SAND2022-4352C

A Variance Deconvolution Approach to Uncertainty Quantification for Monte Carlo Radiation Transport

Kayla Clements[1,2], Gianluca Geraci[2], Aaron Olson[2]
[1]School of Nuclear Science and Engineering, Oregon State University, clemekay@oregonstate.edu
[2]Sandia National Laboratories, Albuquerque, NM

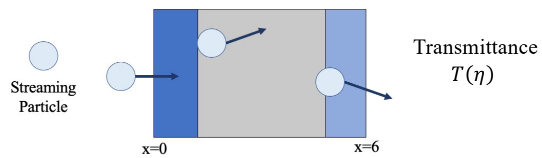
Overview

- Monte Carlo methods used to solve radiation transport problems introduce additional variability that pollutes the variance computed with typical UQ methods.
- We developed an estimator that uses variance deconvolution to remove that additional variability.
- We studied the estimator performance on two representative example problems over different numbers of samples and particle histories.

Introduction

Monte Carlo Methods for Radiation Transport

Cross section – material property that governs interaction probability



To calculate transmittance:

1. Use nuclear data to sample distance to collision event
2. Sample collision events based on cross-section values
3. Track particle until it leaves the system
4. Average behavior of all tracked particles

Finite number of particles N_η → variance from solver

Stochastic Radiation Transport Problem

To perform UQ, we introduce a cross-section as a function of stochastic parameter ξ. For each material region m, total cross-section is:

$$\Sigma_{t,m}(\xi_m) = \Sigma^0_{t,m} + \Sigma^\Delta_{t,m}\,\xi_m$$

Total polluted variance = parametric (ξ) and solver (η) variance

Conclusions

We confirmed via comparison to analytic results that our sample variance estimator accurately takes into account, and removes, the additional variability introduced by the use of Monte Carlo radiation transport solvers. We also performed a numerical campaign to understand the estimator variance trade off between particle histories N_η and UQ samples N_ξ.

Variance Deconvolution

UQ Goal: calculate $\mathbb{V}ar_\xi[T(\xi,\eta)]$

We want the variance of the QoI as function of stochastic input, removing contribution from stochastic solver[1].

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

Apply Law of Total Variance:

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

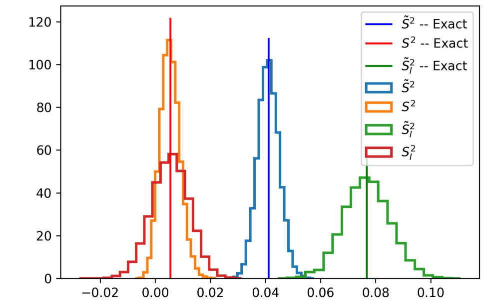
Both $\mathbb{V}ar_\xi[\tilde{T}(\xi,\eta)]$ and $\mathbb{E}_\xi\left[\frac{\sigma^2_\eta}{N_\eta}\right]$ are accessible quantities, so

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

Estimate $S^2 \approx \mathbb{V}ar_\xi[T]$

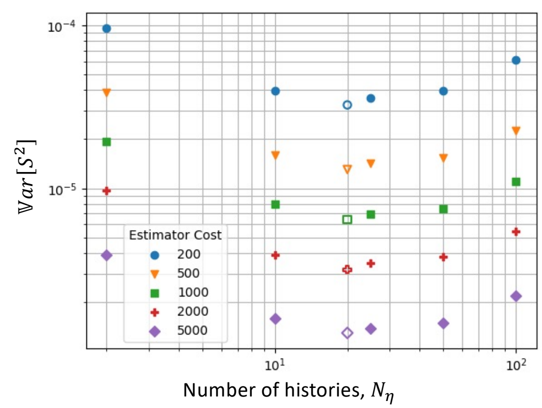
Compare sample estimates of $\mathbb{V}ar_\xi[T]$ and $\mathbb{V}ar_\xi[\tilde{T}(\xi,\eta)]$ to analytic solutions using the p^{th} raw moment for transmittance[1]:

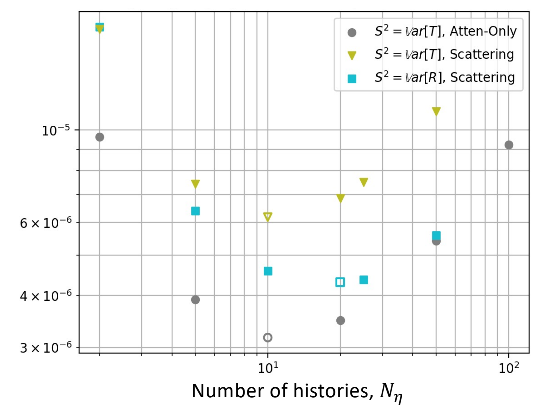
$$\mathbb{E}[T^p] = \prod_{m=1}^{d} exp^{\left[-p\,\Sigma^0_{t,m}\,\Delta x_m\right]}\frac{sinh\left[p\,\Sigma^\Delta_{t,m}\,\Delta x_m\right]}{p\,\Sigma^\Delta_{t,m}\,\Delta x_m}$$



Minimize $\mathbb{V}ar[S^2]$

Comparing where $\mathbb{V}ar[S^2]$ is minimized over 25,000 repetitions for an attenuation-only case (left) and a corresponding case with scattering physics (right), we find that $\mathbb{V}ar[S^2]$ is minimized at different locations for different QoIs, even within one problem[2].





REFERENCES

1. K. CLEMENTS, G. GERACI, and A. J. OLSON, "A Variance Deconvolution Approach to Sampling Uncertainty Quantification for Monte Carlo Radiation Transport Solvers," in "Computer Science Research Institute Summer Proceedings 2021," (2021), Technical Report SAND2022-0653R, pp. 293–307
2. K. CLEMENTS, G. GERACI, and A. J. OLSON, "Numerical Investigation on the Performance of a Variance Deconvolution Estimator," in "Transactions of the American Nuclear Society," (2022), vol. 126. (Accepted).

ACKNOWLEDGEMENTS This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This work was supported by the Center for Exascale Monte-Carlo Neutron Transport (CEMeNT) a PSAAP-III project funded by the Department of Energy, grant number DE-NA003967.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.