Uncertainty quantification of Hamiltonian maps using intrusive polynomial chaos expansion

MSc thesis presentation

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Quantifying uncertainty: the PCE approach

- Many numerical physical models have **stochastic parameters** with uncertainties
  - Example: in a dipole magnet simulation with an **uncertain strength** $k_0 \sim U(a, b)$, the particle possible **output position** is a ***distribution.***
- But: numerical simulations often can only do *"point evalutation"* for specific parameter values $\hat{k}_{0_i}$
- Possible remedies:
  - Sampling-based, Monte Carlo methods: approximate distributions as histograms
  - Polynomial Chaos Expansion

PCE: Idea

- **Polynomial Chaos Expansion:** approximate a **random variable** X with unknown pdf as a **truncated sum of polynomials** of **other random variables** Ξ:

$$
\begin{aligned}
X = f(\Xi) &= \sum_{i=0}^{\infty} x_i \Psi_i(\Xi_j) \\
&\approx \sum_{j=0}^{N_O} x_i \Psi_i(\Xi_j)\,, \quad \Psi_i(\Xi_j) = \sum_{|\alpha|<O} \psi_\alpha \Xi_j^\alpha
\end{aligned}
$$

Find the best approximate distribution *in this polynomial space*, by finding the best coefficients x_i.

PCE: Non-intrusive vs intrusive

- **Non-intrusive:** fit coefficients x_i on empirical X distribution from a dataset or Monte Carlo (MC)
  - Advantages: can use existing simulation code for MC
  - Disadvantages: Not faster than Monte Carlo
- **Intrusive:** the model equations and code are **modified** to solve for the coefficients x_i.
  - Advantages: Very fast, exponential convergence for smooth processes [PS13]
  - Disadvantages: Exponentially increasing number of x_i, need to create the new equations
- Topic of this thesis: **intrusive** methods in **hamiltonian mechanics**.

Polynomial Chaos Expansion: ingredients

- Ingredients:
  - **Germ:** Random variable Ξ with probability distribution $p_\xi(\xi)$, $\xi \in \Omega$, having moments of all orders.
  - **Expected value** over Ξ defines an L_2 **inner product:** $\langle g_1 | g_2 \rangle_\Xi = \langle g_1 \cdot g_2 \rangle_\Xi = \int_\Omega g_1(\xi) g_2(\xi)\, d\,\Xi = \int_\Omega\, g_1(\xi) g_2(\xi)\, p_\xi(\xi) d\xi$
  - **Orthogonal polynomial basis** $\Psi_k(\Xi)$ such that $\langle \Psi_i \cdot \Psi_j \rangle_\Xi = a_i \delta_{ij}$

- Examples:
  - $\Xi \sim U_{(a,b)}$ **uniform: Legendre** polynomials
  - $\Xi \sim \mathcal{N}(\mu, \sigma)$ **gaussian: Hermite** polynomials
  - $\Xi \sim \mathrm{Exp}(\beta)$ **exponential: Laguerre** polynomials
  - etc...

Intrusive methods for differential equations Differential equation for distribution $Y(t)$ with uncertain parameters α_i:

$$Y'(t) = f(Y(t), t\,;\,\alpha_i)$$

1. Substitute the PCE $Y(t) = y_i(t)\Psi_i(\Xi)$ into the model equations (using Einstein notation):

$$y_i'(t)\Psi_i = f\left(y_i(t)\Psi_i,\, t\,;\, \alpha_j\Psi_j\right)$$

2. Galerkin method: multiply with $\Psi_{1\ldots k}$ (test functions):

$$y_i'(t)\Psi_i \cdot \Psi_k = f\left(y_i(t)\Psi_i,\, t\,;\, \alpha_j\Psi_j\right) \cdot \Psi_k$$

3. Take the expected value over Ξ (L_2 Galerkin projection):

$$\begin{aligned} y_i'(t)\left\langle \Psi_i \cdot \Psi_k \right\rangle_\Xi = y_k'(t) &= \left\langle f\left(y_i(t)\Psi_i,\, t\,;\, \alpha_j\Psi_j\right) \cdot \Psi_k \right\rangle_\Xi \\ &= \int_\Omega f\left(y_i(t)\Psi_i,\, t\,;\, \alpha_j\Psi_j\right) \cdot \Psi_k \;\, p_\xi(\xi) d\xi \end{aligned}$$

4. Solve the N_O equations to get the coefficients $y_k(t)$

Setup: Hamilton equations with uncertain parameters $\alpha_i(\Xi)$:

$$\frac{dq_i}{dt}(t) = \frac{\partial H}{\partial p_i}(q,p;\alpha),\ \ \frac{dp_i}{dt}(t) = -\frac{\partial H}{\partial q_i}(q,p;\alpha)$$

The PCE coefficient matrices $Q_{ij}(t),\ P_{ij}(t)$ are defined as $q_i(t) = Q_{ij}(t)\Psi_j$, $p_i(t) = P_{ij}(t)\Psi_j$.

Main result of Hamiltonian PCE: The PCE equations for the coefficients Q_{ij}, P_{ij} are themselves Hamiltonian [PS13]:

$$\frac{dQ_{ij}}{dt} = \frac{\partial \hat{H}}{\partial P_{ij}}(Q,P),\ \ \frac{dP_{ij}}{dt} = -\frac{\partial \hat{H}}{\partial Q_{ij}}(Q,P)$$

where $\hat{H}$ is the Hamiltonian $H(q,p;\alpha)$ averaged over the uncertain PCE variables:

$$\hat{H}(Q,P) = \langle H \rangle_\Xi = \int_\Omega H\left(q_i \leftarrow Q_{ij}\Psi_j(\xi),\ p_i \leftarrow P_{ij}\Psi_j(\xi);\ \alpha(\xi)\right)\ p_\Xi(\xi)d\xi$$

