LA-UR-17-22791
Approved for public release; distribution is unlimited.

Title: Performance Assessment of Cost-Optimized Variance Reduction Parameters in Radiation Shielding Scenarios

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

Intended for: M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, 2017-04-16/2017-04-20 (Jeju, Korea, South)

Issued: 2017-04-06 (Draft)

# Performance Assessment of Cost-Optimized Variance Reduction Parameters in Radiation Shielding Scenarios

Joel A. Kulesza[1,2], Clell J. (CJ) Solomon, Jr.[2],
Brian C. Kiedrowski[1], Edward W. Larsen[1]

[1]University of Michigan, Department of Nuclear Engineering & Radiological Sciences
2355 Bonisteel Blvd., Ann Arbor, MI, 48109
[2]Los Alamos National Laboratory, Monte Carlo Methods, Codes, and Applications Group
P.O. Box 1663, Los Alamos, NM, 87545

jkulesza@umich.edu, csolomon@lanl.gov, bckiedro@umich.edu, edlarsen@umich.edu

American Nuclear Society
International Conference on Mathematics & Computational Methods
April 16–20, 2017

# Acknowledgements

This work is supported by the Department of Energy National Nuclear Security Administration (NNSA) Engineering Campaign 7. 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

# Introduction & Background

**Objective: compare weight-dependent (WD) and -independent (WI) variance reduction (VR) parameter optimization approaches**

- "Traditional" hybrid methods: minimize variance
  - AVATAR (Riper et al., 1997)
  - LIFT (Turner and Larsen, 1997)
  - FW-CADIS (Wagner and Haghighat, 1998)
  - State-of-the-art: FW-CADIS via ADVANTG (Mosher et al., 2015)
- This method: minimize computational cost (i.e., maximize FOM)
  - Computational cost inversely proportional to FOM

$$\widetilde{C}\left(\{VR\}\right) = \widetilde{\sigma}^2\left(\{VR\}\right)\widetilde{\tau}\left(\{VR\}\right) \quad (1)$$

  - Method implemented via COVRT (Solomon et al., 2014)
    - Calculate $\widetilde{\sigma}^2$ and $\widetilde{\tau}$ deterministically
    - Optimize these quantities by varying VR parameters

# Methodology Overview

- Cost-optimized methods are Monte Carlo code agnostic
- Specific implementations are directly related to a Monte Carlo code
  - Descriptions of geometry, materials, tallies, sources, etc.
  - VR technique availability & implementation
    - Weight-dependent vs. weight-independent techniques
  - Performance measure for various physical & computational events
- Basic Steps

1. Solve History-Score Moment Equations
2. Solve Future Time Equations
3. Calculate computational cost, $\widetilde{C}\left(\{VR\}\right) = \widetilde{\sigma}^2\left(\{VR\}\right)\widetilde{\tau}\left(\{VR\}\right)$
4. Vary VR parameters, perform 1–3, compare with previous cost
5. Repeat, as necessary, until $\widetilde{C}\left(\{VR\}\right)$ is minimized

# History-Score-Moment Equations (HSMEs) (1/4)

- Construct & discretize weight-augmented phase space:

$$\boldsymbol{P} = (\boldsymbol{x}, \boldsymbol{\Omega}, E, w) = (\boldsymbol{R}, w) \tag{2}$$

- Define scoring functions and transport kernels
  - How a particle contributes score in $ds$ about $s$ in its next event
    - Examples: $p_{\Sigma}(\boldsymbol{P}, s_{\Sigma})\, ds_{\Sigma}$, $p_C(\boldsymbol{P}, s_C)\, ds_C$
  - How a particle moves through phase space and changes weight
    - Analog emergence (single scattering) kernel example:

$$E(\boldsymbol{P}_0, \boldsymbol{P}_1)\, d\boldsymbol{P}_1 = \delta(x_1 - x_0)\, p(\boldsymbol{\Omega}_0, E_0 \to \boldsymbol{\Omega}_1, E_1) \times \delta(w_1 - w_0)\, dx_1 d\Omega_1 dE_1 dw_1 \tag{3}$$

