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National Laboratories

Deconvolution strategies for efficient parametric variance estimation in stochastic media transport problems

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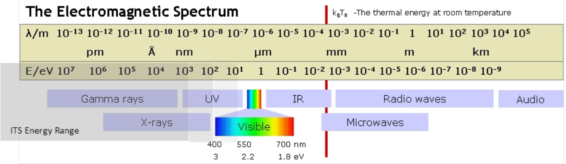

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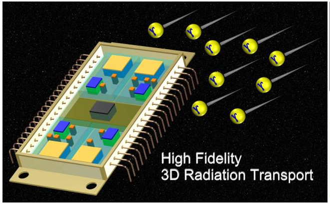
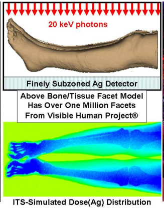
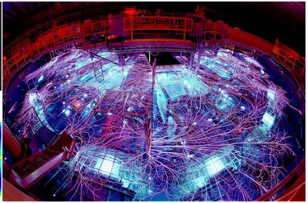






Figures courtesy of Brian Franke and Shawn Pautz

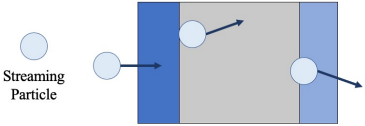
High-fidelity radiation transport modeling and simulation with HPC

- **Severe** simulations **budget constraints**
- **Significant UQ parameter dimensionality** driven by model complexity

Uncertainty Quantification for Monte Carlo Radiation Transport

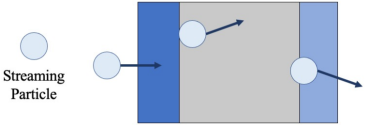
The Challenge of Under-resolved Computations

Input uncertainties ⟶



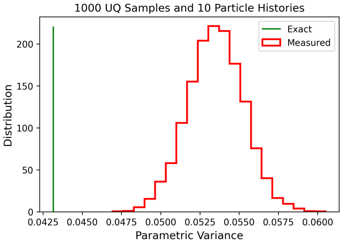
⟶ **Compute statistics**

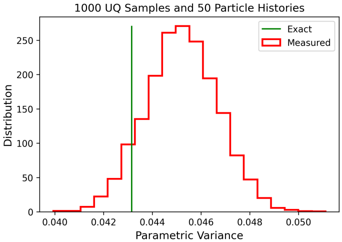
Input uncertainties ⟶

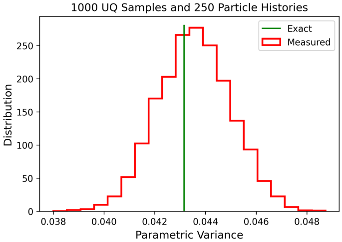


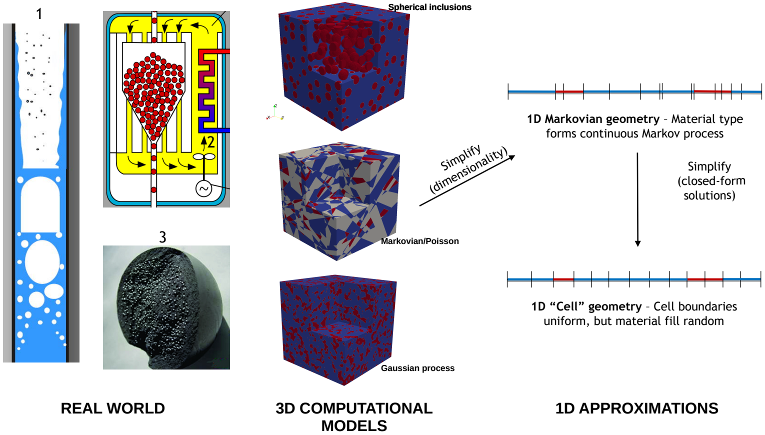
⟶ **Compute statistics**

How much should your MC RT be resolved?









