A Generalized Polynomial Chaos Expansion for High-Dimensional Design Optimization under Dependent Random Variables

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Outline

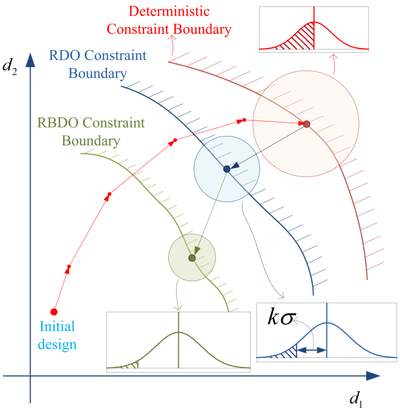
Design under uncertainty

$$\text{Inputs } \mathbf{X} = (X_1, \ldots, X_N) \in \mathbb{R}^N \rightarrow \boxed{\textbf{COMPLEX SYSTEM}} \rightarrow \text{Output } y(\mathbf{X})$$

$\mathbf{X} \sim f_{\mathbf{X}}(\mathbf{x}; \mathbf{d})\,d\mathbf{x}$: Input random variables

$\mathbf{d} \in \mathcal{D} \subseteq \mathbb{R}^M$: Design parameters

RDO: Robust design opt. RBDO: Reliability-based design opt.



RDO
Low variability, insensitive design

RDO + RBDO
(RBRDO)

RBDO
Low risk of failure

Stochastic design optimization

- **RDO**

$$\min_{\mathbf{d}\in\mathcal{D}\subseteq\mathbb{R}^M} \quad c_0(\mathbf{d}) := w_1 \frac{\overbrace{\mathbb{E}_{\mathbf{d}}\left[y_0(\mathbf{X})\right]}^{\text{Mean}}}{\mu_0^*} + w_2 \frac{\overbrace{\sqrt{\text{var}_{\mathbf{d}}\left[y_0(\mathbf{X})\right]}}^{\text{Standard deviation}}}{\sigma_0^*},$$

$$\text{subject to} \quad c_l(\mathbf{d}) := \alpha_l \sqrt{\text{var}_{\mathbf{d}}\left[y_l(\mathbf{X})\right]} - \mathbb{E}_{\mathbf{d}}\left[y_l(\mathbf{X})\right] \le 0, \; l = 1,\cdots,K,$$

$$d_{k,L} \le d_k \le d_{k,U}, \; k = 1,\cdots,M$$

Needs: Statistical moments, design sensitivities of moments

- **RBDO**

$$\min_{\mathbf{d}\in\mathcal{D}\subseteq\mathbb{R}^M} \quad c_0(\mathbf{d}),$$

$$\text{subject to} \quad c_l(\mathbf{d}) := \overbrace{\mathbb{P}_{\mathbf{d}}\left[\mathbf{X} \in \Omega_{\mathbf{d},F,l}\right]}^{\text{Failure probability}} - p_l \le 0, \; l = 1,\cdots,K,$$

$$d_{k,L} \le d_k \le d_{k,U}, \; k = 1,\cdots,M,$$

Needs: Failure probability, design sensitivity of failure probability

Existing methods & limitations

Existing methods

- **Statistical moment analysis**
  - PEM, TSE, TPQ, PCE, PDD, etc.
- **Reliability analysis**
  - FOSM, FORM/SORM, Saddlepoint approx., etc.

Limitations

- Curse of dimensionality: PEM, TPQ, PCE, GPCE
- Low non-linearity of output: PEM, TSE, FOSM, FORM/SORM
- Transformed input from depen. to indepen. (high non-linearity): PEM, TSE, TPQ, PCE, PDD, FOSM, FORM/SORM, Saddlepoint approx.
- Select dependent probability measures: GPCE, GPDD

(Goal) To create robust methods for high-dimensional design opt. under arbitrary, dependent random variables

High-dimensional stochastic design opt.

Transforming input $\mathbf{X}$ to $\mathbf{Z}$ to sidestep update of $\mathbf{X}$ during opt.

