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Sandia National Laboratories

Numerical Investigation on the Performance of a Variance Deconvolution Estimator

Oregon State University

CEMENT

Kayla Clements, Gianluca Geraci, Aaron Olson

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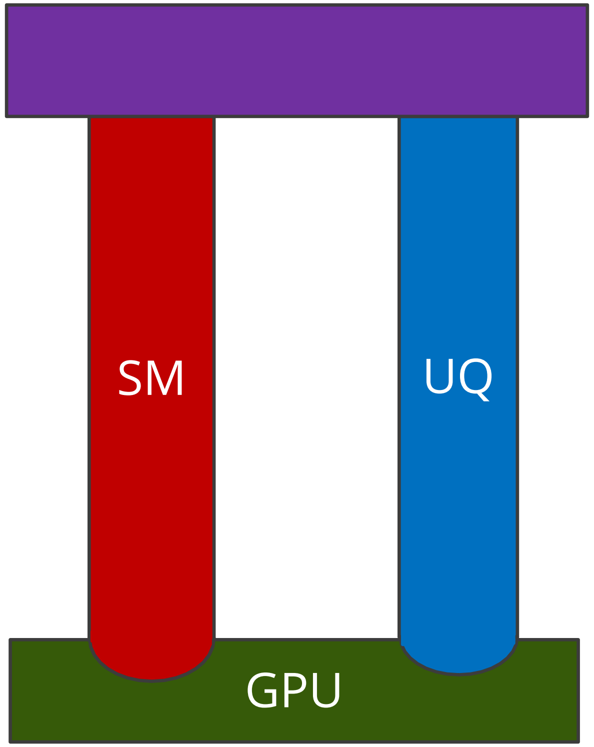
Motivation – Next-Generation Monte Carlo Project

Develop efficient, embedded stochastic media (SM) and uncertainty quantification (UQ) Monte Carlo transport methods for the GPU.

SM in Embeddable UQ methods:

- Notation, expressions, adaptations
- Multi-fidelity acceleration



Embeddable UQ Goals:

- Variance deconvolution
- NISP approach to PCE
- Sampling-based GSA method

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Background – Uncertainty Quantification

- Quantity of interest (QoI): $Q(\xi)$
- p^{th} moment equation
  - $\mathbb{E}\left[Q^p\right] = \frac{1}{N}\sum_{i=1}^{N} Q_i^p$
  - $\mathbb{V}ar[Q] = \mathbb{E}[Q^2] - \mathbb{E}[Q]^2$
- Sampling UQ algorithm:
  1. Sample UQ parameter ξ
  2. Solve for QoI $Q(\xi)$ with existing solver
  3. Repeat for a number of UQ samples
  4. Evaluate statistics, e.g. $\mathbb{E}\left[Q\right]$ and $\mathbb{V}ar[Q]$, over UQ space

