Formal averaging of periodic and quasi-periodic vector fields

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Example (Fermi-Pasta-Ulam problem)

Hamiltonian system with Hamiltonian function

$$egin{array}{rcl} \mathcal{H}(p,ar{p},q,ar{q}) &=& rac{1}{2}(p^Tp+ar{p}^Tar{p})+rac{1}{2\epsilon^2}q^Tq+U(q,ar{q}), \ \mathcal{U}(q,ar{q}) &=& rac{1}{4}\left((ar{q}_1-q_1)^4+(ar{q}_m+q_m)^4
ight) \ &+rac{1}{4}\sum_{j=1}^{m-1}(ar{q}_{j+1}-q_{j+1}-ar{q}_j-q_j)^4. \end{array}$$

We consider m = 3, $\epsilon = 1/100$, and initial values

$$ar{p}(0)=p(0)=ar{q}(0)=\left(egin{array}{c}1\\0\\0\end{array}
ight), \ q(0)=\left(egin{array}{c}\epsilon\\0\\0\end{array}
ight).$$

Solution for the component $q_2(t)$,



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and for n = 0, 1, 2, 3, ...,

 $q_2(2\pi\epsilon n)$

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and for $n = 0, 1, 2, 3, \ldots$,

$$q_2(2\pi\epsilon n)$$
, and $q_2(\frac{\pi\epsilon}{2}+2\pi\epsilon n)$.

Consider a Hamiltonian system

$$\frac{d}{dt}y = J^{-1}\nabla H(y;\epsilon), \quad H(y;\epsilon) := \epsilon^{-1}H^0(y) + R(y),$$

Let $\varphi_{\tau} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ be such that $\varphi_{t/\epsilon}$ is the *t*-flow of that system. Assume that the τ -flow φ_{τ}^{0} of H^{0} is (2π) -periodic. $(H^{0}(y) \text{ and } R(y) \text{ may depend on } \epsilon)$. It can be shown that $\varphi_{2\pi}$ is a near-to-identity map,

Backward error analysis

There exists $\mathcal{H}(Y;\epsilon) = \mathcal{H}_0(Y) + \epsilon \mathcal{H}_1(Y) + \epsilon^2 \mathcal{H}_2(y) + \cdots$,

$$\frac{d}{dt}Y = J^{-1}\nabla \mathcal{H}(Y;\epsilon),$$

such that, $Y(2\pi\epsilon n) = y(2\pi\epsilon n)$ if $Y(0) = y(0) = y_0$.

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$$\mathcal{H}(Y; \epsilon) = \mathcal{H}_0(Y) + \epsilon \mathcal{H}_1(Y) + \epsilon^2 \mathcal{H}_2(y) + \cdots$$
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Example (Fermi-Pasta-Ulam problem)

We consider

$$egin{array}{lll} ilde{\mathcal{H}}(Y,\epsilon) &:= & \mathcal{H}_0(Y) + \epsilon^2 \mathcal{H}_2(Y) + \epsilon^4 \mathcal{H}_4(Y) \ &= & \mathcal{H}(Y;\epsilon) + \mathcal{O}(\epsilon^6), \end{array}$$

and plot the variation $\tilde{\mathcal{H}}(y(t);\epsilon) - \tilde{\mathcal{H}}(y(0);\epsilon)$



Smooth invariant

Under the previous assumtions for

$$\frac{d}{dt}y = J^{-1}\nabla H(y;\epsilon), \quad H(y;\epsilon) := \epsilon^{-1}H^0(y) + R(y)$$

consider $\mathcal{H}(Y; \epsilon) = \mathcal{H}_0(Y) + \epsilon \mathcal{H}_1(Y) + \epsilon^2 \mathcal{H}_2(y) + \cdots$ as before, then $\mathcal{H}(y; \epsilon)$ is a first integral of the original system.

