LA-UR-18-27893
Approved for public release; distribution is unlimited.

Title: A Monte Carlo Importance-splitting Analytic Benchmark

Author(s): Kulesza, Joel A.
Solomon, Clell Jeffrey Jr.
Kiedrowski, Brian C.

Intended for: 20th Topical Meeting of the Radiation Protection & Shielding Division (RPSD-2018), 2018-08-26/2018-08-31 (Santa Fe, New Mexico, United States)

Issued: 2018-08-20 (Draft)

Disclaimer:
Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

A Monte Carlo Importance-splitting Analytic Benchmark

Joel A. Kulesza[1,2], Clell J. Solomon, Jr.[1], and Brian C. Kiedrowski[2]

[1]Los Alamos National Laboratory, Monte Carlo Methods, Codes, and Applications Group
[2]University of Michigan, Dept. of Nuclear Engineering & Radiological Sciences

American Nuclear Society
20th Topical Meeting of the Radiation Protection & Shielding Division
August 27, 2018

Acknowledgements

This work is supported by the Department of Energy National Nuclear Security Administration (NNSA) Advanced Simulation and Computing (ASC) Program. It is also supported by the NNSA under Award Number(s) DE-NA0002576 and in part by the NNSA Office of Defense Nuclear Nonproliferation R&D through the Consortium for Nonproliferation Enabling Capabilities.

Outline

Background & Introduction

Primary objective: Show a procedure to create analytic benchmarks for Monte Carlo mean and variance (e.g., with uncollided importance splitting)

Secondary objective: Reinforce relationship between adjoint and forward transport quantities calculated deterministically and with Monte Carlo

- Analog Monte Carlo: all statistical moments are equal (iff $w_0 = 1$)
- For fair non-analog (using variance reduction) Monte Carlo calculations
  - The first statistical moment, $M_1(\mathbf{P}_0)$, is preserved
  - Higher moments, $M_{m>1}(\mathbf{P}_0)$, are modified
    - Predictable via the History-score Moment Equations (HSMEs)
- Prior work for various variance reduction techniques includes
  - Exponential transform (Sarkar and Prasad, 1979)
  - Importance splitting (Booth and Cashwell, 1979)
  - Weight windows (Solomon et al., 2014)
  - DXTRAN (Kulesza et al., 2018)

Background on History-score Moment Equations (HSMEs)

- History-score Probability Density Function (HSPDF) describes all possible random walks

$$\psi\left(\mathbf{P}_0, s\right) = \psi_{\text{absorption}}\left(\mathbf{P}_0, s\right) + \psi_{\text{scattering}}\left(\mathbf{P}_0, s\right) + \psi_{\text{surf. crossing}}\left(\mathbf{P}_0, s\right) + \cdots$$

- HSMEs compute the statistical moments of the HSPDF

$$M_m\left(\mathbf{P}_0\right) = \int \mathrm{d}s\, s^m\, \psi\left(\mathbf{P}_0, s\right)$$

- Generally, the first two statistical moments are of the most interest
  - $M_1\left(\mathbf{P}_0\right)$ is comparable to the adjoint flux solution for the system
  - $M_2\left(\mathbf{P}_0\right)$ is a flux-like quantity representing the second-scoring moment of histories for a given position in phase space $\mathbf{P}$
- Detector behavior is calculated with inner products and the forward source similar to adjoint transport

$$D_m = \int \mathrm{d}\mathbf{P}_0\, S\left(\mathbf{P}_0\right)\, M_m\left(\mathbf{P}_0\right) \implies \widehat{\mu} = \int \mathrm{d}\mathbf{P}_0\, S\left(\mathbf{P}_0\right)\, M_1\left(\mathbf{P}_0\right)$$

Benchmarking Procedure Overview

1. Define problem of interest and limiting assumptions
2. Construct the HSPDF describing all possible random walks
3. Calculate the first two statistical moments of the HSPDF with the HSMEs
   - Don't forget how lower moments act as sources to higher moments!
4. Compute the Monte Carlo behavior from the two statistical moments