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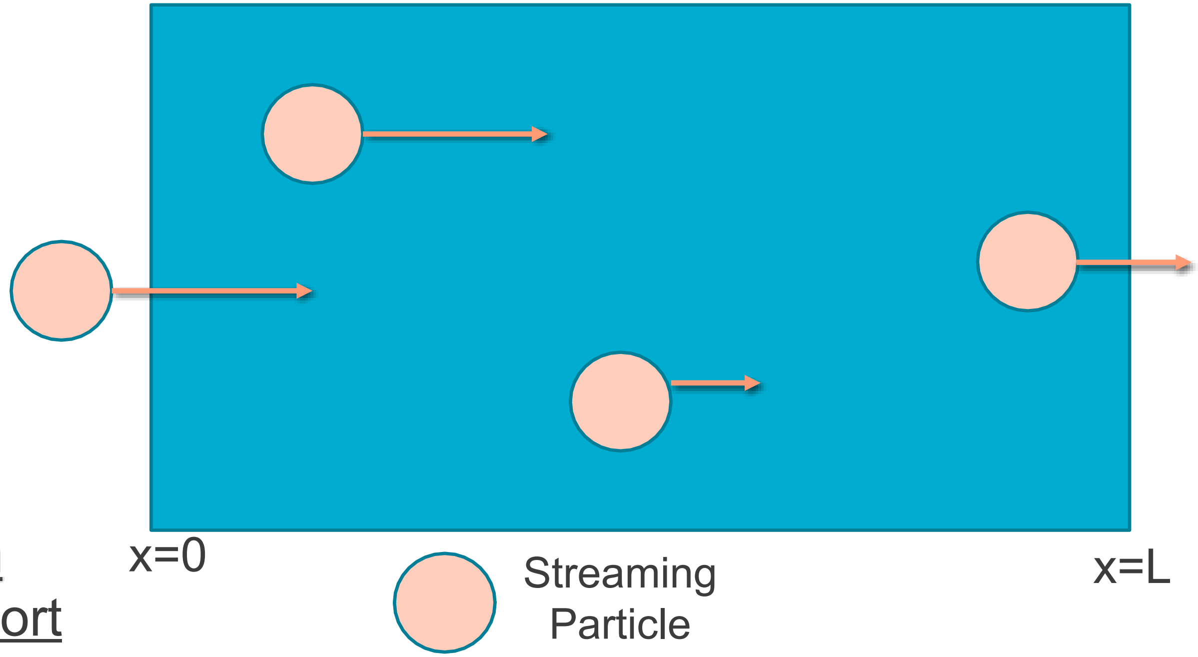
Background – Monte Carlo Particle Transport

$$\mu \frac{\partial \psi(x,\mu)}{\partial x} + \Sigma_t(x)\psi(x,\mu) = 0$$

$$0 \leq x \leq L, \quad -1 \leq \mu \leq 1$$

$$\psi(0,\mu) = 1, \mu \geq 0, \qquad \psi(L,\mu) = 0, \mu > 0$$

$$\Sigma_t(\xi) = \Sigma_t + \Delta\Sigma_t * \xi, \quad \xi \sim U(-1,1)$$



UQ Sampling Algorithm

1. Sample UQ parameter ξ
2. For each $Q(\xi)$:
3. Repeat for number of UQ samples
4. Perform UQ analysis

Monte Carlo Transport

1. Initialize particle
2. Sample distance to next collision
3. Stream particle – boundary? collision?
4. Continue until particle is either absorbed or exits system
5. Start again with a new particle until all particles have finished
6. Repeat for all histories, then average quantities of interest

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Theory – Estimator Statistics

- Uncertain parameter Σ_t

$$\Sigma_t(\xi) = \Sigma_t + \Delta\Sigma_t * \xi,\ \xi \sim U(-1,1)$$

- Parameter uncertainty ξ and Monte Carlo solver uncertainty η

$$f = f(\xi, \eta)$$

$$T(\xi_i) = \mathbb{E}_\eta[f(\xi_i, \eta)] = \frac{1}{N}\sum_{j=1}^{N} f(\xi_i, \eta_j) \approx \frac{1}{N_\eta}\sum_{j=1}^{N_\eta} f(\xi_i, \eta_j) = \tilde{T}(\xi_i)$$

- Average code response

$$\mathrm{E}_\xi[T] = \frac{1}{N}\sum_{i=1}^{N} T_i \approx \frac{1}{N_\xi}\sum_{i=1}^{N_\xi} \tilde{T}(\xi_i)$$

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Theory – Variance Deconvolution I

- Goal: $\mathbb{V}ar[T(\xi)]$

$$= \mathbb{V}ar_\xi[T(\xi,\eta)] \approx \mathbb{V}ar_\xi[\tilde{T}(\xi,\eta)]$$

- Law of total variance

$$\mathbb{V}ar_Y[Z(X,Y)] = \mathbb{V}ar_Y[\mathbb{E}_X[Z]] + \mathbb{E}_Y[\mathbb{V}ar_X[Z]]$$

- Applied to solver response

$$\mathbb{V}ar[\tilde{T}(\xi,\eta)] = \mathbb{V}ar_\xi\left[\mathbb{E}_\eta[\tilde{T}(\xi,\eta)]\right] + \mathbb{E}_\xi\left[\mathbb{V}ar_\eta[\tilde{T}(\xi,\eta)]\right]$$