Real-world examples

- Two-phase flow in **Boiling Water Reactor** nuclear power coolant (1)
- **Pebble distribution** in Pebble-Bed nuclear power reactors (2)
- Distribution of **TRISO fuel** particles in Pebble-Bed pebble (3)
- Raleigh-Taylor **instabilities** in Inertial Confinement Fusion reactors
- **Accident scenarios** in various nuclear power reactor cores

Contributions of this talk:

- How can we obtain accurate parametric variance estimations given a **limited** computational budget for **particle histories**?
- How can we extend this to account for **limited stochastic media realizations**?

Bonus point

- Designed a verification test case, *i.e.* closed form solution for necessary statistics

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Plan and Contributions of the Talk
Focus on Variance and Stochastic Media

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Mathematical Framework

What are the sources of variability/uncertainty?

- **Uncertain parameters**, e.g. cross sections: ξ
- **MC RT (internal) randomness**: η
- **Material arrangements/realizations**: ω

What is the mathematical counterpart of a MC RT simulation?

- **Particle histories** can be interpreted as elementary events: $f = f(\xi, \omega, \eta)$
- **MC RT QoI** can be interpreted as an average of f over the histories with fixed UQ parameters and material arrangements

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

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Problem formulation

We focus on statistics over **material arrangements**

$$\mathbb{P}_{\mathbb{E}}(\xi) \stackrel{\text{def}}{=} \mathbb{E}_{\omega}\left[Q(\xi,\omega)\right],$$

while the UQ analysis aims at evaluating the parametric variance, *i.e.* $\mathbb{V}ar_{\xi}\left[\mathbb{P}_{\mathbb{E}}(\xi)\right]$

Brute force approach

$$\mathbb{V}ar_{\xi}\left[\mathbb{P}_{\mathbb{E}}(\xi)\right] \approx \mathbb{V}ar_{\xi}\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_{\omega}}(\xi)\right],$$

where

$$\mathbb{P}_{\mathbb{E}}(\xi) \approx \frac{1}{N_{\omega}}\sum_{k=1}^{N_{\omega}} \tilde{Q}_{N_{\eta}}(\xi,\omega^{(k)}) \stackrel{\text{def}}{=} \tilde{\mathbb{P}}^{\mathbb{E}}_{N_{\omega}}(\xi).$$

Is this correct/efficient?

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Understanding the Variance Contributions

From the law-of-total variance to deconvolution

$$\text{Definitions}\begin{cases}\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}(\xi) \overset{\text{def}}{=} \dfrac{1}{N_\omega}\displaystyle\sum_{k=1}^{N_\omega} \tilde{Q}_{N_\eta}(\xi, \omega^{(k)}), \\ \tilde{Q}_{N_\eta}(\xi, \omega) \overset{\text{def}}{=} \dfrac{1}{N_\eta}\displaystyle\sum_{j=1}^{N_\eta} f\left(\xi, \omega, \eta^{(j)}\right)\end{cases}$$

Let's start by 'decomposing' the **variance contribution** (law-of-total-variance)

$$\mathbb{V}ar\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right] = \mathbb{V}ar_\xi\left[\mathbb{E}_{\eta,\omega}\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right]\right] + \mathbb{E}_\xi\left[\mathbb{V}ar_{\eta,\omega}\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right]\right]$$

- The expected value estimators are all **unbiased**

$$\mathbb{E}_{\eta,\omega}\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right] = \mathbb{E}_{\eta,\omega}\left[\frac{1}{N_\omega}\sum_{k=1}^{N_\omega}\tilde{Q}_{N_\eta}(\xi, \omega^{(k)})\right] = \frac{1}{N_\omega}\sum_{k=1}^{N_\omega}\mathbb{E}_\omega\left[\mathbb{E}_\eta\left[\tilde{Q}_{N_\eta}(\xi, \omega^{(k)})\right]\right] = \frac{1}{N_\omega}\sum_{k=1}^{N_\omega}\mathbb{P}_{\mathbb{E}}(\xi, \omega) = \mathbb{P}_{\mathbb{E}}(\xi, \omega)$$

