# A Goal-oriented RBM-accelerated generalized Polynomial Chaos Algorithm

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# Reduced Order Methods for UQ problems

Parameterized UQ

- generalized Polynomial Chaos (gPC)
- Monte Carlo Methods
- ...

Reduced Order Methods

- Reduced Basis Methods (RBM)
- Proper Orthogonal Decomposition (POD)
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- Howard C. Elman and Qifeng Liao (2013) Reduced Basis Collocation Methods for Partial Differential Equations with Random Coefficients. SIAM/ASA J. UNCERTAINTY QUANTIFICATION. Vol. 1, pp. 192-217
- Peng Chen, Alfio Quarteroni (2015) A new algorithm for high-dimensional uncertainty quantification based on dimension-adaptive sparse grid approximation and reduced basis methods Journal of Computational Physics 298 176?193
- ...

# generalized Polynomial Chaos

- Parametric PDE:

$$\begin{cases} \mathcal{L}(\boldsymbol{x}, u, \boldsymbol{\mu}) = f(\boldsymbol{x}, \boldsymbol{\mu}), & \forall (\boldsymbol{x}, \boldsymbol{\mu}) \in D \times \Gamma, \\ \mathcal{B}(\boldsymbol{x}, u, \boldsymbol{\mu}) = g(\boldsymbol{x}, \boldsymbol{\mu}), & \forall (\boldsymbol{x}, \boldsymbol{\mu}) \in \partial D \times \Gamma. \end{cases}$$

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- Orthogonal Basis:

$$< \Phi_m(\boldsymbol{\mu}), \Phi_n(\boldsymbol{\mu}) >= \int \Phi_m(\boldsymbol{\mu}) \Phi_n(\boldsymbol{\mu}) \boldsymbol{\rho}(\boldsymbol{\mu}) d\boldsymbol{\mu} = \delta_{m,n}$$

# gPC Basis

$$\Phi_m(\boldsymbol{\mu}) = \phi_{m_1}(\mu_1)...\phi_{m_K}(\mu_K)$$

- Basis function:

| Distribution of $\mu$ | $\phi_m(\mu)$ | Support |
|---|---|---|
| Gaussian | Hermite | $(-\infty, \infty)$ |
| Gamma | Laguerre | $[0, \infty)$ |
| Beta | Jacobi | $[-1, 1]$ |
| Uniform | Legendre | $[-1, 1]$ |

Table 1: Various probability distributions with their corresponding gPC polynomial family and support.

# gPC Coefficients

- Approximation by quadrature rules:

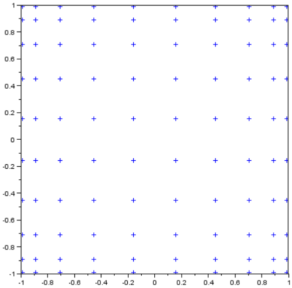
$$\widetilde{u}_m(\boldsymbol{x}) = \int u(\boldsymbol{x}, \boldsymbol{\mu})\Phi_m(\boldsymbol{\mu})\rho(\boldsymbol{\mu})d\boldsymbol{\mu} \approx \sum_{q=1}^{Q} u(\boldsymbol{x}, \boldsymbol{\mu}^q)\Phi_m(\boldsymbol{\mu}^q)w_q$$

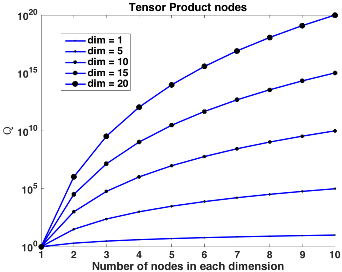
- Solve PDE problem $Q$ times to get $u(x, \boldsymbol{\mu}^q)$

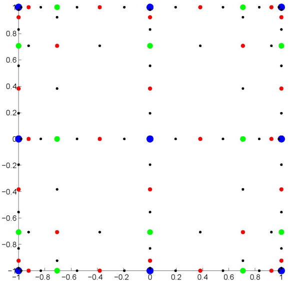
- Our goal:

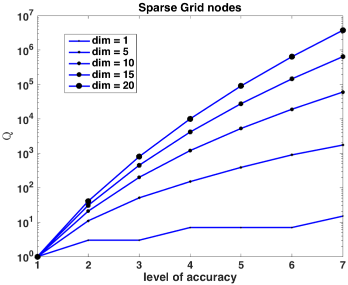
$$\widetilde{u}_m^{RB}(\boldsymbol{x}) = \int u(\boldsymbol{x}, \boldsymbol{\mu})\Phi_m(\boldsymbol{\mu})\rho(\boldsymbol{\mu})d\boldsymbol{\mu} \approx \sum_{q=1}^{Q} u^{RB}(\boldsymbol{x}, \boldsymbol{\mu}^q)\Phi_m(\boldsymbol{\mu}^q)w_q$$

# Computational Challenge







- Parametric problems:

$$\begin{cases} \mathcal{L}(\boldsymbol{x}, u, \boldsymbol{\mu}) = f(\boldsymbol{x}, \boldsymbol{\mu}), & \forall\, (\boldsymbol{x}, \boldsymbol{\mu}) \in D \times \Gamma, \\ \mathcal{B}(\boldsymbol{x}, u, \boldsymbol{\mu}) = g(\boldsymbol{x}, \boldsymbol{\mu}), & \forall\, (\boldsymbol{x}, \boldsymbol{\mu}) \in \partial D \times \Gamma. \end{cases} \tag{1}$$

- How do we solve the PDE (1) at $\boldsymbol{\mu} = \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, ..., \boldsymbol{\mu}_{100000}$?

- $u(\boldsymbol{x}, \boldsymbol{\mu}) \approx c_1(\boldsymbol{\mu}) u(\boldsymbol{x}, \boldsymbol{\mu}_1^*) + c_2(\boldsymbol{\mu}) u(\boldsymbol{x}, \boldsymbol{\mu}_2^*) + ... + c_N(\boldsymbol{\mu}) u(\boldsymbol{x}, \boldsymbol{\mu}_N^*)$

- How do we choose $\boldsymbol{\mu}_1^*, \boldsymbol{\mu}_2^*, ..., \boldsymbol{\mu}_N^*$ ?

# Framework of RBM

- Offline stage: Choose $\boldsymbol{\mu}_1^*, \boldsymbol{\mu}_2^*, ..., \boldsymbol{\mu}_N^*$ by greedy algorithm. The full solution $\{u(\boldsymbol{\mu}_i^*)\}_{i=1}^N$ are computed via classical PDE solver (finite element method, collocation method, etc).

- Online Stage: Evaluate the RB model at any parameter value in the pre-defined parameter range ($\boldsymbol{\mu} \in \Xi$):

$$u^{RB}(\boldsymbol{\mu}) = c_1(\boldsymbol{\mu})u(\boldsymbol{\mu}_1^*) + c_2(\boldsymbol{\mu})u(\boldsymbol{\mu}_2^*) + .. + c_N(\boldsymbol{\mu})u(\boldsymbol{\mu}_N^*)$$

# Greedy Algorithm

- Randomly choose any parameter value in the training set $\Xi$ and set: $RB_1 = span\{u(\boldsymbol{\mu_1})\}, k = 1.$
- Greedy sweep:
  - While $\Delta^{max} < \delta_{tol}$
  - for each $\boldsymbol{\mu} \in \Xi$, solve PDE (1) in $RB_k$ to get $u^k(\boldsymbol{\mu})$;
  - for each $\boldsymbol{\mu} \in \Xi$, compute the error estimate $\Delta^k(\boldsymbol{\mu}) \geq ||u^k(\boldsymbol{\mu}) - u(\boldsymbol{\mu})||_{X_{\mathcal{N}}}$;
  - find the parameter $\boldsymbol{\mu}^{k+1}$ that maximizes the error estimate, set $\Delta^{max} = \Delta^k(\boldsymbol{\mu}^{k+1}), RB_{k+1} = span\{u(\boldsymbol{\mu_1}), ...u(\boldsymbol{\mu_{k+1}})\}$;
  - end