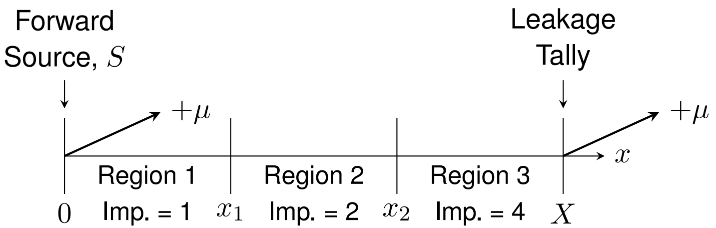
$$\widehat{\mu} = \int \mathrm{d}\mathbf{P}_0 \, S\left(\mathbf{P}_0\right) \, M_1\left(\mathbf{P}_0\right), \tag{1}$$

$$\widehat{\sigma^2} = \int \mathrm{d}\mathbf{P}_0 \, S\left(\mathbf{P}_0\right) \, M_2\left(\mathbf{P}_0\right) - \left(\widehat{\mu}\right)^2 . \tag{2}$$

- This computation can be performed
  - **Analytically with the HSMEs (confirmed numerically herein)**
  - Directly with a forward approach (similar to DSA, Burn (1995))

Motivating Problem Summary

- Integer-only $(2:1)$ splitting
  - Non-integer splitting via additional sampling has been demonstrated previously (Booth and Cashwell, 1979; Solomon et al., 2014)
- Monoenergetic homogeneous pure absorber; $\Sigma_t = \Sigma_a$
- Monodirectional; $0 < \mu \leq 1$
- The previous two items guarantee no importance rouletting
  - Also create the most simple, non-trivial, case for analysis



Analytic Adjoint-transport Approach, M_1, Region 3

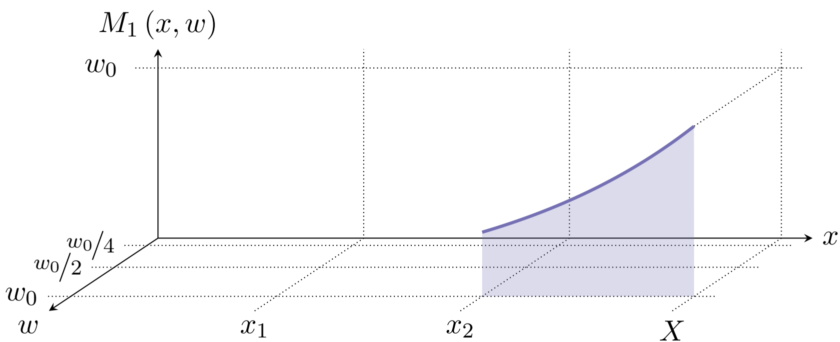
System

$$-\mu\frac{\partial M_1}{\partial x} + \Sigma_t M_1 = 0\,,\; x_2 \le x \le X, \tag{3a}$$

$$M_1\left(X, w\right) = \delta\left(w - w_0\right) \tag{3b}$$

Solution

$$M_1\left(x, w\right) = \delta\left(w - w_0\right)\exp\left(\frac{\Sigma_t}{\mu}\left(x - X\right)\right) \tag{4}$$



Analytic Adjoint-transport Approach, M_1, Region 2

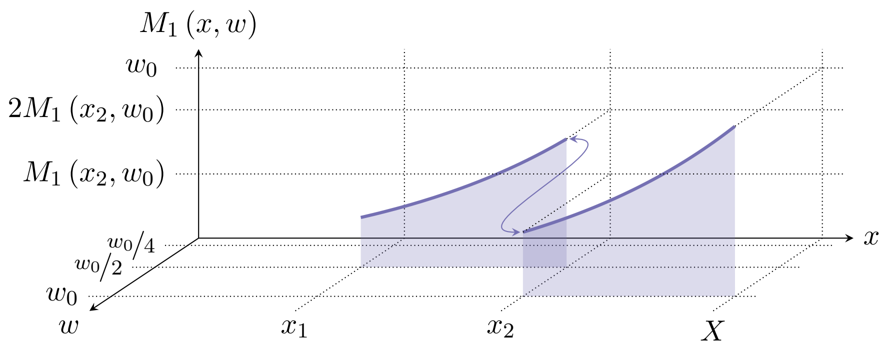
System

$$-\mu \frac{\partial M_1}{\partial x} + \Sigma_t M_1 = 0\,,\; x_1 \le x < x_2, \tag{5a}$$

$$\lim_{\epsilon \to 0^+} M_1 \left(x_2 - \epsilon, w\right) = 2 M_1 \left(x_2, w\right) \delta \left(w - w_0/2\right) / \delta \left(w - w_0\right) \tag{5b}$$

