Impact of Sampling Strategies in the Polynomial Chaos Surrogate Construction for Monte Carlo Transport Applications

Gianluca Geraci and Aaron J. Olson

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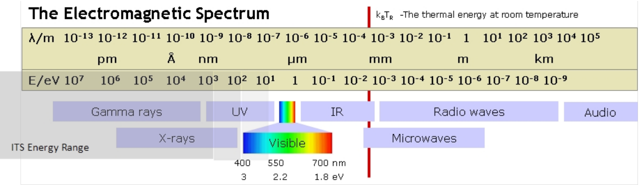
Plan of the talk

- Motivation and background
- Polynomial Chaos Expansion
- Sampling strategies
- Numerical Results
- Concluding Remarks

Motivation and background



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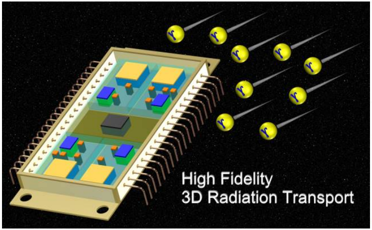
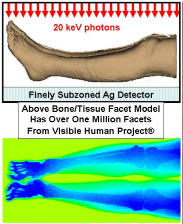
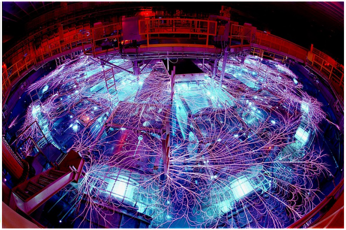




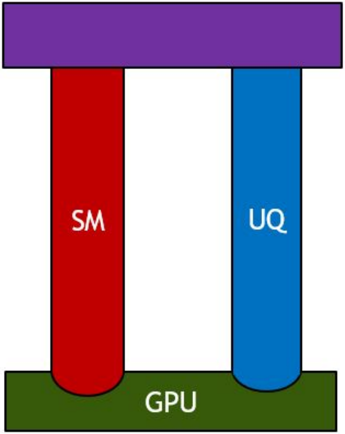


Figures courtesy of Brian Franke and Shawn Pautz

High-fidelity state-of-the-art modeling and simulations with HPC

- **Predictive science** needs Uncertainty Quantification (UQ)
- UQ under **severe** simulations **budget constraints**
- **Significant dimensionality** driven by model complexity

Develop efficient, embedded **Stochastic Media (SM)** and **Uncertainty Quantification (UQ)** Monte Carlo transport methods for the **GPU**.



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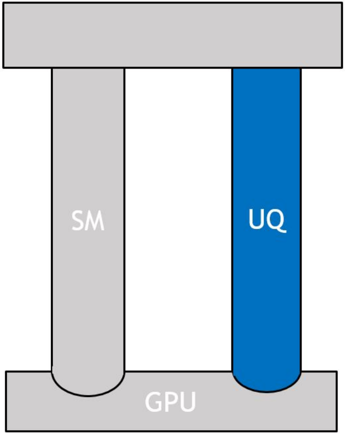


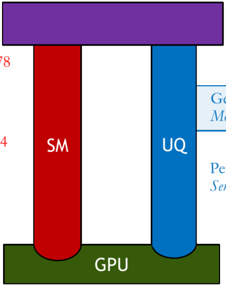
Develop efficient, embedded **Stochastic Media (SM)** and **Uncertainty Quantification (UQ)** Monte Carlo transport methods for the **GPU**.

CLS/LRP for three+ materials — Vu, Paper #33712, *Transport in Stochastic Media I*

Markovian three+ materials — Olson, Paper #33778, *Transport in Stochastic Media I*

CoPS **for generalized mixing** — Davis, Paper #33784, *Transport in Stochastic Media II*

CoPS **memory/runtime efficiency** — Vu, Paper #33614, *Transport in Stochastic Media I*



Geraci, Paper #33671, *Monte Carlo Methods* — **PCE surrogate models**

Petticrew, Paper #33657, *Sensitivity Analysis* — **Global sensitivity analysis**

