Dimension Reduction and Measure Transformation in Stochastic Simulations of Coupled Systems

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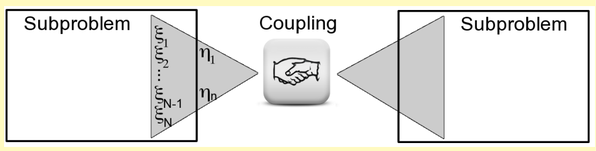
Objectives & Challenges

- Develop UQ for coupled models in Nuclear Reactor Technology.
- Adapt measure of approximation at every handshaking.
- Mitigate mixing of uncertainty at handshaking.
- Develop multiscale quadrature rules.



Problem Definition

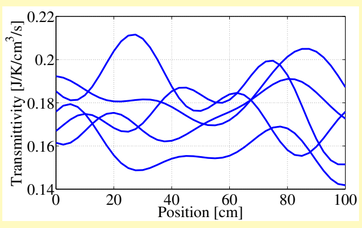
Coupled neutron transport and heat transfer:

$$\frac{d}{dx}\left(D(T(\boldsymbol{\xi}))\frac{d\Phi}{dx}(\boldsymbol{\xi})\right) - \left(\Sigma_a(T(\boldsymbol{\xi}),\boldsymbol{\xi}) - \nu\Sigma_f(T(\boldsymbol{\xi}))\right)\Phi(\boldsymbol{\xi}) = -s, \quad \text{with} \quad \frac{d\Phi}{dx}(0) = \frac{d\Phi}{dx}(L) = 0,$$

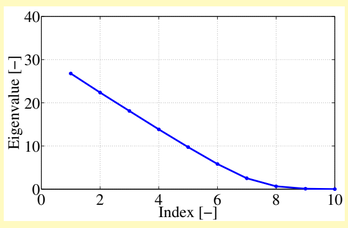
$$\frac{d}{dx}\left(k\frac{dT}{dx}(\boldsymbol{\xi})\right) - h(T(\boldsymbol{\xi}) - T_\infty) = -q(\Phi(\boldsymbol{\xi}), T(\boldsymbol{\xi})), \quad \text{with} \quad \frac{dT}{dx}(0,\boldsymbol{\xi}) = \frac{dT}{dx}(L,\boldsymbol{\xi}) =$$

Absorption cross section random field:

$$\Sigma_a(T,\boldsymbol{\xi}) \equiv \Sigma_a^{\#}\left(T, g(\boldsymbol{\xi})\right) \quad \text{with} \quad g(\boldsymbol{\xi}) = \sum_{i=1}^{N}\sqrt{\lambda_i}\varphi_i\xi_i, \qquad N = 10.$$



Sample paths.



Eigenvalues.

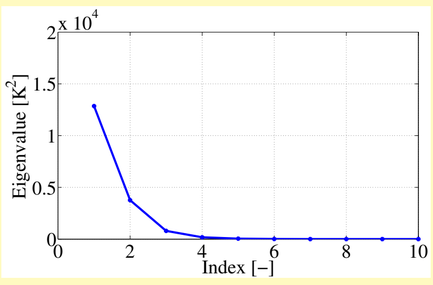
Measure Transformation

Neutron-transport problem:

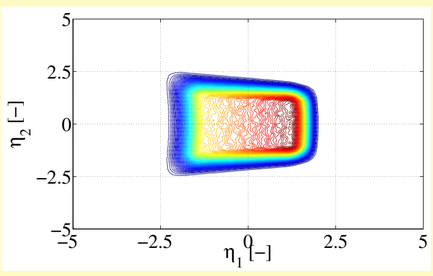
- Solve *the neutron problem* to obtain $q(\boldsymbol{\xi}) = \sum_{|\boldsymbol{\alpha}|=0}^{p} q_{\boldsymbol{\alpha}} H_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$.
- Algorithmic UQ operations with respect to the probability distribution $P_{\boldsymbol{\xi}}$ of $\xi_1, \xi_2, \ldots, \xi_{N-1}, \xi_N$:
  - polynomial chaos $H_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$ orthogonal with respect to $P_{\boldsymbol{\xi}}$,
  - quadrature rule $\{(\boldsymbol{\xi}^{(k)}, w^{(k)}),\ 1 \le k \le r\}$ for integration to $P_{\boldsymbol{\xi}}$.

Coupling region:

- Compute KL decomposition $\hat{q}(\boldsymbol{\xi}) = \underline{q} + \sum_{i=1}^{n}\sqrt{\lambda_i}\varphi_i\eta_i(\boldsymbol{\xi})$.



Joint Probability Density of Interface Random Variables.

