National Laboratories

A Polynomial Chaos Approach for Uncertainty Quantification of Monte Carlo Transport Codes

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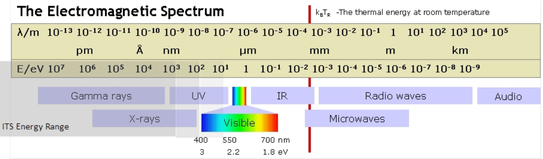
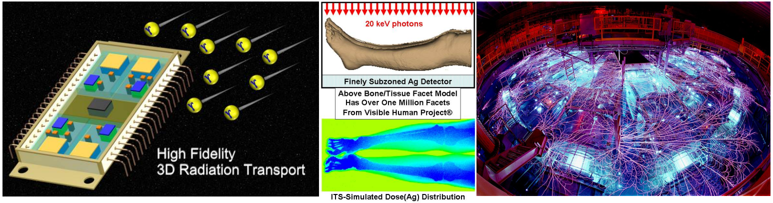
Plan of the talk

- Motivation and Background
- Polynomial Chaos
- Algorithmic Contributions
- Numerical Results
- Summary and Conclusions
- References

Motivation and Background



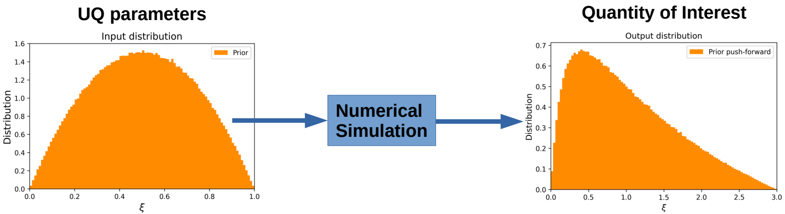
From Opensource Handbook of Nanoscience and Nanotechnology



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

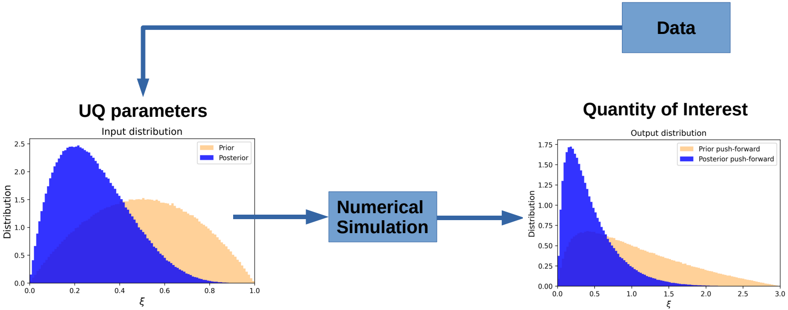


Uncertainty Quantification:

- 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**



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Polynomial Chaos

Polynomial Chaos Expansion
Generalities[1]

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.** $p(\xi)$

Remarks

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

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

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

[1] O. Le Maitre and O. Knio. *Spectral methods for uncertainty quantification. With applications to computational fluid dynamics.* Springer Netherlands, 2010.

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Non-Intrusive Spectral Projection
The case of radiation transport applications

Spectral projection → 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 $\mathbb{E}\left[Q\Psi_k\right]$

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)

$\Downarrow$

Sampling approaches: potentially more suited than quadrature in this context

Sampling Approaches → Monte Carlo

$$\mathbb{E}\left[Q\Psi_k\right] = \int_\Xi Q(\xi)\Psi_k(\xi)\, p(\xi) \mathrm{d}\xi \approx \frac{1}{N_\xi} \sum_{i=1}^{N_\xi} Q(\xi^{(i)})\Psi_k(\xi^{(i)})$$

Q: How do we get the QoI $Q(\xi)$ in a Radiation Transport context?

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Context: NISP via sampling is not new[2], so...
Q: what do we need to know in the **RT context**?
A: The **QoI is not obtained directly**, but as a statistics of elementary events

Assumptions/Notation

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

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

NOTE:

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

In this talk:
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?
Q3: Can this knowledge inform the **PCE construction**?