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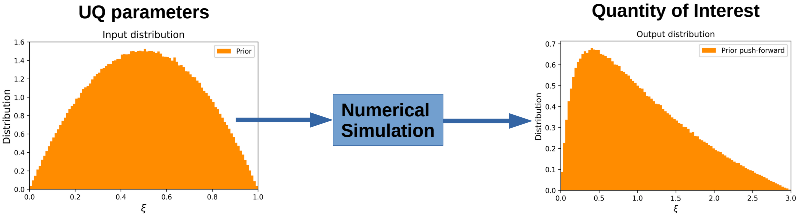
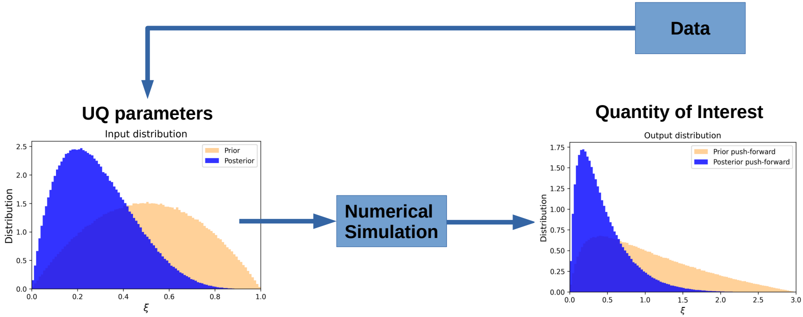
CoPS **on the GPU** — Kersting, Paper #33673, *Monte Carlo Algorithms*



Uncertainty Quantification:

- UQ **main tasks**: **Forward** and **Inverse**
- **Forward UQ:** Propagation of (known) parameter distributions through numerical code



Uncertainty Quantification:

- UQ **main tasks**: **Forward** and **Inverse**
- **Forward UQ:** Propagation of (known) parameter distributions through numerical code
- **Inverse UQ:** Infer posterior distributions from observational data (Bayes rule)

Forward UQ via surrogate modeling:

- Statistics $\longrightarrow$ **large number of QoI realizations**
- Computational burden **can be alleviated** by replacing the original code **with a surrogate**

Polynomial Chaos Expansion (PCE)

Polynomial Chaos

- **UQ parameters:** $\xi \in \Xi \subset \mathbb{R}^d$
- **Joint pdf:** $p(\xi)$ (independent components)
- **QoI:** $Q = Q(\xi) \in \mathbb{R}$
- **Polynomial Chaos Expansion**

$$Q(\xi) = \sum_{k=0}^{\infty} \beta_k \Psi_k(\xi) \approx \sum_{k=0}^{P} \beta_k \Psi_k(\xi) = Q^{PCE}(\xi), \quad \text{with} \quad P + 1 = \frac{(n_0 + d)!}{n_0!\, d!} \quad \text{and}$$

  n_0 being the **total order** of the expansion.

- Polynomial basis Ψ_k is selected to be **orthogonal w.r.t. $p(\xi)$**

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Remarks

- **Statistics can be obtained in close form** or by sampling Q^{PCE} directly, *e.g.*

$$\mathbb{E}\left[Q\right] = \beta_0 \quad \text{and} \quad \mathbb{V}ar\left[Q\right] = \sum_{k=1}^{P} \beta_k^2\, \mathbb{E}\left[\Psi_k^2\right]$$

- **Coefficients evaluation**:
  - **Regression**: L2 (ordinary least-square) or L1 (sparse) minimization
  - **Spectral projection**: multidimensional integration

Spectral projection $\rightarrow$ Non-Intrusive Spectral Projection (NISP)

$$\mathbb{E}\left[\Psi_k \Psi_\ell\right] = \int_\Xi \Psi_k \Psi_\ell \, p(\xi) \mathrm{d}\xi = b_k \delta_{k\ell} \quad \rightarrow \quad \beta_k = \frac{\mathbb{E}\left[Q \Psi_k\right]}{b_k}$$

Our task is the efficient computation of the multi-dimensional integral $\mathbb{E}\left[Q\Psi_k\right]$

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Radiation transport features

- **Large dimensionality**, *i.e.* large number of uncertainty sources, random fields, *etc.*
- **Noisy response** $Q(\xi)$: MC transport solvers (more on this later)

Non-Intrusive Spectral Projection
The case of radiation transport applications

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Sampling approaches: more suited than quadrature in this context

