

Uniform accuracy from geometric high-order averaging

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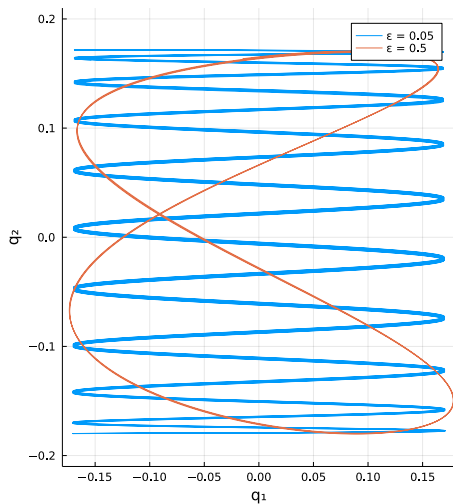
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Outline

- 1 Numerical introduction
- 2 Geometric normal forms
- 3 Uniform accuracy results

Introducing a stiff Hénon-Heiles model



$$\begin{cases} \dot{p}_1 = -\frac{1}{\varepsilon}q_1 - 2q_1q_2 \\ \dot{q}_1 = \frac{1}{\varepsilon}p_1 \\ \dot{p}_2 = -q_2 - q_1^2 + \frac{3}{2}q_2^2 \\ \dot{q}_2 = p_2 \end{cases}$$

Figure: Example trajectory of this Hénon-Heiles model for $t \in [0, 20]$.

Other examples:

- strong magnetic field
- non-linear Schrödinger
- ...

Appropriate numerical methods

$$\partial_t y^\varepsilon = \frac{1}{\varepsilon} A y^\varepsilon + f(y^\varepsilon), \quad y^\varepsilon(0) = y_0 \in X$$

where $\theta \mapsto e^{\theta A}$ is 2π -periodic and $y \mapsto f(y)$ is analytic

Exponential integrators based on the variation of constants

$$y^\varepsilon(t) = e^{tA/\varepsilon} y_0 + \int_0^t e^{(t-s)A} f(y^\varepsilon(s)) ds,$$

Lawson methods RK scheme on the filtered problem

$$u^\varepsilon(t) = e^{-tA/\varepsilon} y^\varepsilon(t), \quad \text{i.e.} \quad \partial_t u^\varepsilon(t) = e^{-\frac{t}{\varepsilon}A} f(e^{\frac{t}{\varepsilon}A} u^\varepsilon).$$

Splitting methods e.g. Strang splitting

$$y_{\ell+1}^\varepsilon = e^{\frac{h}{2\varepsilon}A} \circ e^{hf} \circ e^{\frac{h}{2\varepsilon}A}(y_\ell^\varepsilon)$$

Inner non-stiff method for long-time integration

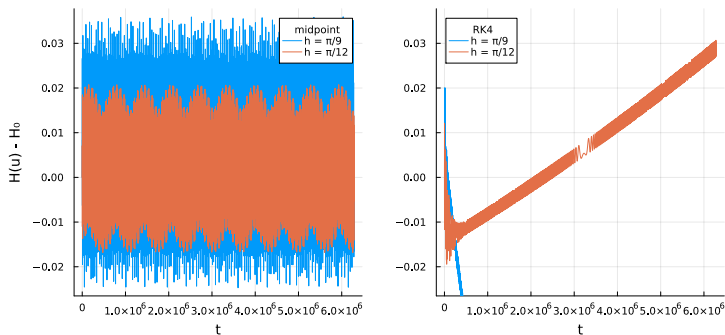


Figure: Energy behaviour of the Strang splitting solution depending on the method to compute e^{hf} with the Hénon-Heiles model.

➔ **preserving structure is key, use the midpoint scheme**

📺 great visuals in introductory video by braintruffle on YouTube

📖 Hairer, Lubich, Wanner – Geometric Numerical Integration (2006)

Order reduction from splitting error

$$e^{\frac{h}{2\varepsilon}A} \circ e^{hf} \circ e^{\frac{h}{2\varepsilon}A} = \exp\left(h\left(\frac{1}{\varepsilon}A + f\right) - \frac{h^3}{24\varepsilon^2}[A + 2\varepsilon f, [A, f]] + \dots\right)$$

where $[f, g] = g'f - f'g$ is the standard Lie bracket of vector fields.