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

Step 2. Sampling approximations

$$\beta_k = \frac{1}{b_k}\mathbb{E}_\xi\left[\mathbb{E}_\eta\left[f(\xi,\eta)\right]\Psi_k(\xi)\right] = \frac{1}{b_k}\frac{1}{N_\xi}\sum_{i=1}^{N_\xi}\left[\mathbb{E}_\eta\left[f(\xi^{(i)},\eta)\right]\Psi_k(\xi^{(i)})\right] = \boxed{\frac{1}{b_k}\frac{1}{N_\xi}\sum_{i=1}^{N_\xi}\left[\frac{1}{N_\eta}\sum_{j=1}^{N_\eta}f(\xi^{(i)},\eta^{(j)})\Psi_k(\xi^{(i)})\right] \overset{\text{def}}{=} \hat{\beta}_k}$$

NOTE: this estimator is unbiased

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The effect of a limited number of histories

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

Q: Can we separate the effect of the MC RT randomness?

Law-of-total variance (and *variance deconvolution*[3])

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

Finally,

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

NOTES:

- The **true variance** is polluted by the (average) **noise** introduced by limited histories

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NISP for Radiation Transport

Variance of the nested MC-MC estimator[4]

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Algorithmic Contributions

- **UQ studies** require the evaluation of second or **higher powers of the coefficients**
- For instance, to evaluate the **variance**[5]

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

- Through NISP we evaluate

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

Q: Can we use the previous expression for $\hat{\beta}_k$ to evaluate β_k^2?
A: Yes, but **the resulting estimator is biased**

$$\mathbb{V}ar\left[\hat{\beta}_k\right] = \mathbb{E}\left[\left(\hat{\beta}_k\right)^2\right] - \left(\overbrace{\mathbb{E}\left[\hat{\beta}_k\right]}^{Unbiased}\right)^2 \implies \mathbb{E}\left[\left(\hat{\beta}_k\right)^2\right] = \left(\beta_k\right)^2 + \overbrace{\mathbb{V}ar\left[\hat{\beta}_k\right]}^{Estimator\ bias}$$

$$= \mathbb{E}\left[\left(\hat{\beta}_k\right)^2\right] - \left(\beta_k\right)^2$$

[5] or the conditional variances in Global Sensitivity Analysis

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Q: Can we use the previous expression for $\hat{\beta}_k$ to evaluate β_k^2?
A: Yes, but **the resulting estimator is biased**

$$\mathbb{V}ar\left[\hat{\beta}_k\right] = \mathbb{E}\left[\left(\hat{\beta}_k\right)^2\right] - \left(\overbrace{\mathbb{E}\left[\hat{\beta}_k\right]}^{Unbiased}\right)^2 \implies \mathbb{E}\left[\left(\hat{\beta}_k\right)^2\right] = \left(\beta_k\right)^2 + \overbrace{\mathbb{V}ar\left[\hat{\beta}_k\right]}^{Estimator\ bias}$$

$$= \mathbb{E}\left[\left(\hat{\beta}_k\right)^2\right] - \left(\beta_k\right)^2$$

[5] or the conditional variances in Global Sensitivity Analysis

- **UQ studies** require the evaluation of second or **higher powers of the coefficients**
- For instance, to evaluate the **variance**[5]

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

- Through NISP we evaluate

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Estimation of Surrogate Variability

- Two **sources of variability** affect the **PC construction** (in our case)
    1. Randomness introduced by **finite sampling in ξ**, i.e., N_ξ
    2. Randomness introduced by **finite sampling in η**, i.e., MC RT noise given by N_η
- We can quantify **#2** by extending **variance deconvolution** to the variance-covariance matrix of the coefficients' estimators

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$$Q\left(\xi=\bar{\xi}\right) \approx \hat{\beta}_0 + \underline{\Psi}^{\mathrm{T}}(\bar{\xi})\underline{\hat{\beta}}_{N_\eta}$$

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\end{aligned}$$

- We have presented the PC expansion with

$$P + 1 = \frac{(n_0 + d)!}{n_0!\, d!} \quad \text{terms}$$

Q: How do we decide the number of terms to retain?

