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Physics-informed Polynomial Chaos Expansion

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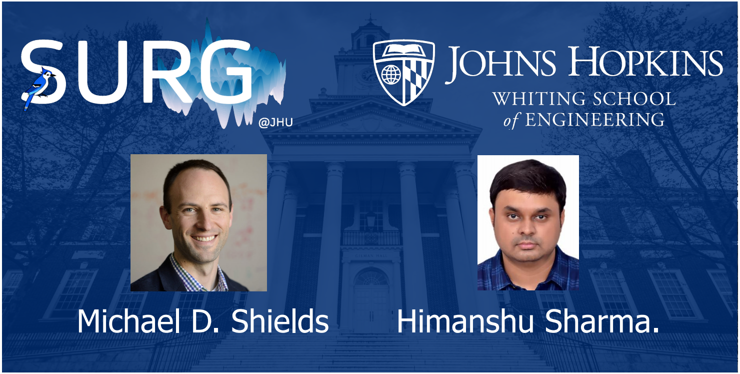
Introduction

- Brno University of Technology, Czech Republic
- Faculty of Civil Engineering, Institute of Structural Mechanics
- Topics of interest: uncertainty quantification (PCE), multi-scale modeling, probabilistic design codes

Introduction

- Collaboration with Johns Hopkins University,
  - members of SURG team (M. D. Shields, H. Sharma)



Acknowledgments

GAČR
CZECH SCIENCE FOUNDATION
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UNITED STATES OF AMERICA
MSEE
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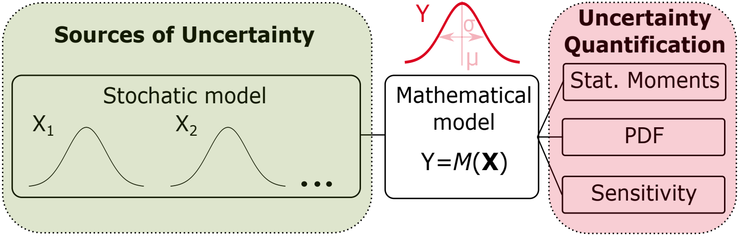
UQ & PCE

Uncertainty quantification

- quantity of interest of a physical system is represented by a costly mathematical model $Y = \mathcal{M}(\mathbf{X})$
- behavior of **real** physical system is **non-linear**
- input variables should be considered as **random** variables $\mathbf{X}$
- uncertainty quantification of $Y = \mathcal{M}(\mathbf{X})$: statistical moments, PDF, sensitivity analysis, estimation of quantiles etc.



Polynomial Chaos Expansion

$$Y = \mathcal{M}(\mathbf{X}) = \sum_{\alpha \in \mathbb{N}^M} \beta_\alpha \Psi_\alpha(\mathbf{X})$$

- deterministic **coefficients** to be computed - β_α
- orthonormal **basis** of multivariate polynomials - $\Psi_\alpha(\mathbf{X})$
- M represents number of input random variables
- multi-index $\alpha = \{\alpha_1, ..., \alpha_M\}$, $\mathcal{A} = \{\alpha \in \mathbb{N}^M\}$

GHANEM R.G., SPANOS P.D. Stochastic finite elements—a spectral approach. Berlin: Springer; 1991

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Orthonormal basis

$$\langle \psi_\alpha, \psi_\beta \rangle = \int \psi_\alpha(\xi)\psi_\beta(\xi)p_\xi(\xi)d\xi = \delta_{\alpha\beta}$$

- multivariate basis functions are orthonormal with respect to the joint PDF p_ξ.
- normalized Hermite polynomials are orthonormal to Gaussian probability measure in the Wiener-Hermite PCE.
- common distributions can be associated to specific type of polynomial (Wiener-Askey scheme).

XIU, D.; KARNIADAKIS, G.: The Wiener-Askey polynomial chaos for stochastic differential equations. J Sci. Comput., 2002, 24(2):619-44.

