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Global Sensitivity Analysis of Fields: A Demonstration for Hydrogen Autoignition

Jonathan Wang, Ph.D. in Theoretical & Applied Mechanics, est. May 2019*
*Habib Najm (8351)**, Mohammad Khalil (8954)**, Jonathan Freund**
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**University of Illinois Urbana-Champaign   **Sandia National Laboratories, CA*

Abstract

Complex chemical mechanisms in combustion models typically involve numerous reactions with uncertain reaction rates; global sensitivity analysis (GSA) facilitates the propagation of uncertainty by reducing the dimensionality of the parameter space. GSA has thus far been focused on scalars; in this work, we employ the Karhunen-Loève expansion (KLE) and polynomial chaos expansion (PCE) to compute Sobol' sensitivity indices for a field. We demonstrate the approach for a simplified problem that mimics autoignition and emphasize that field GSA provides important information that scalar GSA does not. Applications to other combustions systems are also discussed.

Background

- Because propagating uncertainty through large reacting flow simulations is often infeasible with detailed chemical mechanisms, reduced models are typically used.
- Field GSA exposes the nature of the model reduction or neglected uncertainty in a way that scalar GSA does not; for example, it can highlight the region of a flame in which a particular reaction introduces significant uncertainty.
- Field GSA poses a computational and technical challenge: naïvely building PCEs separately at each physical point is expensive and raises questions of how to represent the correlation structure between points.
- The KLE addresses these challenges by providing a compact representation of a stochastic process that preserves correlation structure and establishing a framework in which Sobol' sensitivity indices can be computed from PCEs.

Methods

- The KLE compresses field data by projection onto a deterministic and stochastic basis.

$$F(x,\vec{\xi}) = \sum_{n=1}^{N} \sqrt{\lambda_n}\,\eta_n(\vec{\xi})\,u_n(x)$$

  - $u_n(x)$ are orthogonal eigenvectors (deterministic).
  - $\eta_n(\vec{\xi})$ are uncorrelated random variables (stochastic).

- The PCE efficiently represents a random variable using a smooth distribution.

$$\eta_n(\vec{\xi}) = \sum_{k=0}^{P-1} \eta_{nk}\Psi_k(\vec{\xi})$$

  - $\vec{\xi}$ are (Gaussian) iid germs.
  - $\Psi_k(\vec{\xi})$ are (Hermite) polynomials.
  - η_{nk} are computed by projection with Monte Carlo integration.

- Sobol' indices quantify the relative contribution of uncertainty from each parameter.

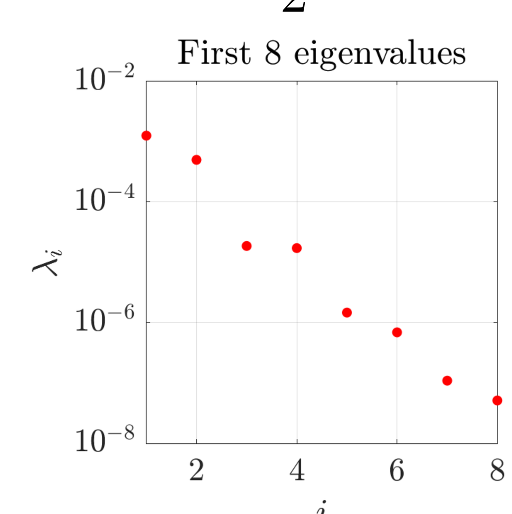
$$\mathcal{S}_i(x) \equiv \frac{\mathrm{V}\left(\mathrm{E}\left(F|\xi_i\right)\right)}{\mathrm{V}\left(F\right)} = \frac{\sum_{\boldsymbol{\alpha}\in\mathbb{I}_i} F_{\boldsymbol{\alpha}}(x)\langle\Psi^2_{\boldsymbol{\alpha}}\rangle}{\sum_{\boldsymbol{\alpha}} F_{\boldsymbol{\alpha}}(x)\langle\Psi^2_{\boldsymbol{\alpha}}\rangle}, \text{ where } F(x,\vec{\xi}) = \sum_{k=0}^{P-1} F_k(x)\Psi_k(\vec{\xi}), \quad F_k(x) = \sum_{n=1}^{N}\sqrt{\lambda_n}\eta_{nk}u_n(x)$$