- 2 germs Ξ_0, Ξ_1 : $\Big[\mathcal{U}(l = 3.5, h = 4.5),\ \mathcal{N}(\mu = 0, \sigma = 1)\Big]$
- Order $O = 3$ expansion, $N_O = \binom{O+2}{O} = 10$ polynomials
- $H(p, q; k_0) = H_2 = \frac{p^2}{2} + k_0 \frac{q^2}{2}$, $k0 \sim \mathcal{U}(l = 3.5, h = 4.5)$
  - The parameter k_0 is one of the germs, Ξ_0
- Resulting PCE Hamiltonian $\hat{H}(Q_i, P_i)$:

$$\hat{H}(P_i, Q_i) = \frac{P_0^2}{2} + \frac{P_1^2}{2} + \frac{P_2^2}{2} + \frac{P_3^2}{2} + \frac{P_4^2}{2} + \frac{P_5^2}{2} + \frac{P_6^2}{2} + \frac{P_7^2}{2} + \frac{P_8^2}{2} + \frac{P_9^2}{2} + \frac{5Q_0^2}{4} + \frac{\sqrt{3}Q_0Q_2}{3} + \frac{5Q_1^2}{4} + \frac{\sqrt{3}Q_1Q_4}{3} + \frac{5Q_2^2}{4} + \frac{2\sqrt{15}Q_2Q_5}{15} + \frac{5Q_3^2}{4} + \frac{\sqrt{3}Q_3Q_7}{3} + \frac{5Q_4^2}{4} + \frac{2\sqrt{15}Q_4Q_8}{15} + \frac{5Q_5^2}{4} + \frac{3\sqrt{35}Q_5Q_9}{35} + \frac{5Q_6^2}{4} + \frac{5Q_7^2}{4} + \frac{5Q_8^2}{4} + \frac{5Q_9^2}{4}$$

$\hat{H}_O$ for each order O of PCE expansion:

- $\hat{H}_0$: $\frac{P_0^2}{2} + \frac{5Q_0^2}{4}$
- $\hat{H}_1$: $\frac{P_0^2}{2} + \frac{P_1^2}{2} + \frac{P_2^2}{2} + \frac{5Q_0^2}{4} + \frac{\sqrt{3}Q_0Q_2}{3} + \frac{5Q_1^2}{4} + \frac{5Q_2^2}{4}$
- $\hat{H}_2$: $\frac{P_0^2}{2} + \frac{P_1^2}{2} + \frac{P_2^2}{2} + \frac{P_3^2}{2} + \frac{P_4^2}{2} + \frac{P_5^2}{2} + \frac{5Q_0^2}{4} + \frac{\sqrt{3}Q_0Q_2}{3} + \frac{5Q_1^2}{4} + \frac{\sqrt{3}Q_1Q_4}{3} + \frac{5Q_2^2}{4} + \frac{2\sqrt{15}Q_2Q_5}{15} + \frac{5Q_3^2}{4} + \frac{5Q_4^2}{4} + \frac{5Q_5^2}{4}$
- $\hat{H}_3$: $\frac{P_0^2}{2} + \frac{P_1^2}{2} + \frac{P_2^2}{2} + \frac{P_3^2}{2} + \frac{P_4^2}{2} + \frac{P_5^2}{2} + \frac{P_6^2}{2} + \frac{P_7^2}{2} + \frac{P_8^2}{2} + \frac{P_9^2}{2} + \frac{5Q_0^2}{4} + \frac{\sqrt{3}Q_0Q_2}{3} + \frac{5Q_1^2}{4} + \frac{\sqrt{3}Q_1Q_4}{3} + \frac{5Q_2^2}{4} + \frac{2\sqrt{15}Q_2Q_5}{15} + \frac{5Q_3^2}{4} + \frac{\sqrt{3}Q_3Q_7}{3} + \frac{5Q_4^2}{4} + \frac{2\sqrt{15}Q_4Q_8}{15} + \frac{5Q_5^2}{4} + \frac{3\sqrt{35}Q_5Q_9}{35} + \frac{5Q_6^2}{4} + \frac{5Q_7^2}{4} + \frac{5Q_8^2}{4} + \frac{5Q_9^2}{4}$
- $\hat{H}_4$: $\frac{P_0^2}{2} + \frac{P_{10}^2}{2} + \frac{P_{11}^2}{2} + \frac{P_{12}^2}{2} + \frac{P_{13}^2}{2} + \frac{P_{14}^2}{2} + \frac{P_1^2}{2} + \frac{P_2^2}{2} + \frac{P_3^2}{2} + \frac{P_4^2}{2} + \frac{P_5^2}{2} + \frac{P_6^2}{2} + \frac{P_7^2}{2} + \frac{P_8^2}{2} + \frac{P_9^2}{2} + \frac{5Q_0^2}{4} + \frac{\sqrt{3}Q_0Q_2}{3} + \frac{5Q_{10}^2}{4} + \frac{5Q_{11}^2}{4} + \frac{\sqrt{3}Q_{11}Q_6}{3} + \frac{5Q_{12}^2}{4} + \frac{2\sqrt{15}Q_{12}Q_7}{15} + \frac{5Q_{13}^2}{4} + \frac{3\sqrt{35}Q_{13}Q_8}{35} + \frac{5Q_{14}^2}{4} + \frac{4\sqrt{7}Q_{14}Q_9}{21} + \frac{5Q_1^2}{4} + \frac{\sqrt{3}Q_1Q_4}{3} + \frac{5Q_2^2}{4} + \frac{2\sqrt{15}Q_2Q_5}{15} + \frac{5Q_3^2}{4} + \frac{\sqrt{3}Q_3Q_7}{3} + \frac{5Q_4^2}{4} + \frac{2\sqrt{15}Q_4Q_8}{15} + \frac{5Q_5^2}{4} + \frac{3\sqrt{35}Q_5Q_9}{35} + \frac{5Q_6^2}{4} + \frac{5Q_7^2}{4} + \frac{5Q_8^2}{4} + \frac{5Q_9^2}{4}$

- The initial distribution $z_i(t=0) = [q_j(0), p_k(0)]$ can be a distribution as well.
- This distribution is PC expanded as well:

$$z_i(0) = Z_{ij}(0)\Psi_j \longleftrightarrow Z_{ij}(0) = \langle z_i(0)|\Psi_j\rangle_\Xi$$

- Example with the harmonic oscillator, using the second germ Ξ_1:
    - A fixed number is a zeroth PC order initial condition: $q_0(0) = 1 \longrightarrow Q_{00}(0) = 1$, remaining $Z_{ij}(0) = 0$
    - First order polynomial $q_0(0) \sim \mathcal{N}(1, 0.2)$: $q_0 = 1 + 0.2\,\Xi_1 \longrightarrow Q_{00} = 1, Q_{01} = 0.2$, remaining $Z_{ij}(0) = 0$
- Ideally, all parameters including initial distributions are independent germs. But, $\longrightarrow$ combinatorial explosion.
- Many $Z_{ij}(0) = 0 \ \longrightarrow$ resulting system is sparse