Solution

1. Evaluate the QoI variance from sampling only (for $N_\eta > 1$), i.e., **variance deconvolution**

$$\mathbb{V}ar\,[Q]^{dec} = \mathbb{V}ar_\xi \left[\tilde{Q}_{N_\eta} \right] - \mathbb{E}_\xi \left[\frac{\sigma_\eta^2}{N_\eta} \right]$$

2. **Re-order PC coefficients** according to their (decreasing) contribution to the variance
3. Select $P_{trim} \leq P$ such that

$$\sum_{k=1}^{P_{trim}} \left[\left(\hat{\beta}_k \right)^2 - \mathbb{V}ar \left[\hat{\beta}_k \right] \right] \leq \mathbb{V}ar\,[Q]^{dec}$$

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Numerical Results

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

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

Analytical solution

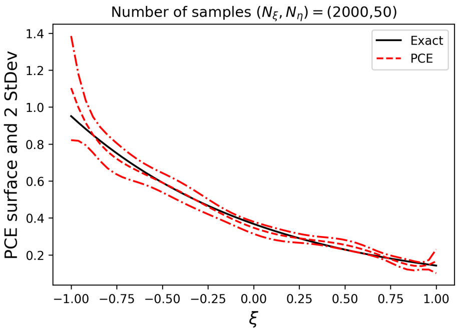
$$T(\xi) = \exp\left[-\sum_{m=1}^{d} \Sigma_{t,m}(\xi_m)\Delta x_m\right] = \exp\left[-\tau(\xi)\right],$$

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

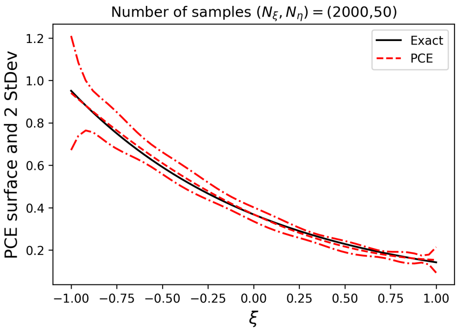
Exact solution (nth raw moment)

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

Radiation transport example
PC variability (and coefficients trim)



(a) PCE W/O Trim (Sample 1)



(b) PCE W/ Trim (Sample 1)

Figure: Two PC repetitions for the 1D attenuation problem (dashed red) with (bottom) and without (top) the expansion trim. Results obtained with $N_\xi = 2000$, $N_\xi = 50$, and $n_0 = 6$. The exact attenuation profile is reported in black.

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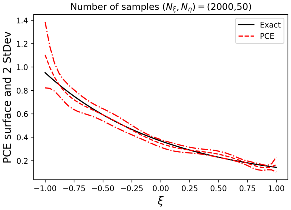

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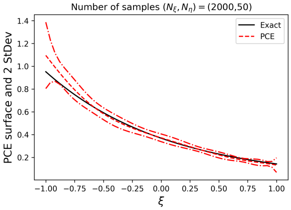
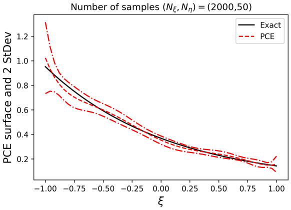
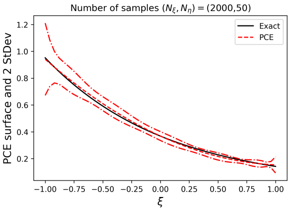


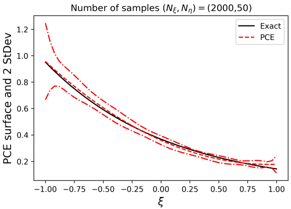
(b) PCE W/O Trim (Sample 2)



