

# Averaging with B-series

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## Example (Fermi-Pasta-Ulam problem)

Hamiltonian system with Hamiltonian function

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2} p_1^T p_1 + \frac{1}{2} (p_2^T p_2 + \omega^2 q_2^T q_2) + U(q_1, q_2),$$

where  $p_1, p_2, q_1, q_2 \in \mathbb{R}^m$  and

$$\begin{aligned} U(q_1, q_2) &= \frac{1}{4} \left( (q_{1,1} - q_{2,1})^4 + (q_{1,m} + q_{2,m})^4 \right) \\ &\quad + \frac{1}{4} \sum_{j=1}^{m-1} (q_{1,j+1} - q_{2,j+1} - q_{1,j} - q_{2,j})^4. \end{aligned}$$

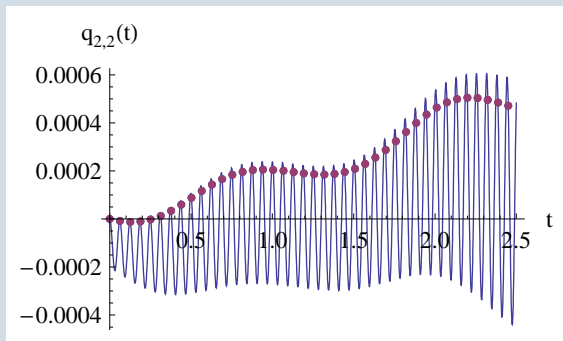
Consider the  $t$ -flow  $\varphi_t : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$  of that Hamiltonian system.

In particular, take  $\epsilon = 2\pi/\omega$ , and consider  $\varphi_\epsilon$ , that advances the solution in one period if the fast oscillations.

## Example (Fermi-Pasta-Ulam problem (cont.))

Component  $q_{2,2}(t)$  for  $m = 3$ ,  $\omega = 100$ , and initial values

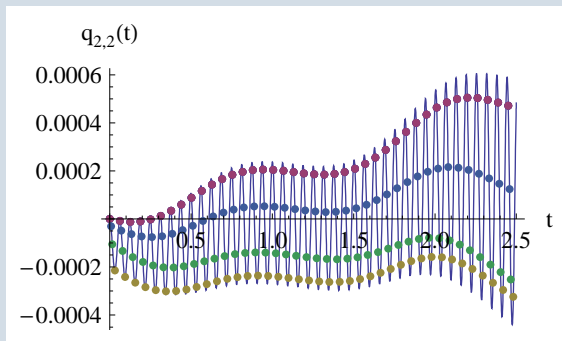
$$p_1(0) = p_2(0) = q_1(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad q_2(0) = \begin{pmatrix} \omega^{-1} \\ 0 \\ 0 \end{pmatrix}.$$



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First rescale time by considering the dimensionless time  $\tau = \omega t$ , and then apply the  $(2\pi)$ -periodic  $\tau$ -dependent change of variables

### Change of variables

$$\begin{aligned}\hat{p}_1 &= p_1, & \hat{p}_2 &= \cos(\tau)p_2 + \omega \sin(\tau)q_2, \\ \hat{q}_1 &= q_1, & \hat{q}_2 &= \cos(\tau)q_2 - \omega^{-1} \sin(\tau)p_2,\end{aligned}$$

(note that at stroboscopic times  $\tau_n = 2\pi n$ , that change of variables reduces to the identity map.)

The transformed system is a time-dependent Hamiltonian system with Hamiltonian function

$$\omega^{-1} \left( \frac{1}{2} \hat{p}_1^T \hat{p}_1 + U(\hat{q}_1, \cos(\tau)\hat{q}_2 + \omega^{-1} \sin(\tau)\hat{p}_2) \right).$$

Clearly, such a system can be written in the form

$$\frac{d}{d\tau} y = \omega^{-1} f_1(y, \tau) + \omega^{-2} f_2(y, \tau) + \omega^{-3} f_3(y, \tau) + \dots$$

# Backward error analysis of highly oscillatory systems

We consider highly oscillatory systems with frequency  $\omega$  that, after time rescaling  $\tau = \omega t$  (and possibly a  $(2\pi)$ -periodic  $\tau$ -dependent change of variables that is the identity map at stroboscopic times  $\tau_n = 2\pi n$ ), can be written as

$$\frac{d}{d\tau}y = f(y, \tau; \omega) := \omega^{-1}f_1(y, \tau) + \omega^{-2}f_2(y, \tau) + \omega^{-3}f_3(y, \tau) + \dots$$

where each  $f_j(y, \tau)$  is smooth in  $y$  and  $2\pi$ -periodic in  $\tau$ .

