Uniform accuracy from geometric high-order averaging

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Outline

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1. Highly-oscillatory problems
   - Behaviour of highly-oscillatory problems
   - Geometric properties of averaging
2. High-order averaging
   - The averaging ansatz and normal forms
   - Well-posedness of the averaged model
   - The quasi-periodic case
3. Numerical experiments
   - Computing the change of variable and the pullback
   - Validation on the Hénon-Heiles model

A more general model

We are concerned with models of the form

$$\partial_t y^\varepsilon = \frac{1}{\varepsilon} A y^\varepsilon + f(y^\varepsilon), \qquad y^\varepsilon(0) = y_0 \in \mathbb{R}^d$$

where $\tau \mapsto e^{\tau A}$ is (quasi-)periodic.

Examples

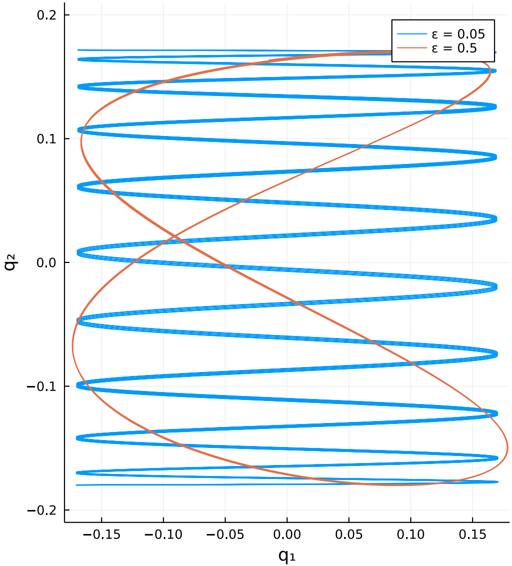
- Discretised non-linear Schrödinger

$$i\partial_t \psi^\varepsilon = -\frac{1}{\varepsilon}\Delta\psi^\varepsilon + |\psi^\varepsilon|^2\psi^\varepsilon$$

- Particle methods for Vlasov equation with stiff magnetic field

$$\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon + \left(E + \frac{1}{\varepsilon} v \times B\right) \cdot \nabla_v f^\varepsilon = 0$$

Introducing the stiff Hénon-Heiles model



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

Figure: Trajectories of the Hénon-Heiles model with initial data $(p_1, p_2, q_1, q_2) = (0.12, 0.12, 0.12, 0.12)$ for $t \in [0, 20]$.

Appropriate numerical methods

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

Exponential integrators based on the integral form

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

Lawson methods RK scheme on the filtered problem

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

Splitting methods e.g. Strang splitting

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

Strang splitting error – Order reduction

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

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

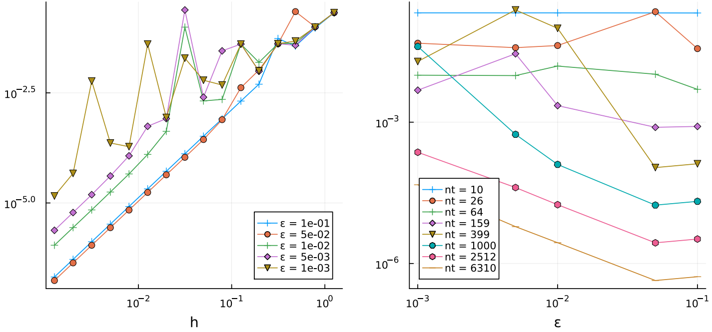


Figure: Error convergence w.r.t. h (left) and ε (right) of the Strang splitting on the Hénon-Heiles model for $t \in [0, 4\pi]$.

Two-scale notions of convergence

$$
\begin{tikzcd}
u^{\varepsilon_0}(t) \arrow[rr, "\varepsilon \to 0"] & {} & u^0(t) \\
(u_\ell^{\varepsilon_0}) \arrow[u, "\mathcal{O}(\Delta t^q)"] \arrow[rr, "\varepsilon \to 0"'] & {} \arrow[u, dashed, "\mathcal{O}(\Delta t^q)", "\text{UA}"'] & (u_\ell^0) \arrow[u, "\mathcal{O}(\Delta t^q)", "\text{AP}"']
\end{tikzcd}
$$