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Theory – Variance Deconvolution II

$$\mathbb{V}ar[\tilde{T}(\xi,\eta)] = \mathbb{V}ar_{\xi}\left[\mathbb{E}_{\eta}[\tilde{T}(\xi,\eta)]\right] + \mathbb{E}_{\xi}\left[\mathbb{V}ar_{\eta}[\tilde{T}(\xi,\eta)]\right]$$

$$\mathbb{V}ar[\tilde{T}(\xi,\eta)] = \mathbb{V}ar_{\xi}[T] + \frac{1}{N_{\eta}}\mathbb{E}_{\xi}[\sigma_{\eta}^{2}]$$

$$\mathbb{V}ar_{\xi}[T] = \mathbb{V}ar[\tilde{T}(\xi,\eta)] - \frac{1}{N_{\eta}}\mathbb{E}_{\xi}[\sigma_{\eta}^{2}]$$

Parametric variance

Total (polluted) variance

Average Monte Carlo solver variance

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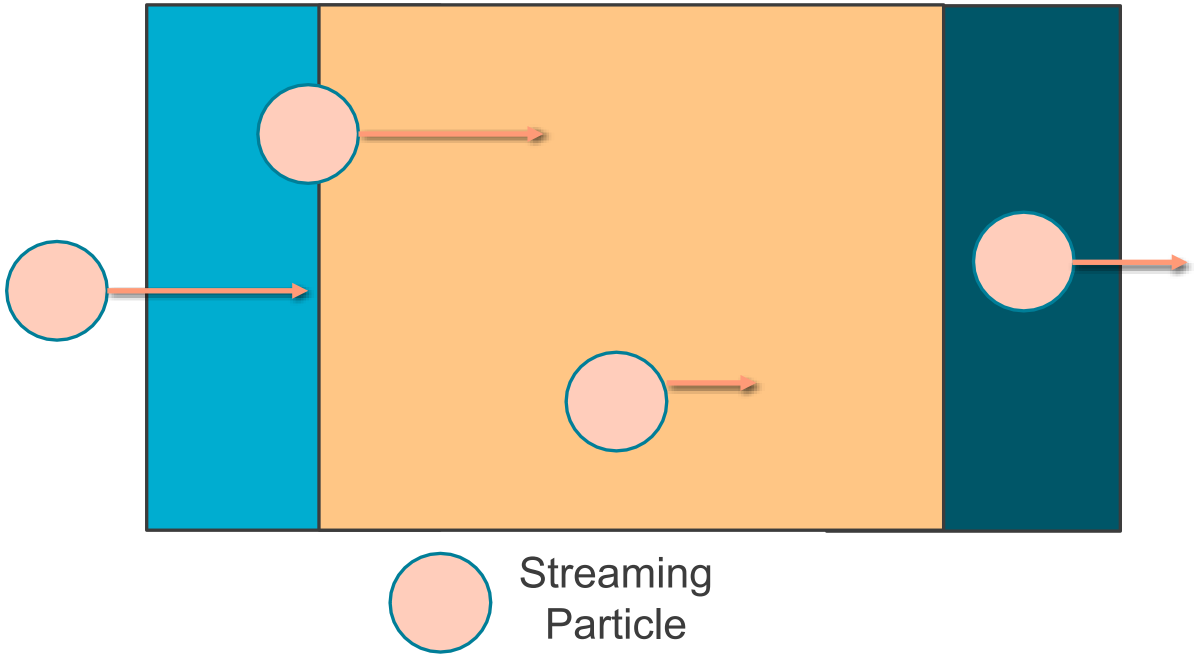
Example – Problem Description

$$\mu \frac{\partial \psi(x,\mu,\xi)}{\partial x} + \Sigma_t(x,\xi)\psi(x,\mu,\xi) = 0$$

$$0 \leq \quad \leq \quad , \qquad -1 \leq \quad \leq 1$$

$$\psi(0,\mu) = 1, \mu \geq 0, \qquad \psi(L,\mu) = 0, \mu > 0$$



$$\Sigma_t(\xi) = \bar{\Sigma}_t + \Delta\Sigma_t * \xi, \qquad \xi \sim U(-1,1)$$

$$c = \Sigma_s/\Sigma_t(\xi) = \bar{c} + \Delta c * \xi, \qquad \xi \sim U(-1,1)$$