- Assemble transport kernels into continuous random walks

# History-Score-Moment Equations (HSMEs) (2/4)

- Analog collision with scattering example:

$$\psi_E\left(\boldsymbol{P}_0, s\right) ds = \int d\boldsymbol{P}_1 T\left(\boldsymbol{P}_0, \boldsymbol{P}_1\right) \int d\boldsymbol{P}_2 \Sigma\left(\boldsymbol{P}_1, \boldsymbol{P}_2\right) \times \int ds_\Sigma p_\Sigma\left(\boldsymbol{P}_2, s_\Sigma\right) \int d\boldsymbol{P}_3 E\left(\boldsymbol{P}_2, \boldsymbol{P}_3\right) \psi\left(\boldsymbol{P}_3, s - s_\Sigma\right) ds \quad (4)$$

- Assemble into history-score probability distribution function $\psi\left(\boldsymbol{P}_0, s\right) ds$

$$\psi\left(\boldsymbol{P}_0, s\right) ds = \sum_i \psi_i\left(\boldsymbol{P}_0, s\right) ds \quad (5)$$

  - Probability of contributing score $ds$ about $s$ from phase space $\boldsymbol{P}_0$

# History-Score-Moment Equations (HSMEs) (3/4)

- The $m$ moments of the history-score distribution are:

$$M_m\left(\boldsymbol{P}_0\right) = \int_{-\infty}^{\infty} s^m \psi\left(\boldsymbol{P}_0, s\right) ds \tag{6}$$

- First moment ($m = 1$) comparable to adjoint integral transport equation
- Associated detector responses (with physical source term $Q\left(\boldsymbol{P}_0\right)$) are:

$$\widetilde{D}_m = \int M_m\left(\boldsymbol{P}_0\right) Q\left(\boldsymbol{P}_0\right) d\boldsymbol{P}_0 \tag{7}$$

- Population variance is:

$$\widetilde{\sigma}^2 = \widetilde{D}_2 - \widetilde{D}_1^2 \tag{8}$$

- Difficulty of solving for $M_{m>1}\left(\boldsymbol{P}_0\right)$ affected by VR techniques used

# History-Score-Moment Equations (HSMEs) (4/4)

- Weight separability with weight-independent VR techniques (Booth and Cashwell, 1979):

$$M_m(\boldsymbol{R}, aw) = a^m M_m(\boldsymbol{R}, w) = a^m w^m M_m(\boldsymbol{R}, w = 1) \tag{9}$$

- This separability shows that weight-independent techniques do not require a discretized weight mesh for any moments
  - Reduced memory requirements
  - Reduced deterministic solver computational time
  - Permits easier incorporation into pre-existing deterministic solver

**Can WI techniques perform as well as WD techniques?**

# Future Time Equations (FTEs) (1/1)

- Construct future time distribution like history-score probability distribution:

$$\Upsilon\left(\boldsymbol{P}_0, \tau\right) d\tau = \sum_t \left[\prod_{n_t=1}^{N_t} \int d\boldsymbol{P}_{n_t} B_{n_t}\left(\boldsymbol{P}_{n_t-1}, \boldsymbol{P}_{n_t}\right) \tau_{n_t}\left(B_{n_t}, \boldsymbol{P}_{n_t}\right)\right] d\tau \tag{10}$$

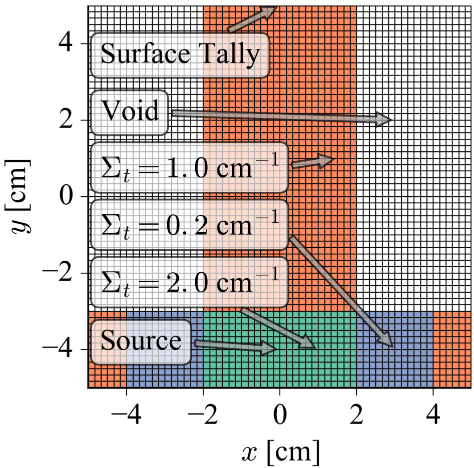
- Each $\tau_{n_t}$ from profiled Monte Carlo code calculations, $\mathcal{O}\left(10^{-7}\ \text{minutes}\right)$
- Similar to history-score-moment distribution, expected future time of particle at $\boldsymbol{P}_0$ is:

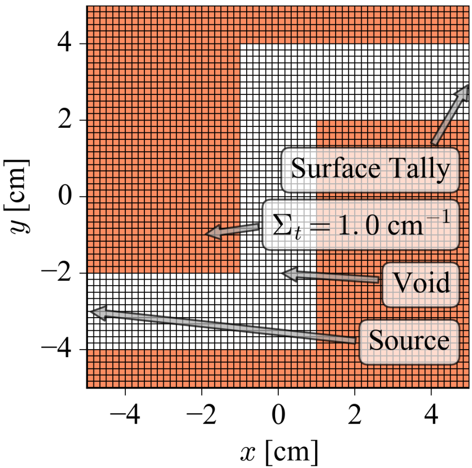
$$\overline{\tau}\left(\boldsymbol{P}_0\right) = \int_0^{\infty} \tau \Upsilon\left(\boldsymbol{P}_0, \tau\right) d\tau \tag{11}$$

- Expected future time of a particle then calculated as:

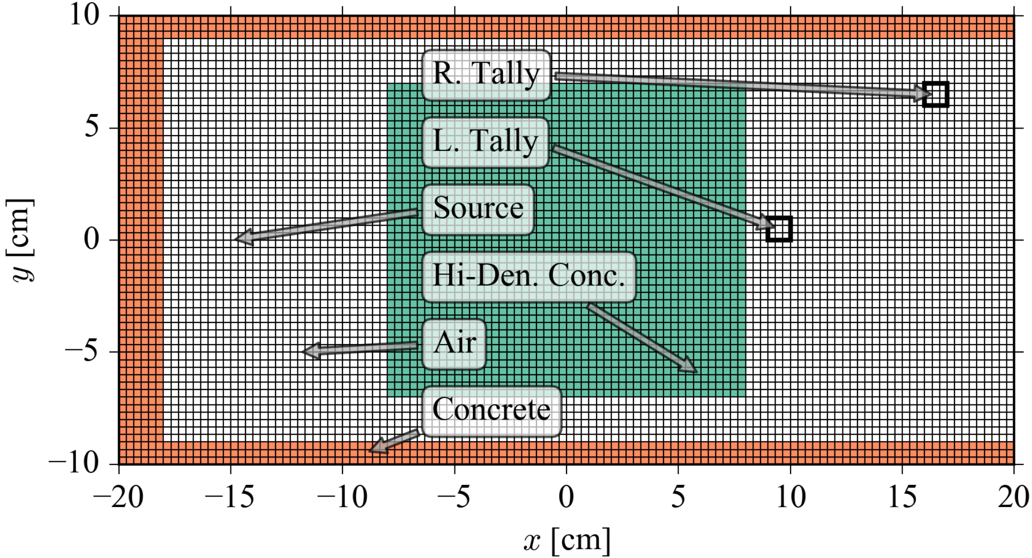
$$\widetilde{\tau} = \int \overline{\tau}\left(\boldsymbol{P}_0\right) Q\left(\boldsymbol{P}_0\right) d\boldsymbol{P}_0 \tag{12}$$