Solution

$$M_1 \left(x, w\right) = 2\delta \left(w - \frac{w_0}{2}\right) \exp\left(\frac{\Sigma_t}{\mu}\left(x - X\right)\right) \tag{6}$$



Analytic Adjoint-transport Approach, M_1, Region 1

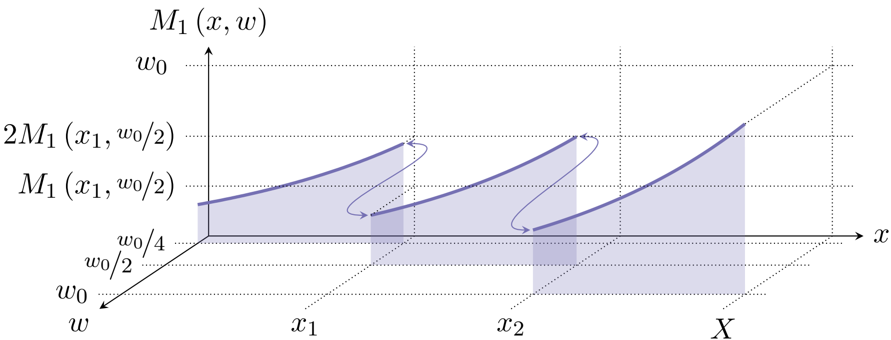
System

$$-\mu\frac{\partial M_1}{\partial x} + \Sigma_t M_1 = 0\,,\ 0 \le x < x_1, \tag{7a}$$

$$\lim_{\epsilon\to 0^+} M_1\left(x_1-\epsilon, w\right) = 2M_1\left(x_1, w\right)\delta\left(w - w_0/4\right)/\delta\left(w - w_0/2\right) \tag{7b}$$

Solution

$$M_1\left(x,w\right) = 4\delta\left(w - \frac{w_0}{4}\right)\exp\left(\frac{\Sigma_t}{\mu}\left(x - X\right)\right) \tag{8}$$



Analytic Adjoint-transport Approach, M_2, Region 3

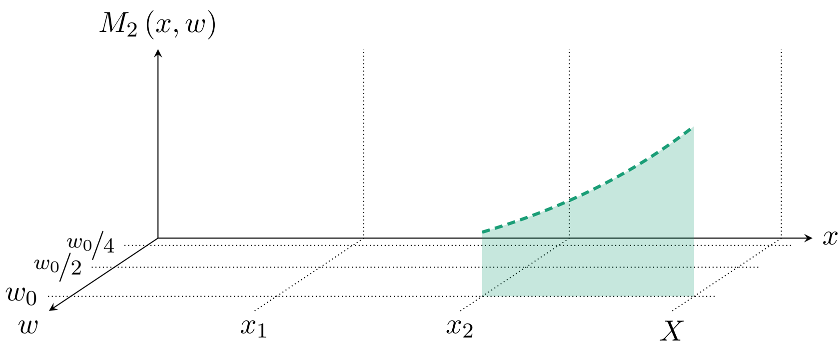
System

$$-\mu\frac{\partial M_2}{\partial x} + \Sigma_t M_2 = 0\,,\; x_2 \leq x \leq X, \tag{9a}$$

$$M_2\left(X, w\right) = \delta\left(w - w_0\right) \tag{9b}$$

Solution

$$M_2\left(x, w\right) = \delta\left(w - w_0\right)\exp\left(\frac{\Sigma_t}{\mu}\left(x - X\right)\right) \tag{10}$$