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

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

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

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

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

Order reduction

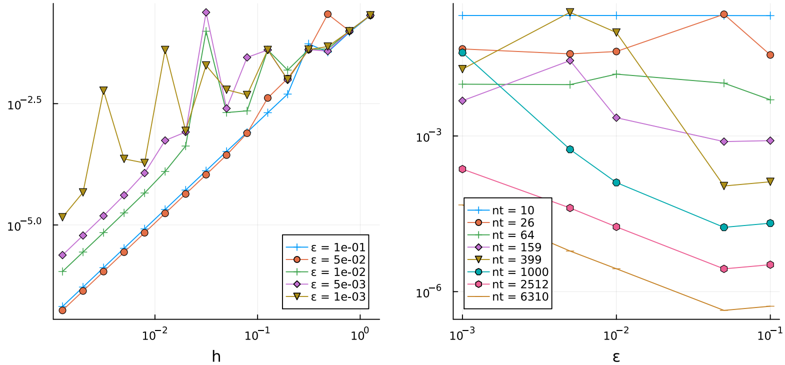


Figure: Error convergence w.r.t. h (left) and ε (right) of the Strang splitting on the Hénon-Heiles model for $t \in [0, 4\pi]$.

Uniform accuracy

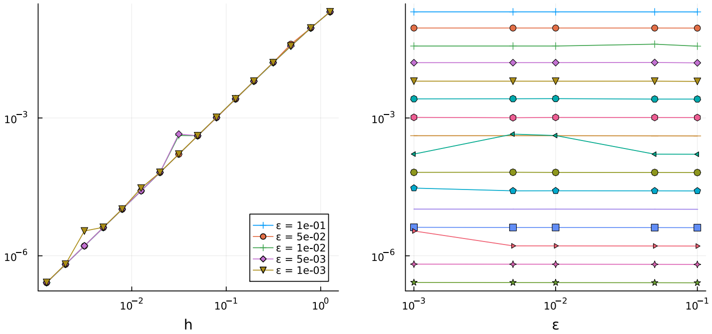


Figure: Error convergence w.r.t. h (left) and ε (right) of the Strang splitting on the first-order averaged Hénon-Heiles model for $t \in [0, 4\pi]$.

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 ...)

Extensions of the averaging approach

- relaxation problems (Castella, Chartier, Lemou, Molmy, LT, ...)
- stochastic case (Laurent, Vilmart)

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

Long-time numerical behaviour

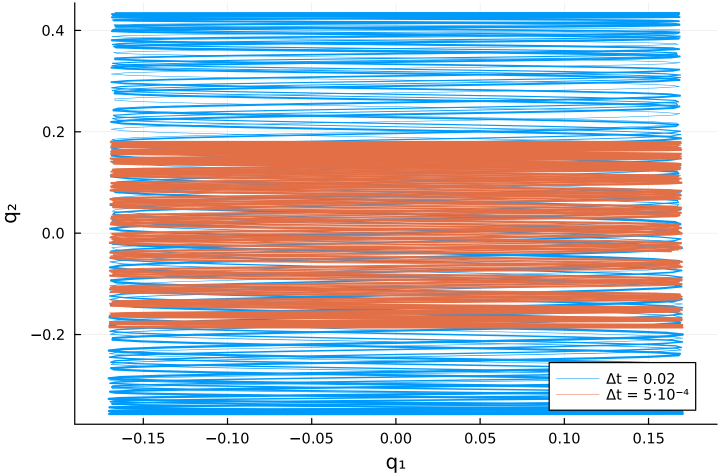


Figure: Trajectory for $t \in [780, 800]$ with $\varepsilon = \pi/100$ for different time steps using the integral RK1 scheme.

The stiff Hénon-Heiles model – Hamiltonian

The system may actually be written in a canonical Hamiltonian form

$$\dot{q} = \nabla_p H(p,q), \qquad \dot{p} = -\nabla_q H(p,q)$$

with the Hamiltonian

$$H(q_1,q_2,p_1,p_2) = \underbrace{\frac{1}{2\varepsilon}\left({p_1}^2 + {q_1}^2\right)}_{\frac{1}{\varepsilon}H_0} + \underbrace{\frac{1}{2}\left({p_2}^2 + {q_2}^2\right) + {q_1}^2 q_2 - \frac{1}{3}{q_2}^3}_{H_1}$$