Orthonormality of PCE

- generally statistical moment of any order is defined as:

$$\langle y^m \rangle = \int \left[f(\mathbf{X})\right]^m p_\xi(\xi)\, d\xi = \int \Big[\sum_{\alpha \in \mathbb{N}^M} \beta_\alpha \Psi_\alpha(\xi)\Big]^m p_\xi(\xi)\, d\xi =$$

$$= \int \sum_{\alpha_1 \in \mathbb{N}^M} \dots \sum_{\alpha_m \in \mathbb{N}^M} \beta_{\alpha_1} \dots \beta_{\alpha_m} \Psi_{\alpha_1}(\xi) \dots \Psi_{\alpha_m}(\xi) p_\xi(\xi)\, d\xi =$$

$$= \sum_{\alpha_1 \in \mathbb{N}^M} \dots \sum_{\alpha_m \in \mathbb{N}^M} \beta_{\alpha_1} \dots \beta_{\alpha_m} \int \Psi_{\alpha_1}(\xi) \dots \Psi_{\alpha_m}(\xi) p_\xi(\xi)\, d\xi$$

- it might be computationally demanding to employ MC
- PCE leads to dramatic simplification of equation due to the orthonormality of basis polynomials

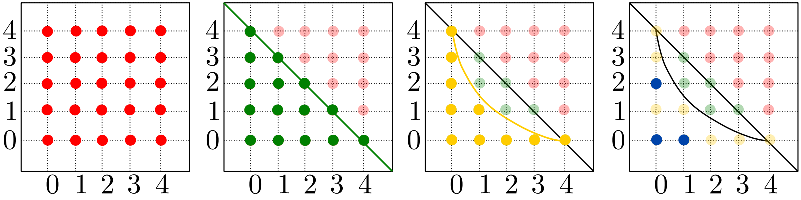
Non-intrusive PCE

- PCE basis is made of polynomials up to a certain degree p
- coefficients by OLS $\rightarrow \mathcal{Y} = \mathcal{M}(\mathbf{X})$ for n_{sim}
- $n_{sim} \geq 3 - 5P$, where $P = \text{card } \mathcal{A}$

$$\boldsymbol{\beta} = (\boldsymbol{\Psi}^T \boldsymbol{\Psi})^{-1} \ \boldsymbol{\Psi}^T \mathcal{Y}$$

$$\boldsymbol{\Psi} = \left\{ \Psi_{ij} = \Psi_j(\xi^{(i)}), i = 1, ..., n, \quad j = 0, ..., P-1 \right\}$$

Tensor product Total pol. order Hyperbolic Sparse solution



Sensitivity analysis: Sobol' indices

- Hoeffding-Sobol' decomposition - Sobol' indices (ANOVA)
- highly efficient derivation of Sobol' indices from PCE
- first order indices

$$S_i = \sum_{\alpha \in \mathcal{A}_i} \frac{\beta_\alpha^2}{Var\left[\tilde{\mathcal{M}}^{PCE}\right]} \qquad \mathcal{A}_i = \left\{\alpha \in \mathbb{N}^M : \alpha_i > 0, \alpha_{j \neq i} = 0\right\}$$

- total indices

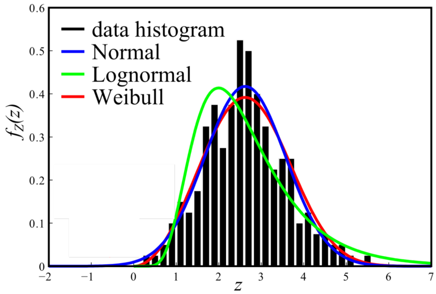
$$S_i^T = \sum_{\alpha \in \mathcal{A}_i^T} \frac{\beta_\alpha^2}{Var\left[\tilde{\mathcal{M}}^{PCE}\right]} \qquad \mathcal{A}_i^T = \left\{\alpha \in \mathbb{N}^M : \alpha_i > 0\right\}$$

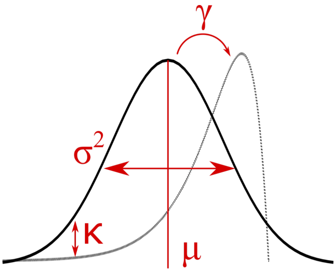
SUDRET, B.: Global sensitivity analysis using polynomial chaos expansions. Reliab Eng and System Safety, 2008, 93: p. 964-979.

SOBOL, I.: Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates. Math and Comput in Simulation 55, 2001, p. 271-280.