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Sampling Strategies

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A: The QoI is not obtained directly, but as a statistics of elementary events

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- **MC transport (internal) randomness**: $\eta \in H \subset \mathbb{R}^{d'}$
- **Particle histories** are interpreted as elementary events: $f = f(\xi, \eta)$
- **RT QoI**: Average of f over the histories for a fixed UQ parameters realization:

$$Q(\xi) = \mathbb{E}_\eta \left[f(\xi, \eta) \right] \overset{MC\ RT}{\approx} \frac{1}{N_\eta} \sum_{j=1}^{N_\eta} f\left(\xi, \eta^{(j)}\right) \overset{\text{def}}{=} \tilde{Q}(\xi)$$

NOTES:

- In the limit of $N_\eta \to \infty$, $\tilde{Q}(\xi) \to Q(\xi)$
- ... but we do have **limited histories**

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- ... but we do have **limited histories**

Questions:
Q1: How do we **propagate the effect** of a limited number of histories?
Q2: What is the **impact of this 'error'** in the PCE coefficients/surrogate?

Step 1. Introducing the MC transport QoI definition:

$$\begin{aligned}\beta_k &= \frac{1}{b_k}\mathbb{E}_\xi\left[Q(\xi)\Psi_k(\xi)\right]\\ &= \frac{1}{b_k}\mathbb{E}_\xi\left[\mathbb{E}_\eta\left[f(\xi,\eta)\right]\Psi_k(\xi)\right]\end{aligned}$$

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Step 2. Sampling approximation:

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$\hat{\beta}_k$ is an unbiased estimator

$$\hat{\beta}_k = \frac{1}{b_k}\frac{1}{N_\xi}\sum_{i=1}^{N_\xi}\left[\frac{1}{N_\eta}\sum_{j=1}^{N_\eta} f(\xi^{(i)}, \eta^{(j)})\Psi_k(\xi^{(i)})\right] = \frac{1}{b_k}\frac{1}{N_\xi}\sum_{i=1}^{N_\xi}\left[\tilde{Q}(\xi^{(i)})\Psi_k(\xi^{(i)})\right]$$

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Variance starting from the noisy RT QoI

$$\mathbb{V}ar\left[\hat{\beta}_k\right] = \frac{1}{b_k^2}\frac{\mathbb{V}ar\left[\tilde{Q}\Psi_k\right]}{N_\xi}$$

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Law of total variance (hint of derivation) – $\mathbb{V}ar\left[\cdot\right] = \mathbb{V}ar\left[\mathbb{E}_\eta\left[\cdot\right]\right] + \mathbb{E}\left[\mathbb{V}ar_\eta\left[\cdot\right]\right]$

$$\begin{aligned}
\mathbb{V}ar\left[\tilde{Q}(\xi;\eta)\Psi_k\right] &= \mathbb{V}ar\left[\mathbb{E}_\eta\left[\tilde{Q}(\xi;\eta)\Psi_k(\xi)\right]\right] + \mathbb{E}\left[\mathbb{V}ar_\eta\left[\tilde{Q}(\xi;\eta)\Psi_k(\xi)\right]\right] \\
&= \mathbb{V}ar\left[\mathbb{E}_\eta\left[f(\xi,\eta)\right]\Psi_k(\xi)\right] + \mathbb{E}\left[\frac{\mathbb{V}ar_\eta\left[f(\xi,\eta)\right]}{N_\eta}\Psi_k^2(\xi)\right] \\
&= \mathbb{V}ar\left[Q(\xi)\Psi_k(\xi)\right] + \mathbb{E}\left[\frac{\sigma_\eta^2(\xi)}{N_\eta}\Psi_k^2(\xi)\right].
\end{aligned}$$

Finally,

$$\boxed{\mathbb{V}ar\left[\hat{\beta}_k\right] = \frac{1}{b_k^2}\frac{\mathbb{V}ar\left[\mathbf{Q}(\xi)\Psi_k(\xi)\right] + \mathbb{E}\left[\frac{\sigma_\eta^{\mathbf{2}}(\xi)}{\mathbf{N}_\eta}\Psi_k^2(\xi)\right]}{N_\xi}}$$

NOTES:

- The **true variance** is polluted by the (average) **noise** introduced by limited histories
- The **noise** is the variance of the inner MC RT estimator

Q: Is there a **best sampling strategy** in this context?

$$\beta_k = \frac{\mathbb{E}\left[Q\Psi_k\right]}{b_k} = \begin{cases} \frac{1}{b_k}\mathbb{E}_\xi\left[\mathbb{E}_\eta\left[f(\xi,\eta)\right]\Psi_k(\xi)\right] \approx \frac{1}{b_k}\frac{1}{N_\xi}\sum_{i=1}^{N_\xi}\left(\frac{1}{N_\eta}\sum_{j=1}^{N_\eta} f(\xi^{(i)},\eta^{(j)})\Psi_k(\xi^{(i)})\right) \triangleq \hat{\beta}_k^n & \text{(Nested)} \\ \frac{1}{b_k}\mathbb{E}\left[f(\xi,\eta)\Psi_k(\xi)\right] \approx \frac{1}{b_k}\frac{1}{N_{real}}\sum_{r=1}^{N_{real}}\left(f(\xi^{(r)},\eta^{(r)})\Psi_k(\xi^{(r)})\right) \triangleq \hat{\beta}_k^d & \text{(Direct)}. \end{cases}$$

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Cost comparison ($N_{real} = N_\xi \times N_\eta$):

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Variance of the MC-MC estimator
Two different sampling strategies: Nested Vs Direct

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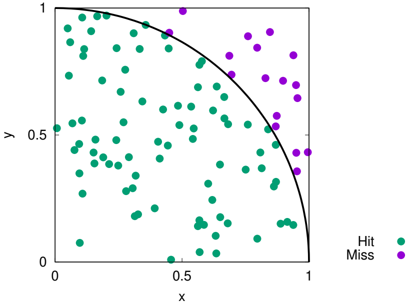
Main Result: $\mathbb{V}ar\left[\hat{\beta}_k^d\right] < \mathbb{V}ar\left[\hat{\beta}_k^n\right]$ for $N_\eta > 1$ (for the same cost)

Valid under the assumption: no start-up cost

Numerical Results

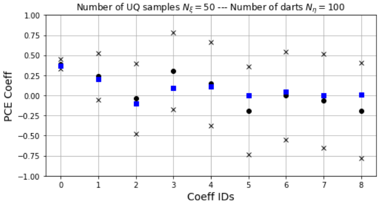


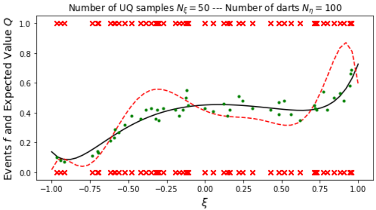
- **Quarter of circle** inscribed in a unitary square
- **UQ parameters:** $\xi \sim \mathcal{U}(-1,1)$
- **Darts:** $\eta = [\eta_x, \eta_y]^{\mathrm{T}}$
- **Elementary evaluation:** $f = 1$ for hit and $f = 0$ otherwise
- **QoI** (area): $Q(\xi) = \mathbb{E}_\eta \left[f(\xi, \eta) \right]$

$$\text{Area}: Q(\xi) = \frac{\pi}{4} r^2(\xi), \quad \text{where} \quad r^2(\xi) = \frac{23 + 3\xi - 18\xi^2 + 12\xi^3 + 17\xi^8}{40}.$$

Finite spectral content (P=8)