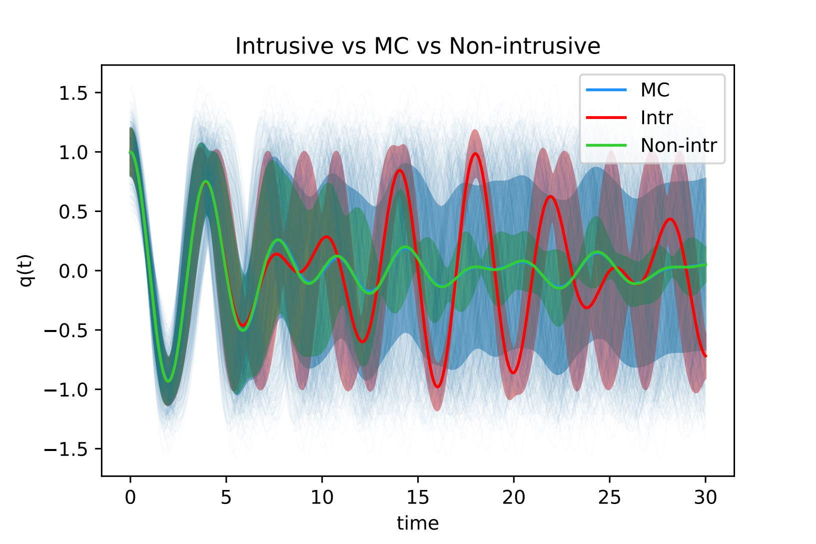
PC mean and variance

- For a PCE random variable $q_i(t) = Q_{ij}(t)\Psi_j$, **closed form** for **mean** and **variance** due to Ψ_i orthogonality:
  - $\mathbb{E}\left(q_0\right)(t) = Q_{0j}(t)\int_{\Omega} 1 \cdot \Psi_j \, d\Xi = Q_{0j}(t)\left\langle \Psi_0, \Psi_j \right\rangle = Q_{00}(t)$
  - $\mathbb{E}\left(q_0^2\right)(t) = \sum_{j=0}^{O} Q_{0j}^2(t)\left\langle \Psi_j, \Psi_j \right\rangle = \sum_{j=0}^{O} Q_{0j}^2(t)$
  - $\mathrm{Var}(q_0)(t) = \mathbb{E}\left(\left(q_0 - \mathbb{E}\left(q_0\right)\right)^2\right)(t) = \sum_{j=0}^{O} Q_{0j}^2(t) - Q_{00}^2(t)$

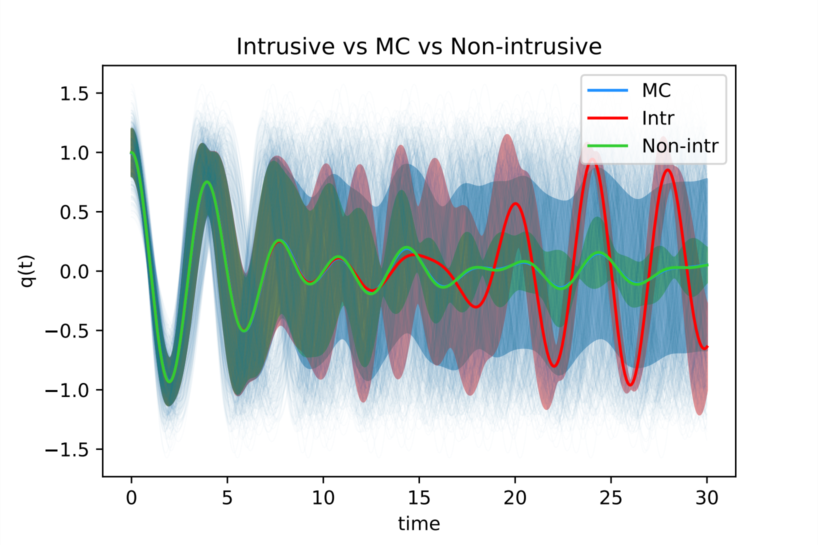
Plot description

- In faint blue *Monte Carlo* realizations of the stochastic system $H(p, q, k_i)$ are plotted. The “empirical” standard deviation band and average $\mu(t) \pm \sigma(t)$ at each time t are shown.
- In red the average $\mathbb{E}\left(q_{H_O}\right)(t)$ and standard deviation $\sqrt{\mathrm{Var}(q_{H_O})}(t)$ for the *intrusive* system solution $q_{H_O}(t)$.
- In green the band obtained from a least squares fit of PCE coefficients Q_{ij} on Monte Carlo samples (*non intrusive* PCE).

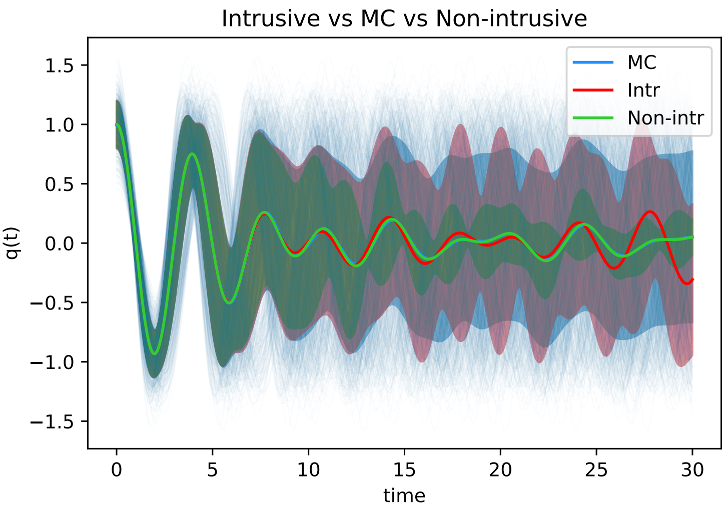
Results: $H_2 = \frac{p^2}{2} + k_0\frac{q^2}{2}$, $k0 \in U(\frac{3}{2}, \frac{7}{2})$, $O = 1$