# Tophat & Three-legged Duct, from Solomon (2010)

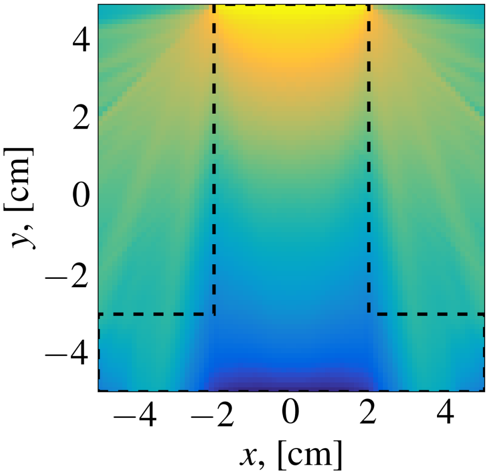


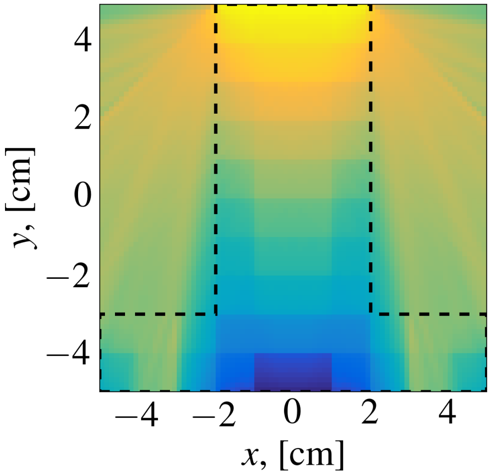
# Mini2Room, inspired by Kulesza et al. (2016)



# Tophat First and Second Moment Solutions

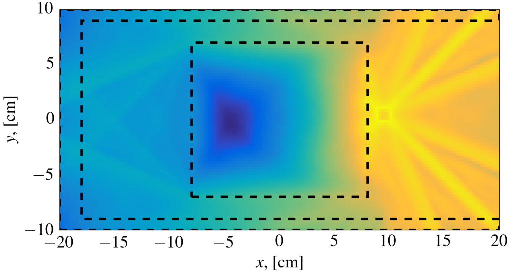



$M_1$

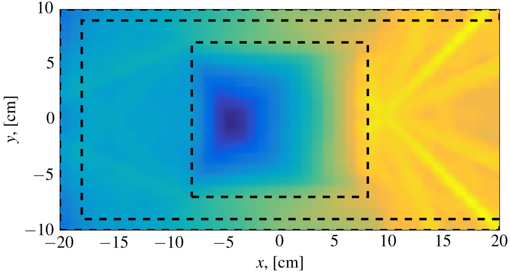



Optimized $M_2$

# Mini2Room First and Second Moment Solutions




$M_1$




Optimized $M_2$

# Tophat & Three-legged Duct Results

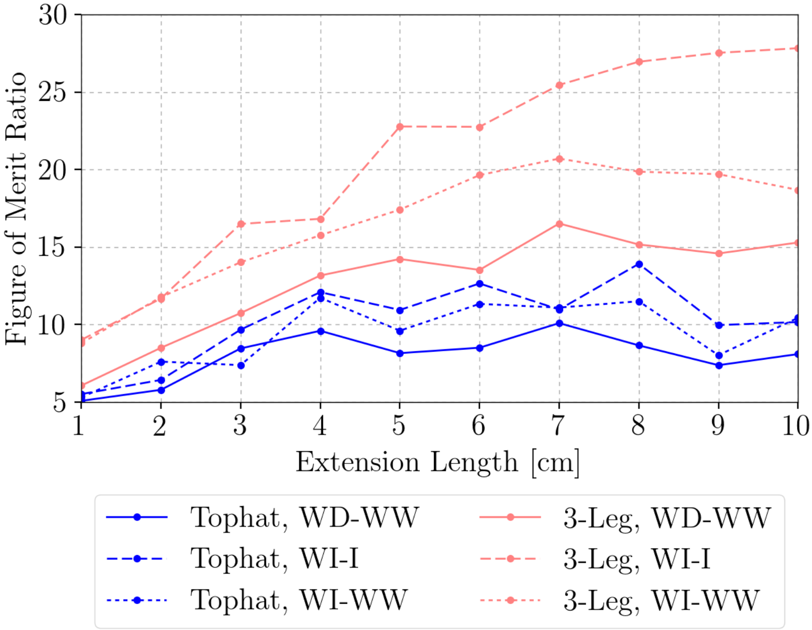
- WI FOM ratio usually as good or better than WD
  - WI ~10× faster
  - WI uses ~100× less memory
- Means approach unity as the quadrature is refined
- Variance & FOM show no substantial change
- Relatively coarse quadrature can be effective
- Iterative optimization depends on relative changes

MCNP FOM Ratios, Higher is Better

| Geometry | WD-WW[a] | WI-I[b] | WI-WW[c] |
|---|---|---|---|
| TH[d] | 3.46 | 3.53 | 5.78 |
| TLD[e] | 7.26 | 7.26 | 6.77 |