- **Law-of-total-variance** can be applied **recursively**

$$\mathbb{V}ar_{\eta,\omega}\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right] = \mathbb{V}ar_\omega\left[\mathbb{E}_\eta\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right]\right] + \mathbb{E}_\omega\left[\mathbb{V}ar_\eta\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right]\right] = \ldots = \frac{\mathbb{V}ar_\omega\left[Q(\xi, \omega)\right]}{N_\omega} + \frac{\mathbb{E}_\omega\left[\frac{\sigma^2_\eta(\xi,\omega)}{N_\eta}\right]}{N_\omega},$$

Finally, we get

$$\mathbb{V}ar\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right] = \mathbb{V}ar_\xi\left[\mathbb{P}_{\mathbb{E}}\right] + \mathbb{E}_\xi\left[\frac{\mathbb{V}ar_\omega\left[Q(\xi, \omega)\right]}{N_\omega}\right] + \mathbb{E}_\xi\left[\frac{\mathbb{E}_\omega\left[\frac{\sigma^2_\eta(\xi,\omega)}{N_\eta}\right]}{N_\omega}\right]$$

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Understanding the Variance Contributions
From the law-of-total variance to deconvolution

Definitions
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Understanding the Variance Contributions
Contributions interpretation

What are the sources of variability/uncertainty?

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$$\underbrace{\mathbb{V}ar\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right]}_{\text{Polluted variance}} = \underbrace{\mathbb{V}ar_\xi\left[\mathbb{P}_{\mathbb{E}}\right]}_{\text{Parametric variance}} + \underbrace{\mathbb{E}_\xi\left[\frac{\mathbb{V}ar_\omega\left[Q(\xi,\omega)\right]}{N_\omega}\right]}_{\text{Stochastic media}} + \underbrace{\mathbb{E}_\xi\left[\frac{\mathbb{E}_\omega\left[\frac{\sigma^2_\eta(\xi,\omega)}{N_\eta}\right]}{N_\eta}\right]}_{\text{MC RT}}$$

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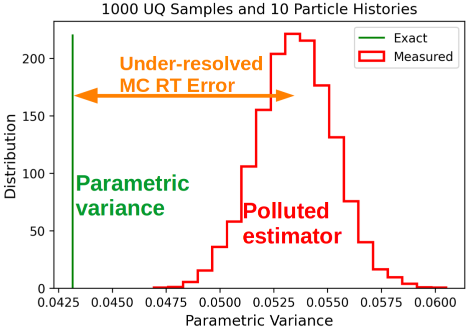

Variance deconvolution recipe:

1 Measure the **polluted variance**

$$\mathbb{V}ar\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right] \rightarrow \tilde{S}^2 = \frac{1}{N_\xi - 1}\sum_{i=1}^{N_\xi}\left(\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}(\xi^{(i)}) - \frac{1}{N_\xi}\sum_{q=1}^{N_\xi}\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}(\xi^{(q)})\right)^2$$

2 Measure the **under-resolved statistics**

$$\mathbb{E}_\xi\left[\frac{\mathbb{V}ar_\omega\left[Q(\xi,\omega)\right]}{N_\omega}\right] + \mathbb{E}_\xi\left[\frac{\mathbb{E}_\omega\left[\sigma^2_\eta(\xi,\omega)\right]}{N_\omega N_\eta}\right]$$

$$\rightarrow \Delta S^2 = \frac{1}{N_\omega N_\xi}\sum_{i=1}^{N_\xi}\left[\frac{1}{N_\omega}\sum_{k=1}^{N_\omega}\left(\tilde{Q}_{N_\eta}(\xi^{(i)},\omega^{(k)}) - \frac{1}{N_\omega}\sum_{q=1}^{N_\omega}\tilde{Q}_{N_\eta}(\xi^{(i)},\omega^{(q)})\right)^2\right]$$

