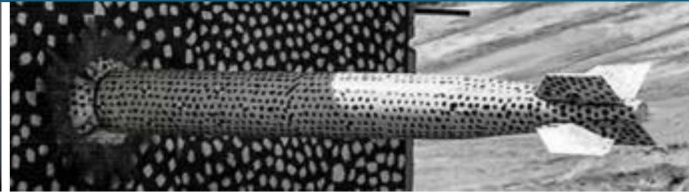
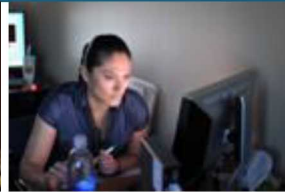




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SAND2019-6232C

Calculation of Parametric Variance using Variance Deconvolution



PRESENTED BY

Aaron Olson



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Introduction



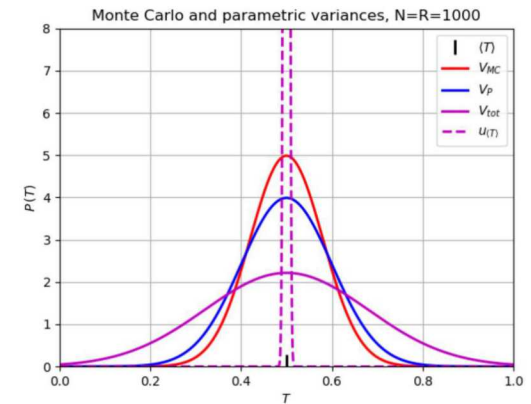
Big idea:

- Can compute **parametric variance** by computing **total variance** and **Monte Carlo variance** and taking the difference:

$$V_P = V_{tot} - V_{MC}$$

Two implementations of idea:

- VAriance DEconvolution (VADE) – non-intrusive
- Embedded VAriance DEconvolution (EVADE) – intrusive



Why Care:

- Often want V_P , but with Monte Carlo transport solver V_{MC} gets mixed in, need a way to separate, especially for small N
- Computational efficiency gains
- Groundwork for stochastic media model yielding variance caused by mixing

Mean, Variance, and Uncertainty



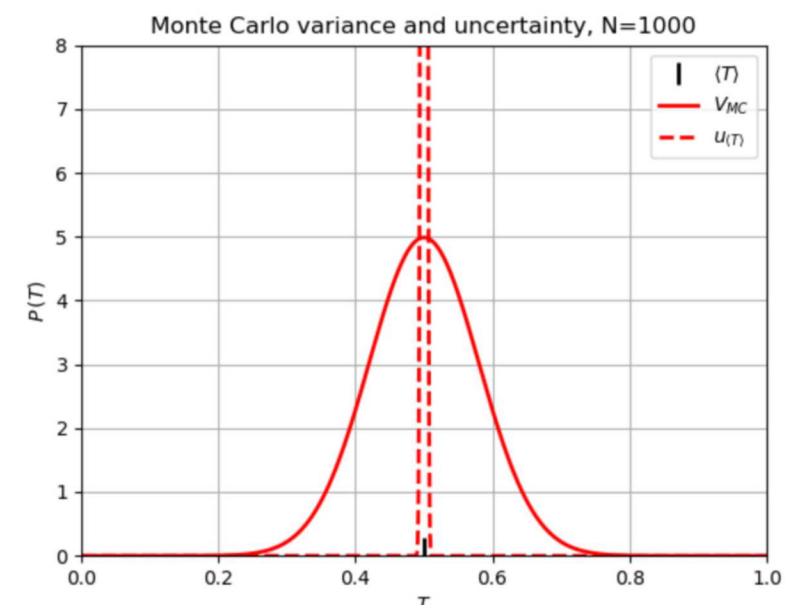
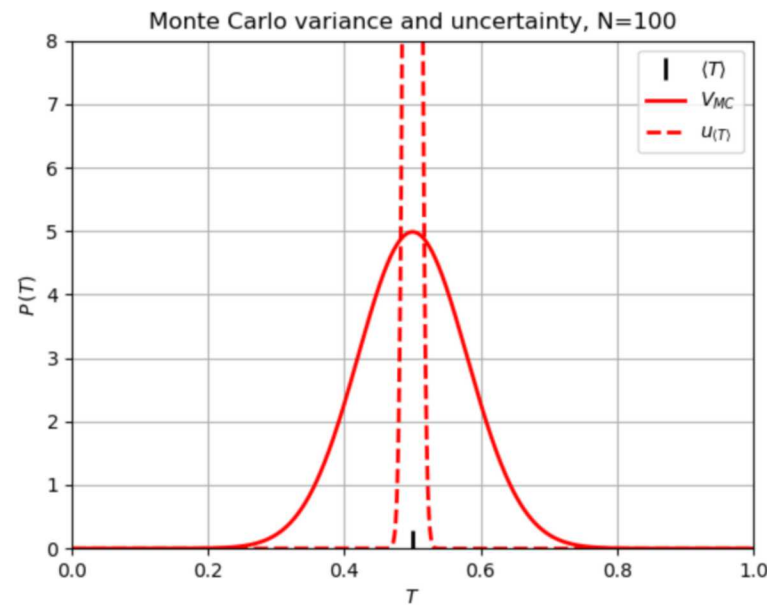
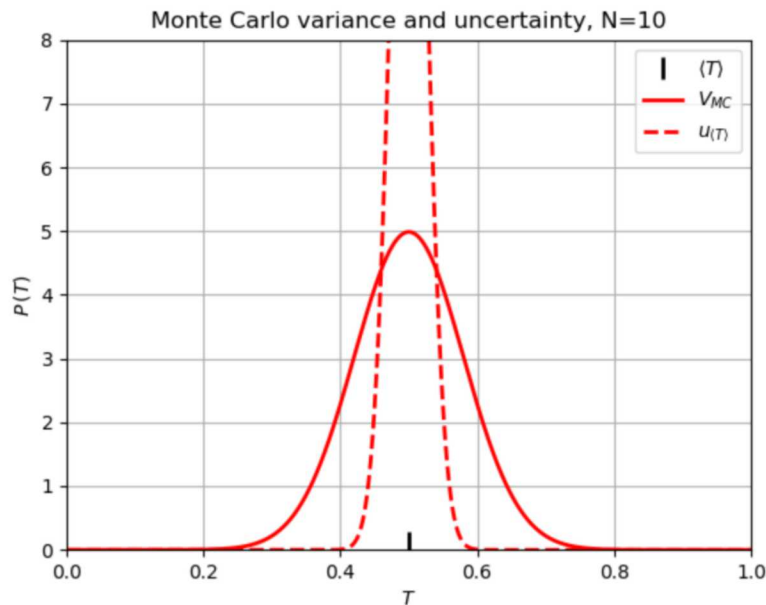
Monte Carlo transport is a stochastic process that yields **variance** even if problem is deterministic