# Goal-oriented RBM

- gPC Coefficents

$$\widetilde{u}_m(\boldsymbol{x}) = \int u(\boldsymbol{x}, \boldsymbol{\mu})\Phi_m(\boldsymbol{\mu})\rho(\boldsymbol{\mu})d\boldsymbol{\mu} \approx \sum_{q=1}^{Q} u(\boldsymbol{x}, \boldsymbol{\mu}^q)\Phi_m(\boldsymbol{\mu}^q)w_q$$

$$\widetilde{u}_m^{RB}(\boldsymbol{x}) = \int u(\boldsymbol{x}, \boldsymbol{\mu})\Phi_m(\boldsymbol{\mu})\rho(\boldsymbol{\mu})d\boldsymbol{\mu} \approx \sum_{q=1}^{Q} u^{RB}(\boldsymbol{x}, \boldsymbol{\mu}^q)\Phi_m(\boldsymbol{\mu}^q)w_q$$

- Weighted a posteriori error estimate:

$$\Delta^w(\boldsymbol{\mu}) = \Delta(\boldsymbol{\mu}_q)\sqrt{|w_q|}$$

# Motivation of $\Delta^w(\boldsymbol{\mu}) = \Delta(\boldsymbol{\mu}_q)\sqrt{|w_q|}$

- Error:

$$||\widetilde{u}_m(\mathbf{x}) - \widetilde{u}_m^{RB}(\mathbf{x})||_{l^2} \leq \sum_{q=1}^{Q} ||u(\mathbf{x}, \boldsymbol{\mu}^q) - u^{RB}(\mathbf{x}, \boldsymbol{\mu}^q)||_{l^2} |\Phi_m(\boldsymbol{\mu}^q) w_q|$$
$$\leq \sum_{q=1}^{Q} \Delta(\boldsymbol{\mu}^q) |\Phi_m(\boldsymbol{\mu}^q) w_q|$$
$$= \sum_{q=1}^{Q} \Delta(\boldsymbol{\mu}^q)\sqrt{|w_q|} |\Phi_m(\boldsymbol{\mu}^q)\sqrt{|w_q|}|$$

- Find $\sum_{q=1}^{Q} (\Phi_m(\boldsymbol{\mu}^q))^2 |w_q|) \leq C$ and define $\Delta^w(\boldsymbol{\mu}^q) = \Delta(\boldsymbol{\mu}^q)\sqrt{|w_q|}$

- Control the error by tolerance:

$$||\widetilde{u}_m(\mathbf{x}) - \widetilde{u}_m^{RB}(\mathbf{x})||_{l^2} \leq \sqrt{(\sum_{q=1}^{Q} (\Delta^w(\boldsymbol{\mu}^q))^2)(\sum_{q=1}^{Q} (\Phi_m(\boldsymbol{\mu}^q))^2 |w_q|)}$$
$$\leq \delta_{tol} \times C$$

# Error Analysis

## Theorem (J.-Chen-Narayan)

*Given an $M$-term gPC projection and an $N$-dimensional reduced basis approximation, the error in the quantity of interest computed from the RBM-gPC approximation $u_M^N$, and that computed from the truth gPC approximation $u_M$ is*

$$\left\| \mathcal{F}\left[u_M^N\right] - \mathcal{F}\left[u_M\right] \right\|_{X_{\mathcal{N}}} \leq C_{\mathrm{Lip}}\, C_{Q,M}\, \delta_{tol},$$