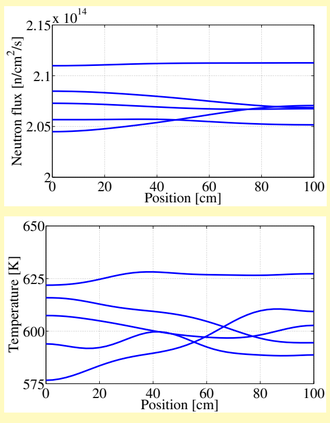


Eigenvalues of Covariance Operator of Solution.

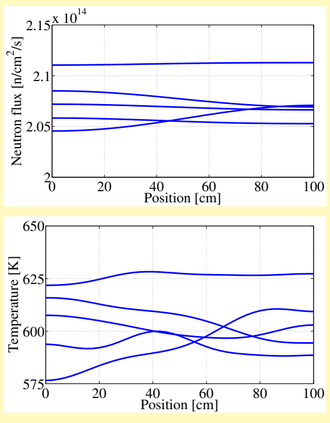
Heat-transfer problem:

- Solve *the heat problem* to obtain $T(\boldsymbol{\eta}) = \sum_{|\tilde{\boldsymbol{\alpha}}|=0}^{\tilde{p}} T_{\tilde{\boldsymbol{\alpha}}} H_{\tilde{\boldsymbol{\alpha}}}(\boldsymbol{\eta})$.
- Algorithmic UQ operations with respect to the probability distribution $P_{\boldsymbol{\eta}}$ of $\eta_1, \ldots, \eta_n$:
  - polynomial chaos $H_{\tilde{\boldsymbol{\alpha}}}(\boldsymbol{\eta})$ orthogonal with respect to $P_{\boldsymbol{\eta}}$,
  - quadrature rule $\{(\boldsymbol{\eta}^{(k)}, \tilde{w}^{(k)}),\ 1 \le k \le \tilde{r}\}$ for integration to $P_{\boldsymbol{\eta}}$.
- Typical benefits: (1) fewer polynomial chaos (2) fewer quadrature nodes.

Comparison of Sample Paths of Solution



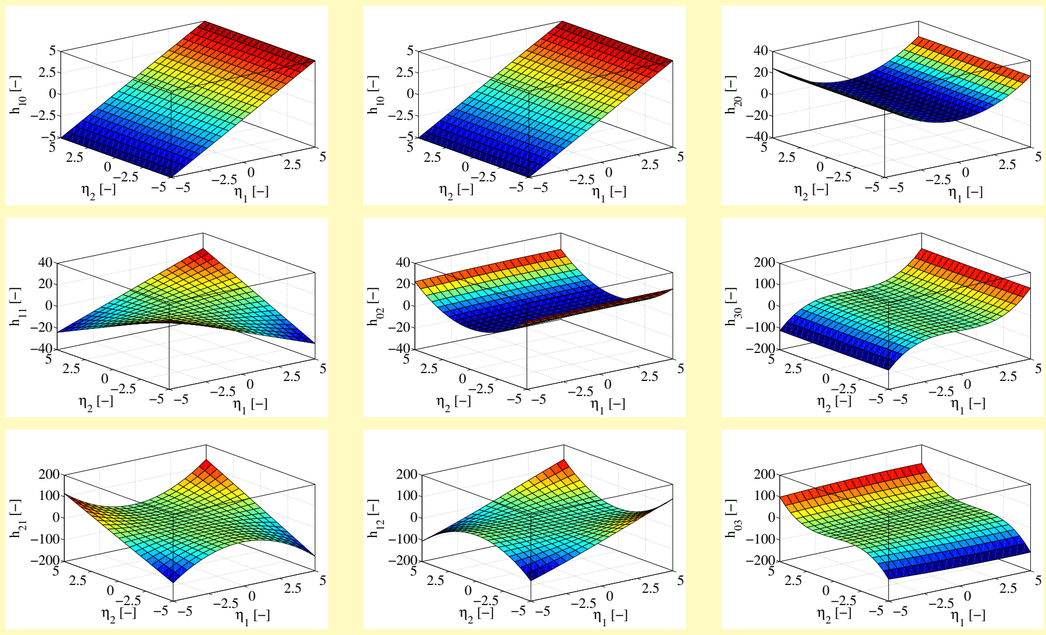
Elementary Implementation



Implementation with Dimension Reduction

Orthogonal Polynomials with Respect to η

Gram-Schmidt procedure using $P_{\boldsymbol{\eta}}$ as measure: variables:



Multiscale Quadrature

Given, explicit dependence of η on ξ, find efficient quadrature for:

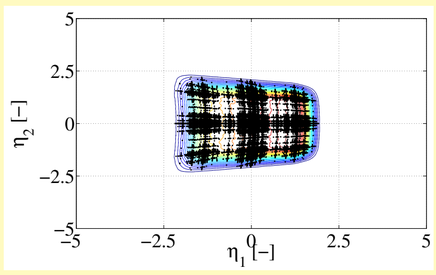
$$I(f) = \int_{\mathbb{R}^n} f(\boldsymbol{\eta})dP_{\boldsymbol{\eta}}, \qquad \boldsymbol{\eta} \in \mathbb{R}^n \quad \boldsymbol{\xi} \in \mathbb{R}^N \quad N >> n$$

In fine scale description: Quadrature in $\mathbb{R}^N$

$$I(f) \approx Q(f) = \sum_{k=1}^{R} f(\boldsymbol{\eta}^{(k)})w^{(k)}, \quad \boldsymbol{\eta}^{(k)} \equiv \boldsymbol{\eta}(\boldsymbol{\xi}^{(k)}) \in \mathbb{R}^n, \quad w^{(k)} \in \mathbb{R}.$$

Enforcing equality for a class of functions π:

$$\int_{\mathbb{R}^n} \pi(\boldsymbol{\eta})dP_{\boldsymbol{\eta}} = \sum_{k=1}^{R} \pi(\boldsymbol{\eta}^{(k)})w^{(k)}, \quad \forall \pi \in \mathcal{P}_p^n.$$



Quadrature points relative to initial measure.

In coarse scale:

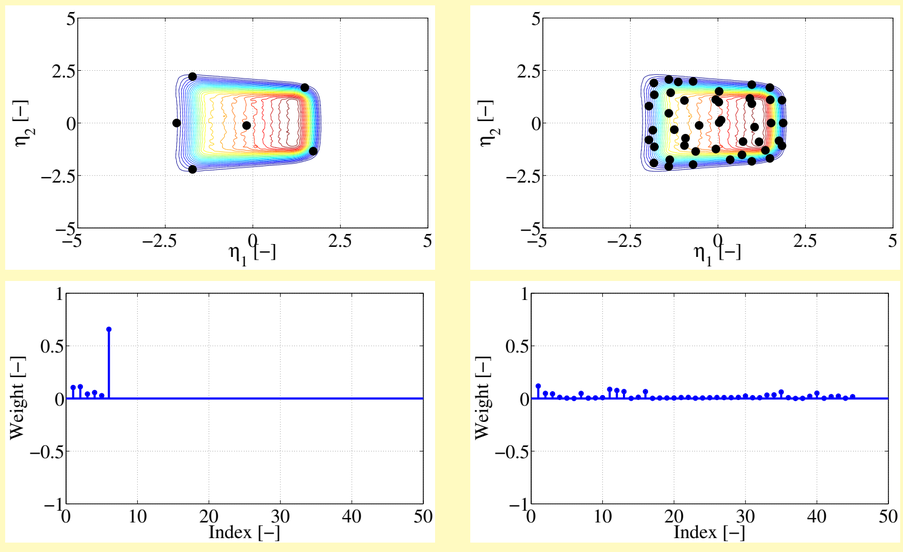
$$\boxed{\min_{\boldsymbol{w}} |\boldsymbol{w}|_{L^1} = \sum_{k=1}^{R}|w_k|, \text{ subject to } \boldsymbol{A}\boldsymbol{w} = \boldsymbol{b}, \quad \hat{\boldsymbol{w}} \in \mathbb{R}^r}$$

where:

$$\boldsymbol{w} = \begin{bmatrix} w_1 & w_2 & \ldots & w_{R-1} & w_R \end{bmatrix}^{\mathrm{T}},$$

$$\boldsymbol{b} = \begin{bmatrix} \int_{\mathbb{R}^n}\pi_1(\boldsymbol{\eta})dP_{\boldsymbol{\eta}} & \ldots & \int_{\mathbb{R}^n}\pi_r(\boldsymbol{\eta})dP_{\boldsymbol{\eta}} \end{bmatrix}^{\mathrm{T}},$$

$$\boldsymbol{A} = \begin{bmatrix} \pi_1(\boldsymbol{\eta}^{(1)}) & \pi_1(\boldsymbol{\eta}^{(2)}) & \ldots & \pi_1(\boldsymbol{\eta}^{(R-1)}) & \pi_1(\boldsymbol{\eta}^{(R)}) \\ \vdots & \vdots & & \vdots & \vdots \\ \pi_r(\boldsymbol{\eta}^{(1)}) & \pi_r(\boldsymbol{\eta}^{(2)}) & \ldots & \pi_r(\boldsymbol{\eta}^{(R-1)}) & \pi_r(\boldsymbol{\eta}^{(R)}) \end{bmatrix}.$$



Quadrature points and weights relative to adapted measure.

Acknowledgment

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