Consider  $\psi : \mathbb{R}^d \rightarrow \mathbb{R}^d$  such that  $\psi(y(0)) = y(2\pi)$ ,

- The map  $\psi$  is as a smooth near-to-identity map,
- $f_j(\cdot, \tau)$  is  $(2\pi)$ -periodic  $\Rightarrow y(\tau_n) = \psi^n(y(0))$  for  $\tau_n = 2\pi n$ ,
- $\psi$  is symplectic if  $f$  is Hamiltonian.

## Backward error analysis for the near-to-identity map $\psi$

Given

$$\frac{d}{d\tau}y = \omega^{-1}f_1(y, \tau) + \omega^{-2}f_2(y, \tau) + \omega^{-3}f_3(y, \tau) + \dots \quad (1)$$

there exists

$$\frac{d}{d\tau}\bar{y} = \omega^{-1}\bar{f}_1(\bar{y}) + \omega^{-2}\bar{f}_2(\bar{y}) + \omega^{-3}\bar{f}_3(\bar{y}) + \dots \quad (2)$$

such that formally,  $y(2\pi n) = \bar{y}(2\pi n)$  for the solutions  $y(\tau)$  and  $\bar{y}(\tau)$  of (1) and (2) with  $\bar{y}(0) = y(0)$ .

If (1) is Hamiltonian, then (2) is Hamiltonian with

$$\bar{H}(y) = \omega^{-1}\bar{H}_1(y) + \omega^{-2}\bar{H}_2(y) + \omega^{-3}\bar{H}_3(y) + \dots$$

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In averaging theory [Sanders, Verhulst, Murdock 2007], obtaining

$$\frac{d}{d\tau}\bar{y} = \omega^{-1}\bar{f}_1(\bar{y}) + \omega^{-2}\bar{f}_2(\bar{y}) + \omega^{-3}\bar{f}_3(\bar{y}) + \dots \quad (3)$$

from the original HOS system is called **stroboscopic averaging**.

### High order averaging

There exists a formal  $(2\pi)$ -periodic change of variables  $y = K(\bar{y}, \tau)$  that transforms the original system

$$\frac{d}{d\tau}y = \omega^{-1}f_1(y, \tau) + \omega^{-2}f_2(y, \tau) + \omega^{-3}f_3(y, \tau) + \dots$$

into the autonomous system (3).

The change of variables  $y = K(\bar{y}, \tau)$  is not unique. Typical choices

- $K(\bar{y}, 0) = \bar{y}$ : Stroboscopic averaging,
- $\int_0^{2\pi} K(\bar{y}, \tau) d\tau = \bar{y}$ .

## B-series

We will be dealing with B-series-like expansions of the form

$$B(\alpha, y) = \alpha_{\emptyset} y + \sum_{u \in \mathcal{T}} \frac{\omega^{-|u|}}{\sigma(u)} \alpha_u F_u(y),$$

where  $\mathcal{T}$  is a set of indices, and for each  $u \in \mathcal{T}$ ,

- $\alpha_u \in \mathbb{R}$  are the coefficients of the B-series,
- $F_u : \mathbb{R}^D \rightarrow \mathbb{R}^D$  is the *elementary differential*,
- $|u| \in \mathbb{Z}^+$  is the *degree (or order)* of  $u$ ,
- $\sigma(u)$  is *some normalization factor*.

In standard B-series (Hairer and Wanner 1974),  $\mathcal{T}$  is the set of rooted trees, and  $\sigma(u)$  is the symmetry number of the tree  $u$ .