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$$\mathbb{V}ar_\xi\left[\mathbb{P}_{\mathbb{E}}\right] \rightarrow S^2 = \tilde{S}^2 - \Delta S^2$$

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3. Get the **parametric variance** by difference

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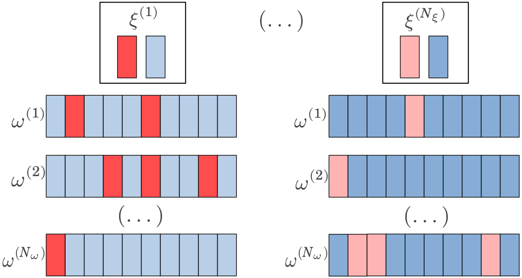
Numerical Results



Material	$\Sigma^0_{t,m}$ [cm^{-1}]	$\Sigma^\Delta_{t,m}$ [cm^{-1}]	p_m
A	1.0	0.95	0.05
B	0.4	0.25	0.95

Table: Uncertain cross sections properties

- 1D slab, neutral particle, **absorption-only** mono-energetic steady state radiation transport
- Normally incident beam with unitary magnitude
- **Random cross sections** $(m = A, B)$: $\Sigma_{t,m}(\xi_m) = \Sigma^0_{t,m} + \Sigma^\Delta_{t,m}\xi_m$, where $\xi_A, \xi_B \sim \mathcal{U}(-1, 1)$
- Total number of **material sections**: $N_{tot} = 10$ (with $\Delta x = 0.15$ cm)
- The **QoI** is the **transmittance**

Transmittance: $T(\xi,\omega) = \exp\left[-\tau(\xi,\omega)\right]$, where

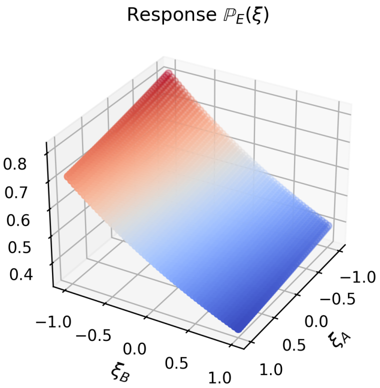
Slab optical thickness: $\tau(\xi,\omega) = \Delta x\left(N_A(\omega)\Sigma_{t,A}(\xi_A) + N_B(\omega)\Sigma_{t,B}(\xi_B)\right)$

Material distribution: $N_A(\omega) \sim \mathcal{B}(N_{tot}, P_A)$, where $N_A(\omega) + N_B(\omega) = N_{tot}$

$$\mathbb{P}_{\mathbb{E}}(\xi) = \mathbb{E}_\omega\left[T(\xi,\omega)\right]$$

$$= \exp\left[-N_{tot}\Delta x \Sigma_{t,B}(\xi_B)\right]\sum_{x=0}^{N_{tot}} B_\omega(x)\exp\left[-x\Delta x(\Sigma^{\Delta}_{t,A}\xi_A - \Sigma^{\Delta}_{t,B}\xi_B)\right]$$

$$B_\omega(x) \stackrel{\text{def}}{=} \frac{N_{tot}!}{x!\,(N_{tot}-x)!}p_A^x\,(1-p_A)^{(N_{tot}-x)}\exp\left[-2x\Delta x(\Sigma^0_{t,A} - \Sigma^0_{t,B})\right]$$



$$\mathbb{V}ar_{\xi}\left[\mathbb{P}_{\mathbb{E}}\right] = \mathbb{E}_{\xi}\left[\mathbb{P}_{\mathbb{E}}(\xi)^2\right] - \left(\mathbb{E}_{\xi}\left[\mathbb{P}_{\mathbb{E}}(\xi)\right]\right)^2$$