Analytic Adjoint-transport Approach, M_2, Region 2

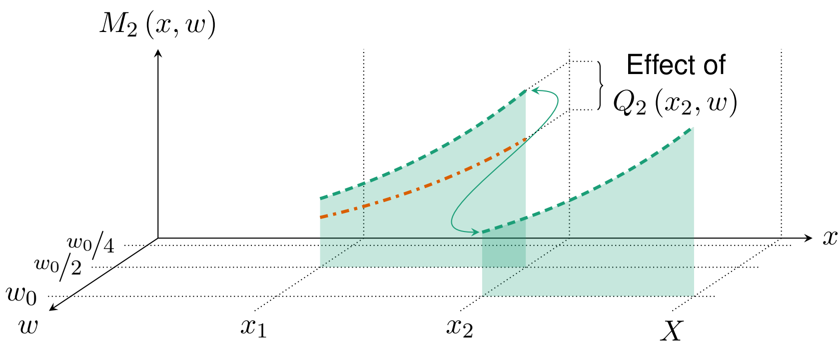
System

$$-\mu \frac{\partial M_2}{\partial x} + \Sigma_t M_2 = 0\,,\; x_1 \le x < x_2, \tag{11a}$$

$$\lim_{\epsilon \to 0^+} M_2\left(x_2 - \epsilon, w\right) = 2 M_2\left(x_2, w\right) \frac{\delta\left(w - w_0/2\right)}{\delta\left(w - w_0\right)} + \underbrace{2\left[M_1\left(x_2, w\right)\right]^2}_{Q_2(x_2,w)} \tag{11b}$$

Solution

$$M_2\left(x, w\right) = 2\delta\left(w - \frac{w_0}{2}\right) \exp\left(\frac{\Sigma_t}{\mu}\left(x - X\right)\right)\left[1 + \exp\left(\frac{\Sigma_t}{\mu}\left(x_2 - X\right)\right)\right] \tag{12}$$



Analytic Adjoint-transport Approach, M_2, Region 1

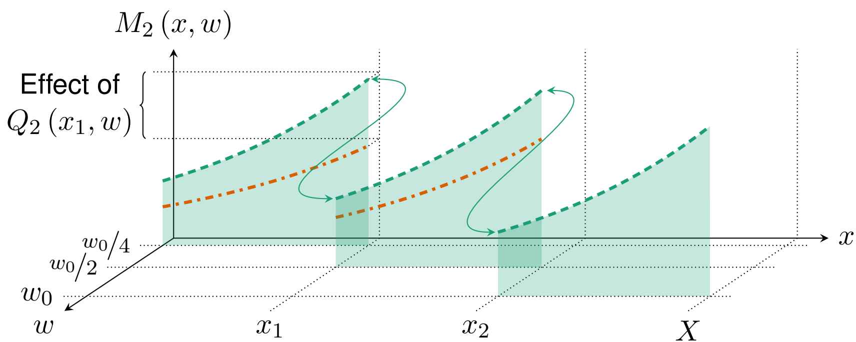
System

$$-\mu \frac{\partial M_2}{\partial x} + \Sigma_t M_2 = 0\,,\; 0 \le x < x_1\,, \tag{13a}$$

$$\lim_{\epsilon \to 0^+} M_2\left(x_1 - \epsilon, w\right) = 2 M_2\left(x_1, w\right) \frac{\delta\left(w - w_0/4\right)}{\delta\left(w - w_0/2\right)} + 2\left[M_1\left(x_1, w\right)\right]^2 \tag{13b}$$

Solution

$$M_2\left(x, w\right) = 4\delta\left(w - \frac{w_0}{4}\right) \exp\left(\frac{\Sigma_t}{\mu}\left(x - X\right)\right)\left[1 + 2\exp\left(\frac{\Sigma_t}{\mu}\left(x_1 - X\right)\right) + \exp\left(\frac{\Sigma_t}{\mu}\left(x_2 - X\right)\right)\right] \tag{14}$$



Overview of Solution Methods

- Analytically compute $M_1(x)$ and $M_2(x)$:

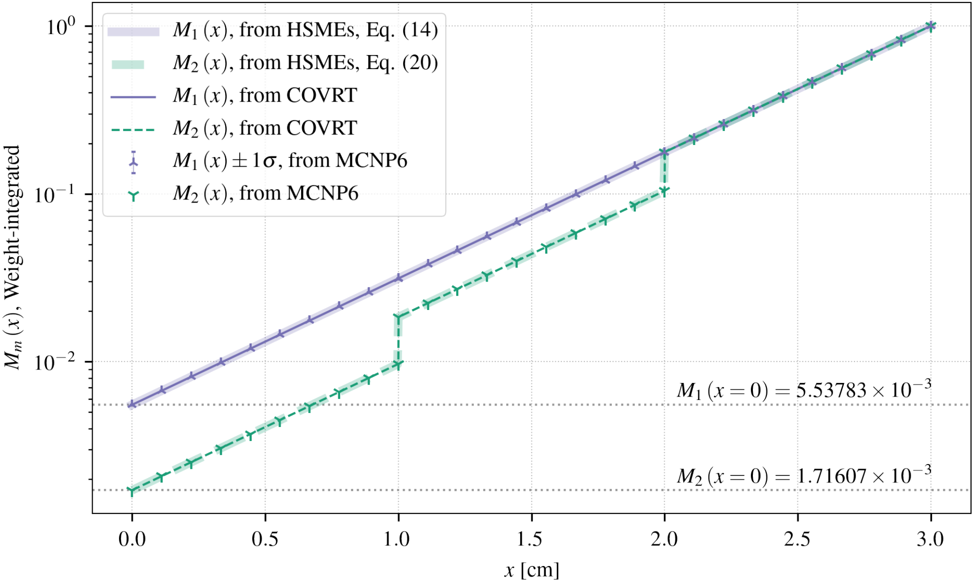
$$M_1(x=0) = \exp\left(-3\sqrt{3}\right) \approx 5.53783 \times 10^{-3} \quad (15)$$

and

$$\begin{aligned} M_2(x=0) & \\ &= \frac{1}{4}\exp\left(-5\sqrt{3}\right)\left(2+\exp\left(\sqrt{3}\right)+\exp\left(2\sqrt{3}\right)\right) \\ &\approx 1.71607 \times 10^{-3}. \end{aligned} \quad (16)$$

- Numerically with a single COVRT calculation
- Numerically with a series of forward MCNP calculations
  - Yields "correct" value at $x = 0$
  - Provides sanity check along traverse in $0 < x < 2$

Moment Traverses



Summary & Future Work

- Summary:
  - Demonstrated a procedure to predict Monte Carlo mean *and* variance
    - This work focuses on a HSME-based approach
    - Alternative approaches are available
  - Showed relationship between adjoint/forward deterministic and Monte Carlo solutions for both mean *and* variance
- Future work:
  - Develop analytic benchmark with scattering (also importance rouletting)
    - Already available numerically (just ask), but not analytically
    - Must “iterate” scattering source to convergence
  - Identify other scenarios of interest and define corresponding benchmarks

Questions?

Contact Information

Joel A. Kulesza
Office: +1 (505) 667-5467
Email: jkulesza@lanl.gov

Clell J. Solomon, Jr.
Office: +1 (505) 665-5720
Email: csolomon@lanl.gov

Brian C. Kiedrowski
Office: +1 (734) 615-5978
Email: bckiedro@umich.edu

Backup Slides

References

P. K. Sarkar and M. A. Prasad, “Prediction Of Statistical Error And Optimization Of Biased Monte Carlo Transport Calculations,” *Nuclear Science and Engineering*, vol. 70, no. 3, pp. 243–261, Jun. 1979. [Online]. Available: http://www.ans.org/pubs/journals/nse/a_20146

T. E. Booth and E. D. Cashwell, “Analysis Of Error In Monte Carlo Transport Calculations,” *Nuclear Science and Engineering*, vol. 71, no. 2, pp. 128–142, Aug. 1979. [Online]. Available: http://www.ans.org/pubs/journals/nse/a_20404

