

$$E_1^j = c_j[b_1, ..., b_1, b_2] + c_{j+1}[b_1, ..., b_1, b_1, b_2] + \cdots$$

We can use additional exponentials to cancel the lowest order terms of E_1^j or to remove its first singularities

Separable Problem:

$$\dot{\mathbf{x}} = C(t)\mathbf{x} + D(t)\mathbf{x}$$

with $[C(t), D(t)] = 0$. Then, we can consider the graded free Lie algebra generated by

$\{c_1, d_1, c_2, d_2, c_3, d_3\}$ with $b_i = c_i + d_i, \ i = 1, 2, 3$ and $[c_i, c_j] = [d_i, d_j] = 0$.

$$\begin{aligned}
\Omega \;=\; & c_1 + d_1 + \frac{1}{12}c_3 + \frac{1}{12}d_3 - \frac{1}{12}[c_1, d_2] - \frac{1}{12}[d_1, c_2] \\
& + \frac{1}{240}[c_2, d_3] + \frac{1}{240}[d_2, c_3] \\
& + \frac{1}{360}\big([c_1, c_1, d_3] + [c_1, d_1, c_3] + [d_1, c_1, d_3] + [d_1, d_1, c_3]\big) \\
& - \frac{1}{240}\big([c_2, c_1, d_2] + [c_2, d_1, c_2] + [d_2, c_1, d_2] + [d_2, d_1, c_2]\big) \\
& + \frac{1}{720}\big([c_1, c_1, c_1, d_2] + [c_1, c_1, d_1, c_2] + [c_1, d_1, c_1, d_2] \\
& \quad + [c_1, d_1, d_1, c_2] + [d_1, c_1, c_1, d_2] + [d_1, c_1, d_1, c_2] \\
& \quad + [d_1, d_1, c_1, d_2] + [d_1, d_1, d_1, c_2]\big) + \mathcal{O}(h^7).
\end{aligned}$$

$\exp\big(\Omega\big)$ can be approximated by

$$\prod_{i=1}^{m} \exp\left(\alpha_{i,1}c_1 + \alpha_{i,2}c_2 + \alpha_{i,3}c_3\right) \exp\left(\beta_{i,1}d_1 + \beta_{i,2}d_2 + \beta_{i,3}d_3\right)$$

Fourth-order: easy

Sixth-order: very complicate

For the particular case

$$\dot{\mathbf{x}} = C\mathbf{x} + D(t)\mathbf{x}$$

the problem simplifies

$$\begin{aligned}\Omega &= c_1 + d_1 + \frac{1}{12}d_3 - \frac{1}{12}[c_1,d_2] + \frac{1}{360}\big([c_1,c_1,d_3] + [d_1,c_1,d_3]\big) \\ &\quad - \frac{1}{240}\big([d_2,c_1,d_2]\big) + \frac{1}{720}\Big([c_1,c_1,c_1,d_2] + [c_1,d_1,c_1,d_2] \\ &\quad + [d_1,c_1,c_1,d_2] + [d_1,d_1,c_1,d_2]\Big) + \mathcal{O}(h^7).\end{aligned}$$

and sixth-order methods can be obtained. Other cases can also be considered.

On the other hand, for the autonomous case

$$\dot{\mathbf{x}} = C\mathbf{x} + D\mathbf{x}$$

many efficient splitting methods are known

$$e^{C+D} = \prod_{i=1}^{m} e^{\alpha_i C}\ e^{\beta_i D}$$

Then, for our composition

$$\prod_{i=1}^{m} \exp\left(\alpha_{i,1}c_1 + \alpha_{i,2}c_2 + \alpha_{i,3}c_3\right)\exp\left(\beta_{i,1}d_1 + \beta_{i,2}d_2 + \beta_{i,3}d_3\right)$$

we can take $\alpha_{i,1} = \alpha_i,\ \beta_{i,1} = \beta_i$ which solve many (the most complicate) order conditions

Hamiltonian Systems

This is just a particular, but very important, case. Let us consider $H(\mathbf{q},\mathbf{p},t) : \mathbb{R}^{2l} \times \mathbb{R} \to \mathbb{R}$, where $\mathbf{q}$, $\mathbf{p} \in \mathbb{R}^l$, the Hamilton eqs. are

$$\frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}}; \qquad \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}}$$

or, equivalently

$$\frac{d}{dt}\left\{ \begin{array}{c} \mathbf{q} \\ \mathbf{p} \end{array} \right\} = \left(\begin{array}{cc} 0 & I \\ -I & 0 \end{array} \right) \left\{ \begin{array}{c} \frac{\partial H}{\partial \mathbf{q}} \\ \frac{\partial H}{\partial \mathbf{p}} \end{array} \right\}$$