Scaling: $\mathbf{Z} = \mathrm{diag}[r_1, \ldots, r_N]\mathbf{X}$

$$\mathbb{E}_{\mathbf{d}}[Z_{i_k}] = \mathbb{E}_{\mathbf{d}}[X_{i_k}] r_{i_k} = \underbrace{d_k}_{\text{varied}} \, r_{i_k} = \underbrace{g_k}_{\text{fixed}}$$

Alternative formulation of RDO

$$\begin{aligned} \min_{\mathbf{d}\in\mathcal{D}\subseteq\mathbb{R}^M} \quad & c_0(\mathbf{d}) := w_1 \frac{\mathbb{E}_{\mathbf{g}(\mathbf{d})}[h_0(\mathbf{Z};\mathbf{r})]}{\mu_0^*} + w_2 \frac{\sqrt{\mathrm{var}_{\mathbf{g}(\mathbf{d})}[h_0(\mathbf{Z};\mathbf{r})]}}{\sigma_0^*}, \\ \text{subject to} \quad & c_l(\mathbf{d}) := \alpha_l \sqrt{\mathrm{var}_{\mathbf{g}(\mathbf{d})}[h_l(\mathbf{Z};\mathbf{r})]} - \mathbb{E}_{\mathbf{g}(\mathbf{d})}[h_l(\mathbf{Z};\mathbf{r})] \le 0, \\ & l = 1, \ldots, K, \; d_{k,L} \le d_k \le d_{k,U}, \; k = 1, \ldots, M. \end{aligned}$$

Alternative formulation of RBDO

$$\begin{aligned} \min_{\mathbf{d}\in\mathcal{D}\subseteq\mathbb{R}^M} \quad & c_0(\mathbf{d}), \\ \text{subject to} \quad & c_l(\mathbf{d}) := \mathbb{P}_{\mathbf{g}(\mathbf{d})}\left[\mathbf{Z} \in \bar{\Omega}_{F,l}(\mathbf{d})\right] - p_l \le 0, \; l = 1, \ldots, K, \\ & d_{k,L} \le d_k \le d_{k,U}, \; k = 1, \ldots, M. \end{aligned}$$

High-dimensional UQ analysis

Dimensionally decomposed GPCE (Lee and Rahman 2023)

$$h(\mathbf{Z};\mathbf{r}) \simeq h_{S,m}(\mathbf{Z};\mathbf{r}) = \sum_{i=1}^{L_{N,S,m}} C_i(\mathbf{r})\Psi_i(\mathbf{Z};\mathbf{g}), \quad L_{N,S,m} := \sum_{s=1}^{S} \binom{N}{s}\binom{m}{s}$$

$\Psi_i(\mathbf{Z};\mathbf{g})$=Multivariate ON poly. basis (non-tensor products)

$C_i(\mathbf{r})$=Expansion coefficients

- Dimension-wise decomposition
- Ability to select safely and effectively basis functions

Computational cost (DD-GPCE vs. *regular* GPCE)

m=3

N	DD-GPCE S=1	DD-GPCE S=2	Regular GPCE
10	31	166	286
20	61	631	1,771
40	121	2,461	12,341

Ex. if $N = 40$, $S = 1$, $m = 3$,

(DD-GPCE) $L_{40,1,3} = 121$

(regular GPCE) $L_{40,3} = 12,341$

regular GPCE: $L_{N,m} := \dfrac{(N+m)!}{N!m!}$

High-dimensional UQ analysis

Three-step algorithm to generate multivariate ON

For $u \subseteq \{1,\ldots,N\}$, $0 \le S \le N$, consider **multi-index set**

$$\{\mathbf{j} = (\mathbf{j}_u, \mathbf{0}_{-u}) \in \mathbb{N}_0^N : \mathbf{j}_u \in \mathbb{N}^{|u|},\ |u| \le |\mathbf{j}_u| \le m,\ 0 \le |u| \le S\},$$
$$|\mathbf{j}_u| := j_{i_1} + \cdots + j_{i_{|u|}},\ \mathbf{j}^{(1)},\ldots,\mathbf{j}^{(L_{N,S,m})},\ \mathbf{j}^{(1)} = \mathbf{0}.$$