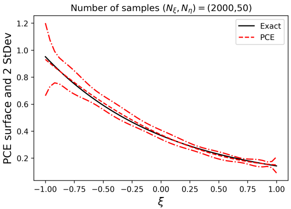
(c) PCE W/O Trim (Sample 3)



(d) PCE W/ Trim (Sample 1)



(e) PCE W/ Trim (Sample 2)



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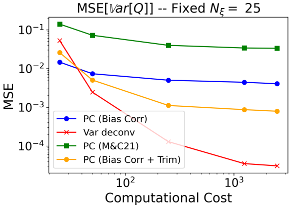
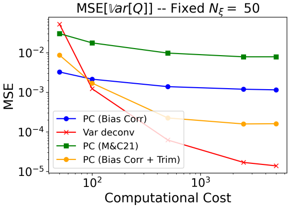
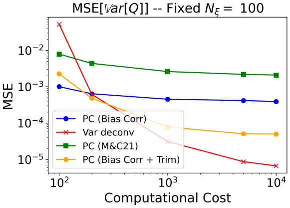


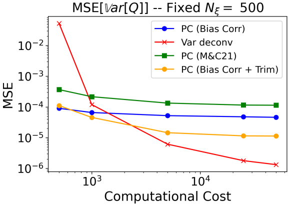
(a) $N_\xi = 25$



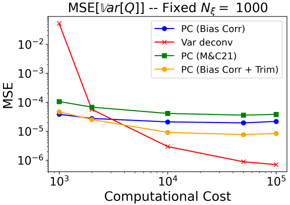
(b) $N_\xi = 50$



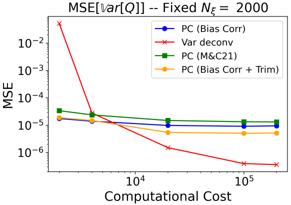
(c) $N_\xi = 100$



(d) $N_\xi = 500$



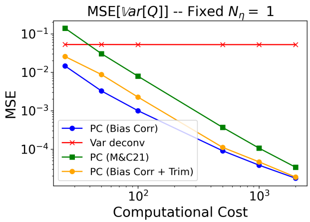
(e) $N_\xi = 1000$



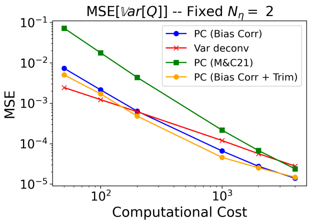
(f) $N_\xi = 2000$

Figure: MSE for the estimated variance obtained with $1\,500$ independent repetitions with an increasing number of UQ samples N_ξ and $N_\eta = [1, 2, 10, 50, 100]$.

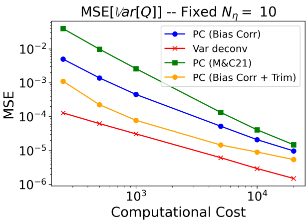
Radiation transport example
QoI variance – increasing N_η