Definition – Hamiltonian structure

A vector field $(\theta, y) \mapsto g(y)$ is said to be *Hamiltonian* if there exists $(\theta, y) \mapsto H(y) \in \mathbb{R}$ such that

$$g(y) = J^{-1}\, \nabla H(y) \quad \text{where} \quad J^{-1} = \begin{pmatrix} 0 & -I_d \\ I_d & 0 \end{pmatrix}.$$

The midpoint scheme – Energy drift

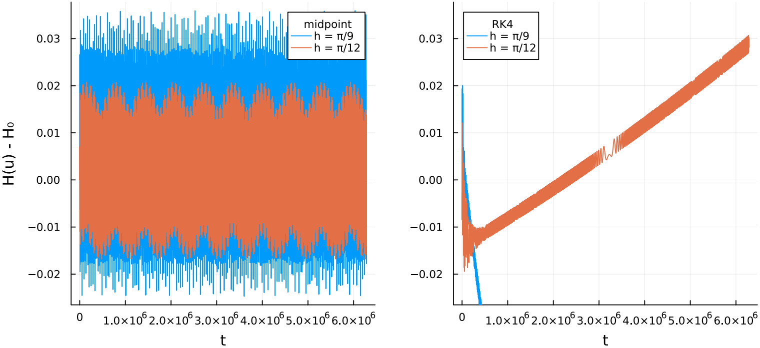


Figure: Energy deviation over time depending on the scheme used to approximate e^{hf} in the Strang splitting.

🎞 great visuals in introductory video by braintruffle on YouTube

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

Lie group & algebra

In general, it is important to respect the correspondence

$$\text{Lie algebra } \mathfrak{g} \quad \underset{\text{tangent}}{\overset{\exp}{\rightleftarrows}} \quad \text{Lie group } \mathfrak{G}$$

Examples

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

⚠ Only some operations preserve structure ⚠

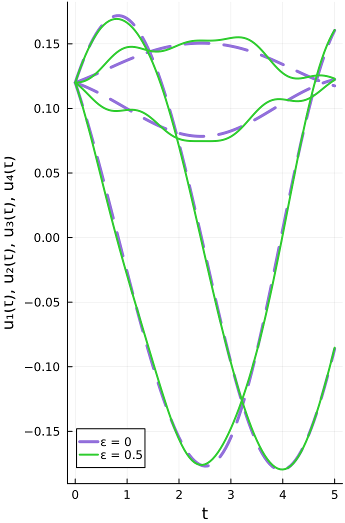
e.g. for $g \in \mathfrak{g}$ and $\phi \in \mathfrak{G}$,

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

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

Outline

Filtering out the oscillations



Introduce the "filtered" problem on

$$u^\varepsilon(t) = e^{-tA/\varepsilon} y^\varepsilon(t),$$

and the filtered vector field can be defined as

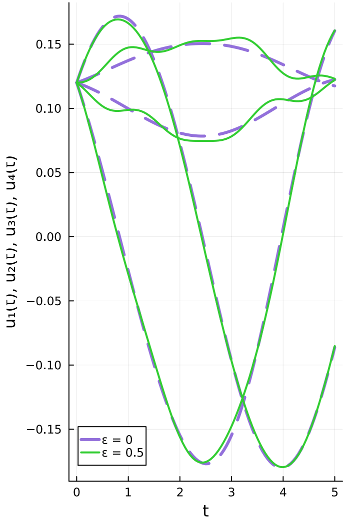
$$f \triangleleft e^{\theta A} = e^{-\theta A} f\left(e^{\theta A} u\right) := g_\theta$$

where $(\theta, u) \mapsto g_\theta(u)$ is periodic w.r.t. θ and

$$\partial_t u^\varepsilon(t) = g_{t/\varepsilon}\left(u^\varepsilon(t)\right).$$

⚠ $|\partial_t^{k+1} u^\varepsilon(t)| = \mathcal{O}(1/\varepsilon^k)$ therefore the order of numerical schemes is still limited

The averaging ansatz



Limit behaviour

The main dynamics are dictated by the *non-stiff* problem

$$u^\varepsilon(t) = u_0 + \int_0^t \widehat{g}_0\big(u^\varepsilon(s)\big)\mathrm{d}s + \mathcal{O}(\varepsilon),$$

with $\widehat{g}_0$ the θ-average vector field.