Problem Parameters				Scattering Parameters	
	x_R	$\Sigma^0_{t,m}$	$\Sigma^\Delta_{t,m}$	$c^0_{s,m}$	$c^\Delta_{s,m}$
m = 1	2.0	0.90	0.70	0.50	0.40
m = 2	5.0	0.15	0.12	0.50	0.40
m = 3	6.0	0.60	0.50	0.50	0.40

Table I: 1D attenuation problem parameters.

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Example – Solver Algorithm

1. Determine number of realizations N_ξ and number of histories N_η
2. For *i* = 1:N_ξ
   a) Sample ξ and calculate $\Sigma_t(\xi_i)$
   b) For *j* = 1: N_η
      - Run simulation to compute $f(\xi_i, \eta_j)$
   c) Calculate $\tilde{T}(\xi_i) = \frac{1}{N_\eta}\sum_{j=1}^{N_\eta} f(\xi_i, \eta_j)$
   d) Calculate $\sigma_\eta^2(\xi^{(i)}) \approx \frac{1}{N_\eta - 1}\sum_{j=1}^{N_\eta}\left(f(\xi^{(i)}, \eta^{(j)}) - \frac{1}{N_\eta}\sum_{s=1}^{N_\eta}\tilde{f}(\xi^{(i)}, \eta^{(s)})\right)^2$
3. Calculate average of stochastic noise over the whole parameter space: $\mathbb{E}\left[\sigma_\eta^2\right] \approx \frac{1}{N_\xi}\sum_{i=1}^{N_\xi}\sigma_\eta^2(\xi^{(i)})$
4. Calculate sample variance of solutions from Monte Carlo simulations over parameter space:

$$\mathbb{V}ar_\xi[\tilde{T}(\xi, \eta)] \approx \frac{1}{N_\xi - 1}\sum_{j=1}^{N_\xi}\left(\tilde{T}(\xi_i) - \tilde{T}_{avg}\right)^2$$

5. Solve for the true variance over the parameter space by removing the average stochastic MC noise from the measured solution variance:

$$\mathbb{V}ar_\xi[T] = \mathbb{V}ar[\tilde{T}(\xi, \eta)] - \frac{1}{N_\eta}\mathbb{E}_\xi[\sigma_\eta^2]$$

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Results – Attenuation Only

Sampling estimator: $S_T^2 \approx \mathbb{V}ar_{\xi}[T]$			
	Benchmark	Deconvolved	Analytic
$\mathbb{E}[T]$	8.915E-2	8.870E-2	8.378E-2
S_T^2	5.789E-3	5.768E-3	5.505E-3

Table II. Mean QoI and parametric variance.

- Benchmark: $N_\eta = 10^5, N_\xi = 10^3$ $(C = 10^8)$
- Variance deconvolution: $N_\eta = 10^1, N_\xi = 10^3$ $(C = 10^4)$