If we denote $\mathbf{x} = (\mathbf{q},\mathbf{p})$, it corresponds to the particular case $\mathbf{f} = -J\dfrac{\partial H}{\partial \mathbf{x}}$

Lie bracket $\quad \Rightarrow \quad$ Poisson bracket

The Hamiltonian

$$\boxed{H = T(\mathbf{p},t) + V(\mathbf{q},t)}$$

appears in many problem: is time-dependent + separable

The Poisson brackets destroy the separability
$\Rightarrow$ Use of composition Magnus integrators

NUMERICAL EXAMPLES: HAMILTONIAN SYSTEMS

Perturbed oscillator by a plane wave

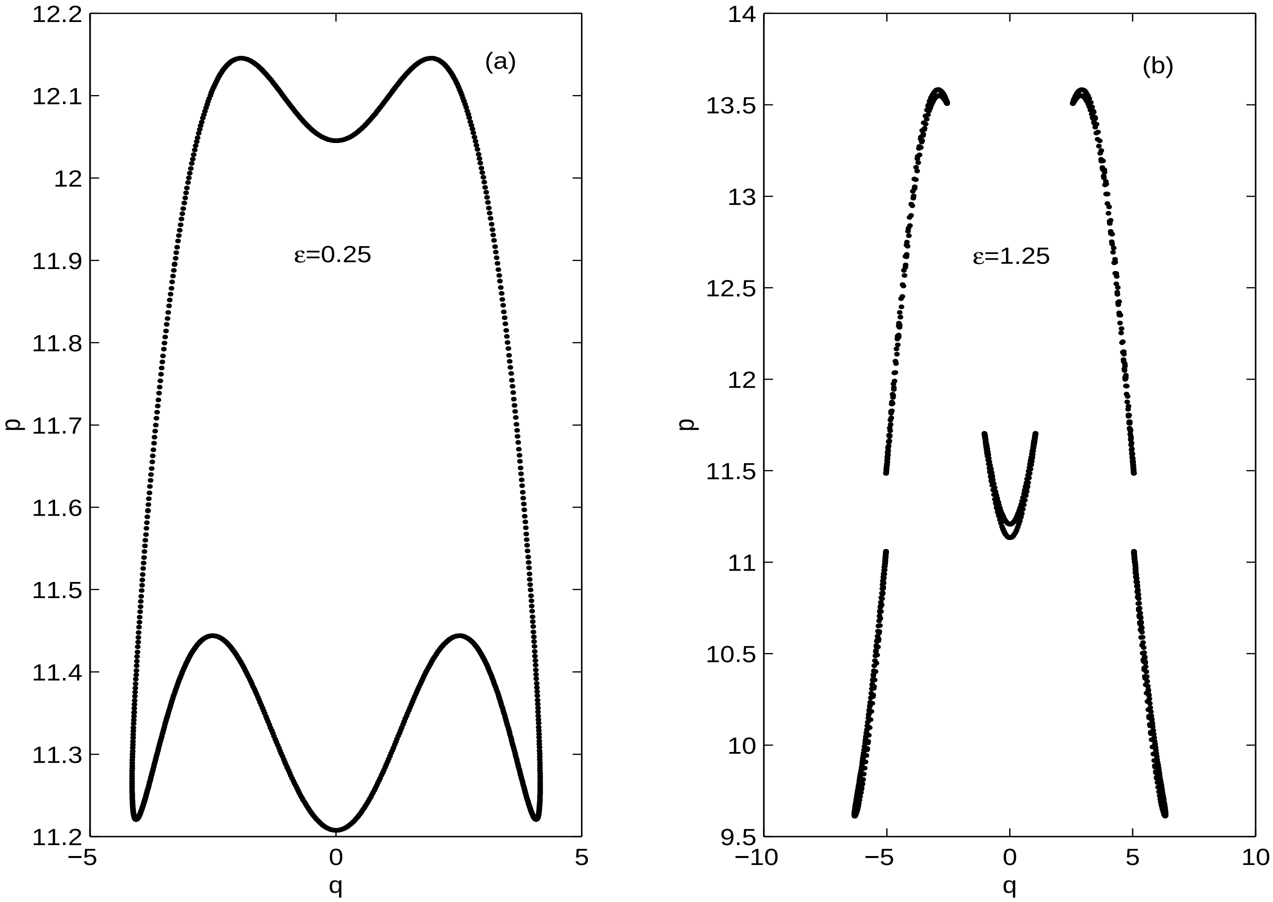
$$H = \frac{1}{2}(p^2 + q^2) + \varepsilon\,(\cos(q)g_1(t) + \sin(q)g_2(t))$$