Averaging

Decompose the solution u^ε as

$$u^\varepsilon(t) = \Phi^\varepsilon_{t/\varepsilon} \circ \exp(tG^\varepsilon) \circ \left(\Phi^\varepsilon_0\right)^{-1}(u_0)$$

with $(\theta, u) \mapsto \Phi^\varepsilon_\theta(u) = \mathrm{id} + \mathcal{O}(\varepsilon)$ a periodic change of variable and $u \mapsto G^\varepsilon(u)$ a non-stiff vector field.

The method of Lie series

Homological equation since $u^\varepsilon(t) = \Phi^\varepsilon_{t/\varepsilon} \circ e^{tG^\varepsilon} \circ (\Phi^\varepsilon_0)^{-1}(u_0)$ with $\partial_t u^\varepsilon = g_{t/\varepsilon}(u^\varepsilon)$,

$$\partial_\theta \Phi^\varepsilon_\theta = \varepsilon \left(g_\theta \circ \Phi^\varepsilon_\theta - D\Phi^\varepsilon_\theta \cdot G^\varepsilon \right)$$

➔ refine Φ^ε with a fixed point ⚠ but there is no structure here!

Lie series Construct generators $\varepsilon a^{[k]} = \mathcal{O}(\varepsilon^k)$ such that

$$\Phi^{[n]}_\theta = \exp\left(\varepsilon\, a^{[n]}_\theta\right) \circ \ldots \circ \exp\left(\varepsilon\, a^{[1]}_\theta\right),$$

with $\Phi^{[0]} = \mathrm{id}$, closure $\widehat{a}^{[k]}_0 = 0$ and the iterations

$$\partial_\theta a^{[n+1]}_\theta = \left(D\Phi^{[n]}_\theta\right)^{-1} \left(g_\theta \circ \Phi^{[n]}_\theta - \tfrac{1}{\varepsilon} \partial_\theta \Phi^{[n]}_\theta \right) - G^{[n+1]} = \mathcal{O}(\varepsilon^n),$$

👍 every element is in the Lie algebra

Averaging as a higher-order filtering

$$y^{\varepsilon}(t) \xleftarrow{e^{\theta A}} u^{\varepsilon}(t) \xleftarrow{\exp\left(\varepsilon a_{\theta}^{[1]}\right)} v^{[1]}(t) \xleftarrow{\exp\left(\varepsilon a_{\theta}^{[2]}\right)} \dots$$

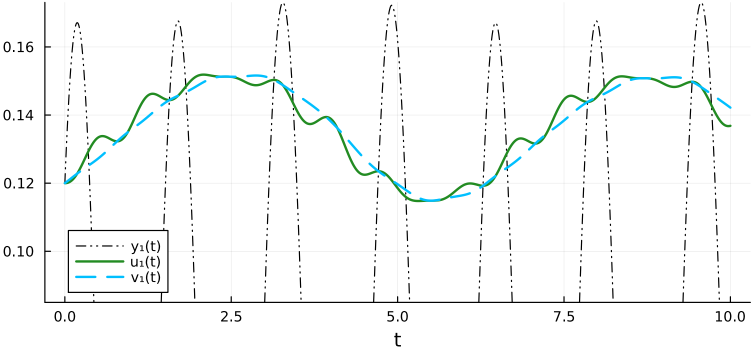


Figure: Original, filtered and first-order pulled-back solutions for $\varepsilon = 0.25$.

The pullback approach

Knowing the change of variable $\Phi^{[n]}$, we define

$$v^{[n]}(t) = \left(\Phi^{[n]}_{t/\varepsilon}\right)^{-1}(u^{\varepsilon}(t)),$$

which satisfies the new differential equation

$$\begin{aligned}\partial_t v^{[n]}(t) &= (D\Phi^{[n]}_{t/\varepsilon})^{-1}\left(g_{t/\varepsilon} \circ \Phi^{[n]} - \tfrac{1}{\varepsilon}\partial_\theta \Phi^{[n]}\right) \\ &= G^{[n+1]}\big(v^{[n]}(t)\big) + \partial_\theta a^{[n+1]}_{t/\varepsilon}\big(v^{[n]}(t)\big) \\ &=: g^{[n]}_{t/\varepsilon}\big(v^{[n]}(t)\big)\end{aligned}$$

the oscillations are now small

Because $a^{[n+1]} = \mathcal{O}(\varepsilon^n)$, the new vector field satisfies (formally)

$$|\partial_t^{k+1} v(t)| = \mathcal{O}(1/\varepsilon^{\min(0,k-n)}).$$

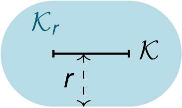
Assumptions – Analyticity and complex expansions