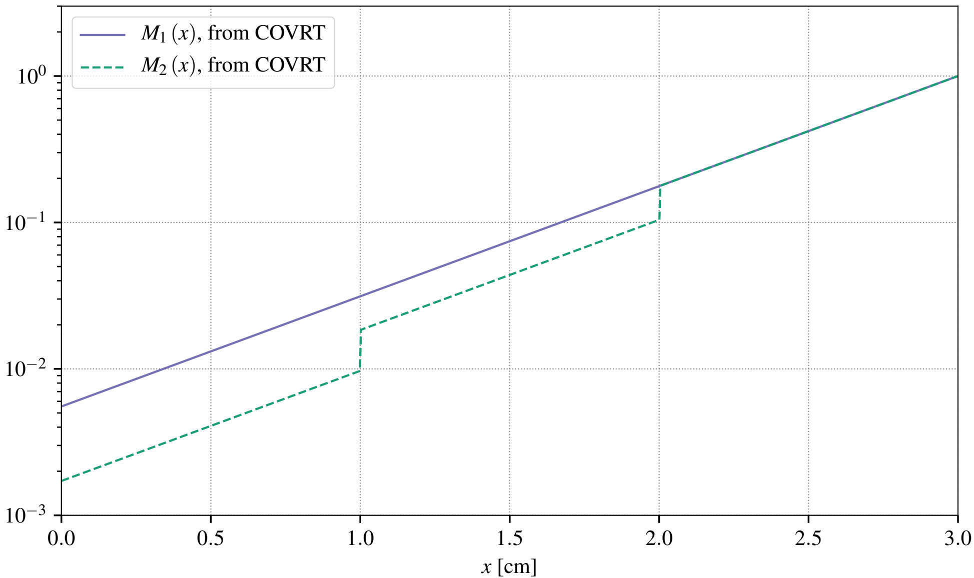
C. J. Solomon, A. Sood, T. E. Booth, and J. K. Shultis, “A Priori Deterministic Computational-Cost Optimization Of Weight-Dependent Variance-Reduction Parameters For Monte Carlo Neutral-Particle Transport,” *Nuclear Science and Engineering*, vol. 176, no. 1, pp. 1–36, Jan. 2014. [Online]. Available: http://www.ans.org/pubs/journals/nse/a_35436

References

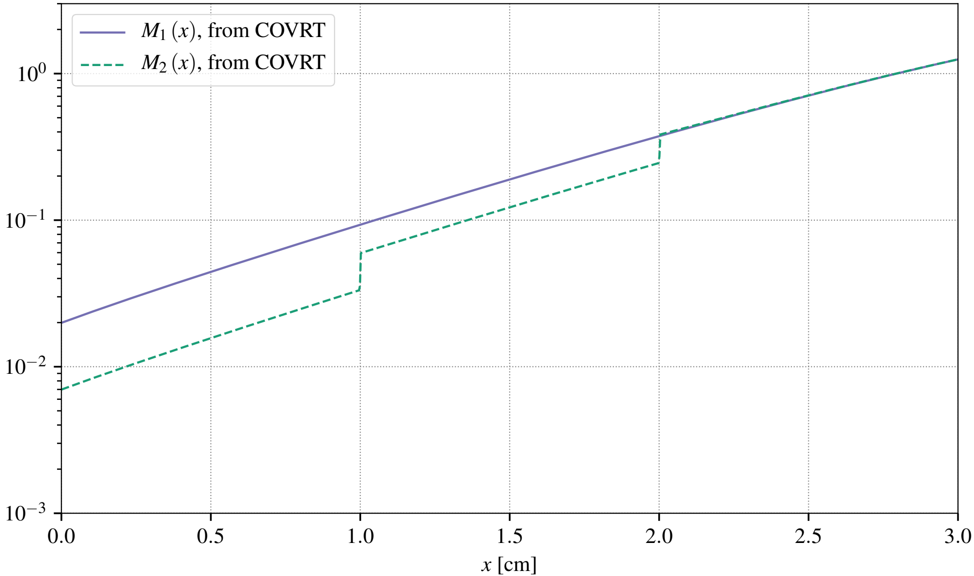
J. A. Kulesza, C. J. Solomon, and B. C. Kiedrowski, “Progress in Deterministically Predicting Tally Variance with DXTRAN Regions,” in *Proceedings of Advances in Nuclear Nonproliferation Technology and Policy Conference (ANTPC2018)*. Wilmington, NC, USA; September 23–27: American Nuclear Society, 2018.