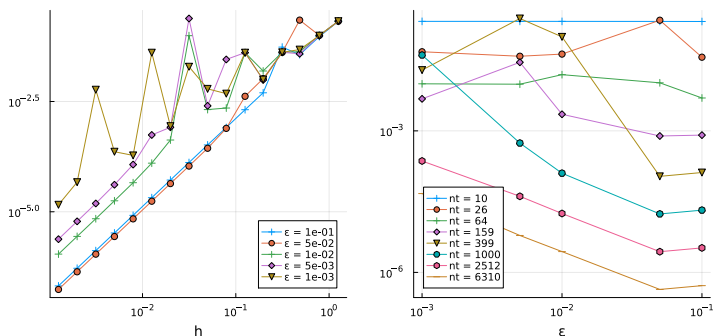
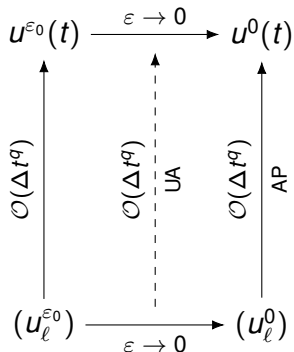


Figure: Error convergence w.r.t. h (left) and ε (right) of the Strang splitting on the Hénon-Heiles model for $t \in [0, 4\pi]$.

Two-scale notions of convergence



Definition – Order of convergence

A method of order q is said to be *uniformly accurate* (UA) if its uniform order of convergence is not degraded, i.e. if

$$\sup_{0 < \varepsilon \leq \varepsilon_0} \max_{0 \leq \ell \leq N} |y^\varepsilon(t_\ell) - y_\ell^\varepsilon| = \mathcal{O}(\Delta t^q).$$

We say a method is *asymptotic preserving* (AP) if

$$\lim_{\varepsilon \rightarrow 0^+} \max_{0 \leq \ell \leq N} |y^\varepsilon(t_\ell) - y_\ell^\varepsilon| = \mathcal{O}(\Delta t^q).$$

These notions may depend on the initial conditions (e.g. near-equilibrium).

Some literature

Different approaches

- high-order averaging (Castella, Chartier, Lemou, Méhats, LT ...)
- asymptotic preserving (AP) schemes (Dimarco, Jin, Pareschi, Toscani, ...)
- exponential integrators (Hochbruck, Lubich, Ostermann, Schratz ...)
- exact splitting (Bernier, Casas, Crouseilles, Li...)

Extensions of the averaging approach

- relaxation problems (Castella, Chartier, Lemou, Molmy, LT, ...)
- using neural networks (Bouchereau)
- stochastic case (Busnot-Laurent, Vilmart)

In some regard, also related to: homogenization, Chapman-Enskog expansion, non-linear geometric optics...

The principle of normal forms

Error of Strang splitting

$$e^{\frac{h}{2\varepsilon}A} \circ e^{hf} \circ e^{\frac{h}{2\varepsilon}A} = \exp\left(h\left(\frac{1}{\varepsilon}A + f\right) - \frac{h^3}{24\varepsilon^2}[A + 2\varepsilon f, [A, f]] + \dots\right)$$

→ easy if the vector field commute

Normal forms ansatz Find a change of variables Φ_ε such that

$$\exp(t/\varepsilon A + f) = \Phi_\varepsilon \circ \exp(t/\varepsilon A + tF_\varepsilon) \circ \Phi_\varepsilon^{-1}, \quad [A, F_\varepsilon] = 0.$$

Homological equation Derivating w.r.t. t , we find

$$[A, \Phi_\varepsilon] = \Phi_\varepsilon' A - A\Phi_\varepsilon = \varepsilon f \circ \Phi_\varepsilon - \varepsilon \Phi_\varepsilon' F_\varepsilon.$$

→ invert $\text{ad}_A := [A, \cdot]$ to refine Φ_ε with a fixed point¹

¹Chartier et al. *FoCM* (2020), Chartier et al. *IMA J. Numer. Anal.* (2021)

The effect of the change of variables

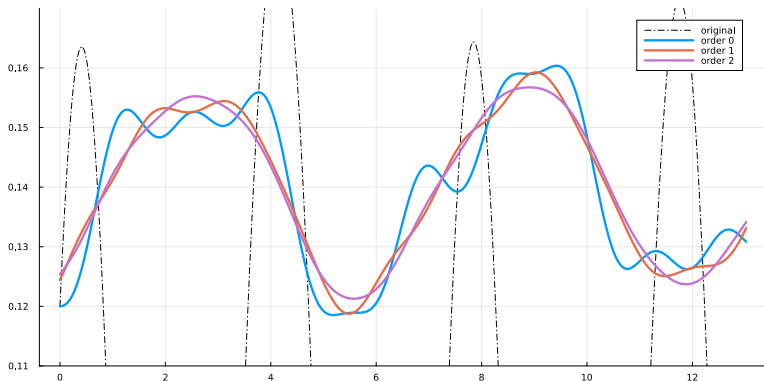


Figure: First component of the solutions $e^{-t/\varepsilon A} \Phi_\varepsilon^{-1}(y(t))$ of the stiff Hénon-Heiles model with $\varepsilon = 0.6$ for different orders of approximation of Φ_ε .