Verification test
PCE coefficients





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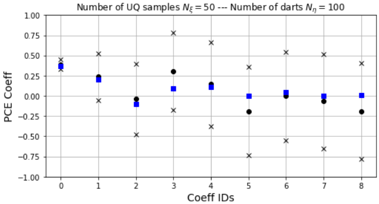
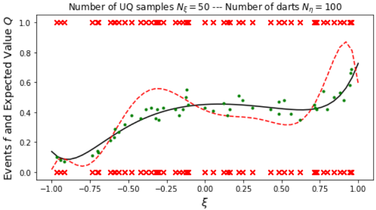
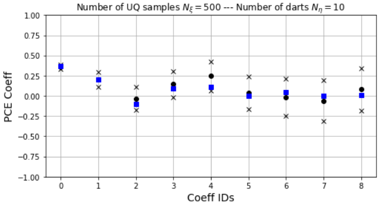
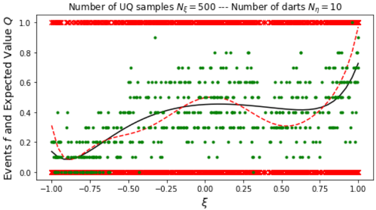
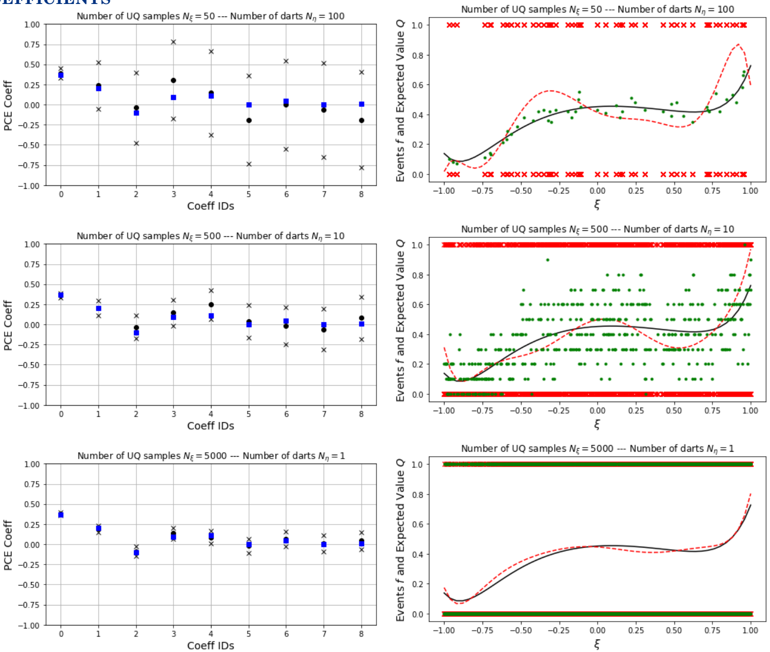








Verification test
PCE coefficients



- 1D slab, neutral particle, **absorption-only** mono-energetic steady state radiation transport
- Normally incident beam with unitary magnitude
- **Random** material **cross sections**: $\Sigma_{t,m}(\xi_m) = \Sigma_{t,m}^{0} + \Sigma_{t,m}^{\Delta}\xi_m$, where $\xi_m \sim \mathcal{U}(-1,1)$
- The **QoI** is the **transmittance**: $T(\xi) = \psi(L,1,\xi)$

$$\mu \frac{\partial \psi(x,\mu,\xi)}{\partial x} + \Sigma_t(x,\xi)\psi(x,\mu,\xi) = 0, \quad \text{where} \quad 0 \leq x \leq L;$$

Analytical solution:

$$T(\xi) = \exp\left[-\sum_{m=1}^{d} \Sigma_{t,m}(\xi_m)\Delta x_m\right] = \exp\left[-\tau(\xi)\right],$$

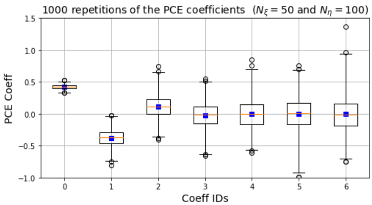
- **Uncertain slab optical thickness:** $\tau(\xi)$
- mth **material thickness:** Δx_m

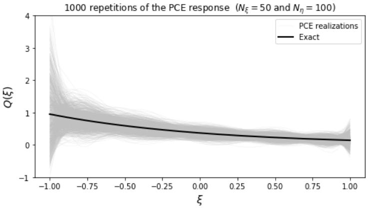
Exact solution (nth raw moment)

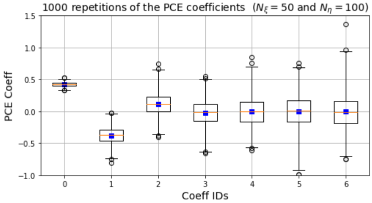
$$\mathbb{E}\left[T^n\right] = \int_{[-1,1]^d} T^n(\xi)p(\xi)\,\mathrm{d}\xi = \prod_{m=1}^{d} \exp\left[-n\Sigma_{t,m}^{0}\Delta x_m\right] \frac{\sinh\left[n\Sigma_{t,m}^{\Delta}\Delta x_m\right]}{n\Sigma_{t,m}^{\Delta}\Delta x_m}.$$