1. Create **monomial basis**

$$\mathbf{P}_{S,m}(\mathbf{z}) = (\mathbf{z}^{\mathbf{j}^{(1)}},\ldots,\mathbf{z}^{\mathbf{j}^{(L_{N,S,m})}})^\intercal$$

2. Estimate **monomial moment matrix**

$$\mathbf{G}_{S,m} := \mathbb{E}_{\mathbf{g}}[\mathbf{P}_{S,m}(\mathbf{Z})\mathbf{P}_{S,m}^\intercal(\mathbf{Z})]$$

3. Conduct **Whitening transformation**

$$(\Psi_1(\mathbf{z},\mathbf{g}),\ldots,\Psi_{L_{N,S,m}}(\mathbf{z};\mathbf{g}))^\intercal = \mathbf{Q}_{S,m}^{-1}\mathbf{P}_{S,m}(\mathbf{z}),\ \ \mathbf{G}_{S,m} = \mathbf{Q}_{S,m}\mathbf{Q}_{S,m}^\intercal$$

High-dimensional UQ analysis

DD-GPCE (Lee and Rahman 2021)

$$h(\mathbf{Z};\mathbf{r}) \simeq h_{S,m}(\mathbf{Z};\mathbf{r}) = \sum_{i=1}^{L_{N,S,m}} C_i(\mathbf{r})\Psi_i(\mathbf{Z};\mathbf{g}), \quad L_{N,S,m} := \sum_{s=1}^{S} \binom{N}{s}\binom{m}{s}$$

- **First two moments**

$$\mathbb{E}_{\mathbf{g}}\left[h_{S,m}(\mathbf{Z};\mathbf{r})\right] = C_1(\mathbf{r}) = \mathbb{E}_{\mathbf{g}}\left[h(\mathbf{Z})\right]$$

$$\mathrm{var}_{\mathbf{g}}[h_{S,m}(\mathbf{Z};\mathbf{r})] = \sum_{i=2}^{L_{N,S,m}} C_i^2(\mathbf{r})$$

- **Failure probability**

$$\mathbb{P}_{\mathbf{g}(\mathbf{d})}\left[\mathbf{Z} \in \bar{\Omega}_{F,S,m}\right] := \int_{\bar{\mathbb{A}}^N} I_{\bar{\Omega}_{F,S,m}}(\mathbf{z}) f_{\mathbf{Z}}(\mathbf{z};\mathbf{g})\, d\mathbf{z} := \mathbb{E}_{\mathbf{g}}\left[I_{\bar{\Omega}_{F,S,m}}(\mathbf{Z})\right]$$

$$= \lim_{\bar{L}\to\infty} \frac{1}{\bar{L}} \sum_{l=1}^{\bar{L}} I_{\bar{\Omega}_{F,S,m}}(\mathbf{z}^{(l)}),$$

$$I_{\bar{\Omega}_{F,S,m}}(\mathbf{z}) = \begin{cases} 1, & \mathbf{z} \in \bar{\Omega}_{F,S,m}, \\ 0, & \mathbf{z} \notin \bar{\Omega}_{F,S,m}. \end{cases}$$

High-dimensional design sensitivity analysis

Sensitivities of first two moments

$$\frac{\partial \mathbb{E}_{\mathbf{g}}[h_{S,m}(\mathbf{Z})]}{\partial d_k} = \frac{\partial g_k}{\partial d_k} \sum_{i=2}^{L_{\min}} C_i(\mathbf{r}) D_{k,j}(\mathbf{g}), \;\; L_{\min} = \min(L_{N,S,m}, L_{N,S',m'})$$

$$\frac{\partial \mathbb{E}_{\mathbf{d}}[h_{S,m}^2(\mathbf{Z})]}{\partial d_k} = \frac{\partial g_k}{\partial d_k} \sum_{i_1=1}^{L_{N,S,m}} \sum_{i_2=1}^{L_{N,S,m}} \sum_{i_3=2}^{L_{N,S',m'}} C_{i_1}(\mathbf{r}) C_{i_2}(\mathbf{r}) D_{k,i_3}(\mathbf{g}) T_{i_1 i_2 i_3}$$