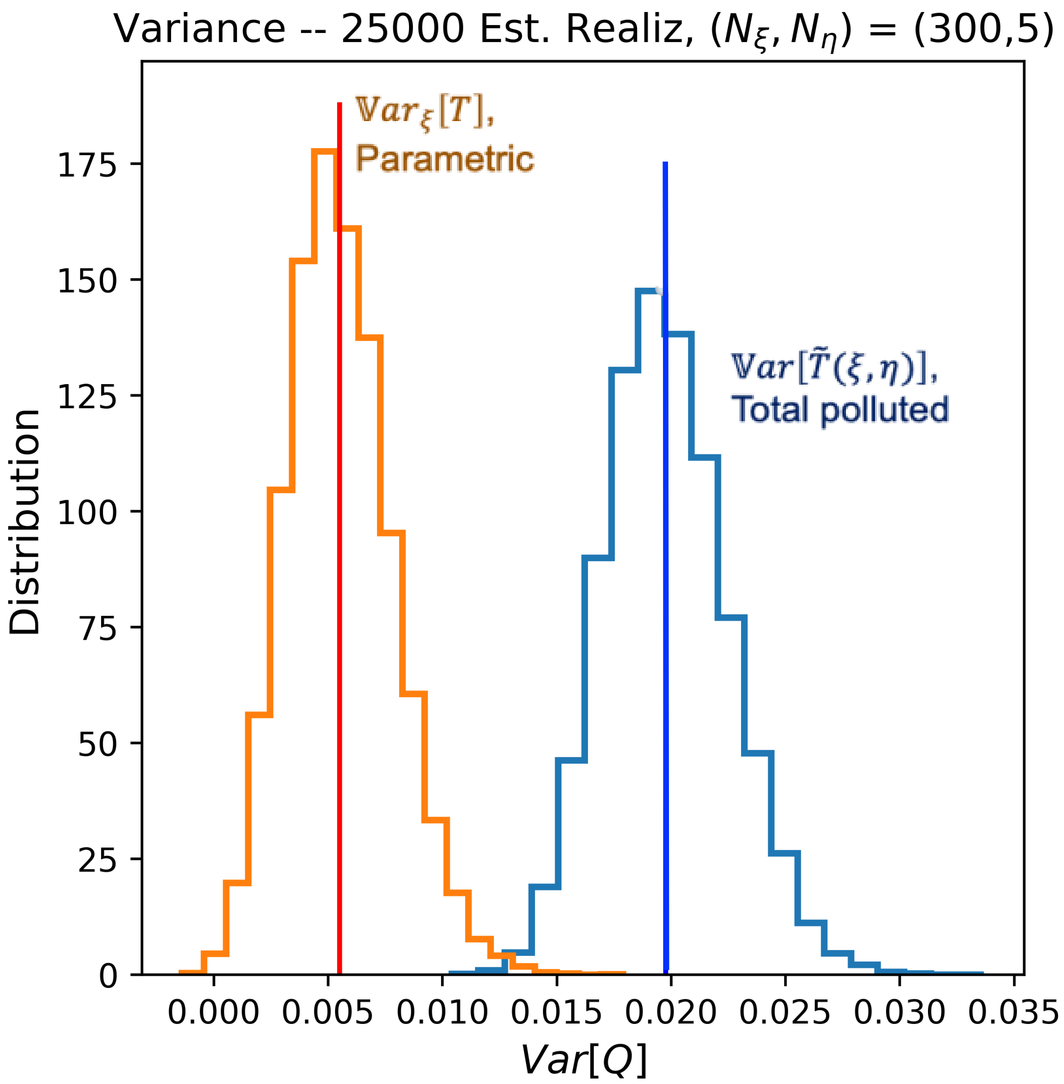

Figure I: 1D radiation transport problem (m=3). 25,000 variance deconvolution repetitions.