Higher moments and Sensitivity

- Sobol indices consider only the first 2 moments
- Higher statistical moments: shape of PDF
- Monte Carlo (LHS) needs thousands of simulations
- Efficient alternative? → Polynomial Chaos Expansion

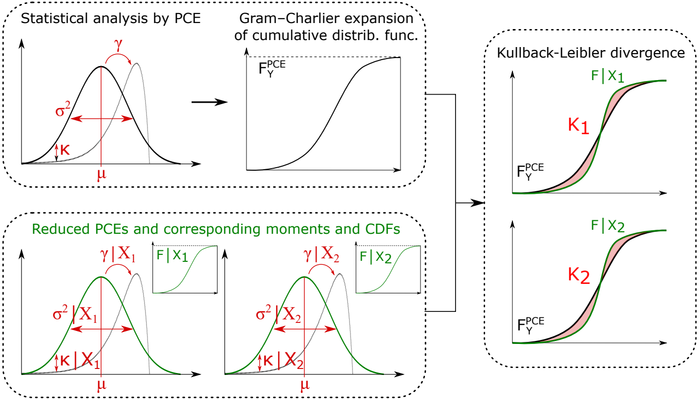




NOVÁK, L. On Distribution-Based Global Sensitivity Analysis by Polynomial Chaos Expansion. *Computers & Structures*, 2022

Distribution-based SA

- Conditional moments → conditional CDFs
- Generalization of Sobol indices for PCE



NOVÁK, L. On Distribution-Based Global Sensitivity Analysis by Polynomial Chaos Expansion. *Computers & Structures*, 2022

Physically Constrained PCE

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PC^2: Physically Constrained PC

- Orthonormal basis in PCE
  - Analytical form (fast evaluation) $\rightarrow$ easy derivation
  - Efficient for UQ (statistical and sensitivity analysis)
- Physical constraints
  - Combination of data ($\mathbf{X}$, $\mathcal{M}(\mathbf{X}) = \mathcal{Y}$) and equality constraints
  - Boundary conditions: Dirichlet, Neumann, Mixed, etc.
  - constrained by PDE/ODE in virtual samples (discrete)
- Efficient optimization?
  - Karush–Kuhn–Tucker conditions & Lagrange multipliers
  - Normal equations $\rightarrow$ constrained least squares

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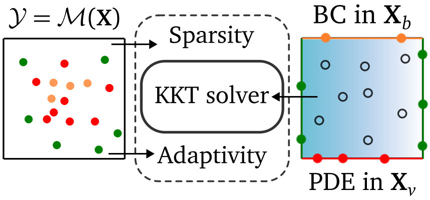
Lagrange multipliers, KKT

- P unknown deterministic coefficients β
- n_{sim} samples in experimental design $\Psi(\mathbf{X})$, $\mathcal{Y}$
- n_{BC} boundary conditions $\mathcal{B}\left[\Psi(\mathbf{X}_b)\right]$,$\mathbf{c}_b$
- $n_{\text{v}} = P - n_{\text{BC}}$ virtual samples $\mathcal{L}\left[\Psi(\mathbf{X}_v)\right]$,$\mathbf{c}_v$

$$\begin{aligned} \min \quad & \|\Psi(\mathbf{X})\beta - \mathcal{Y}\|^2 \\ \text{s.t.} \quad & \mathcal{B}[\Psi(\mathbf{X}_b)]\beta = \mathbf{c_b} \\ & \mathcal{L}[\Psi(\mathbf{X}_v)]\beta = \mathbf{c_v} \end{aligned}$$

$$\underbrace{\begin{bmatrix} \mathbf{\Psi}^T\mathbf{\Psi} & \boldsymbol{A}^T \\ \boldsymbol{A} & \mathbf{0} \end{bmatrix}}_{\text{KKT matrix}} \begin{bmatrix} \beta \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{\Psi}^T\mathcal{Y} \\ \boldsymbol{c} \end{bmatrix}$$



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Wave Equation

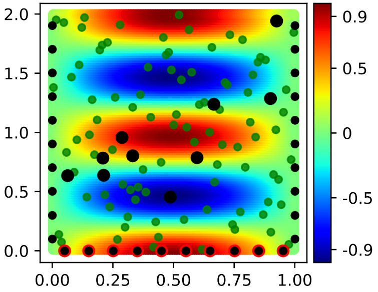
- Solution of the model $\mathcal{M}(\mathbf{X})$

- Dirichlet $\begin{cases} y(0,t) = y(1,t) = 0 \\ y(x,0) = \sin(\pi x) \end{cases}$

- Neumann $\dfrac{\partial y(x,0)}{\partial t} = 0$

- Virtual $\dfrac{\partial^2 y(x,t)}{\partial t^2} = 4\dfrac{\partial^2 y(x,t)}{\partial x^2}$

The code is available here.