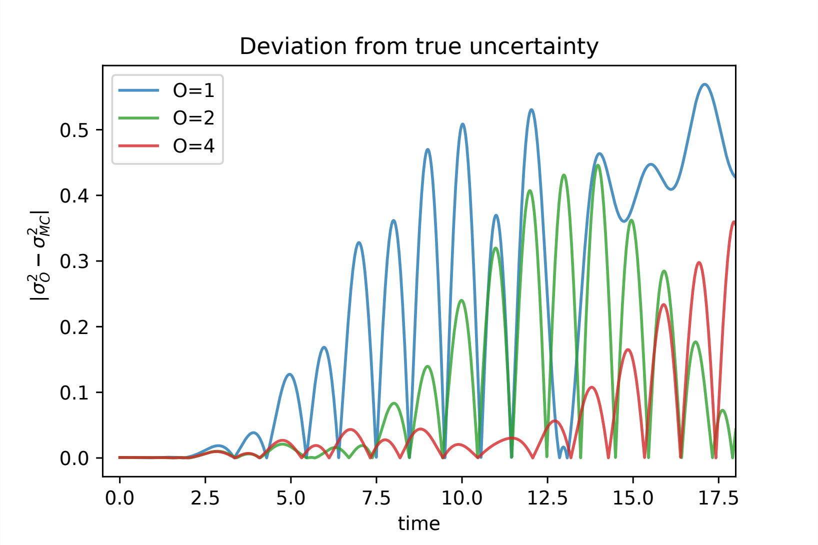


Results: $H_2 = \frac{p^2}{2} + k_0\frac{q^2}{2}$, $k0 \in U(\frac{3}{2}, \frac{7}{2})$, $O = 2$



RESULTS: $H_2 = \frac{p^2}{2} + k_0\frac{q^2}{2}$, $k0 \in U(\frac{3}{2}, \frac{7}{2})$, $O = 4$

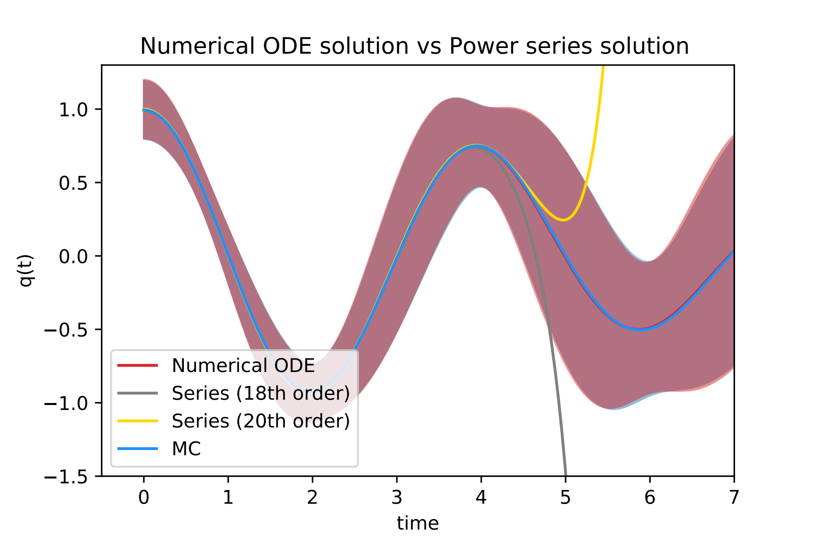


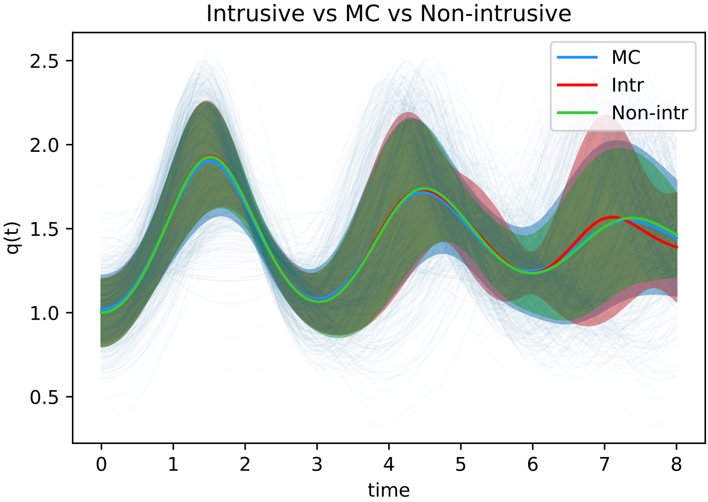

Deviation from true uncertainty
O=1
O=2
O=4
$|\sigma_O^2 - \sigma_{MC}^2|$
0.0
0.1
0.2
0.3
0.4
0.5
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
time

- The numerical solution of the intrusive ODE is in red, and Monte Carlo in blue.
- In yellow and gray the (time) order $T = 18, 20$ truncated exponential map, which will be a polynomial of degree T in t, is used to calculate coefficients $Z_{\text{Exp}}(t) = (Q_{\text{Exp}}, P_{\text{Exp}})(t)$. From them the average and error band are calculated as shown before.

$$
\begin{aligned}
Z_{\text{Exp}}(t) &= M(t, Z(0)) \\
\mathrm{I}(Z) &= \text{Identity map}(Z_i) := [Q_0, \ldots, Q_m, P_0, \ldots, P_m] \\
M(t, Z(0)) &= \left(e^{-t:\hat{H}_O:}\, \mathrm{I} \right)\Big|_{Z(0)} \\
&\approx \left(\mathrm{I} + \frac{(-t)^1}{1!}[\hat{H}_O, \mathrm{I}] + \ldots + \frac{(-t)^T}{T!}[\hat{H}_O, [\hat{H}_O, \ldots, \mathrm{I}]] \right)\Big|_{Z(0)}
\end{aligned}
$$