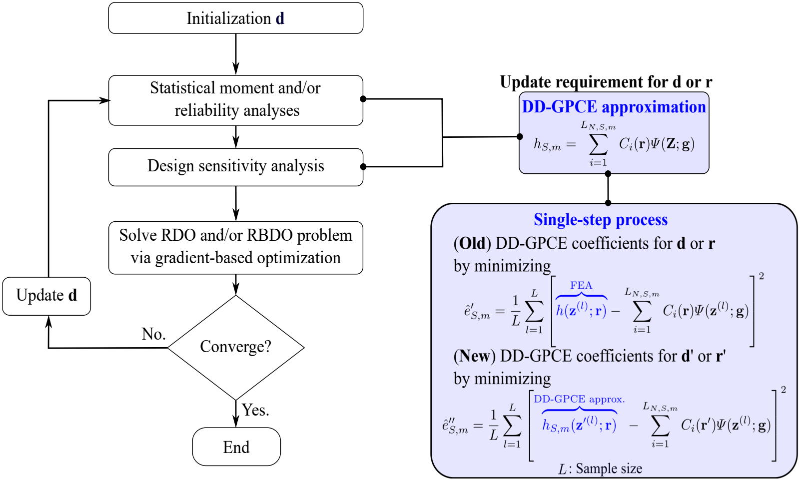
$$T_{i_1 i_2 i_3} = \mathbb{E}_{\mathbf{g}}\left[\prod_{p=1}^{3} \Psi_{i_p}(\mathbf{Z};\mathbf{g})\right], \;\; s_{k,S',m'}(\mathbf{Z};\mathbf{g}) = \sum_{i=2}^{L_{N,S',m'}} D_{k,i}(\mathbf{g}) \Psi_i(\mathbf{Z};\mathbf{g})$$

Design sensitivities of failure probability

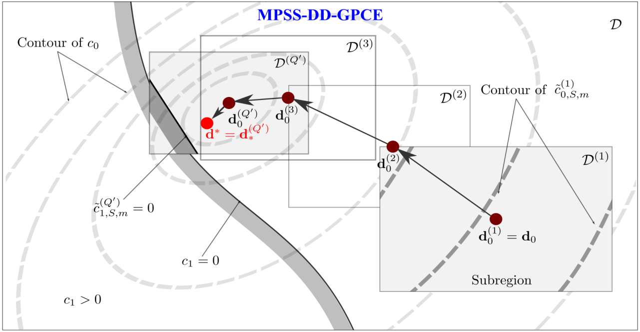
$$\frac{\partial \mathbb{P}_{\mathbf{g}}\left[\mathbf{Z} \in \bar{\Omega}_{F,S,m}\right]}{\partial d_k} = \frac{\partial g_k}{\partial d_k} \lim_{\bar{L}\to\infty} \frac{1}{\bar{L}} \sum_{l=1}^{\bar{L}} \left[I_{\bar{\Omega}_{F,S,m}}(\mathbf{z}^{(l)}) s_k(\mathbf{z}^{(l)};\mathbf{g}) \right]$$

High-dimensional design optimization

Single-step DD-GPCE



High-dimensional design optimization



Local stochastic design optimization problem solved by single-step process

Local RDO

$$\min_{\mathbf{d}\in\mathcal{D}^{(q')}\subseteq\mathbb{R}^M} \tilde{c}^{(q')}_{0,S,m}(\mathbf{d}) := w_1 \frac{\mathbb{E}_{\mathbf{g}}[\tilde{h}^{(q')}_{0,S,m}(\mathbf{Z};\mathbf{r})]}{\mu_0^*} + w_2 \frac{\sqrt{\operatorname{var}_{\mathbf{g}}[\tilde{h}^{(q')}_{0,S,m}(\mathbf{Z};\mathbf{r})]}}{\sigma_0^*},$$

$$\text{subject to } \tilde{c}^{(q')}_{l,S,m}(\mathbf{d}) := \alpha_l \sqrt{\operatorname{var}_{\mathbf{g}}[\tilde{h}^{(q')}_{l,S,m}(\mathbf{Z};\mathbf{r})]} - \mathbb{E}_{\mathbf{g}}[\tilde{h}^{(q')}_{l,S,m}(\mathbf{Z};\mathbf{r})] \le 0,$$