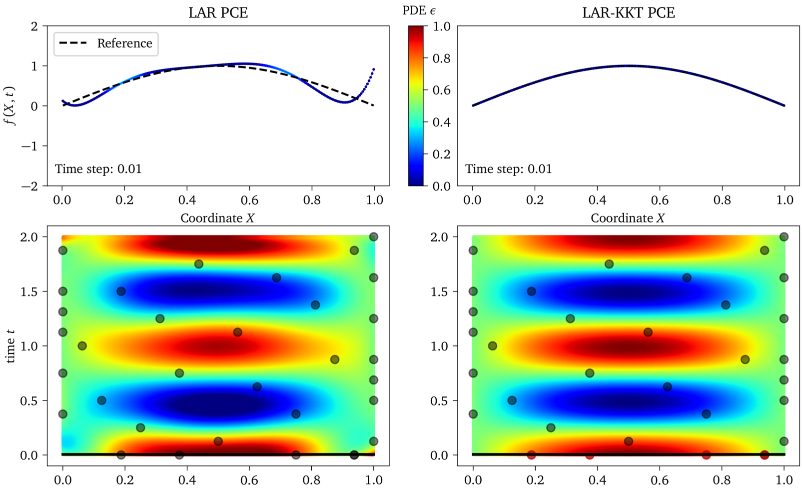
●● standard LAR PCE

●●●● PC^2 based on KKT (LAR)

→ iterative algorithm

$p \in [12, 14]$

Wave Equation: Results



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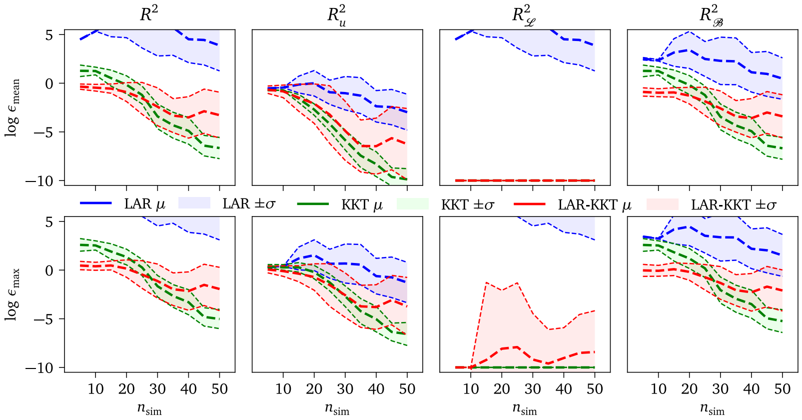
Wave Equation: Convergence Plots



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PC^2 for random PDEs

PC^2 & UQ for PDEs

given stochastic PDE:

$$\mathcal{L}(\mathbf{x}, t, \mathcal{X}(\omega); u(\mathbf{x}, t, \mathcal{X}(\omega))) = f(\mathbf{x}, t, \mathcal{X}(\omega)), \quad \forall \mathbf{x} \in \mathcal{D}, t \in \mathcal{T}, \omega \in \Omega$$
$$\mathcal{B}(\mathbf{x}, t, \mathcal{X}(\omega); u(\mathbf{x}, t, \mathcal{X}(\omega))) = g(\mathbf{x}, t, \mathcal{X}(\omega)), \quad \forall \mathbf{x} \in \partial\mathcal{D}, t \in \mathcal{T}, \omega \in \Omega$$