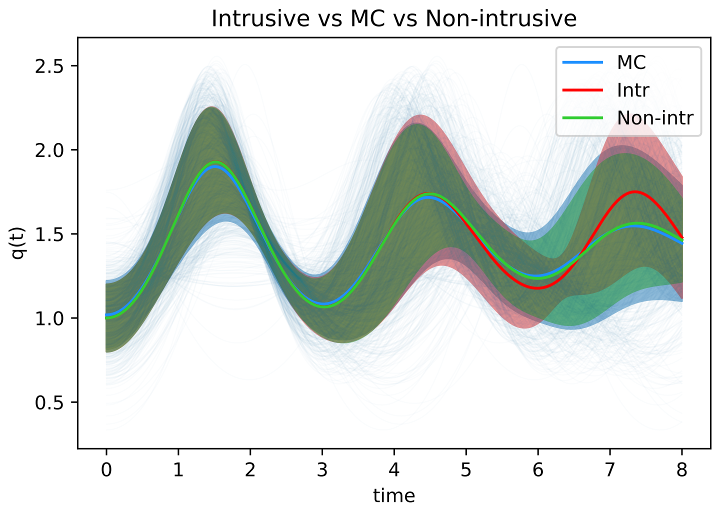
Results: $H_2 = \frac{p^2}{2} + k_0\frac{q^2}{2}$, $k0 \in U(\frac{3}{2}, \frac{7}{2})$, $O = 4$



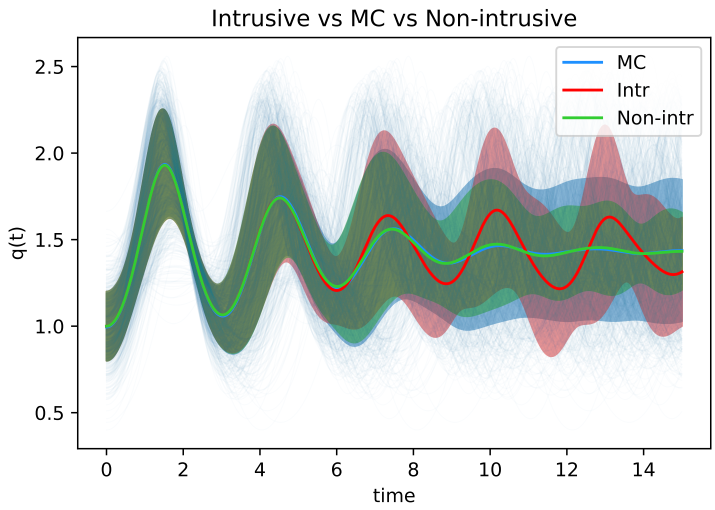

Intrusive vs MC vs Non-intrusive
MC
Intr
Non-intr
q(t)
time
2.5
2.0
1.5
1.0
0.5
0
1
2
3
4
5
6
7
8

RESULTS: $H_4 = \frac{p^2}{2} - k_0\frac{q^2}{2} + \frac{q^4}{4}$, $k0 \in U(\frac{3}{2}, \frac{7}{2})$, $O = 2$

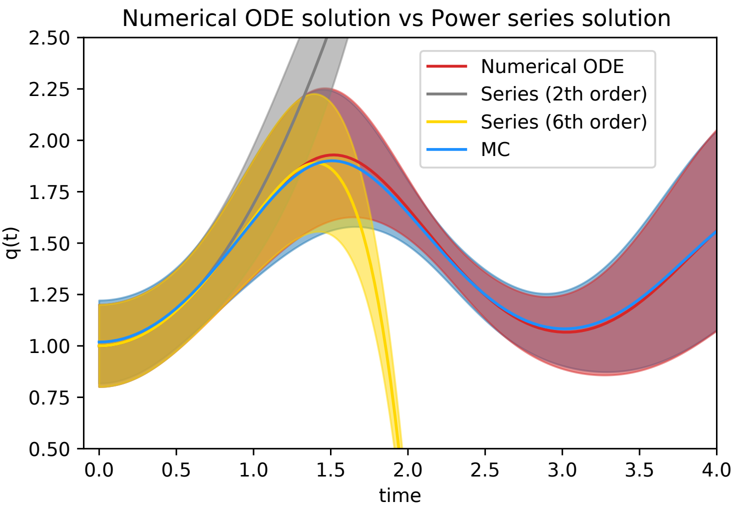
ETH zürich



RESULTS: $H_4 = \frac{p^2}{2} - k_0\frac{q^2}{2} + \frac{q^4}{4}$, $k0 \in U(\frac{3}{2}, \frac{7}{2})$, $O = 3$



Results: $H_4 = \frac{p^2}{2} - k_0\frac{q^2}{2} + \frac{q^4}{4}$, $k0 \in U(\frac{3}{2}, \frac{7}{2})$, $O = 2$



- Hamiltonian of FODO cell:

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}} + \frac{1}{6}\left(k_3 x^3 - k_2 x y^2\right) + \frac{\delta}{\beta_0}. \tag{1}$$

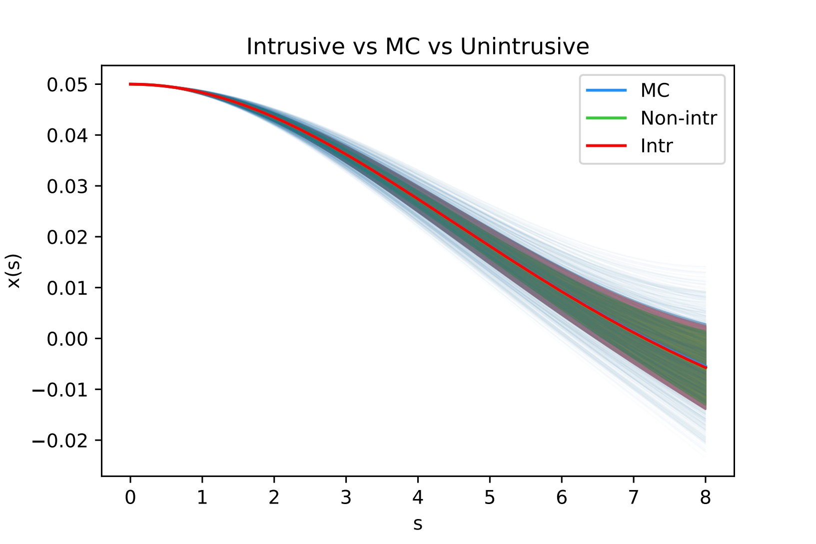
- Third-order expansion:

$$H \approx -\frac{k_2 x y^2}{6} + \frac{k_3 x^3}{6} + \frac{p_x^2}{2\sqrt{\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}}} - \frac{p_x^2\delta}{2\beta_0\left(\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}\right)^{\frac{3}{2}}} +$$