❓ does this preserve geometric properties? ❓

Lie group & algebra

In general, it is important to respect the correspondence

$$\text{Lie algebra } \mathfrak{g} \quad \begin{array}{c} \xrightarrow{\text{exp}} \\ \xleftarrow{\text{tangent}} \end{array} \quad \text{Lie group } \mathfrak{G}$$

Examples

- **vector fields** \leftrightarrow **flows**
- Hamiltonian \leftrightarrow symplectic
- divergence-free \leftrightarrow volume-preserving

⚠ Only some operations preserve structure ⚠

e.g. for $f, g \in \mathfrak{g}$ and $\phi \in \mathfrak{G}$,

$$g \circ \phi := (\phi')^{-1} \cdot g \circ \phi \in \mathfrak{g}.$$

$$[f, g] := g'f - f'g \in \mathfrak{g}.$$

Geometric homological equation

From a generator Setting $\Phi_\varepsilon = \exp(\varepsilon b_\varepsilon)$, then the homological equation is transformed

$$\begin{aligned} \Phi'_\varepsilon A - A\Phi_\varepsilon &= \varepsilon(f \circ \Phi_\varepsilon - \Phi'_\varepsilon F_\varepsilon) \\ &\quad \updownarrow \times (\Phi'_\varepsilon)^{-1} \\ A - A \circ \exp(\varepsilon b_\varepsilon) &= \varepsilon(f \circ \exp(\varepsilon b_\varepsilon) - F_\varepsilon) \end{aligned}$$

➔ build a generator $b^{[n]} = c^{[1]} + \dots + c^{[n]} = b_\varepsilon + \mathcal{O}(\varepsilon^{n+1})$

Pre-Lie / Magnus interpretation $g_1 \triangleright g_2 = [\text{ad}_A^\dagger g_1, g_2]$. Writing $b = \text{ad}_A^\dagger g$, the homological equation is²

$$\frac{e^{\varepsilon g \triangleright} - I}{\varepsilon g \triangleright} g = e^{\varepsilon g \triangleright} f - F_\varepsilon.$$

Performing “geometric” iterations

The modified variable Setting $\phi^{[n]}(v(t)) = y(t)$, we can separate the **oscillations**, the **drift** and the **residue** $r^{[n]} = \mathcal{O}(\varepsilon^{n+1})$,

$$\partial_t v = \left(\frac{1}{\varepsilon} A + f \right) \circ \phi_\varepsilon(v) = \frac{1}{\varepsilon} Av + F^{[n]}(v) + r^{[n]}(v)$$

the coupling is now small!

Hori's iterations Build a generator $b^{[n]} = c^{[1]} + \dots + c^{[n]}$ with

$$[A, \varepsilon c^{[k+1]}] = \varepsilon r^{[k]} = \underbrace{A \circ e^{\varepsilon b^{[k]}} - A + \varepsilon f \circ e^{\varepsilon b^{[k]}}}_{g^{[k]}} - \underbrace{\varepsilon F^{[k]}}_{\Pi_A g^{[k]}}.$$

In practice the pseudo-inverse ad_A^\dagger is computed using the Fourier coefficients of $\theta \mapsto g \circ e^{\theta A} = e^{-\theta A} \cdot g \circ e^{\theta A}$,

$$\text{ad}_A^\dagger g = \sum_{\alpha \neq 0} \frac{1}{i\alpha} \widehat{g}_\alpha.$$

Order reduction from splitting error

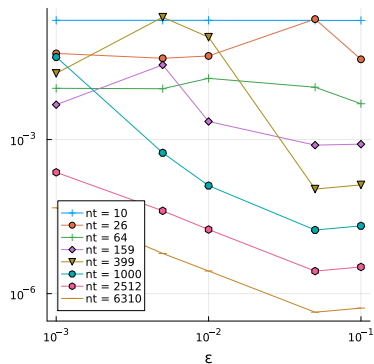
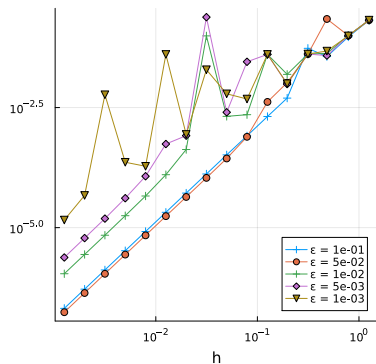


Figure: Error convergence w.r.t. h (left) and ϵ (right) of the Strang splitting on the Hénon-Heiles model for $t \in [0, 4\pi]$.