- random vector $\mathcal{X} \subset \{\mathbf{x}, t, \mathcal{X}\}$
- Basis of reduced PCE:

$$\mathcal{A}_{\mathcal{X}} = \{\boldsymbol{\alpha} \in \mathcal{A} : \alpha_k \neq 0 \leftrightarrow k \in \mathbf{u}\}, \quad \mathbf{u} = \{\mathrm{i} \in \mathrm{I} : \xi_i \in \mathcal{X}\}$$

- Local mean and variance:

$$\mathbb{E}[u|\mathbf{x}, t] = \beta_0 + \sum_{\boldsymbol{\alpha} \in \mathcal{A}_{\sim\mathcal{X}}} \beta_{\boldsymbol{\alpha}}$$
$$\sigma^2_{[u|\mathbf{x},t]} = \sum_{\boldsymbol{\alpha} \in \mathcal{A}_{\mathcal{X}}} \beta^2_{\boldsymbol{\alpha}}$$

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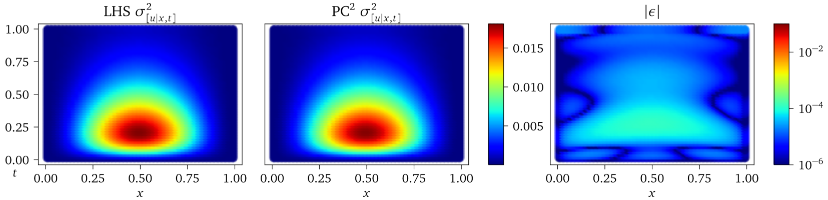
Heat Equation with Random $\mathcal{D}$

$$\frac{\partial f(x,t)}{\partial t} = \mathcal{D}\frac{\partial^2 f(x,t)}{\partial x^2}, \qquad x \in [0,1], \quad t \in [0,1], \quad \mathcal{D} \sim \mathcal{U}[0.2, 0.8]$$

$$f(0,t) = f(1,t) = 0, \qquad f(x,0) = \sin(\pi x)$$

- PC^2 based on 90 $\mathbf{X}_{\mathrm{BC}}$ and $\mathbf{X}_{\mathrm{v}}$ ($n_{sim} = 0$)



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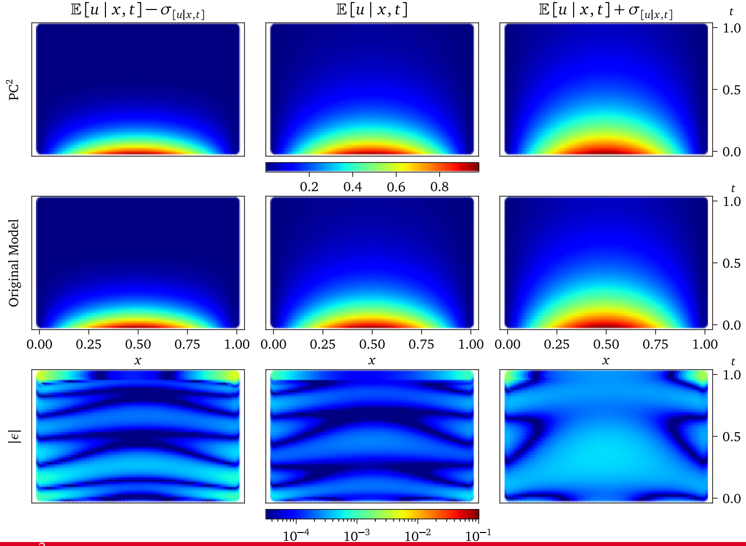
Mean and Quantiles



PC^2 for stochastic PDEs

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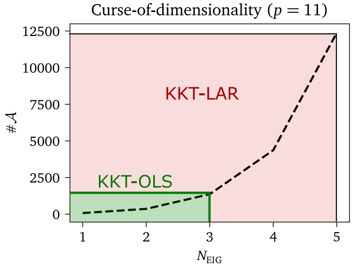
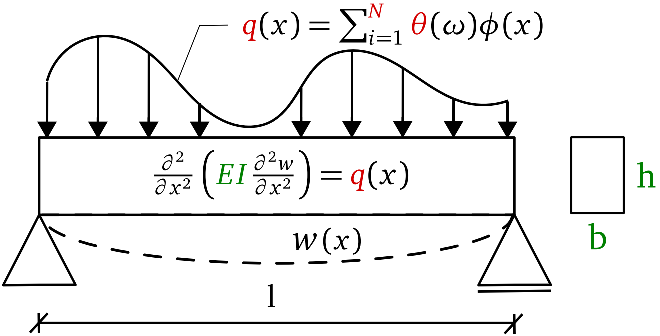
Random vs. Stochastic PDEs