K. W. Burn, “Extending The Direct Statistical Approach To Include Particle Bifurcation Between The Splitting Surfaces,” *Nuclear Science and Engineering*, vol. 119, no. 1, pp. 44–79, Jan. 1995. [Online]. Available: http://www.ans.org/pubs/journals/nse/a_24070

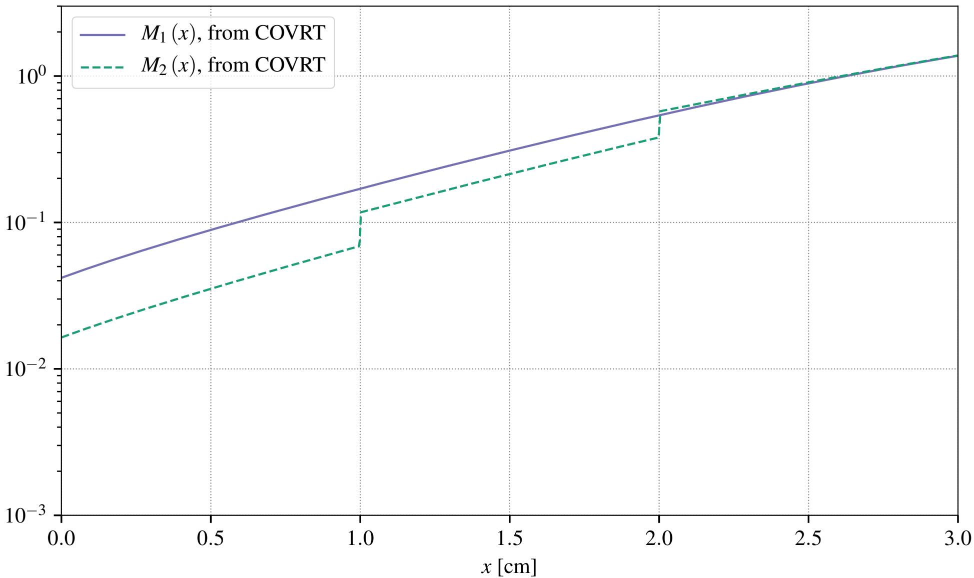
Demo: $M_1(x)$ and $M_2(x)$, 0 Collisions, $\Sigma_t = \Sigma_s =$ 1 cm^{-1}



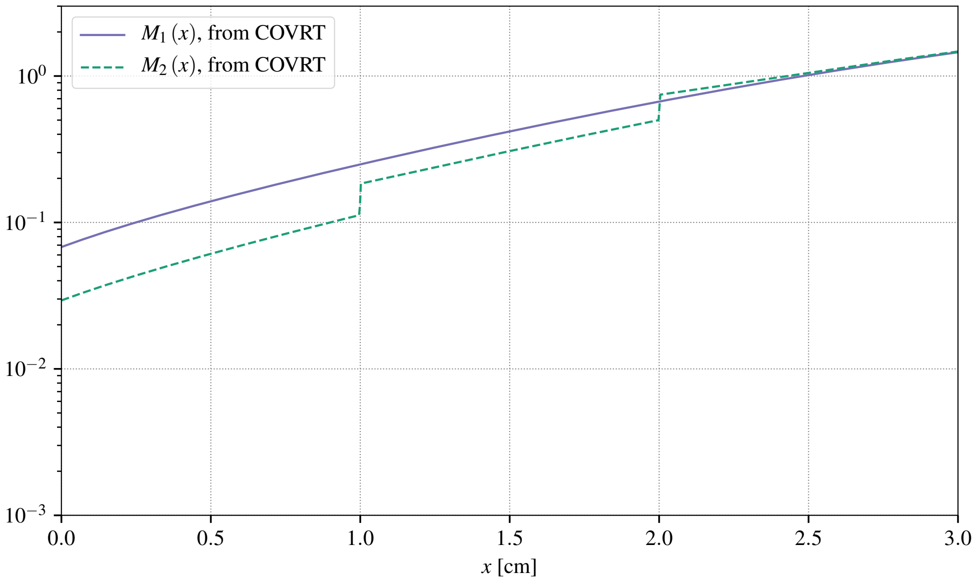
Demo: $M_1(x)$ and $M_2(x)$, 1 Collision, $\Sigma_t = \Sigma_s = 1$ cm[-1]