Results – Transmittance vs. Reflectance

$N_\xi \times N_\eta = 2000$

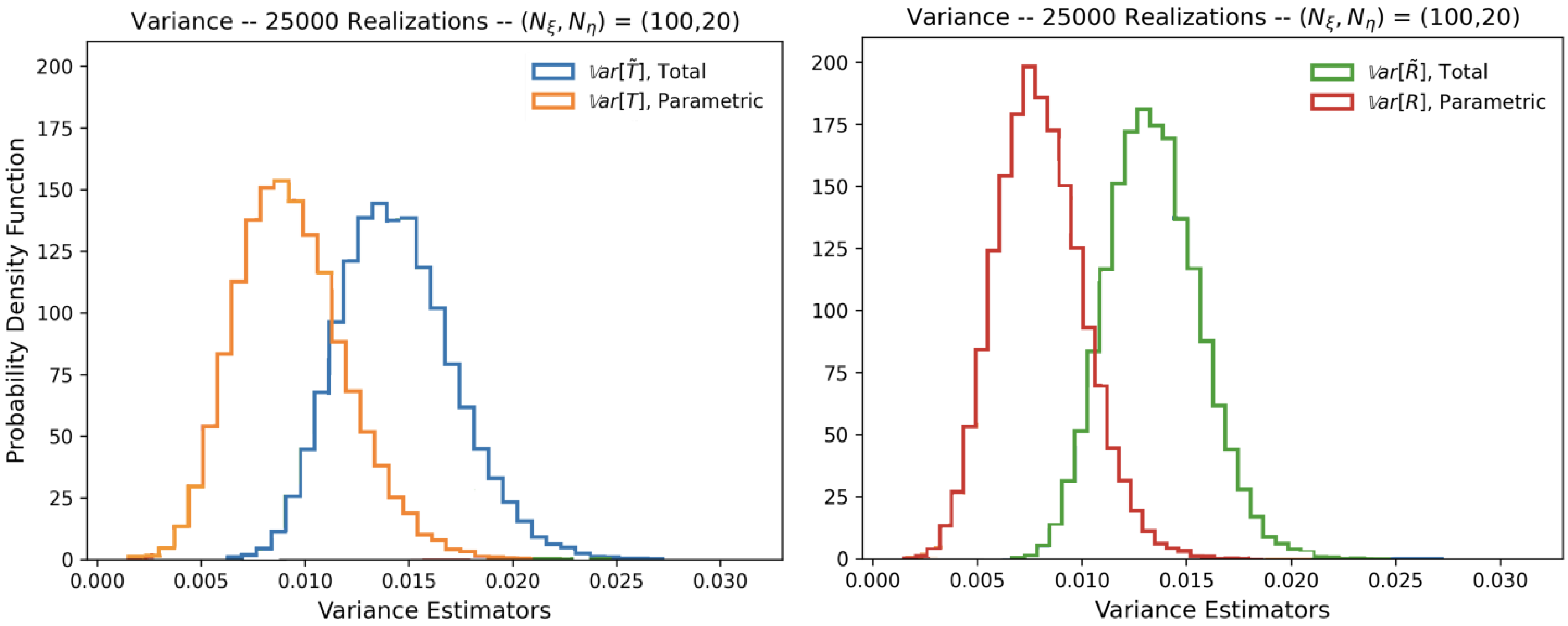

Figure II: Variance deconvolution results for transmittance (left) and reflectance (right) in a problem with scattering.

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Numerical Study

- Sampling estimator $S^2 \approx \mathbb{V}ar_{\xi}[T]$ is unbiased
- Total estimator cost $\mathrm{C} = N_{\xi} \times N_{\eta}$
- Goal: accurate estimate of S^2