We denote  $\mathcal{T}_j = \{u \in \mathcal{T} : |u| = j\}$ , so that

$$B(\alpha, y) = \alpha_{\emptyset} y + \sum_{j \geq 1} \omega^{-j} \sum_{u \in \mathcal{T}_j} \frac{\alpha_u}{\sigma(u)} F_u(y).$$

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## Assumption

For each pair  $(u, v) \in \mathcal{T}_j \times \mathcal{T}_k$ , there exist  $w_1, \dots, w_m \in \mathcal{T}_{j+k}$  and  $\lambda_1, \dots, \lambda_m \in \mathbb{R}$  such that

$$\left( \frac{\partial}{\partial y} F_u(y) \right) F_v(y) = \sum_{j=1}^m \lambda_j F_{w_j}(y).$$

Let us denote  $\mathcal{F} = \{\emptyset\} \cup \{u_1 \cdots u_m : u_1, \dots, u_m \in \mathcal{T}\}$ .

Let  $\mathbb{R}^{\mathcal{F}}$  be the set of real functions  $\mathcal{F} \rightarrow \mathbb{R}$ . Consider also

- $\mathbf{g} = \{\beta \in \mathbb{R}^{\mathcal{F}} : \beta_{\emptyset} = 0, \beta_{uv} = 0 \text{ if } u, v \in \mathcal{F}/\{\emptyset\}\}$ .
- $\mathcal{G} = \{\alpha \in \mathbb{R}^{\mathcal{F}} : \alpha_{\emptyset} = 1, \alpha_{uv} = \alpha_u \alpha_v \text{ if } u, v \in \mathcal{F}\}$ .

## Theorem

Under the assumption above, there exists a binary operation

$$\begin{aligned}\mathbb{R}^{\mathcal{F}} \times \mathbb{R}^{\mathcal{F}} &\rightarrow \mathbb{R}^{\mathcal{F}} \\ (\alpha, \beta) &\mapsto \alpha\beta\end{aligned}$$

where for each  $u \in \mathcal{F}$ ,  $\exists v_j, w_j \in \mathcal{F}/\{\emptyset\}$  such that

$$(\alpha\beta)_u = \beta_{\emptyset}\alpha_u + \alpha_{\emptyset}\beta_u + \sum_{j=1}^m \alpha_{v_j}\beta_{w_j},$$

with  $|v_j| + |w_j| = |u|$  satisfying that

- $B(\beta, B(\alpha, y)) = B(\alpha\beta, y)$  if  $\alpha \in \mathcal{G}$
- $\frac{\partial}{\partial y} B(\alpha, y) \cdot B(\beta, y) = B(\beta\alpha, y)$  if  $\beta \in \mathfrak{g}$ .

- $\mathcal{G}$  has with that binary operation a group structure, and
- $\mathfrak{g}$  has a pre-Lie algebra structure, and also a Lie algebra structure with  $[\alpha, \beta] := \alpha\beta - \beta\alpha$ .

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# Averaging in terms of B-series

Consider a nonautonomous  $(2\pi)$ -periodic ODE written in the form

$$\frac{d}{d\tau}y = B(\beta(\tau), y), \quad \text{where } \beta(\tau) \in \mathfrak{g} \text{ and } \beta(\tau + 2\pi) = \beta(\tau).$$

Its solutions  $y(\tau)$  can be expanded as  $y(\tau) = B(\alpha(\tau), y(0))$  with  $\alpha(\tau) \in \mathcal{G}$ , where

$$\frac{d}{d\tau}B(\alpha(\tau), y(0)) = B(\beta(\tau), B(\alpha(\tau), y(0))), \quad B(\alpha(0), y(0)) = y(0).$$

That certainly holds if

$$\forall u \in \mathcal{T}, \quad \frac{d}{d\tau}\alpha(\tau)_u = (\alpha(\tau)\beta(\tau))_u, \quad \alpha(0)_u = 0,$$

or more compactly,

$$\frac{d}{d\tau}\alpha(\tau) = \alpha(\tau)\beta(\tau), \quad \alpha(0) = I,$$

which uniquely determines  $\alpha(\tau) \in \mathcal{G}$  in terms of  $\beta(\tau) \in \mathfrak{g}$ .