[a] WD COVRT → Weight Windows
[b] WI COVRT → Importances
[c] WI COVRT → Importances → Weight Windows
[d] Tophat
[e] Three-legged Duct

# Extended Tophat & Three-legged Duct FOM Ratios



# Mini2Room Comparison with ADVANTG

- ADVANTG ($S_4$, 27 neutron groups), FOM: 3.0
- COVRT ($S_4$, 2, 4, 8, and 27 neutron groups), FOMs: 15, 6.3, 3.8, 6.5
  - Varying FOM due to multi-group COVRT calculations collapsed to one-group importances
  - A variety of collapsing schemes were explored, but none gave consistent or consistently improved FOMs
- ADVANTG time: 8 seconds, MCNP time: 65 hours
  - Long-running histories in MCNP drove time up
- COVRT time: 0.3, 1.0, 5.3, 48.0 hours, MCNP time: 34–116 minutes
  - COVRT time scales linearly with workload
    - Multiple optimization passes for each energy group

# Summary & Future Work

- Demonstrated the effectiveness of cost-optimized VR parameters
- Optimized WI techniques can be as, or more, effective than WD
  - Significant savings in deterministic runtime & memory requirements
- Varying levels of agreement between mean and variance values
  - Optimization depends on relative changes
- Highly angle-dependent problems challenge these methods
- Value in creating hybrid radiation transport method benchmark suite
- Extension of history-score-moment and future-time equations to DXTRAN

# Questions?

Contact Information

Joel A. Kulesza
Mobile: +1 (734) 223–7312 Email: jkulesza@umich.edu

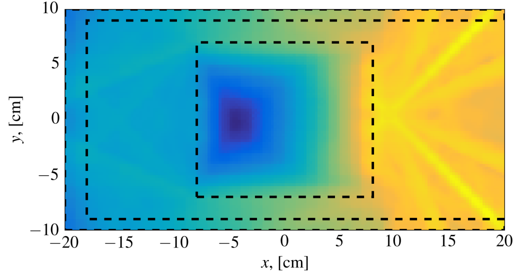
CJ Solomon
Office: +1 (505) 665–5720 Email: csolomon@lanl.gov

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

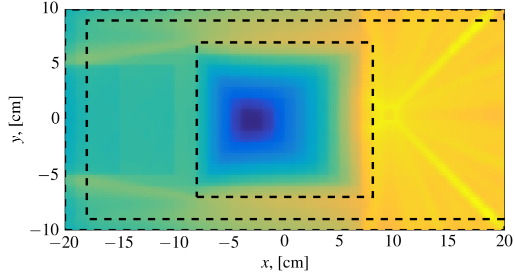
Edward W. Larsen
Office: +1 (734) 936–0124 Email: edlarsen@umich.edu