Indeed, for $t_n = 2\pi\epsilon n$, n = 1, 2, ...

$$H(Y(t_n); \epsilon) = H(y(t_n); \epsilon) =$$
Const

and by a interpolating argument, $H(Y(t); \epsilon) = \text{Const}$, and thus

$$\{H,\mathcal{H}\}\equiv 0.$$

Numerical integration of HOS with ϵ -independent time-steps

Integrate the smooth system

$$\frac{d}{dt}Y = J^{-1}\nabla H(Y;\epsilon), \quad Y(0) = y_0$$

instead of the highly oscillatory one. Different options

- Symbolic-numeric algorithms using explicit knowledge of ${\cal H}$
- Purely numerical schemes that try to approximate Y(t) by using H as input (HMSM, ...).

Motivated by that, we aim at

- Obtaining formulae for $\mathcal{H}(Y; \epsilon)$ and its solutions Y(t)
- Such formulae should be as explicit as possible and
- Of universal character

Time-dependent $(2\pi\epsilon)$ -periodic change of variables

Let φ_{τ}^{0} be the τ -flow of H^{0} , consider

$$y = \varphi_{t/\epsilon}^0(\hat{y}).$$

Notice that for $t_n = 2\pi\epsilon n$, it reduces to the identity map.

The system with $H(y; \epsilon) = \epsilon^{-1} H^0(y) + R(y)$ is transformed into a non-autonomous Hamiltonian system with $\hat{H}(\hat{y}, t/\epsilon)$, where

$$\hat{\mathcal{H}}(\hat{y}, au) := \mathcal{R}(arphi^{0}_{ au}(\hat{y})) = \sum_{k \in \mathbb{Z}} e^{ik au} \hat{\mathcal{H}}_{k}(\hat{y}).$$

 $(\varphi_{\tau}^{0}(\hat{y}) \text{ is } (2\pi)\text{-periodic in } \tau)$. Clearly,

$$rac{d}{dt}\hat{y} = \sum_{k\in\mathbb{Z}} e^{ikt/\epsilon} f_k(\hat{y}).$$

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From now on, we consider systems of that general form. The $f_k(\hat{y})$ may depend on ϵ , but not reflected in the notation ϵ , $\epsilon \in \{0, \infty\}$

Standard high order averaging [Sanders, Verhulst, Murdock 2007]

Under suitable assumptions on the HOS

$$rac{d}{dt}y = \sum_{k\in\mathbb{Z}}e^{ikt/\epsilon}f_k(y).$$

there exists a formal $(2\pi\epsilon)$ -periodic change of variables $y = K(Y, t/\epsilon)$ that transforms the original HOS into the *(averaged)* autonomous equations

$$\frac{d}{dt}Y = F(Y;\epsilon) := F_0(Y) + \epsilon F_1(Y) + \epsilon^2 F_2(Y) + \cdots$$

The change of variables $y = K(Y, \tau)$ is not unique:

• Stroboscopic averaging: K(Y, 0) = Y, which implies $Y(2\pi\epsilon n) = y(2\pi\epsilon n)$ for all $n \in \mathbb{Z}$.

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$$\int_0^{2\pi} K(Y,\tau) d\tau = Y$$
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Stroboscopic averaging of HOS autonomous Hamiltonian systems

Back to the HOS Hamiltonian system $H(y) = e^{-1}H^0(y) + R(y)$, the $(2\pi\epsilon)$ -periodic change of variables

$$\varphi = \varphi_{t/\epsilon}^0(K(Y, t/\epsilon))$$

transforms the original HOS autonomous Hamiltonian H into a smooth autonomous Hamiltonian \mathcal{H} .

Comments:

- The smooth Hamiltonian \mathcal{H} is exactly the same as that derived from backward error analysis applied to $\varphi_{2\pi\epsilon}$.
- The (stroboscopically) averaged system of general HOS

$$rac{d}{dt}y = \sum_{k\in\mathbb{Z}}e^{ikt/\epsilon}f_k(y).$$

can also be derived from backward error analysis applied to the near-identity map ψ such that $\psi(y(0)) = y(2\pi\epsilon)$ for any solution y(t).

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We next focus on obtaining, using standard techniques in numerical analysis (B-series, ...), universal formulae for the averaging of non-autonomous periodic HOS.