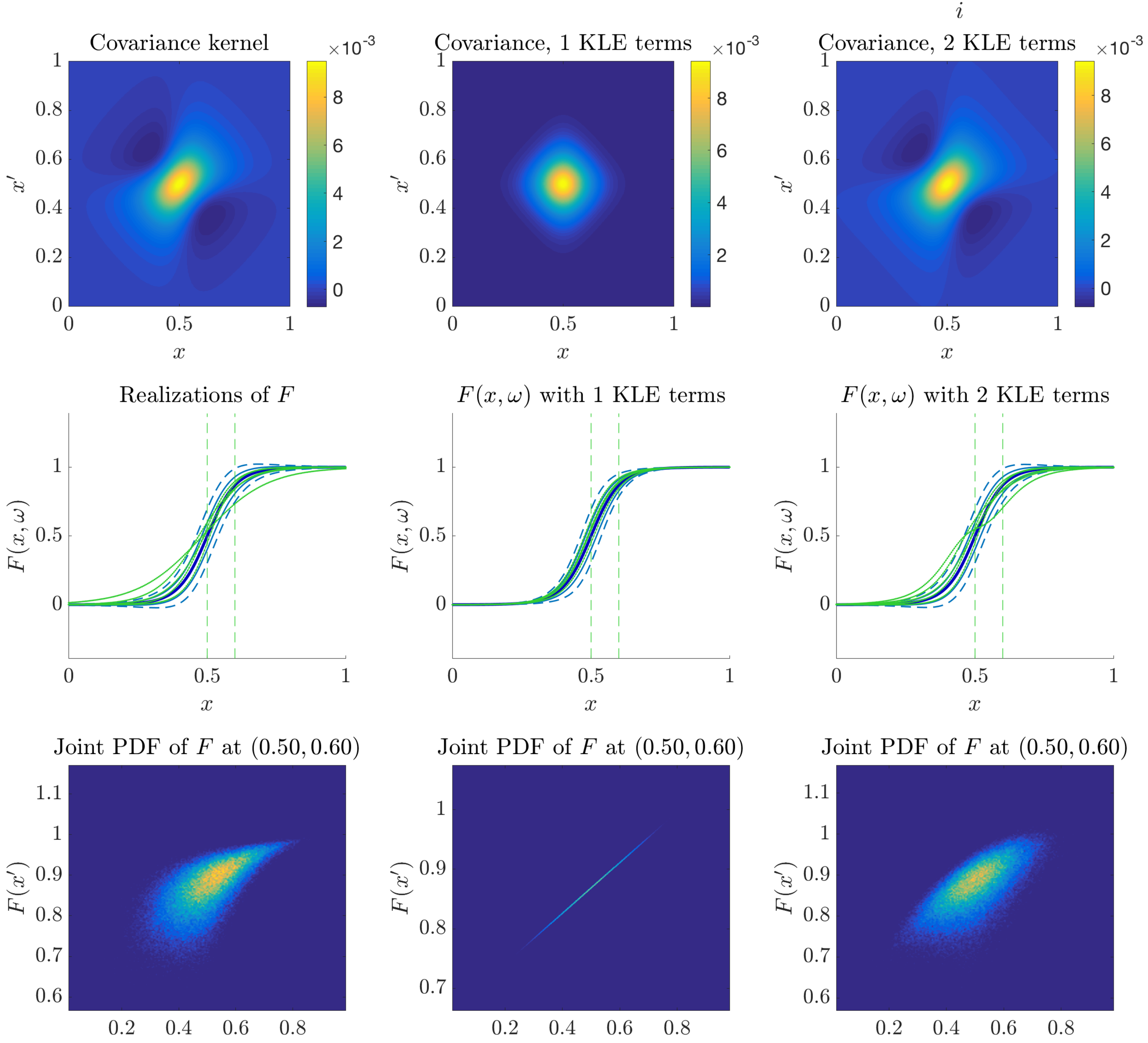
Results

$$F(x;\vec{\xi}) = \frac{a}{2}\tanh\left(r(x-b)+c\right);\; b\sim\mathcal{N}(0.5,0.02);\; r\sim\mathcal{N}(10,2)$$

Karhunen-Loève expansion (KLE):

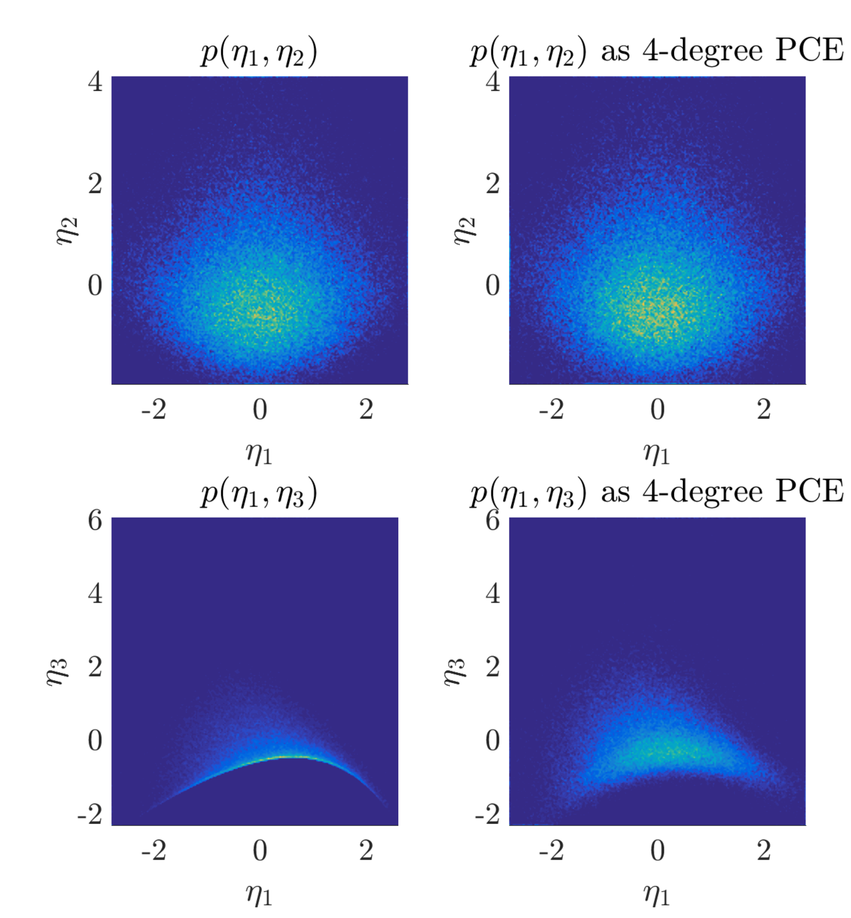
- The KLE modes decay exponentially, and the KLE is able to recover the covariance kernel with only the first two terms.
- However, accurately representing the full stochastic behavior of F—in particular, the joint PDFs—requires additional terms.