# Backup Slides

# Mini2Room Optimized Second Moment, $S_4$ vs. $S_{12}$

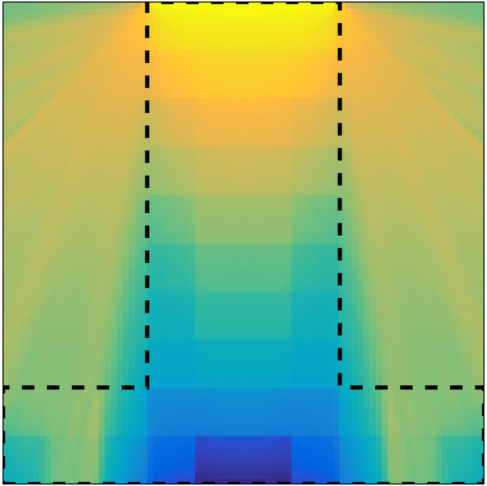



Optimized $M_2$, $S_4$

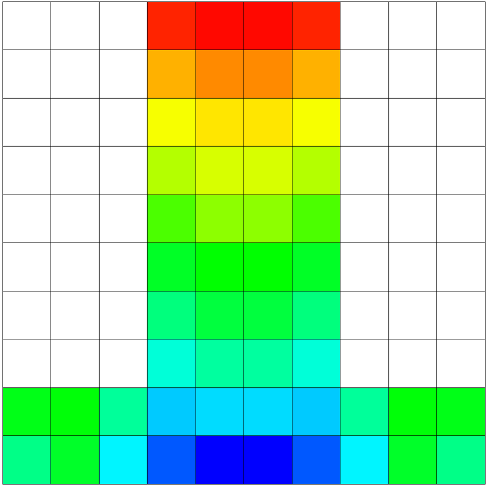



Optimized $M_2$, $S_{12}$

# Tophat Second Moment & Importances

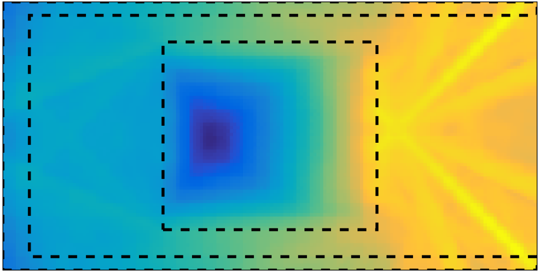


Optimized $M_2$

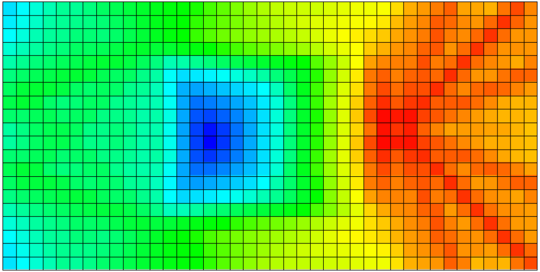


Optimized Importances

# Mini2Room Second Moment & Importances



Optimized $M_2$



Optimized Importances

# References

Booth, T. E., Cashwell, E. D., 1979. Analysis Of Error In Monte Carlo Transport Calculations. Nuclear Science and Engineering 71 (2), 128–142.

Kulesza, J. A., Kiedrowski, B. C., Larsen, E. W., 2016. Application Of Automated Weight Window Generation Techniques To Modeling The Detection Of Shielded Nuclear Material. In: Proceedings of Advances in Nuclear Nonproliferation Technology and Policy Conference (ANTPC). American Nuclear Society, Santa Fe, NM, USA.

Mosher, S. W., Johnson, S. R., Bevill, A. M., Ibrahim, A. M., Daily, C. R., Evans, T. M., Wagner, J. C., Johnson, J. O., Grove, R. E., November 2015. ADVANTG—An Automated Variance Reduction Parameter Generator. Tech. Rep. ORNL/TM-2013/416, Rev. 1, Oak Ridge National Laboratory, Oak Ridge, TN, USA.

Riper, K. A. V., Urbatsch, T. J., Soran, P. D., Parsons, K., Morel, J. E., McKinney, G. W., Lee, S. R., Crotzer, L. A., Alcouffe, R., Brinkley, F. W., Booth, T. E., Anderson, J., 1997. AVATAR — Automatic Variance Reduction In Monte Carlo Calculations. Tech. Rep. LA-UR-97-0919, Los Alamos National Laboratory.

# References

Solomon, C. J., 2010. Discrete-Ordinates Cost Optimization Of Weight-Dependent Variance Reduction Techniques For Monte Carlo Neutral Particle Transport. Ph.D. thesis, Kansas State University.

Solomon, C. J., Sood, A., Booth, T. E., Shultis, J. K., 2014. A Priori Deterministic Computational-Cost Optimization Of Weight-Dependent Variance-Reduction Parameters For Monte Carlo Neutral-Particle Transport. Nuclear Science and Engineering 176 (1), 1–36.

Turner, S. A., Larsen, E. W., September 1997. Automatic Variance Reduction for Three-Dimensional Monte Carlo Simulations by the Local Importance Function Transform—I: Analysis. Nuclear Science and Engineering 127 (1), 22–35.

Wagner, J. C., Haghighat, A., 1998. Automated Variance Reduction Of Monte Carlo Shielding Calculations Using The Discrete Ordinates Adjoint Function. Nuclear Science and Engineering 128, 186–208.