with

$$g_1(t) = \sum_{i=1}^{k} \cos(w_k t), \qquad g_2(t) = \sum_{i=1}^{k} \sin(w_i t)$$

$$\begin{cases} q_0 = 0 & p_0 = 11{,}2075 \\ \omega_i = i\omega_0 & \omega_0 = 1/10 \\ k = 10 & \varepsilon = 0{,}25 - 1{,}25 \end{cases}$$

We are interested in the Poincaré section and consider different methods. We start with a large time-step, h and repeat the computations reducing h until we get the correct picture. For this time-step we measure the computational cost



	$\varepsilon = 0{,}25$		$\varepsilon = 1{,}25$	
	CPU	N	CPU	N
2EXq	4.00	38	7.70	74
3EXq	4.90	58	10.6	121
S^*	8.50	38	15.6	71
S_{RKN}	10.7	48	14.8	68
RK4	12.0	152	26.5	331

Given the time step $h = 2\pi/N$ we show the minimum value of N such that $\delta < 10^{-3}$. For these values we calculated the CPU time in seconds.

The Duffing Problem

$$\ddot{\mathbf{q}} = A(t)\dot{\mathbf{q}} - \nabla_q V(\mathbf{q}, t)$$

or, equivalently

$$\dot{M} = A(t)M$$

$$\frac{d}{dt}\left\{ \begin{array}{c} \mathbf{q} \\ \mathbf{p} \end{array} \right\} = \left(\begin{array}{cc} 0 & M \\ -M^{-1} & 0 \end{array} \right) \left\{ \begin{array}{c} \nabla_q V(\mathbf{q}, t) \\ \mathbf{p} \end{array} \right\}$$

The one-dimensional equation

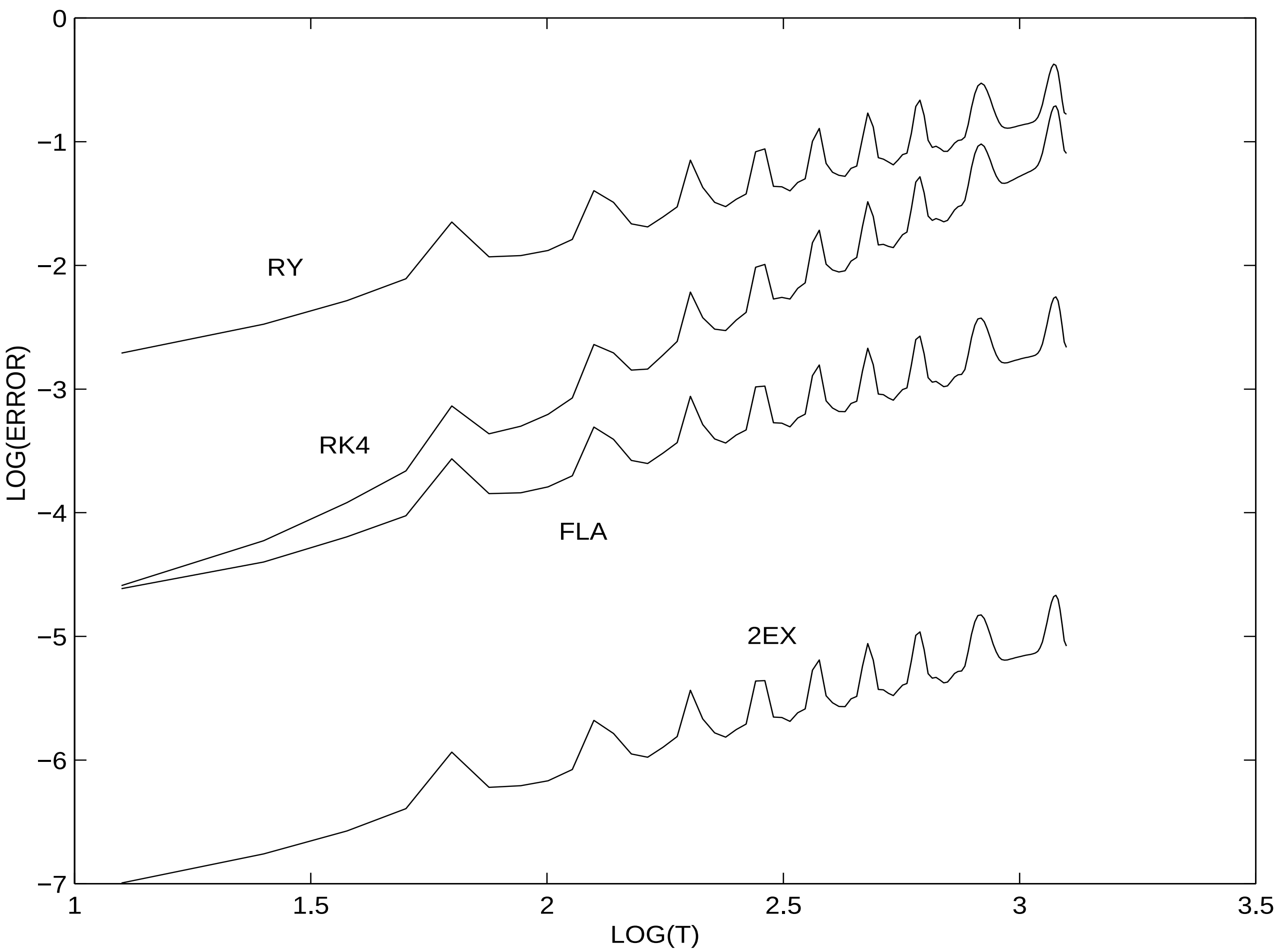
$$\ddot{q} = \epsilon \dot{q} + q - q^3 + \delta \cos(wt)$$