Radiation transport

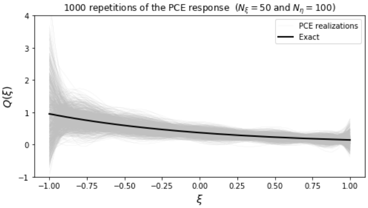
Case 1: Single material section – PCE coefficients



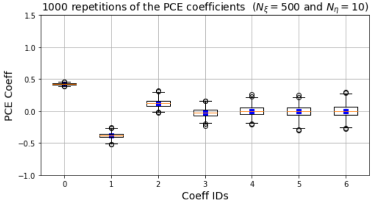




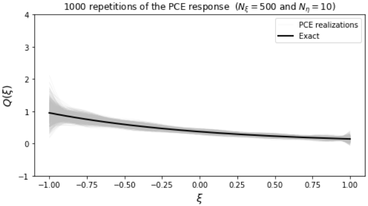
1000 repetitions of the PCE coefficients ($N_\xi = 50$ and $N_\eta = 100$)
PCE Coeff
Coeff IDs



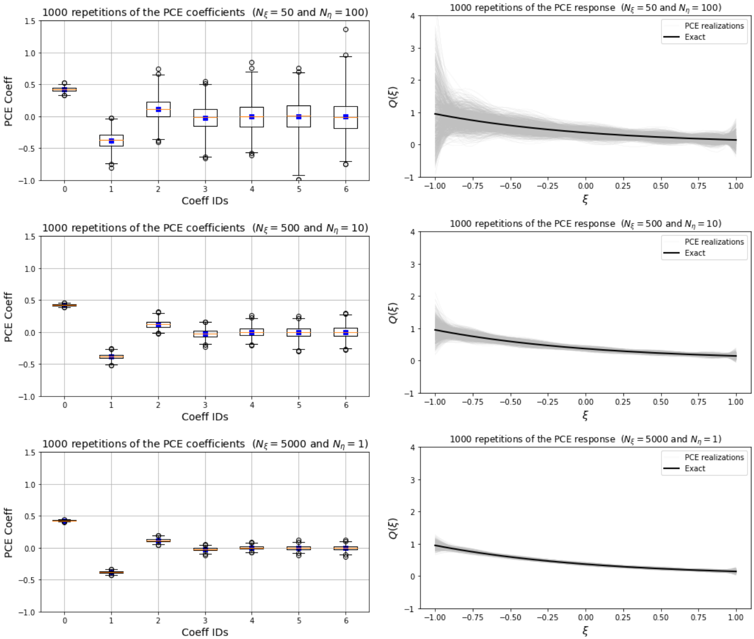
1000 repetitions of the PCE response ($N_\xi = 50$ and $N_\eta = 100$)
PCE realizations
Exact
$Q(\xi)$
ξ



1000 repetitions of the PCE coefficients ($N_\xi = 500$ and $N_\eta = 10$)
PCE Coeff
Coeff IDs



1000 repetitions of the PCE response ($N_\xi = 500$ and $N_\eta = 10$)
PCE realizations
Exact
$Q(\xi)$
ξ



1000 repetitions of the PCE coefficients ($N_\xi = 50$ and $N_\eta = 100$)
PCE Coeff
Coeff IDs
1000 repetitions of the PCE response ($N_\xi = 50$ and $N_\eta = 100$)
PCE realizations
Exact
$Q(\xi)$
ξ
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PCE realizations
Exact
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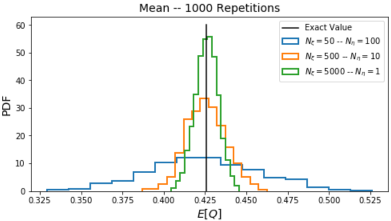
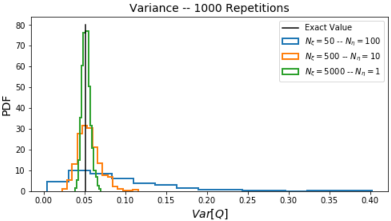
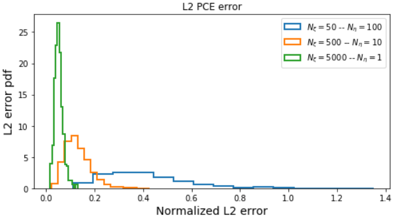
1000 repetitions of the PCE coefficients ($N_\xi = 5000$ and $N_\eta = 1$)
PCE Coeff
Coeff IDs
1000 repetitions of the PCE response ($N_\xi = 5000$ and $N_\eta = 1$)
PCE realizations
Exact
$Q(\xi)$
ξ