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# Averaging in terms of B-series coefficients

## Theorem

Given a  $(2\pi)$ -periodic  $\beta(\tau) \in \mathfrak{g}$ , there exist  $\bar{\beta} \in \mathfrak{g}$ ,  $\bar{\alpha}(\tau) \in \mathcal{G}$ , and a  $(2\pi)$ -periodic  $\kappa(\tau) \in \mathcal{G}$  such that

$$\alpha(\tau) = \bar{\alpha}(\tau)\kappa(\tau), \quad \frac{d}{d\tau}\bar{\alpha}(\tau) = \bar{\alpha}(\tau)\bar{\beta}, \quad \bar{\alpha}(0) = I.$$

Furthermore, it holds that

$$\frac{d}{d\tau}\kappa(\tau) = \kappa(\tau)\bar{\beta} - \beta(\tau)\kappa(\tau).$$

$$\bar{\beta}_u = \int_0^{2\pi} \beta(\tau)_u d\tau - \sum_{j=1}^m \int_0^{2\pi} (\kappa(\tau)_{v_j} \bar{\beta}_{w_j} - \beta(\tau)_{v_j} \kappa(\tau)_{w_j}) d\tau,$$

$$\kappa(\tau)_u = \tau \bar{\beta}_u - \int_0^\tau \beta(\sigma)_u d\sigma + \sum_{j=1}^m \int_0^\tau (\kappa(\sigma)_{v_j} \bar{\beta}_{w_j} - \beta(\sigma)_{v_j} \kappa(\sigma)_{w_j}) d\sigma.$$

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## Alternative algorithm

Given  $\beta(\tau) \in \mathfrak{g}$ ,

- Find  $\alpha(\tau) \in \mathcal{G}$  such that

$$\frac{d}{d\tau} \alpha(\tau) = \alpha(\tau)\beta(\tau), \quad \alpha(0) = I.$$

- For each  $u \in \mathcal{T}$ , obtain  $\bar{\alpha}(\tau)_u$  as the polynomial of degree  $|u|$  that interpolates  $\alpha(\tau)_u$  for  $\tau = 2\pi n$ ,  $n \in \mathbb{Z}$ ,
- Obtain  $\bar{\beta}$  as

$$\bar{\beta}_u = \left. \frac{d}{d\tau} \bar{\alpha}(\tau)_u \right|_{\tau=0}.$$

Last two steps of the algorithm are equivalent to applying numerical differentiation formulae with data  $\alpha(\tau)_u$  for  $\tau = 2\pi n$ ,  $n \in \mathbb{Z}$ .

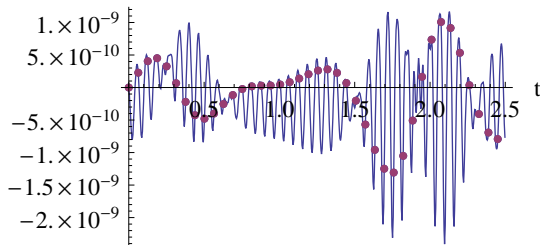
# Applications (work in progress)

- Practical computation of several terms of the higher order averaged equations (possible application beyond numerical analysis)
- Numerical methods that accurately approximate averaged solutions (oscillatory solution can always be recovered locally):
  - 1 Integration of averaged equations obtained by combining microintegration and numerical differentiation
  - 2 B-series methods designed to fit the B-series expansion of the solution of the averaged equations (splitting methods, RK-like methods...

## Example (Fermi-Pasta-Ulam problem)

Variation  $\bar{H}(y(t)) - \bar{H}(y(0))$  of the averaged Hamiltonian

$$\bar{H}_1(y) + \omega^{-2}\bar{H}_3(y) + \omega^{-4}\bar{H}_5(y).$$



Actually, it can be proven that formally,  $\{H, \bar{H}\} = 0$ , so that  $\bar{H}$  is a formal invariant of the original problem. Hence,

$$\tilde{I}(p_1, p_2, q_1, q_2) := H(p_1, p_2, q_1, q_2) - \bar{H}(p_1, p_2, q_1, q_2)$$

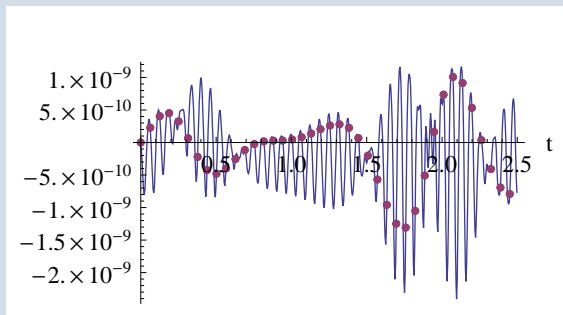
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