*where $C_{Lip}$ is the Lipschitz constant, and $C_{Q,M}$ is a constant independent of $u$, defined by*

$$C_{Q,M} = \sum_{m=1}^{M} B_{Q,m} \left|\mathcal{F}[\Phi_m(\boldsymbol{\mu})]\right|, B_{Q.m} = \sqrt{\sum_{q=1}^{Q} (\Phi_m(\boldsymbol{\mu}^q))^2 |w_q|}, \delta_{tol} = \sqrt{\frac{1}{Q} \sum_{q=1}^{Q} \left[\Delta_N^w(\boldsymbol{\mu}^q)\right]^2}$$

# Numerical Results

- Problem:

$$\begin{cases} -\nabla \cdot (a(\boldsymbol{x}, \boldsymbol{\mu}) \nabla u(\boldsymbol{x}, \boldsymbol{\mu})) = f & \text{in} \quad D \times \boldsymbol{\Gamma}, \\ u(\boldsymbol{x}, \boldsymbol{\mu}) = 0 & \text{on} \quad \partial D \times \boldsymbol{\Gamma}. \end{cases}$$

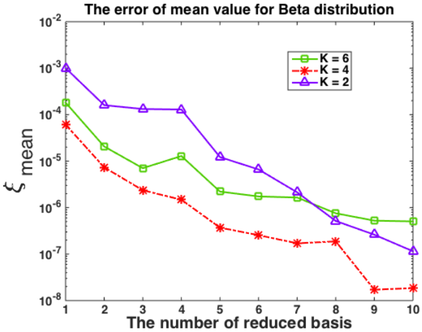
The diffusion coefficient $a(\boldsymbol{x}, \boldsymbol{\mu})$ is defined as:

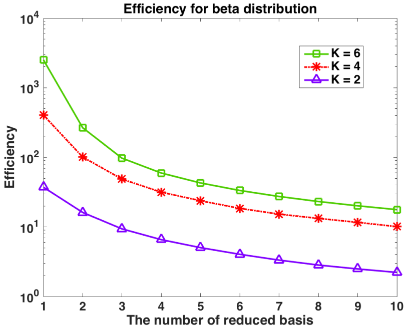
$$a(\boldsymbol{x}, \boldsymbol{\mu}) = A + \sum_{k=1}^{K} \frac{\cos(30 * \mu_k - 1)}{k^2} \cos(kx) \sin(ky),$$

- Number of Quadrature nodes:

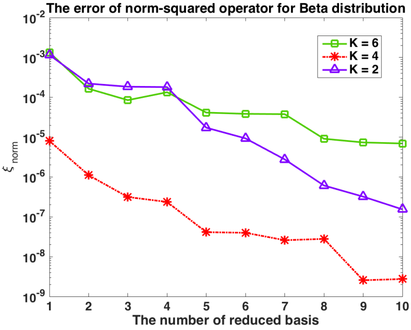
| K | 2 | 4 | 6 |
|---|---|---|---|
| Q(K) | 1,600 | 22,401 | 367,041 |

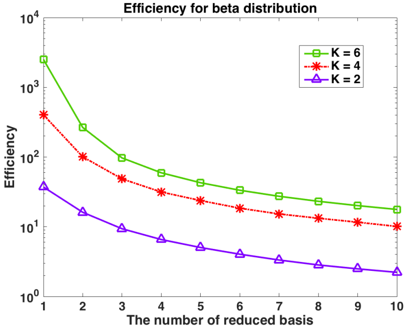
# Mean Value: $\mathcal{F} = \mathbb{E}$



# $L^2_\rho - norm$ squared: $\mathcal{F} = ||.||^2_{L^2_\rho}$



# Conclusion and Reference

- Conclusion
  - We designed, analyzed, and tested a unified, goal-oriented reduced basis method to accelerate the gPC-approximation of parameterized PDEs.
  - As the dimension of the parameter increases, the proposed algorithm is more efficient for the problem we tested.
- Reference

  - J., Chen, Narayan, *A unified, goal-oriented, hybridized reduced basis method and generalized polynomial chaos algorithm for partial differential equations with random inputs*, arXiv:1601.00137. Under revision.

Question?