Local RBDO

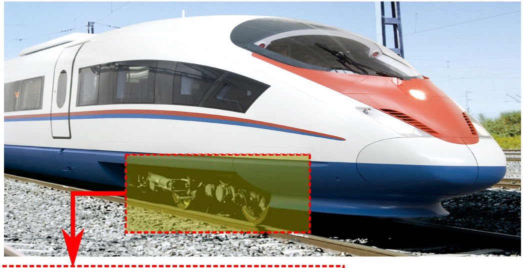
$$\min_{\mathbf{d}\in\mathcal{D}^{(q')}\subseteq\mathbb{R}^M} \tilde{c}^{(q')}_{0,S,m}(\mathbf{d})$$

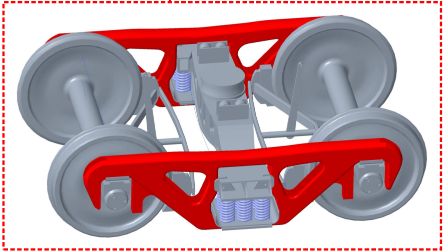
$$\text{subject to } \tilde{c}^{(q')}_{l,S,m}(\mathbf{d}) := \mathbb{P}_{\mathbf{g}}[\mathbf{Z} \in \tilde{\bar{\Omega}}^{(q')}_{F,l,S,m}(\mathbf{d})] - p_l \le 0,$$

$$d_k \in \left[d^{(q')}_{k,0} - \beta^{(q')}_k \frac{(d_{k,U} - d_{k,L})}{2},\ d^{(q')}_{k,0} + \beta^{(q')}_k \frac{(d_{k,U} - d_{k,L})}{2} \right],$$

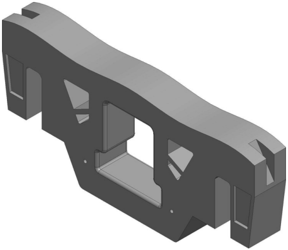
$$l = 1,\ldots,K;\ k = 1,\ldots,M.$$

Example: Train bogie side frame





Train bogie assembly



Bogie side frame

Example: Problem statement

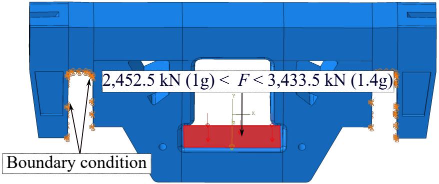
$$\min_{\mathbf{d}\in\mathcal{D}} \quad c_0(\mathbf{d}) := \frac{\mathbb{E}_{\mathbf{d}}[y_0(\mathbf{X})]}{\mathbb{E}_{\mathbf{d}_0}[y_0(\mathbf{X})]}$$

$$\text{subject to} \quad c_1(\mathbf{d}) := \mathbb{P}_{\mathbf{d}}[y_1(\mathbf{X}) < 0] - \Phi(-3) \le 0$$

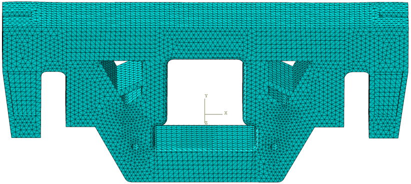
$$y_0(\mathbf{X}) = \rho \int_{\mathcal{D}'(\mathbf{X})} d\mathcal{D}'$$

$$y_1(\mathbf{X}) = \log\left[\frac{N_1(\mathbf{X})}{1\times 10^7}\right]$$

Cast steel
Density=7,800 kg/m^3
Elastic molulus=203 GPa
Poisson's ratio=0.3
Fatigue strength coefficient=1,332 MPa
Fatigue strength exponent=-0.1085
Fatigue ductility coefficient=0.375
Fatigue ductiliy exponent=-0.6354