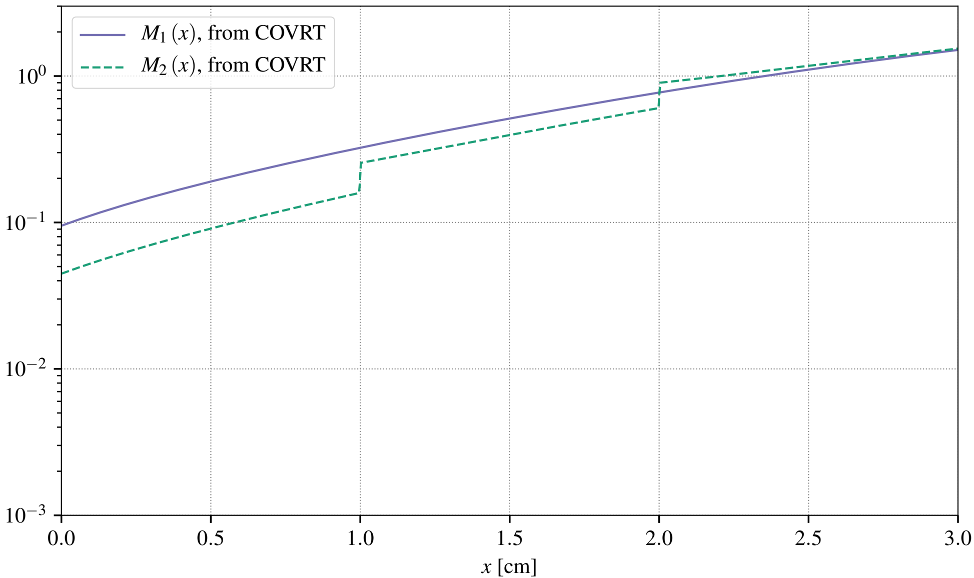
Demo: $M_1(x)$ and $M_2(x)$, 2 Collisions, $\Sigma_t = \Sigma_s = 1$ cm^{-1}



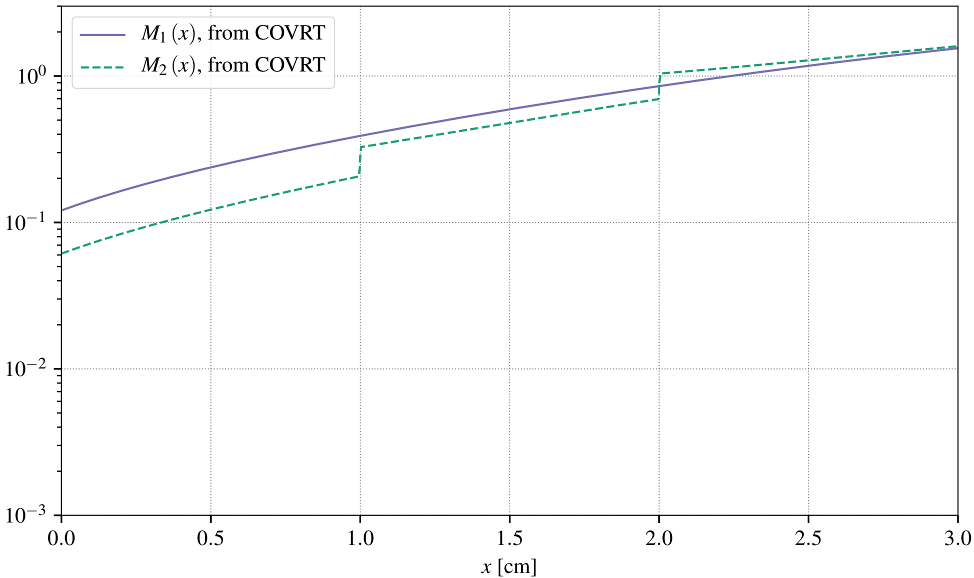
Demo: $M_1(x)$ and $M_2(x)$, 3 Collisions, $\Sigma_t = \Sigma_s = 1$ cm^{-1}



Demo: $M_1(x)$ and $M_2(x)$, 4 Collisions, $\Sigma_t = \Sigma_s = 1$ cm^{-1}



Demo: $M_1(x)$ and $M_2(x)$, 5 Collisions, $\Sigma_t = \Sigma_s = 1$ cm^{-1}



Demo: $M_1(x)$ and $M_2(x)$, 50 Collisions, $\Sigma_t = \Sigma_s = 1$ cm^{-1}