- Random PDEs:
  - low number of random variables M (parameters of PDEs)
  - no *curse-of-dimensionality* $\rightarrow$ **KKT-OLS**
- Stochastic PDEs:
  - a stochastic process (random field) in PDEs
  - decomposition of the stochastic process (KLE)
  - potentially high M (N_{EIG} eigen modes) and p (higher modes)
  - *curse-of-dimensionality* $\rightarrow$ **KKT-LAR**

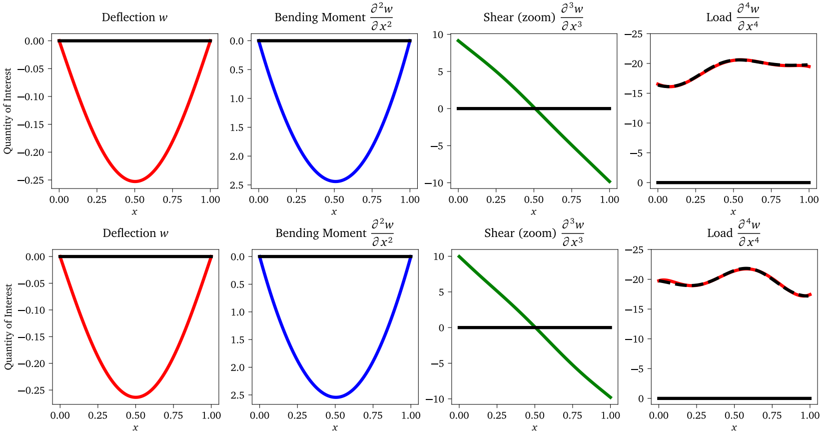


Stochastic Euler Beam

- $EI = const. = 1$, KLE: $q(x) = \sum_{i=1}^{N} \sqrt{\lambda_i}\theta_i(\omega) f_i(x)$
- truncation: $N \in [1, 2, .., 5]$
- PC^2 based on only $\mathbf{X}_{\mathrm{BC}}$ and $\mathbf{X}_{\mathrm{v}}$ $(n_{sim} = 0)$



PC^2 random realizations



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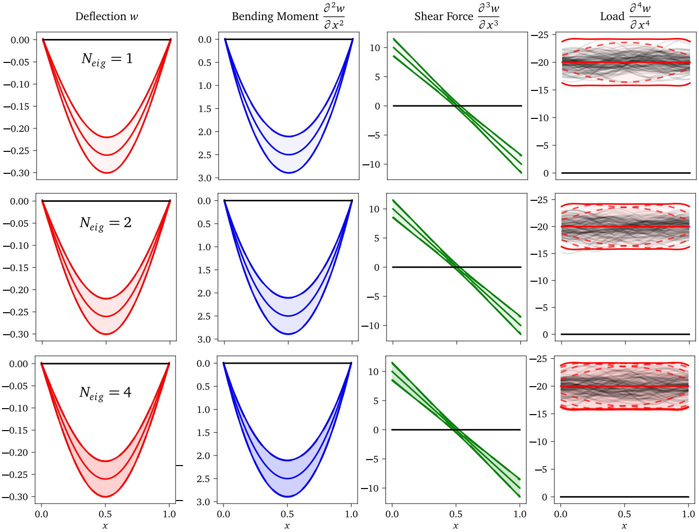
PC² UQ & Derivatives