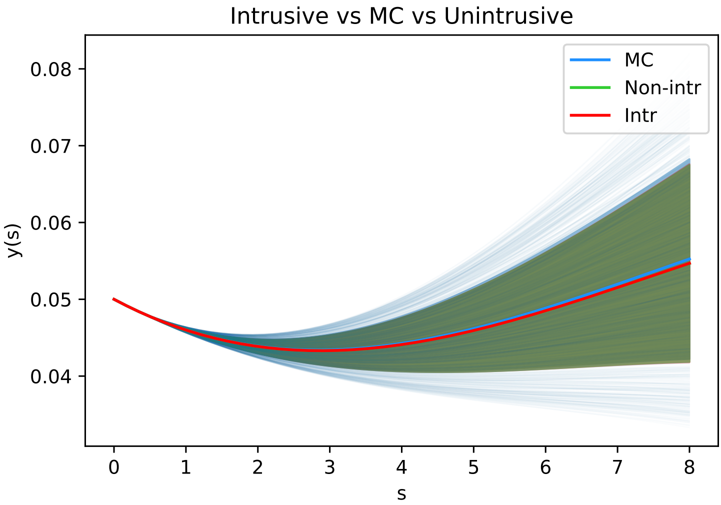
$$\frac{p_y^2}{2\sqrt{\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}}} - \frac{p_y^2\delta}{2\beta_0\left(\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}\right)^{\frac{3}{2}}} + \frac{\delta^2\left(-1 + \frac{1}{\beta_0^2\left(\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}\right)}\right)}{2\sqrt{\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}}} +$$

$$\delta\left(\frac{1}{\beta_0} - \frac{1}{\beta_0\sqrt{\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}}}\right) - \sqrt{\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}} + \frac{\delta^3\left(1 - \frac{1}{\beta_0^2\left(\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}\right)}\right)}{2\beta_0\left(\frac{1}{\beta_0^2} - \frac{1}{\beta_0^2\gamma_0^2}\right)^{\frac{3}{2}}}$$

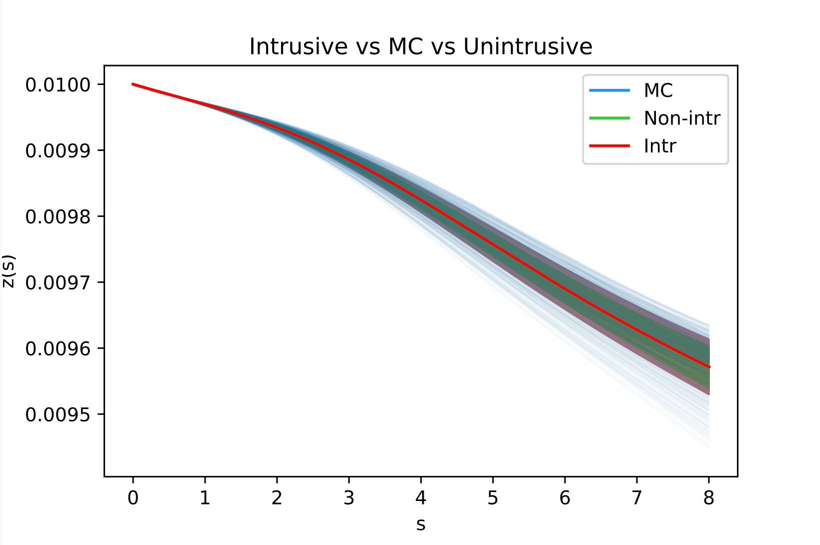
- Setting the design parameter $\beta_0 = \frac{99}{100}$ $(\to \gamma_0 \approx 7.09)$:
$$H = -\frac{k_2 x y^2}{6} + \frac{k_3 x^3}{6} - \frac{50 p_x^2 \delta}{99} + \frac{p_x^2}{2} - \frac{50 p_y^2 \delta}{99} + \frac{p_y^2}{2} - \frac{9950 \delta^3}{970299} + \frac{199 \delta^2}{19602} - 1$$
- $\hat{H}$ PCE example, PCE expansion order $O = 1$:
  - Germs: Ξ_i : $\left[k_2 \sim \mathcal{U}(l = 1.5, h = 3.5),\ k_3 \sim \mathcal{U}(l = 3.0, h = 4.0)\right]$
  - $\hat{H}_1 = -\frac{50 P_{0,0}^2 P_{2,0}}{99} + \frac{P_{0,0}^2}{2} - \frac{100 P_{0,0} P_{0,1} P_{2,1}}{99} - \frac{100 P_{0,0} P_{0,2} P_{2,2}}{99} - \frac{50 P_{0,1}^2 P_{2,0}}{99} + \frac{P_{0,1}^2}{2} - \frac{50 P_{0,2}^2 P_{2,0}}{99} + \frac{P_{0,2}^2}{2} - \frac{50 P_{1,0}^2 P_{2,0}}{99} + \frac{P_{1,0}^2}{2} - \frac{100 P_{1,0} P_{1,1} P_{2,1}}{99} - \frac{100 P_{1,0} P_{1,2} P_{2,2}}{99} - \frac{50 P_{1,1}^2 P_{2,0}}{99} + \frac{P_{1,1}^2}{2} - \frac{50 P_{1,2}^2 P_{2,0}}{99} + \frac{P_{1,2}^2}{2} - \frac{9950 P_{2,0}^3}{970299} + \frac{199 P_{2,0}^2}{19602} - \frac{9950 P_{2,0} P_{2,1}^2}{323433} - \frac{9950 P_{2,0} P_{2,2}^2}{323433} + \frac{199 P_{2,1}^2}{19602} + \frac{199 P_{2,2}^2}{19602} + \frac{7 Q_{0,0}^3}{12} + \frac{\sqrt{3} Q_{0,0}^2 Q_{0,1}}{12} + \frac{7 Q_{0,0} Q_{0,1}^2}{4} + \frac{7 Q_{0,0} Q_{0,2}^2}{4} - \frac{5 Q_{0,0} Q_{1,0}^2}{12} - \frac{\sqrt{3} Q_{0,0} Q_{1,0} Q_{1,2}}{9} - \frac{5 Q_{0,0} Q_{1,1}^2}{12} - \frac{5 Q_{0,0} Q_{1,2}^2}{12} + \frac{\sqrt{3} Q_{0,1}^3}{20} + \frac{\sqrt{3} Q_{0,1} Q_{0,2}^2}{12} - \frac{5 Q_{0,1} Q_{1,0} Q_{1,1}}{6} - \frac{\sqrt{3} Q_{0,1} Q_{1,1} Q_{1,2}}{9} - \frac{\sqrt{3} Q_{0,2} Q_{1,0}^2}{18} - \frac{5 Q_{0,2} Q_{1,0} Q_{1,2}}{6} - \frac{\sqrt{3} Q_{0,2} Q_{1,1}^2}{18} - \frac{\sqrt{3} Q_{0,2} Q_{1,2}^2}{10} - 1$