B-series expansion of solution of the HOS

For the solutions of $\dot{y} = \sum_{k} e^{ikt/\epsilon} f_k(y)$,

$$y(t) = y(0) + \sum_{u \in \mathcal{T}} \frac{\alpha_u(t)}{\sigma_u} \mathcal{F}_u(y(0)),$$

 ${\mathcal T}$ is the set of rooted trees labelled by $k\in {\mathbb Z}$, and for each $u\in {\mathcal T}$,

- the coefficients $\alpha_u(au)$ are linear combinations of $t^j e^{ikt/\epsilon}$,
- The elementary differentials $\mathcal{F}_u : \mathbb{R}^d \to \mathbb{R}^d$ are smooth, $(\sigma_u \in \mathbb{Z} \text{ is a normalization factor.})$

Elementary coefficients

$$\alpha_u(t) = \int_0^t e^{ikt'/\epsilon} \alpha_{u_1}(t') \cdots \alpha_{u_m}(t') dt', \quad u = [u_1 \cdots u_m]_k.$$

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Examples for rooted trees with less than 4 vertices

u	$\mathcal{F}_u(y)$	$\alpha_u(t)$
k	$f_k(y)$	$\int_0^t e^{rac{ikt_1}{\epsilon}} dt_1$
	$f_m'(y)f_k(y)$	$\int_{0}^{t}\int_{0}^{t_{2}}e^{rac{i(kt_{1}+mt_{2})}{\epsilon}}dt_{1}dt_{2}$
(m) (l)	$f_{\ell}'(y)f_m'(y)f_k(y)$	$\int_0^t \int_0^{t_3} \int_0^{t_2} e^{\frac{i(kt_1+mt_2+\ell t_3)}{\epsilon}} dt_1 dt_2 dt_3$
m k	$f_{\ell}^{\prime\prime}(y)(f_m(y),f_k(y))$	$\int_0^t \int_0^{t_2} e^{rac{i(kt_1+mt_1+\ell t_2)}{\epsilon}} dt_1 dt_2$

For each $u \in \mathcal{T}$, $\alpha_u(t) = \alpha_u(t, t/\epsilon)$, with

$$lpha_u(t, au) = \sum_{k\in\mathbb{Z}} lpha_u^k(t) e^{ik au},$$

where each $\alpha_u^k(t)$ is a polynomial in t.

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m k	$f_{\ell}''(y)(f_m(y),f_k(y))$	$\int_0^t \int_0^{t_2} e^{rac{i(kt_1+mt_1+\ell t_2)}{\epsilon}} dt_1 dt_2$

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Relation with modulated Fourier series

For any solution of $\dot{y} = \sum_k e^{ikt/\epsilon} f_k(y)$,

$$\begin{split} y(t) &= y(0) + \sum_{u \in \mathcal{T}} \frac{\alpha_u(t, t/\epsilon)}{\sigma_u} \,\mathcal{F}_u(y(0)), \\ &= y(0) + \sum_{u \in \mathcal{T}} \sum_{k \in \mathbb{Z}} \frac{\alpha_u^k(t)}{\sigma_u} \, e^{ikt/\epsilon} \,\mathcal{F}_u(y(0)), \\ &= y(0) + \sum_{k \in \mathbb{Z}} \left(\sum_{u \in \mathcal{T}} \frac{\alpha_u^k(t)}{\sigma_u} \,\mathcal{F}_u(y(0)) \right) \, e^{ikt/\epsilon} \\ &= y^0(t) + \sum_{k \in \mathbb{Z} \setminus \{0\}} e^{ikt/\epsilon} z^k(t). \end{split}$$

Modulated Fourier series versus B-series approach

In the case of exact solution of the Hamiltonian system with $H(y; \epsilon) = \epsilon^{-1} H^0(y) + R(y)$:

 Modulated Fourier approach [Hairer& Lubich 2000]: Expand exact solution y(t) in the form

$$y(t) = y^0(t) + \sum_{k \in \mathbb{Z} \setminus \{0\}} e^{ikt/\epsilon} z^k(t)$$

by Taylor-expanding R(y) around $y^0(t)$.