- “Monte Carlo variance”: V_{MC}
 - constant for problem/solver combo (“variance reduction” reduces this)
- “Monte Carlo uncertainty”: u_{MC}
 - decreases with more samples (histories)

“Monte Carlo statistical uncertainty”
 “Standard deviation of the mean”
 “Standard error of the mean”

$$u_{MC} = \frac{\sqrt{V_{MC}}}{\sqrt{N}}$$

“Monte Carlo variance”
 “Variance of the distribution”
 “Leading coefficient of convergence”



Figures demonstrate that u_{MC} shrinks with more histories (10, 100, 1000) whereas V_{MC} is constant for a problem/solver combination

Monte Carlo, Parametric, and Total Variances

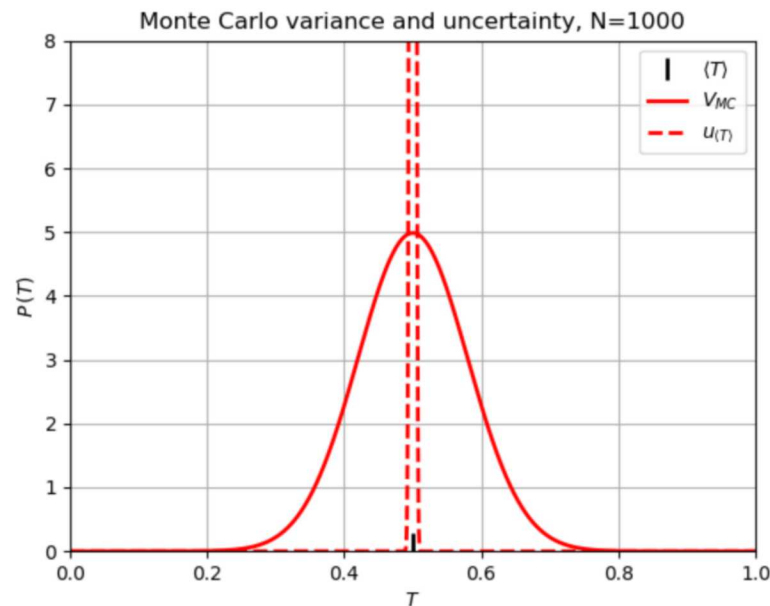


Monte Carlo can be used as **transport solver** or to resolve the **effects of random parameters**

- “**MC**” – Monte Carlo transport solver, “**N**” – number of histories per realization
- “**P**” – randomness described by input parameters, “**R**” – number of randomly sampled realizations