can be obtained from the Hamiltonian

$$\boxed{H = e^{-\epsilon t}\frac{p^2}{2} + e^{\epsilon t}\left(\frac{q^4}{4} - \frac{q^2}{2} - \delta \cos(\omega t) q\right)}$$

which is separable in two time-dependent parts, being both of them solvable. The evaluation of the time-dependent functions is the most computational costly part

$$
\begin{cases} q_0 = 1{,}75 & p_0 = 0 \\ \epsilon = \frac{1}{10000} & \delta = \frac{1}{1000} \\ \omega = \frac{1}{2} \end{cases}
$$



Errors in positions for different splitting methods and the two-exponential CMI. Time step chosen such that all methods require the same computational cost.

The Schrödinger Equation

$$i\frac{\partial}{\partial t}u(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + V(x,t)\right)u(x,t)$$

Spatial semidiscretisation

$$u(x,t) \longrightarrow \mathbf{u}(t) = \left\{\begin{array}{c} u(x_0,t) \\ u(x_1,t) \\ \vdots \\ u(x_N,t) \end{array}\right\}.$$

Then, we have to solve

$$i\mathbf{u}_t = \mathbf{H}(t)\mathbf{u}$$

with $\mathbf{H} \in \mathcal{C}^{N\times N}$ hermitic (usually real and symmetric). If we consider

$$\mathbf{u} = \mathbf{q} + i\mathbf{p}$$

then

$$\frac{d}{dt}\left\{\begin{array}{c} \mathbf{q} \\ \mathbf{p} \end{array}\right\} = \left(\begin{array}{cc} 0 & \mathbf{H}(t) \\ -\mathbf{H}(t) & 0 \end{array}\right)\left\{\begin{array}{c} \mathbf{q} \\ \mathbf{p} \end{array}\right\}$$

$$V(x,t) = D(1-e^{-\alpha x})^2 + xf(t)$$

$i)$ $f(t) = G\cos(wt)$ Laser field

$ii)$ $f(t) = \frac{Gw}{\cosh^2(F\sqrt{w}t)}$ Collision with an atom

Conclusions

- The time and the coordinates in the vector-field $\mathbf{f}(\mathbf{x}, t)$ play different roles on the evolution of the system for many problems $\Rightarrow$ it is convenient to treat them differently

- We have generalized the Magnus integrators for linear systems to be used in non-linear problems

- Composition Magnus integrators can be used in tandem with other geometric integrators (of different order). An important case being the splitting methods for separable systems. The final methods are still Geometric Integrators

- Additional stages can be considered for optimization purposes

Work in Progress

- To analyze the efficiency of fourth-order methods optimized following different criterions

- To build different sixth-order composition Magnus integrators and to analyze their performances

- To consider particular cases, like the separable problem, and to build efficient composition methods for them

- To look for interesting problems where these methods can be of interest (polynomial vector-fields, linear non-homogeneous systems, Riccati equation, separable Hamiltonian systems, some oscillatory problems, etc.)