Our approach: Expand ŷ(t) = φ_{-t/ε}(y(t)) as a B-series in terms of the Fourier modes Ĥ_k of

$$\hat{H}(\hat{y}, au) := R(arphi_{ au}^{\mathsf{0}}(\hat{y})) = \sum_{k \in \mathbb{Z}} e^{ikt/\epsilon} \hat{H}_k(\hat{y}).$$

Averaging with B-series

There exist $\bar{\beta}_u, \bar{\alpha}_u(t), \kappa_u(\tau), u \in \mathcal{T}$, $(\bar{\alpha}_u(t) \text{ polynomial}, \kappa_u(\tau) (2\pi)$ -periodic) such that for any solution y(t) of the HOS

$$y(t) = K(Y(t), t/\epsilon), \quad \frac{d}{dt}Y(t) = F(y(t)),$$

where

$$F(Y) = \sum_{u \in \mathcal{T}} \frac{\overline{\beta}_u}{\sigma_u} \mathcal{F}_u(Y),$$

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$$K(Y, \tau) = Y + \sum_{u \in \mathcal{T}} \frac{\kappa_u(\tau)}{\sigma_u} \mathcal{F}_u(Y),$$

Not unique (but uniquely determined for prescribed $\kappa_u(0)$, $u \in \mathcal{T}$).

That is, $\alpha(t,\tau) = \bar{\alpha}(t)\kappa(\tau)$ with $\frac{d}{dt}\bar{\alpha}(t) = \bar{\alpha}(t)\bar{\beta}$.

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Stroboscopic averaging: K(Y,0) = Y

So that $Y(2\pi n\epsilon) = y(2\pi n\epsilon)$. Thus, $\kappa(0) = 1$ which implies $\bar{\alpha}(0) = 1$, and

$$ar{lpha}_u(t) = lpha_u(t,0), \quad \kappa_u(au) = lpha_u(0, au), \quad ar{eta}_u = \left. rac{d}{dt} ar{lpha}_u(t)
ight|_{t=0}$$

Classical' averaging: $\frac{1}{2\pi} \int_0^{2\pi} K(Y, \tau) d\tau = Y$ $Y(2\pi n\epsilon) \neq y(2\pi n\epsilon)$. We have $\frac{1}{2\pi} \int_0^{2\pi} \kappa(\tau) d\tau = \mathbb{1}$, and thus $\bar{\alpha}_u(t) = 1/(2\pi) \int_0^{2\pi} \alpha_u(t, \tau) d\tau, \quad \kappa_u(\tau) = (\bar{\alpha}(0)^{-1} \alpha(0, \tau))_u$ $\bar{\beta}_u = \frac{d}{dt} \bar{\alpha}(t) \Big|_{t=0}$.

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Given $\omega \in \mathbb{R}^{d}$ non-resonant and $\theta(t) = \theta_{0} + \omega t$,

$$rac{d}{dt}y:=f(y, heta(t))=\sum_{k\in\mathbb{Z}^d}e^{i(k\cdot heta(t))}f_k(y),\quad,\quad y(0)=y_0,$$

Expansion of solutions of quasi-periodic vector fields

$$y(t) = y_0 + \sum_{w \in \mathcal{W}} \alpha_w(t, \theta(t)) f_w(y_0),$$

where \mathcal{W} is the set of 'words' $w = k_1 \cdots k_r$ on the alphabet \mathbb{Z}^d ,

$$\alpha_{k_1\cdots k_r}(t) = \int_0^t \int_0^{t_r} \cdots \int_0^{t_2} e^{i\omega \cdot (k_1 t_1 + \cdots + k_r t_r)} dt_1 \cdots dt_r,$$

$$f_{k_1\cdots k_r}(y) = \frac{\partial}{\partial y} f_{k_2\cdots k_r}(y) f_{k_1}(y),$$

In particular, $f_{mk} = f'_k f_m$, $f_{\ell m k} = f''_k (f_m, f_\ell) + f'_k f'_m f_\ell$.