Intrusive vs MC vs Unintrusive
MC
Non-intr
Intr
x(s)
0.05
0.04
0.03
0.02
0.01
0.00
−0.01
−0.02
s
0
1
2
3
4
5
6
7
8

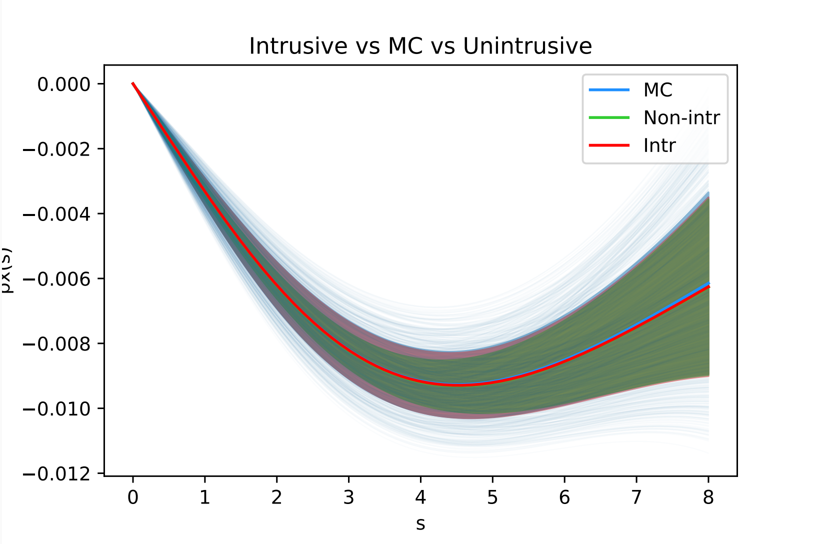
FODO, $O = 2$, $y(s)$



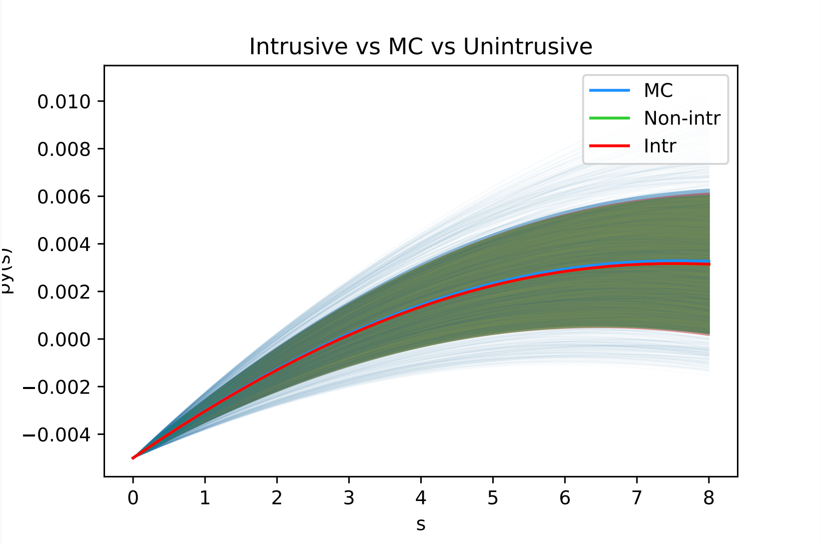
Intrusive vs MC vs Unintrusive
MC
Non-intr
Intr
0.08
0.07
0.06
0.05
0.04
y(s)
0
1
2
3
4
5
6
7
8
s

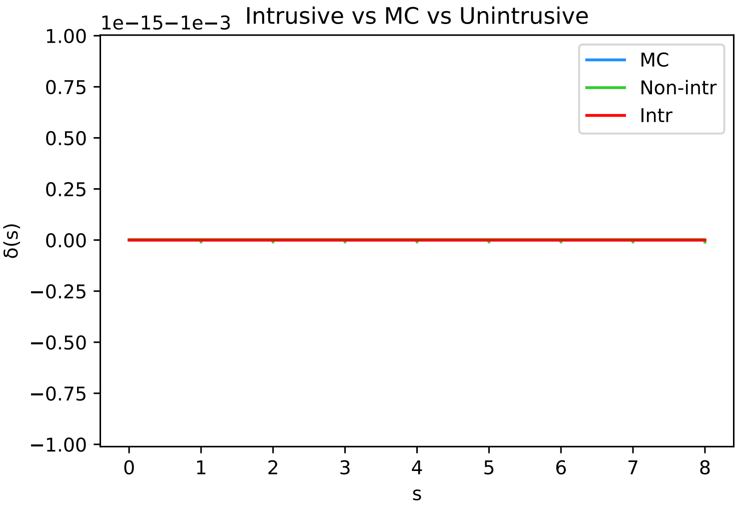

Intrusive vs MC vs Unintrusive
0.0100
0.0099
0.0098
0.0097
0.0096
0.0095
z(s)
0
1
2
3
4
5
6
7
8
s
MC
Non-intr
Intr