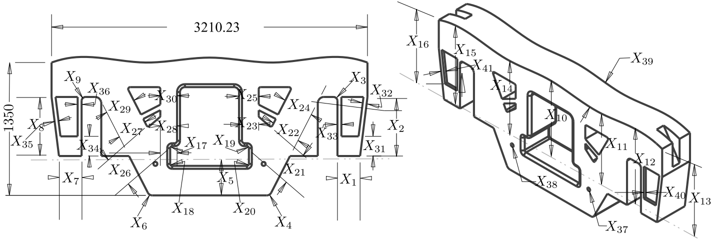


Vertical load F and boundary conditions



Tetrahedral mesh comprising 157,647 elements

Example: Random input

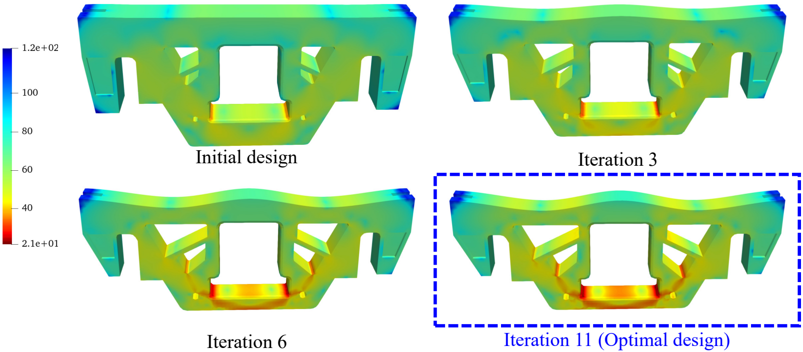


Random variable	Mean	Standard deviation	Probability distribution
X_k	d_k	$0.02\,d_k$	Lognormal
		$k = 1, \ldots, 41$	

Correlation coefficients=0.4 among $X_1, \ldots, X_{41}$

k	$d_{l,0}$ mm	$d_{l,L}$ mm	$d_{l,U}$ mm	k	$d_{l,0}$ mm	$d_{l,L}$ mm	$d_{l,U}$ mm	k	$d_{l,0}$ mm	$d_{l,L}$ mm	$d_{l,U}$ mm
1	230	80	250	15	900	800	900	29	300	100	300
2	600	400	600	16	900	850	900	30	200	100	200
3	40	30	50	17	20	10	30	31	200	100	200
4	50	50	100	18	20	10	50	32	40	20	40
5	500	330	500	19	20	10	30	33	40	20	40
6	50	50	100	20	20	10	50	34	200	100	200
7	230	80	250	21	300	100	300	35	40	20	40
8	600	400	600	22	300	100	300	36	40	20	40
9	40	30	50	23	200	100	200	37	30	30	40
10	900	850	900	24	300	100	300	38	30	30	40
11	900	750	900	25	200	100	200	39	400	300	400
12	900	800	900	26	300	100	300	40	30	30	60
13	900	850	900	27	300	100	300	41	30	30	60
14	900	750	900	28	200	100	200				

Example: Shape design results



MPSS-DD-GPCE leads to RBDO of the bogie side frame, reducing the mean of mass by 50.39 % via 4,980 FEA.

Conclusion

- A novel design optimization method is based on DD-GPCE for statistical moment and reliability analyses of a high-dimensional complex response under dependent input random variables.
- A new sensitivity method yields the second-moments, failure probability, and design sensitivities simultaneously.
- MPSS-DD-GPCE can handle industrial-scale design problems with high-dimensions.

Lee, D. and Rahman, S. (2023) *High-Dimensional Stochastic Design Optimization under Dependent Random Variables by a Dimensionally Decomposed Generalized Polynomial Chaos Expansion*
Int. J. Uncertainty Quantification, Vol. 13, pp.23-59