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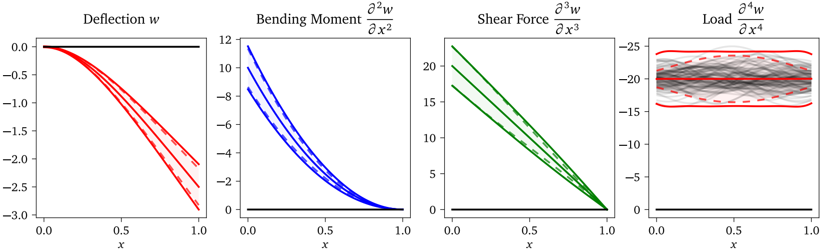
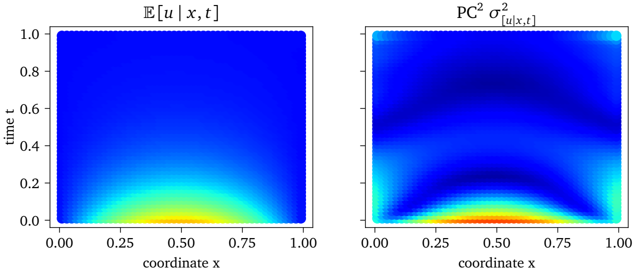
PC^2 Cantilever Beam ($N_{EIG} = 1$)



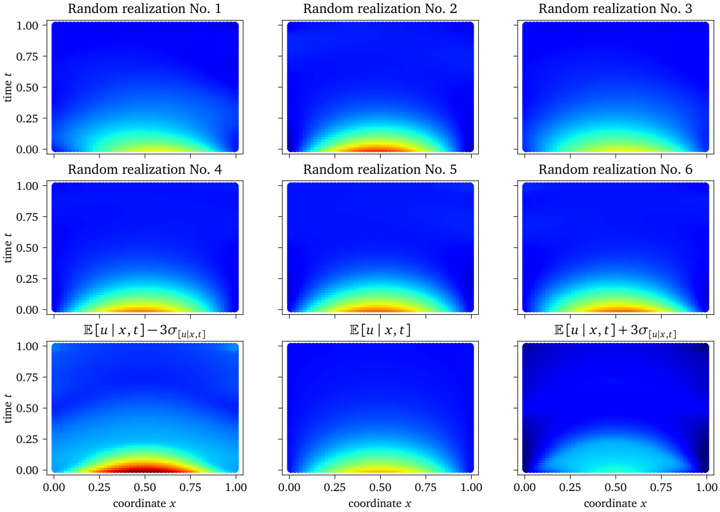
Heat Equation with Stochastic Process

$$\frac{\partial f(x,t)}{\partial t} = \mathcal{D}\frac{\partial^2 f(x,t)}{\partial x^2}, \qquad x \in [0,1], \quad t \in [0,1], \quad \mathcal{D} = 0.5$$

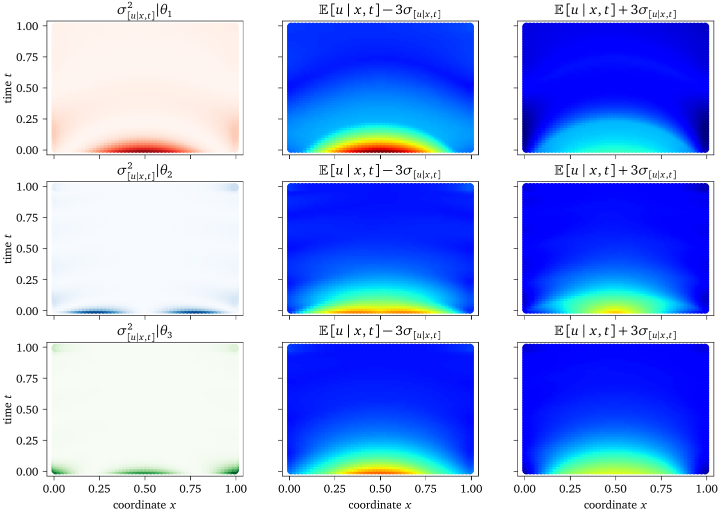
$$f(0,t) = f(1,t) = 0, \qquad f(x,0) = A(x) = \sum_{i=1}^{N} \theta(\omega)\phi(x)$$



PC^2 Heat Equation: Statistics



PC^2 Heat Equation: Sensitivity



PC^2 is available in UQPy!

- available on the Python Package Index (PyPI) and Conda:
  Quick Guide for Installation of Jupyterlab and Anaconda
- version control through git (requires Python 3):
  https://github.com/SURGroup/UQpy
- Examples & Documentation:
  https://uqpyproject.readthedocs.io/en/latest/

Conclusions

- physically constrained PCE for scientific machine learning
- physical constraints significantly improve convergence
- coefficients β estimated by constrained least squares
- construction of PC^2 is computationally efficient
  - $\rightarrow$ adaptive p, q algorithms
  - $\rightarrow$ sparse solvers (e.g. LARs)
- PC^2 for UQ of random and stochastic PDEs
- PC^2 is available in UQPy!