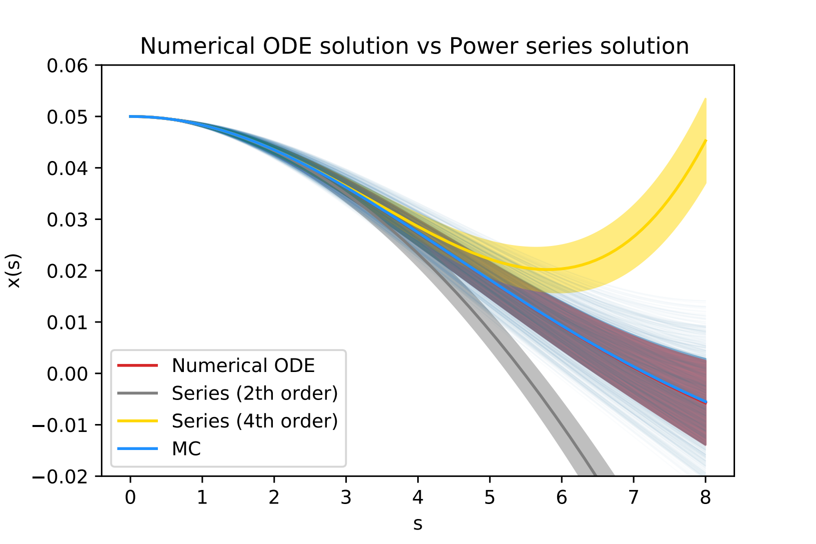
FODO, $O = 2$, $p_x(s)$


Intrusive vs MC vs Unintrusive
MC
Non-intr
Intr
0.000
−0.002
−0.004
−0.006
−0.008
−0.010
−0.012
px(s)
0
1
2
3
4
5
6
7
8
s

ETH zürich


Intrusive vs MC vs Unintrusive
MC
Non-intr
Intr
0.010
0.008
0.006
0.004
0.002
0.000
−0.002
−0.004
py(s)
0
1
2
3
4
5
6
7
8
s


Intrusive vs MC vs Unintrusive
1e−15−1e−3
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
δ(s)
0
1
2
3
4
5
6
7
8
s
MC
Non-intr
Intr


Numerical ODE solution vs Power series solution
0.06
0.05
0.04
0.03
0.02
0.01
0.00
−0.01
−0.02
x(s)
0
1
2
3
4
5
6
7
8
s
Numerical ODE
Series (2th order)
Series (4th order)
MC

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Tools

- Polynomial chaos package `chaospy`
- Python symbolic algebra package `sympy`
- Numerical computations with `numpy`, `scipy`
- Parallelization with `dask`, scalable parallel python library (laptop $\longrightarrow$ cluster)

Script

- Automatically generate the PC equations in multidimensional models, at any order O, for any number/kind of germs Ξ
- Convert in `numpy` functions with `sympy.lambdify`, solve with `scipy`
- Compare with Monte Carlo and non-intrusive PC fit
- Create exponential map at order T

Numerical issues

- `chaospy` floating-point calculations of polynomial coefficients and norms are not fully accurate and orthogonal $\rightarrow$ leads to problems in symbolic integration
  - I implemented the Gram-Schmidt algorithm in `sympy` to orthogonalize the polynomials over a given measure $\mathcal{P}_{\Xi}(\xi)$
- `chaospy` numerical integration when calculating the variance quickly diverges from exact sum-of-square coefficients result
  - Variance has been calculated exactly from coefficients $\mathcal{P}_{\Xi}(\xi)$

Parallelization

- Split $\int_{\Omega} f(\xi) d\Xi = \int_{\Omega} f_1(\xi) d\Xi \ + \ \int_{\Omega} f_2(\xi) d\Xi \ + \ldots$
- Launch several `dask` jobs to integrate the pieces in parallel, sum the result
  - But: `sympy.integrate` issues (”cannot find polynomial root”)

- Many autodifferentiation libraries, not many for integration
- Code transform: attempts with `zygote.jl`, Google's `jax`

Numerical quadrature approach

- Approximate $\langle f(\Xi)\rangle = \int_\Omega f(\xi) p_\Xi(\xi) d\xi \approx \sum_i w_i f(\xi_i)$
- `chaospy.generate_quadrature(o, dist)` can be used to return w_i, ξ_i for a given order of integration and distribution.
- $\dot{Z} = \mathbb{J}\frac{\partial \hat{H}}{\partial Z}$ becomes $\dot{Z} = \sum_i w_i \mathbb{J}\frac{\partial H_{\mathrm{PCE}}}{\partial Z}(\xi_i)$ where

$$H_{\mathrm{PCE}}(Z, \Xi) = H\left(Z_{ij}\Psi_j(\Xi);\ \alpha(\Xi)\right) \tag{2}$$

$$\hat{H}(Z) = \langle H_{\mathrm{PCE}}\rangle_\Xi \tag{3}$$

- Quite slow (slower than MC), but does not require symbolic integration to get $\hat{H}$
- `DA`/autodiff version possible?

- Intrusive polynomial chaos works well for short-medium times. Higher order $\to$ longer times.
- Easy to run into curse of dimensionality from number of germs/degree $\to$ MC then better
- Cannot track model average in general [PS13]
    - From theory: best (Galerkin minimum error) solution is not symplectic, so it cannot come from intrusive methods [PS13]
- Sparseness: if many initial coefficients $Z_{ij}(0) = 0$, system lives in submanifold.
    - $O = 4$ order harmonic PC system with 0th (pointwise) initial conditions equivalent to $O = 2$ system in # of nonzero coefficients!
- Symplectification. Possibility: Cremona maps [Bla02]. Is the tradeoff long term stability/precision worth it?

- Understand/exploit sparseness, from integration to equations
- Better, parallel, symbolic integrals. Wolfram `mathematica`?
- Export equations to better numerical frameworks (`diffeq.jl`)
- Hybrid approach? PCE + Monte Carlo + Data + ML + ...
- Analysis of numerical quadrature in PCE. Good speed/accuracy tradeoff possible? Then $\longrightarrow$ can connect with existing numerical frameworks (`DA`)
- Non-independent germs
- Analysis of symplectification and long term behaviour
- Non-polynomial basis functions e.g. wavelet (related: Fourier frequency space)?
- Quantum mechanics: PC expansion of density matrix?

Sergio Blanes, *Symplectic maps for approximating polynomial hamiltonian systems*, Physical Review E **65** (2002), no. 5, 056703.

J. M. Pasini and T. Sahai, *Polynomial chaos based uncertainty quantification in hamiltonian and chaotic systems*, 52nd IEEE Conference on Decision and Control, 2013, pp. 1113–1118.