where

$$\mathbb{E}_{\xi}\left[\mathbb{P}_{\mathbb{E}}(\xi)\right] = \exp\left[-N_{tot}\Delta x \Sigma_{t,B}^{0}\right]\left(\sum_{x=0}^{N_{tot}} B_{\omega}(x)(x)\frac{\sinh\left[x\Delta x\Sigma_{t,A}^{\Delta}\right]}{x\Delta x\Sigma_{t,A}^{\Delta}}\frac{\sinh\left[N_{tot}\Delta x\Sigma_{t,B}^{\Delta}\left(1-\frac{x}{N_{tot}}\right)\Delta x\Sigma_{t,A}^{\Delta}\right]}{N_{tot}\Delta x\Sigma_{t,B}^{\Delta}\left(1-\frac{x}{N_{tot}}\right)\Delta x\Sigma_{t,A}^{\Delta}}\right),$$

and

$$\mathbb{E}_{\xi}\left[\mathbb{P}_{\mathbb{E}}(\xi)^2\right] = \exp\left[-2N_{tot}\Delta x \Sigma_{t,B}^{0}\right]\left(\sum_{x=0}^{N_{tot}} B_{\omega}(x)^2\frac{\sinh\left[2x\Delta x\Sigma_{t,A}^{\Delta}\right]}{2x\Delta x\Sigma_{t,A}^{\Delta}}\frac{\sinh\left[2N_{tot}\Delta x\Sigma_{t,B}^{\Delta}\left(1-\frac{x}{N_{tot}}\right)\right]}{2N_{tot}\Delta x\Sigma_{t,B}^{\Delta}\left(1-\frac{x}{N_{tot}}\right)}\right.$$
$$\left.+2\sum_{x=0}^{N_{tot}}\sum_{y=x+1}^{N_{tot}} B_{\omega}(x)B_{\omega}(y)\frac{\sinh\left[(x+y)\Delta x\Sigma_{t,A}^{\Delta}\right]}{(x+y)\Delta x\Sigma_{t,A}^{\Delta}}\frac{\sinh\left[2N_{tot}\Delta x\Sigma_{t,B}^{\Delta}\left(1-\frac{x+y}{2N_{tot}}\right)\right]}{2N_{tot}\Delta x\Sigma_{t,B}^{\Delta}\left(1-\frac{x+y}{2N_{tot}}\right)}\right)$$

Radiation transport

1D transport in stochastic media with uncertain properties

N_η	N_ω	$\mathcal{C}$	MSE(S^2)	MSE($\tilde{S}^2$)	Diff. [%]
2	2	400	1.7313e-4	3.6084e-3	95.20
	4	800	4.0763e-5	9.1886e-4	95.56
	8	1600	1.3829e-5	2.3302e-4	94.06
	16	3200	6.3738e-6	6.0617e-5	89.48
	32	6400	3.6007e-6	1.7405e-5	79.31
4	2	800	5.1799e-5	9.4397e-4	94.51
	4	1600	1.4986e-5	2.4136e-4	93.79
	8	3200	6.6362e-6	6.3906e-5	89.61
	16	6400	3.7136e-6	1.7990e-5	79.35
	32	12800	2.5651e-6	5.9639e-6	56.99
8	2	1600	1.9071e-5	2.5549e-4	92.53
	4	3200	7.0521e-6	6.6686e-5	89.42
	8	6400	3.8521e-6	1.9329e-5	80.07
	16	12800	2.5911e-6	6.2441e-6	58.50
	32	25600	2.1348e-6	3.0310e-6	29.57

N_η	N_ω	$\mathcal{C}$	MSE(S^2)	MSE($\tilde{S}^2$)	Diff. [%]
16	2	3200	8.2811e-6	7.4708e-5	88.91
	4	6400	3.9833e-6	2.0705e-5	80.76
	8	12800	2.6616e-6	6.7252e-6	60.42
	16	25600	2.1034e-6	3.0990e-6	32.12
	32	51200	1.8296e-6	2.0513e-6	10.81
32	2	6400	4.7911e-6	2.5362e-5	81.11
	4	12800	2.8784e-6	8.0892e-6	64.42
	8	25600	2.0873e-6	3.3810e-6	38.26
	16	51200	1.8619e-6	2.1960e-6	15.21
	32	102400	1.7596e-6	1.8532e-6	5.05

Table: MSE (based on $5,000$ repetitions) for the parametric variance estimator, with (S^2) and without ($\tilde{S}^2$) deconvolution, $N_\xi = 100$ UQ samples and several choices of random material realizations N_ω and particle histories N_η. The total cost for each estimator is $\mathcal{C} = N_\xi \times N_\omega \times N_\eta$.