L. Novák, H. Sharma, M. D. Shields, Physics-Informed Polynomial Chaos Expansions, arXiv:2309.01697

Comparison to PINNs

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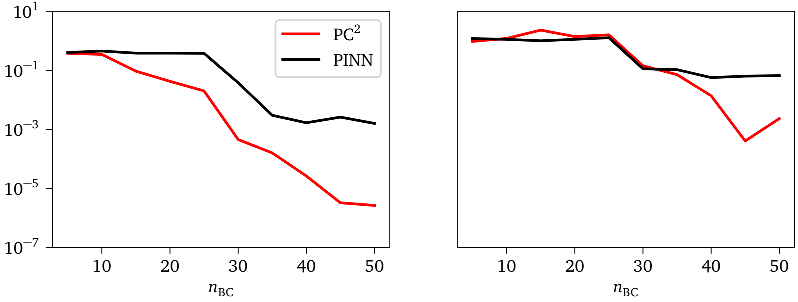
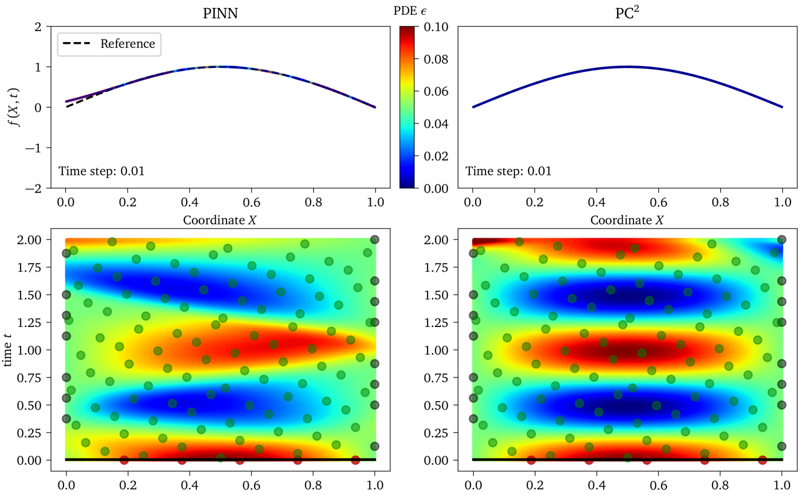
Preliminary Results: PINNs

- Pilot comparison to PINNs: deterministic wave equation
- Only BC samples and virtual samples



Preliminary Results: PINNs



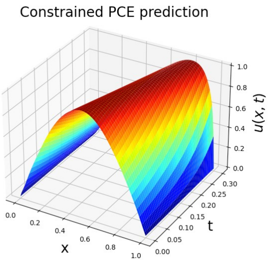
Non-linear PDEs & Non-equality Constraints

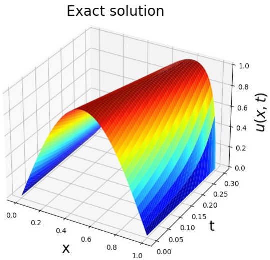
Preliminary Results: Burger's Equation

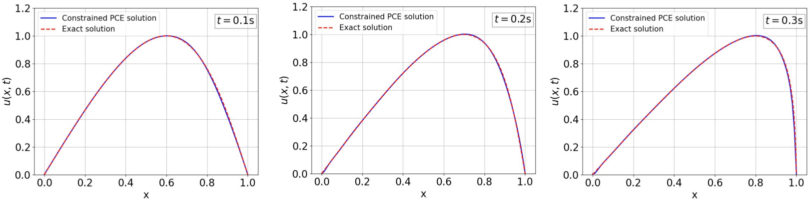
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0.001\frac{\partial^2 u}{\partial x^2},$$

$$x \in [0,1]$$
$$t \in [0,0.3]$$

$$BC: u(0,t) = u(1,t) = 0$$
$$IC: u(x,0) = \sin(\pi x)$$







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