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In particular, $f_{mk} = f'_k f_m$, $f_{\ell mk} = f''_k (f_m, f_\ell) + f'_k f'_m f_\ell$.

Indeed, consider for each $k \in \mathbb{Z}^d$, the Lie operator associated to f_k ,

$$E_k = \sum_{i=1}^{d'} f_k^i \frac{\partial}{\partial y^i}, \text{ so that } f_{k_1 \cdots k_r} = E_{k_1} \cdots E_{k_r} [\mathrm{id}],$$

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Linear non-autonomous quasi-periodic differential equation

$$\frac{d}{dt}\Phi_t = \Phi_t \sum_{k \in \mathbb{Z}^d} e^{ik \cdot \theta(t)} E_k, \quad \Phi_0 = I.$$

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Recursive formulae for $\alpha_w(t,\theta)$

If $r \in \mathbb{Z}^+$, $k \in \mathbb{Z}^d - \{0\}$, $l \in \mathbb{Z}^d$, and $w \in \mathcal{W} \cup \{\emptyset\}$

$$\begin{aligned} \alpha_{k}(t,\theta) &= \frac{i}{k \cdot \omega} (e^{i(k \cdot \theta_{0})} - e^{i(k \cdot \theta)}), \\ \alpha_{0r}(t,\theta) &= \frac{t^{r}}{r!}, \\ \alpha_{0rk}(t,\theta) &= \frac{i}{k \cdot \omega} (\alpha_{0r-1k}(t,\theta) - \alpha_{0r}(t,\theta)e^{i(k \cdot \theta)}), \\ \alpha_{klw}(t,\theta) &= \frac{i}{k \cdot \omega} (\alpha_{lw}(t,\theta) - \alpha_{(k+l)w}(t,\theta)), \\ \alpha_{0rklw}(t,\theta) &= \frac{i}{k \cdot \omega} (\alpha_{0r-1klw}(t,\theta) - \alpha_{0r(k+l)w}(t,\theta)). \end{aligned}$$

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Formal high order averaging: Find a factorization

$$I + \sum_{w \in \mathcal{W}} \alpha_w(t, \theta) E_w = \left(I + \sum_{w \in \mathcal{W}} \bar{\alpha}_w(t) E_w\right) \left(I + \sum_{w \in \mathcal{W}} \kappa_w(\theta) E_w\right)$$
$$\frac{d}{dt} \left(I + \sum_{w \in \mathcal{W}} \bar{\alpha}_w(t) E_w\right) = \left(I + \sum_{w \in \mathcal{W}} \bar{\alpha}_w(t) E_w\right) \left(\sum_{w \in \mathcal{W}} \bar{\beta}_w E_w\right).$$

Or more compactly,

$$\alpha(t,\theta) = \bar{\alpha}(t)\kappa(\theta), \quad \frac{d}{dt}\bar{\alpha}(t) = \bar{\alpha}(t)\bar{\beta}.$$

Pseudo-stroboscopic averaging: $\kappa(\theta_0) = 1$

$$ar{lpha}_w(t) = lpha_w(t, heta_0), \quad \kappa_w(heta) = lpha_w(0, heta), \quad ar{eta}_w = \left. rac{d}{dt} ar{lpha}_w(t)
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 Pseudo-stroboscopic averaging for quasi-periodic problems

We get $y(t) = K(Y(t), \theta(t))$, $(\theta(t) = \theta_0 + \omega t)$, where

$$\frac{d}{dt}Y=F(Y), \quad Y(0)=y_0,$$

with

$$\begin{split} &\mathcal{K}(Y,\theta) &= Y + \sum_{w \in \mathcal{W}} \kappa_w(\theta) f_w(Y), \\ &\mathcal{F}(Y) &= \sum_{w \in \mathcal{W}} \bar{\beta}_w f_w(Y), \\ &\mathcal{Y}(t) &= y_0 + \sum_{w \in \mathcal{W}} \bar{\alpha}_w(t) f_w(y_0). \end{split}$$