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- For fixed N_ξ and N_η, **MSE decreases** if N_ω increases

N_η	N_ω	$\mathcal{C}$	MSE(S^2)	MSE($\tilde{S}^2$)	Diff. [%]
	2	400	1.7313e-4	3.6084e-3	95.20
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- For a given cost $\mathcal{C} = N_\xi \times N_\eta \times N_\omega$, **MSE increases** if N_η increases

N_η	N_ω	$\mathcal{C}$	MSE(S^2)	MSE($\tilde{S}^2$)	Diff. [%]
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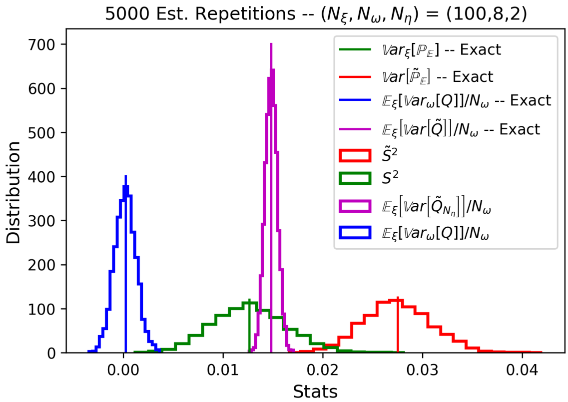
- The difference between S^2 and S **decreases** if $\mathcal{C} = N_\xi \times N_\omega \times N_\eta$ increases



$$\mathbb{V}ar\left[\tilde{\mathbb{P}}^{\mathbb{E}}_{N_\omega}\right] = \mathbb{V}ar_\xi\left[\mathbb{P}_\mathbb{E}\right] + \underbrace{\mathbb{E}_\xi\left[\frac{\mathbb{V}ar_\omega\left[Q(\xi,\omega)\right]}{N_\omega}\right] + \mathbb{E}_\xi\left[\frac{\mathbb{E}_\omega\left[\frac{\sigma_\eta^2(\xi,\omega)}{N_\eta}\right]}{N_\omega}\right]}_{\frac{\mathbb{E}_\xi\left[\mathbb{V}ar\left[\tilde{Q}_{N_\eta}(\xi,\omega)\right]\right]}{N_\omega}}$$

Closing remarks

Conclusions

- Uncertainty Quantification for MC RT requires a characterization of **all sources of variability**
- In the presence of stochastic media **removing the MC RT variability is unattainable**
- The use of the **law-of-total-variance** provides a rigorous approach for efficient and accurate statistics evaluation with under-resolved MC RT computations $\rightarrow$ *variance deconvolution*

Future work

- Extension to **higher-order moments** over the stochastic media realizations, *i.e.* $\mathbb{V}ar_{\omega}[T]$
- **Optimal sample allocation** strategies can be built (*in principle*) from pilot computations
- **Multifidelity** sampling approaches can be built from/for this framework[1]
- Recursive use of variance deconvolution can allow for **statistics beyond variance**, *e.g.* conditional variances (Sobol' indices)

Link with other contributions at ANS

- *Numerical Investigation on the Performance of a Variance Deconvolution Estimator*,
  Presented by: Kayla Clements – Tomorrow in the Uncertainty Quantification and Machine Learning session

[1] G. Geraci and A. J. Olson. "Exploration of Multifidelity UQ Methods for Monte Carlo Radiation Applications in Stochastic Media". In: *SIAM Conference on Uncertainty Quantification (SIAM22)*. 2022.

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References

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