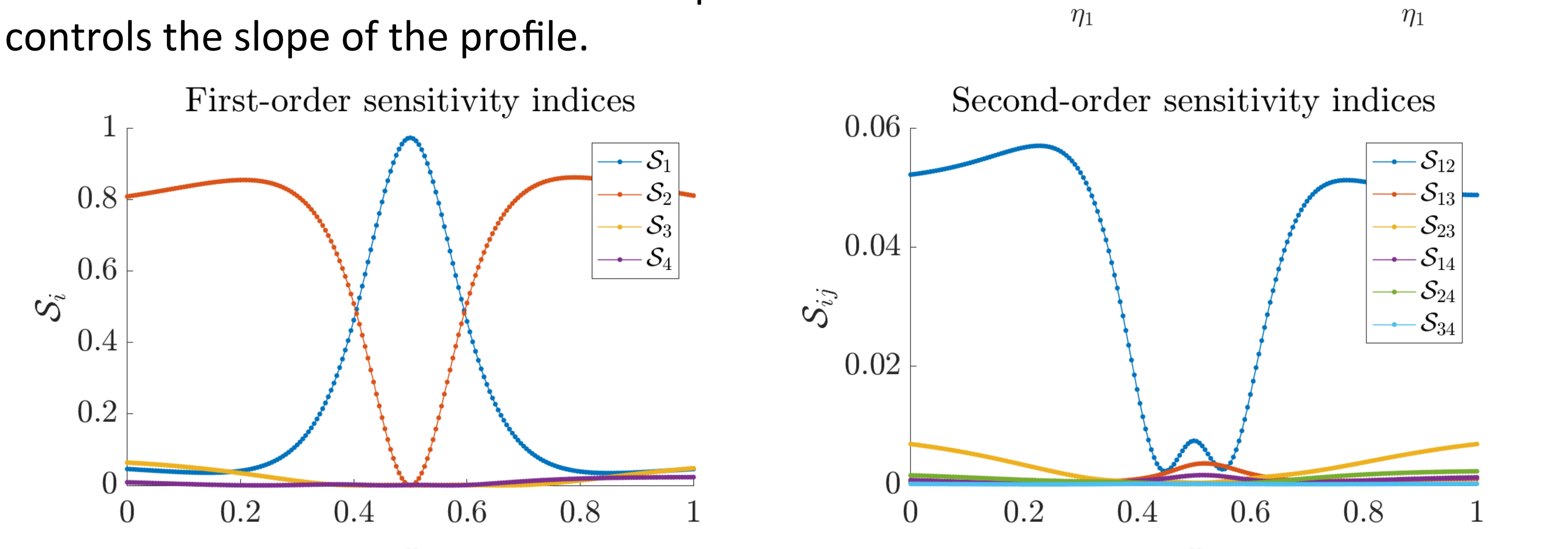
Polynomial chaos expansion (PCE):

- Expanding a process with two independent stochastic inputs results in two independent KL modes.
- The sharp features of the PDFs are difficult for the PCE to resolve and suggest a strong dependence between higher KLE modes. It is yet unclear what that relationship is or how it should be interpreted.



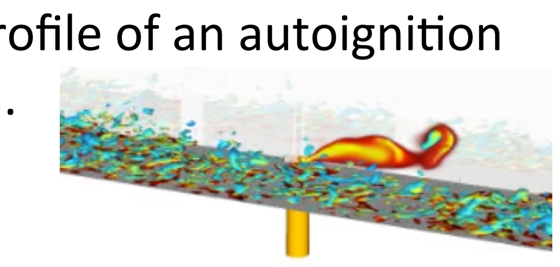
Sobol' sensitivity indices:

- b controls the location of the inflection point.
- r controls the slope of the profile.



Conclusions and Future Work

- This approach for field GSA is demonstrated for a simplified problem, but deciding where to truncate the expansion requires further investigation into the dependence among the KLE modes.
- Field GSA is more informative than scalar GSA in that it indicates not only the parameters that contribute most to the uncertainty of a prediction, but also where that contribution takes place in the physical domain.
- This method is now being applied to the temperature-time profile of an autoignition simulation using a reduced hydrogen combustion mechanism.
- Future work includes application to 2D and 3D multiphysics simulations to study plasma-assisted combustion.



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