For given cost, find N_{ξ} and N_{η} that minimize $\mathbb{V}ar[S^2]$

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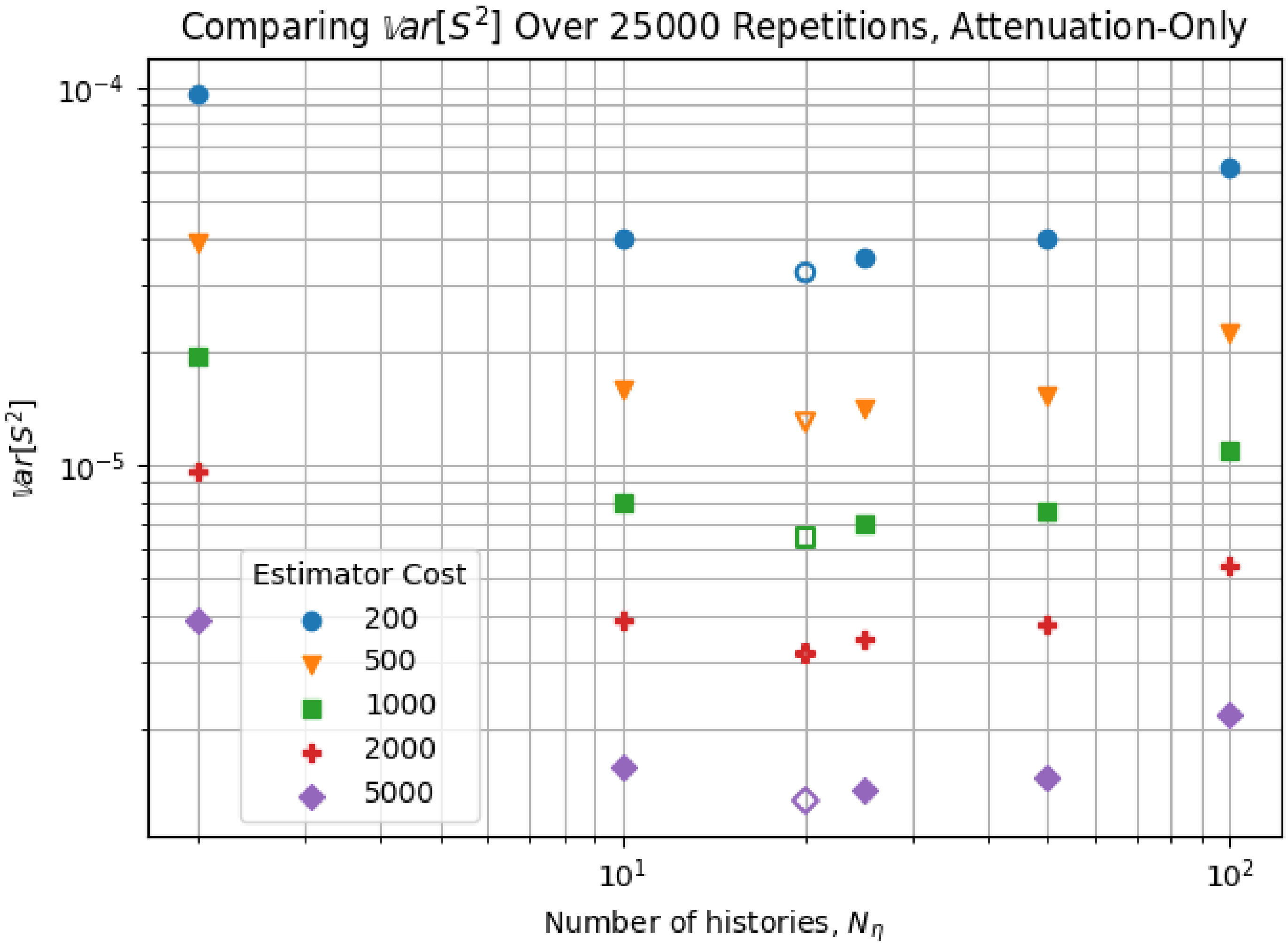
Numerical Study Results – Attenuation Only



Total estimator cost

$C = N_\xi \times N_\eta$

Figure III. $\mathbb{V}ar[S^2]$ as a function of N_η for a variety of total estimator costs, log-log plot. Unfilled point is minimum $\mathbb{V}ar[S^2]$.