Recursion for coefficients of averaged equation

$$\begin{split} \bar{\beta}_{k} &= 0, \quad \bar{\beta}_{0} = 1, \quad \bar{\beta}_{0^{r+1}} = 0, \\ \bar{\beta}_{0^{r}k} &= \frac{i}{k \cdot \omega} (\bar{\beta}_{0^{r-1}k} - \bar{\beta}_{0^{r}} e^{i(k \cdot \theta_{0})}), \\ \bar{\beta}_{klw} &= \frac{i}{k \cdot \omega} (\bar{\beta}_{lw} - \bar{\beta}_{(k+l)w}), \\ \bar{\beta}_{0^{r}klw} &= \frac{i}{k \cdot \omega} (\bar{\beta}_{0^{r-1}klw} - \bar{\beta}_{0^{r}(k+l)w}), \end{split}$$

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where $\beta_k(\theta) = e^{ik \cdot \theta}$ and $\beta_w(\theta) = 0$ for $w = k_1 \cdots k_r$ with r > 1. If $\alpha(t, \theta) = \bar{\alpha}(t)\kappa(\theta)$, then

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B-series expansion of exact solution of quasi-periodic ODEs

$$y(t) = B(\alpha(t), y_0), \text{ where } \alpha_u(t) = \alpha_u(t, \theta(t)) = \sum_{w \in \mathcal{W}_u} \alpha_w(t, \theta(t)).$$

Averaging formulae in B-series form

$$Y(t) = B(\bar{\alpha}(t), y_0), \quad \dot{Y} = B(\bar{\beta}, Y), \quad Y(t) = B(\kappa(\theta(t)), Y(t)),$$

• Quasi-stroboscopic averaging:

$$\bar{\alpha}(t) = \alpha(t, \theta_0), \quad \bar{\beta} = \left. \frac{d}{dt} \bar{\alpha}(t) \right|_{t=0}, \quad \kappa(\theta) = \alpha(0, \theta).$$

• Classical averaging:

$$\bar{\alpha}(t) = \int_{\mathcal{T}^d} \alpha(t,\theta) \, d\theta, \quad \bar{\beta} = \left. \frac{d}{dt} \bar{\alpha}(t) \right|_{t=0},$$
$$\kappa(\theta) = \bar{\alpha}(0)^{-1} \alpha(0,\theta).$$

Future work

- Prove rigorous results (bound independently the coefficients and the smooth *y*-dependent maps),
- Study approximate preservarion of formal invariants of HOS,
- Analyze existing numerical methods for highly oscillatory systems
- Desing and analyze new numerical methods. In particular, heterogenous multiscale methods based on

microintegration+ numerical evaluation of averaged equations+ macrointegration

Algebraic/geometric properties of exact solution

For $u_1, u_2, u_3 \in \mathcal{T}$

- $\alpha_{u_1 \circ u_2} + \alpha_{u_2 \circ u_1} = \alpha_{u_1} \alpha_{u_2}$, \rightarrow symplectic for each fixed t, τ .
- In addition

$$\alpha_{u_1 \circ u_2 u_3} + \alpha_{u_2 \circ u_1 u_3} + \alpha_{u_3 \circ u_1 u_2} = \alpha_{u_1} \alpha_{u_2} \alpha_{u_3}.$$

Hence, for each fixed t, τ , it represents the 1-flow of a vector field in the Lie algebra generated by the f_k .

- Classical averaging does not preserve the properties of $\alpha(t,\tau)$: $\frac{1}{(2\pi)} \int_0^{2\pi} (\alpha_{u_1 \circ u_2}(t,\tau) + \alpha_{u_2 \circ u_1}(t,\tau)) d\tau$ $\neq \frac{1}{(2\pi)^2} \left(\int_0^{2\pi} \alpha_{u_1}(t,\tau) d\tau \right) \left(\int_0^{2\pi} \alpha_{u_2}(t,\tau) d\tau \right)$

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