CASE 1: Single material section – Statistics

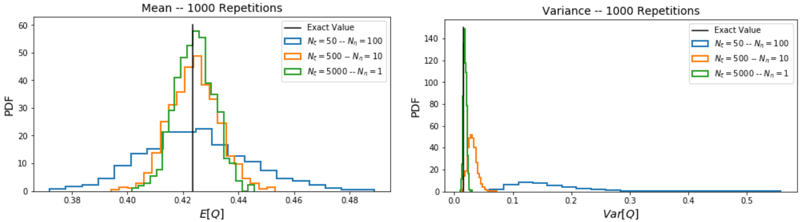






PCE stat	Exp. Value			CoV			Exact Value
N_η	1	10	100	1	10	100	
Mean	4.260E-1	4.257E-1	4.240E-1	1.642E-2	2.766E-2	7.784E-2	4.258E-1
Variance	5.209E-2	5.548E-2	8.396E-2	9.557E-2	2.412E-1	6.538E-1	5.151E-2
L^2 error	5.217E-2	1.293E-01	3.968E-01	3.358E-01	4.052E-1	4.207E-1	–

Table: **1D Radiation transport ($d = 1$): Statistics for the distributions.**



PCE stat N_η	Exp. Value 1	Exp. Value 10	Exp. Value 100	CoV 1	CoV 10	CoV 100	Exact Value
Mean	4.241E-1	4.241E-1	4.242E-1	1.634E-2	2.079E-2	4.497E-2	4.240E-1
Variance	1.832E-2	3.106E-2	1.605E-1	1.426E-1	2.600E-1	4.069E-1	1.546E-2

Table: **1D Radiation transport ($d = 3$): Statistics for the distributions.**

Concluding Remarks

Summary:

- **Hybrid Sampling-PCE methods** are promising thanks to their **scalability**
- Direct sampling (ξ, η) has **provably less variance** than a nested approach
- CIs for PCE coefficients can be propagated to obtain/**estimate surrogate variability**
- **Radiation Transport** is a particular instance of **stochastic solvers** (other examples are cybersecurity, turbulent/combustion flows, subscale modelling etc.)

1 G. Geraci, L.P. Swiler, B.J. Debusschere, *Multifidelity UQ Sampling for Stochastic Simulations*, 16th U.S. National Congress on Computational Mechanics, 2021.

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Work-in-progress

- Law-of-total variance, as derived here, allows for a **variance deconvolution**

2 K.B. Clements, G. Geraci and A.J. Olson, *A Variance deconvolution approach to sampling UQ for Monte Carlo radiation transport solvers*, Computer Science Research Institute Summer Proceedings, 2021. (*in preparation*)

- PCE is amenable for **Global Sensitivity Analysis** and high-order decomposition

3 M. Merritt, G. Geraci, M. Eldred and T. Portone, *Hybrid multilevel Monte Carlo - polynomial chaos method for global sensitivity analysis*, Computer Science Research Institute Summer Proceedings, 2020

4 G. Geraci, P.M. Congedo, R. Abgrall and G. Iaccarino, *High-order statistics in global sensitivity analysis: decomposition and model reduction* Computer Methods in Applied Mechanics and Engineering, 2016

- Extension of the **model cost** w.r.t initialization for each ξ (in coll. with Kayla Clements, OSU)
- Extension to **other sources of uncertainty and additional physics** (in coll. Kayla Clements, OSU)
- Efficient **parallelization on GPUs** (in coll. with Kerry Bossler and Luke Kersting, SNL and Kayla Clements, OSU)

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