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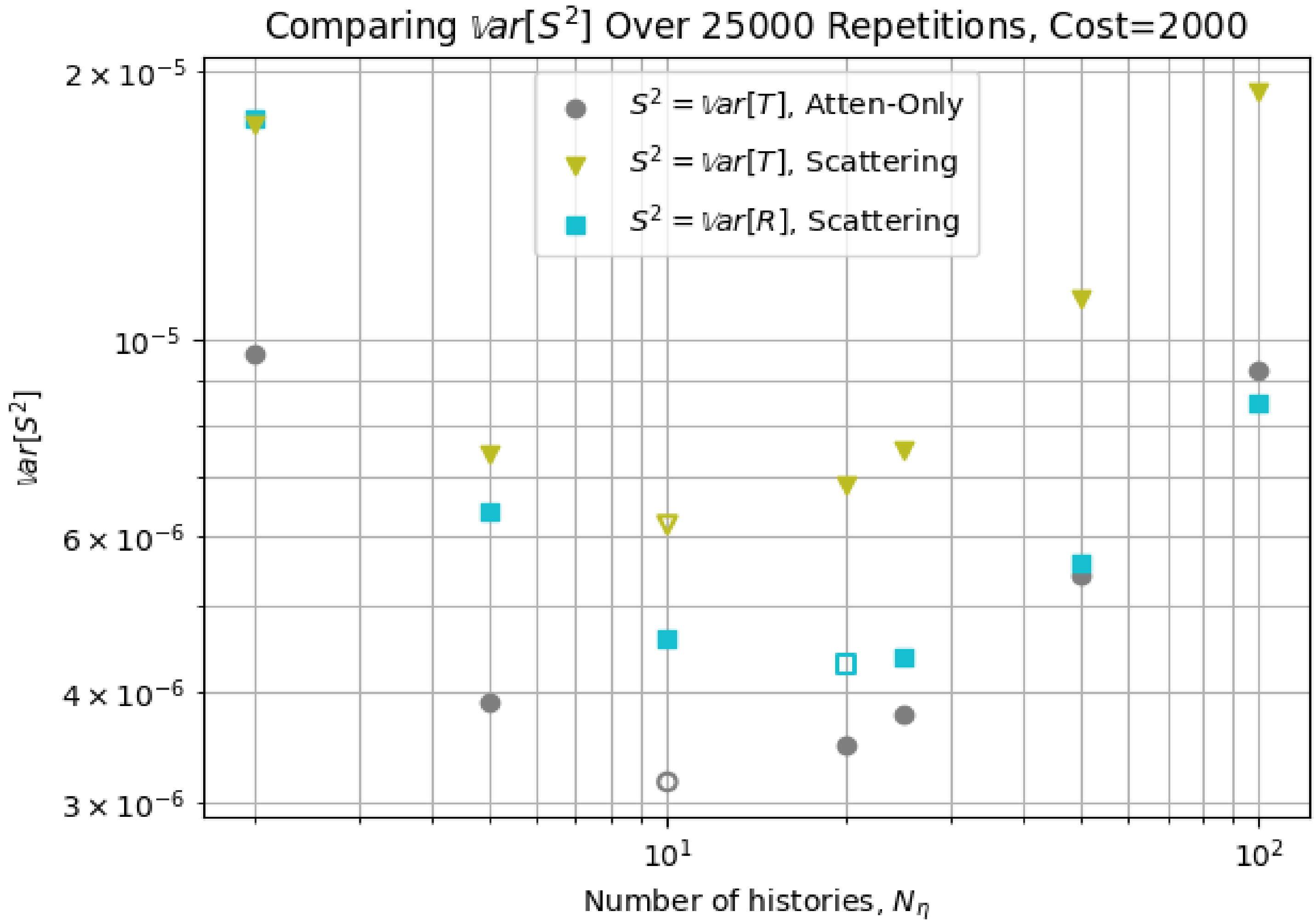
Numerical Study Results – Transmittance vs. Reflectance



Total estimator cost
$C = N_\xi \times N_\eta = 2000$

Figure IV. $\mathbb{V}ar[S^2]$ as a function of N_η for the attenuation-only and scattering cases. Log-log plot, estimator cost $N_\xi \times N_\eta = 2000$. Unfilled point is minimum $\mathbb{V}ar[S^2]$.

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Conclusions and Future Goals

- "De-polluted" total variance by removing contribution from Monte Carlo transport solver
- Performed a numerical campaign to understand the estimator variance trade off between particle histories N_η and UQ samples N_ξ
- Found that $\mathbb{V}ar[S^2]$ is minimized at different locations for different QoIs, even within one problem

Future/Related work:

- Use variance deconvolution to efficiently compute Sobol Indices for Monte Carlo solvers
- Working towards closed-form solution to allow estimation of a cost distribution that minimizes $\mathbb{V}ar[S^2]$ that takes re-sampling cost into account
- Related work – G. Geraci and A.J. Olson, "Deconvolution strategies for efficient parametric variance estimation in stochastic media transport problems," Transport Methods Technical Session

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Questions?

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