Validation on the Hénon-Heiles model

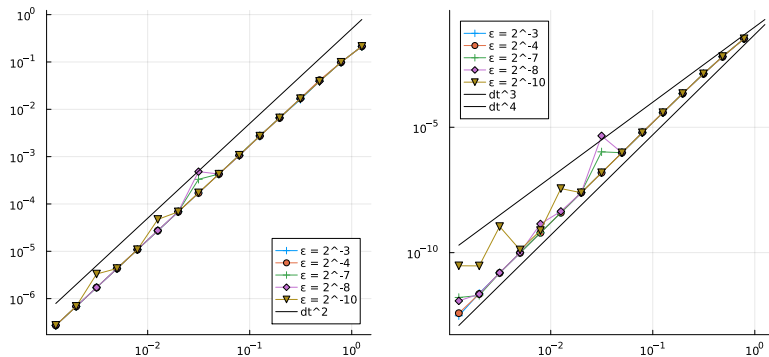


Figure: Error convergence w.r.t. h after the order 1 (left) and order 2 (right) asymptotic expansion, using the Strang and triple-jump (order 4) methods respectively.

Using the midpoint rule

Compute the flow in a structure-preserving manner,

$$\exp(\varepsilon \mathbf{b}^{[n]}) \approx \phi^{[n]} := \text{id} + \varepsilon \mathbf{b}^{[n]} \left(\frac{1}{2} (\text{id} + \phi^{[n]}) \right)$$

⚠ Only for $n \leq 2$ because $\phi^{[n]} = \exp(\varepsilon \mathbf{b}^{[n]}) + \mathcal{O}(\varepsilon^3)$

Derivatives To compute $f \circ \phi^{[n]} = (D\phi^{[n]})^{-1} f \circ \phi^{[n]}$, we use

$$f \circ \phi^{[n]}(v) = f(u) - D\mathbf{b}^{[n]} \left(\frac{1}{2} (u + v) \right) \cdot f \circ \phi^{[n]}(v)$$

with $u = \phi^{[n]}(v)$, or an approximation of it.

- ➔ fixed-point, computing the jacobian-vector product (jvp) with automatic differentiation in forward mode

Long-time behaviour

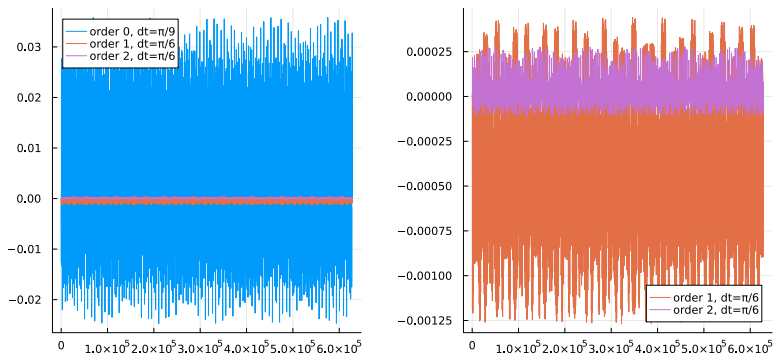


Figure: Energy evolution depending on the order of asymptotic expansion, with $\varepsilon = 0.05$.

Summary

$$\exp(t/\varepsilon \mathbf{A} + f) = \Phi_\varepsilon \circ \exp(t/\varepsilon \mathbf{A} + t\mathbf{F}_\varepsilon) \circ \Phi_\varepsilon^{-1}, \quad [\mathbf{A}, \mathbf{F}_\varepsilon] = 0.$$

- systematic, AD-based high-order averaging procedure
- 👍 *modified problems* solvable with uniform accuracy
- 👍 naturally preserve some geometric properties
- 👎 costly at high order (N_θ^n)

Future work

- automatic symbolic computations of b_ε
- study precisely the splitting error
- use the Magnus formulation to improve speed
- quasi-periodic case

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Thank you for you attention!