Assumptions

- The operator A generates a known 2π-periodic group $\theta \mapsto e^{\theta A}$
- For all ε small enough, the solution stays in some $\mathcal{K}$ for $t \in [0, 1]$

Introduce the complex extensions of $\mathcal{K}$ as

$$\mathcal{K}_r := \{u + \tilde{u}, \quad (u, \tilde{u}) \in \mathcal{K} \times X_{\mathbb{C}}, |\tilde{u}|_{\mathbb{C}} \leq r\}.$$



Assumption – Analyticity

There exists some $R > 0$ such that the vector field $(\theta, u) \mapsto g_\theta(u)$ is of class C^μ w.r.t. θ and u-analytic in $\mathcal{K}$, of radius everywhere greater than $2R$. Furthermore,

$$\sup_{(\theta,u)\in\mathbb{T}\times\mathcal{K}_{2R}} |g_\theta(u)| =: \|g\|_{2R} \leq M.$$

Well-posedness of averaging

The homological equation is “solved” iteratively with the relation

$$\partial_\theta a_\theta^{[n+1]} = g^{[n]} - \widehat{g}_0^{[n]}, \quad \text{and} \quad \Phi^{[0]} = \mathrm{id},$$

with $g^{[n]} = (D\Phi^{[n]})^{-1}\left(g_\theta \circ \Phi^{[n]} - \frac{1}{\varepsilon}\partial_\theta \Phi^{[n]}\right)$.

Well-posedness and accuracy of the averaging procedure

There exists $\varepsilon_0 > 0$ such that for all $n \in \mathbb{N}$, the averaging procedure is well defined for $0 < \varepsilon \leq \varepsilon_n := \frac{\varepsilon_0}{n+1}$. Specifically,

$$\|\Phi^{[n]} - \mathrm{id}\,\| \lesssim \frac{\varepsilon}{\varepsilon_n}, \qquad \|g^{[n]}\| \lesssim 1, \qquad \|g^{[n]} - \widehat{g}_0^{[n]}\| \lesssim \left(\frac{\varepsilon}{\varepsilon_n}\right)^n.$$

Their derivatives w.r.t. θ are of the same size, i.e. respectively $\mathcal{O}(\varepsilon)$, $\mathcal{O}(1)$ and $\mathcal{O}(\varepsilon^n)$ up to order μ.

Well-posedness of the pullback problem

When differentiating the new problem

$$\partial_t v^{[n]}(t) = G^{[n+1]}\big(v^{[n]}(t)\big) + \partial_\theta a_{t/\varepsilon}^{[n+1]}\big(v^{[n]}(t)\big)$$

the oscillations get divided by ε, but are small enough to not generate stiffness!

Theorem – Uniform accuracy (Chartier, Lemou, Méhats, Vilmart 2021)

This problem is non-stiff up to its $(n+1)$-th derivative and can therefore be solved with uniform accuracy up to order n for standard schemes and order $n+1$ with integral schemes. In other words, we may obtain

$$|v(t_\ell) - v_\ell| \leq C\Delta t^{n+1}$$

with C independent of ε.

Multi-frequency homological equation

Multiple frequencies $(\omega_1, \dots, \omega_s)$ such that there is a decomposition

$$e^{\tau A} = \sum_{\alpha \in \mathbb{Z}^s} e^{i\alpha\cdot\omega} \hat{P}_\alpha$$

then identify the multi-phase vector field

$$(\theta, u) \in \mathbb{T}^s \times \mathcal{K} \mapsto g_\theta(u) \qquad \text{s.t.} \qquad g_{\omega\tau} = f \triangleleft e^{\tau A}.$$

Homological equation The iterations are now

$$\sum_i \omega_i \frac{\partial}{\partial \theta_i} a_\theta^{[n+1]} = g_\theta^{[n]} - \widehat{g}_0^{[n]}$$

which is integrated in Fourier space for $\alpha \in \mathbb{Z}^s$, $\alpha \neq 0$,

$$\hat{a}_\alpha^{[n+1]} = \frac{1}{i(\alpha\cdot\omega)} \widehat{g}_\alpha^{[n]}$$

⚠ small divisors!