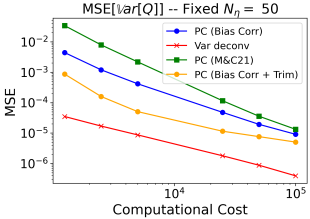
(a) $N_\eta = 1$



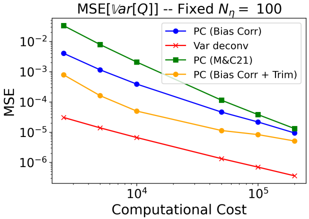
(b) $N_\eta = 2$



(c) $N_\eta = 10$



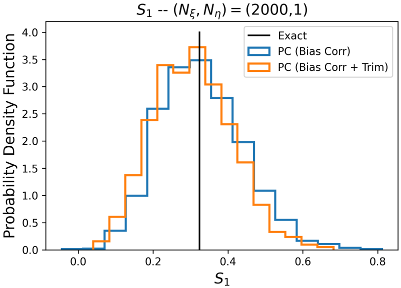
(d) $N_\eta = 50$



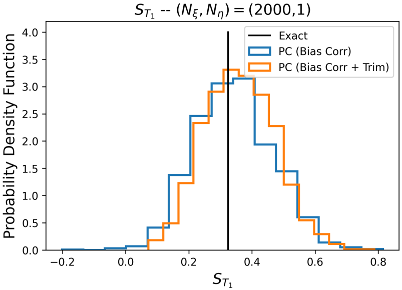
(e) $N_\eta = 100$

Figure: MSE for the estimated variance obtained with $1\,500$ independent repetitions with an increasing number of particles N_η (per UQ sample) and $N_\xi = [25, 50, 100, 500, 1\,000, 2\,000]$.

Radiation transport example
Beyond Moments – Global Sensitivity Analysis



(a) Sensitivity index S_1



(b) Total sensitivity index S_{T_1}

Figure: Sensitivity index S_1 (a) and total sensitivity index S_{T_1} (b) obtained with the PC with bias correction and bias correction and expansion trim.

Summary and Conclusions

Summary

- We explored the **efficient contruction of PC surrogates** for UQ in **radiation transport** applications
- We demonstrated how to **manage the noise contributed by the MC RT** solver in the PC
- Several **algorithmic refinements** improved previous version[6] of the algorithm

Ongoing

- Accounting for the **re-start cost** as

$$\mathcal{C}_{tot} = N_\xi \left(\mathcal{C}_\xi + \mathcal{C}_\eta N_\eta \right)$$

- We have extended the theory to account for it, but this **should be included in the comparisons**

Conclusions

- Managing MC RT noise in PC seems to be both feasible and efficient
- Nevertheless, **additional work is needed to rigorously compare and assess the effectiveness of this tool** with other approaches, e.g., variance deconvolution (see Kayla's talk about GSA)

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THANKS!

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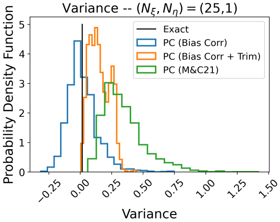
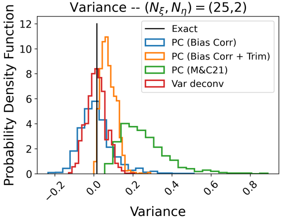
Additional Material

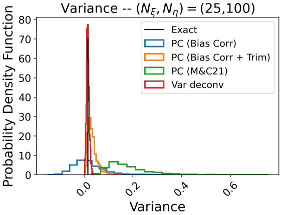
QoI variance – PDFs and Variance Deconvolution



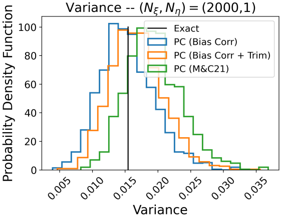
(a) $(N_\xi, N_\eta) = (25, 1)$



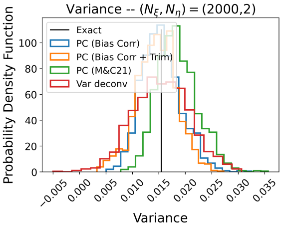
(b) $(N_\xi, N_\eta) = (25, 2)$



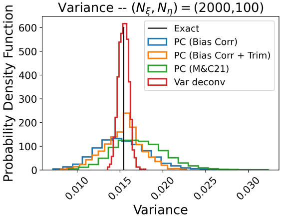
(c) $(N_\xi, N_\eta) = (25, 100)$



(d) $(N_\xi, N_\eta) = (2000, 1)$



(e) $(N_\xi, N_\eta) = (2000, 2)$



(f) $(N_\xi, N_\eta) = (2000, 100)$

Figure: Probability density functions for the estimated variance with PCE and variance deconvolution.