Multi-frequency homological equation

Assumption - Strong non-resonance

The frequencies are strongly non-resonant: there exist $c_D, \nu > 0$ such that for all $\alpha \in \mathbb{Z}^s \setminus \{0\}$

$$|\alpha \cdot \omega| \geq c_D |\alpha|^{-\nu}.$$

- Quantifies the small divisors: if g is H^μ_θ, then $g^{[n]}$ is $H^{\mu - n\nu}_\theta$.

Corollary – Well-posedness under strong non-resonance

If $(\theta, u) \mapsto g_\theta(u)$ is analytic w.r.t. θ with radius 2μ, then the previous results hold for

$$0 < \varepsilon \leq \varepsilon_n := \frac{\varepsilon_0}{(n+1)^{1+\nu}}.$$

Additionally, the maps are analytic with radius μ.

Outline

Using the midpoint rule

Compute the flow in a structure-preserving manner,

$$\exp\left(\varepsilon a_\theta^{[n]}\right) \approx \phi_\theta^{[n]} := \mathrm{id} + \varepsilon a_\theta^{[n]}\left(\tfrac{1}{2}(\mathrm{id} + \phi_\theta^{[n]})\right)$$

❓ Will this impact uniform accuracy?
➡ Only for $n \geq \varepsilon^3$ because $\phi^{[n]} = \exp\left(\varepsilon a^{[n]}\right) + \mathcal{O}(\varepsilon)^3$

Derivatives

$$\begin{aligned}
\tfrac{1}{\varepsilon}\partial_\theta \phi_\theta^{[n]} &= \partial_\theta a_\theta^{[n]}\left(\tfrac{1}{2}(\mathrm{id} + \phi_\theta^{[n]})\right) + \tfrac{1}{2}\varepsilon D a_\theta^{[n]}\left(\tfrac{1}{2}(\mathrm{id} + \phi_\theta^{[n]})\right) \cdot \tfrac{1}{\varepsilon}\partial_\theta \phi_\theta^{[n]} \\
&= \left(g_\theta^{[n-1]} - \langle g^{[n-1]}\rangle\right)\left(\tfrac{1}{2}(\mathrm{id} + \phi_\theta^{[n]})\right) \\
&\quad + \tfrac{1}{2}\varepsilon D a_\theta^{[n]}\left(\tfrac{1}{2}(\mathrm{id} + \phi_\theta^{[n]})\right) \cdot \tfrac{1}{\varepsilon}\partial_\theta \phi_\theta^{[n]}
\end{aligned}$$

➡ fixed-point for $\frac{1}{\varepsilon}\partial_\theta \phi_\theta^{[n]}$, computing the jacobian-vector product (jvp) with automatic differentiation

Validation on the Hénon-Heiles model

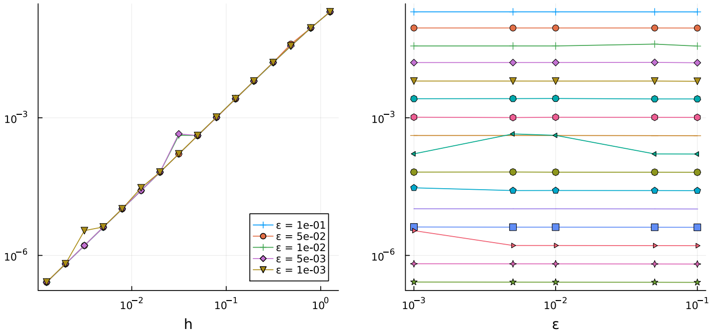


Figure: Error convergence w.r.t. h (left) and ε (right) of the Strang splitting on the first-order averaged Hénon-Heiles model for $t \in [0, 4\pi]$.

Summary

Starting from an ansatz

$$u^\varepsilon(t) = \Phi^\varepsilon_{t/\varepsilon} \circ \exp(tG^\varepsilon) \circ \left(\Phi_0^{[n]}\right)^{-1}(u_0)$$

with Φ^ε periodic and G^ε non-stiff, we derived

- a systematic high-order averaging procedure
- a framework which extends fairly naturally to other contexts
- *modified problems* solvable with uniform accuracy
- and which naturally preserve some geometric properties

However, some obvious limitations remain:

- the computational cost increases exponentially with the order n
- this may not be suited for low-regularity problems

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Thank you for you attention!