If no parametric randomness

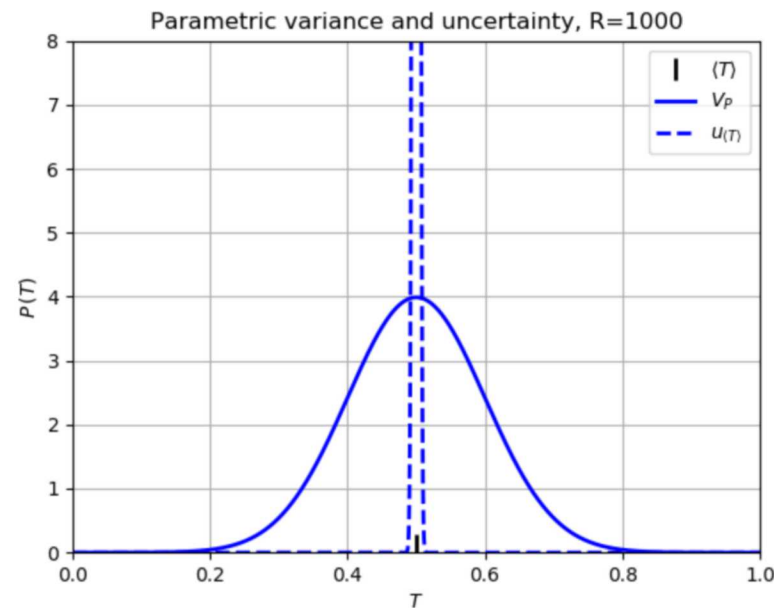
$$u_{MC} = \frac{\sqrt{V_{MC}}}{\sqrt{N}}$$



Monte Carlo variance and uncertainty

If no solver uncertainty

$$u_P = \frac{\sqrt{V_P}}{\sqrt{R}}$$

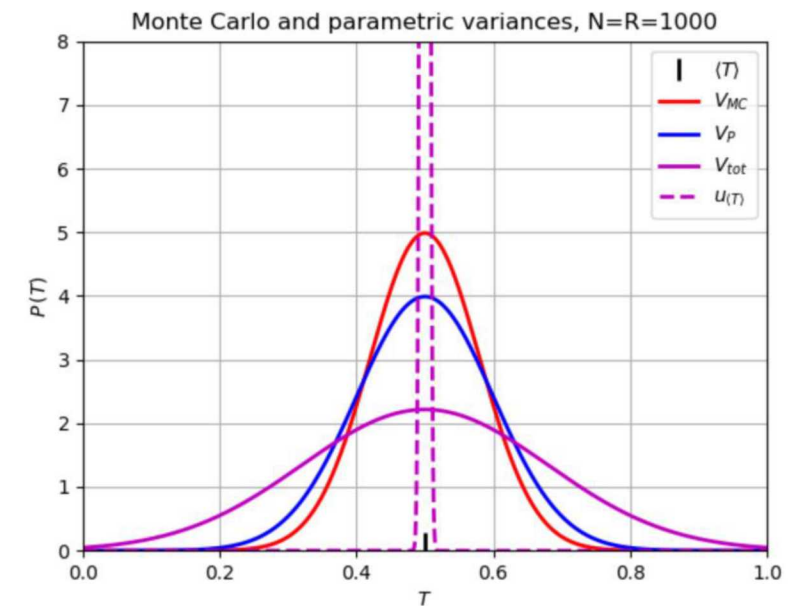


Parametric variance and uncertainty

If parametric randomness and solver uncertainty

$$u_{tot}^2 = u_{MC}^2 + u_P^2$$

$$V_{tot} = V_{MC} + V_P$$



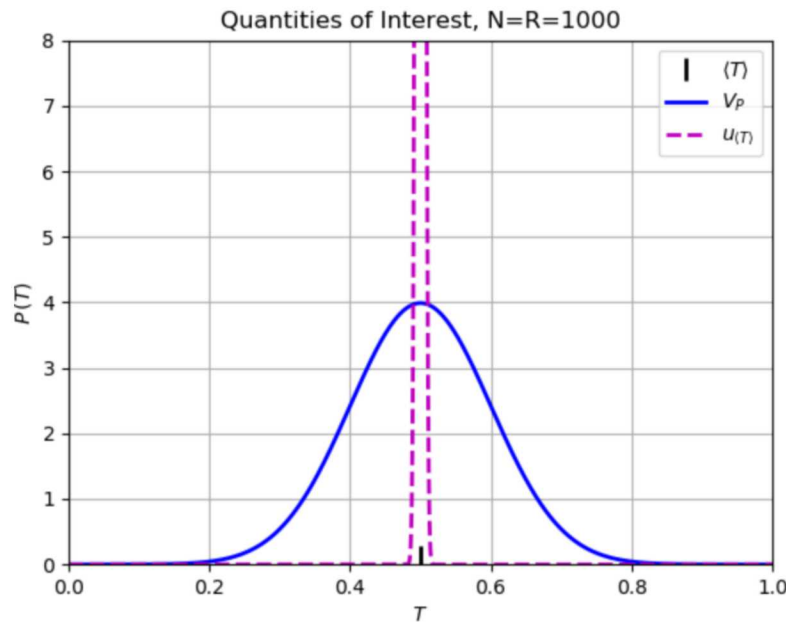
Total variance and uncertainty

Deconvolution of Variances for Parametric Variance



What we really want:

- $\langle T \rangle \pm u_{tot}$
- $V_P \pm u_{V_P}$



Common quantities of interest

Main idea:

- Solve for V_{tot} and V_{MC} separately and deconvolve to get V_P ($V_P = V_{tot} - V_{MC}$)

Supporting ideas:

- Use batches to get u_{tot} and u_{V_P}
- Expand analytic/semi-analytic benchmarks for test problems
- $N=1$ convenient path to solving V_{tot} (naturally convolves variances)
- $N=2$ yields accurate estimates and is efficient

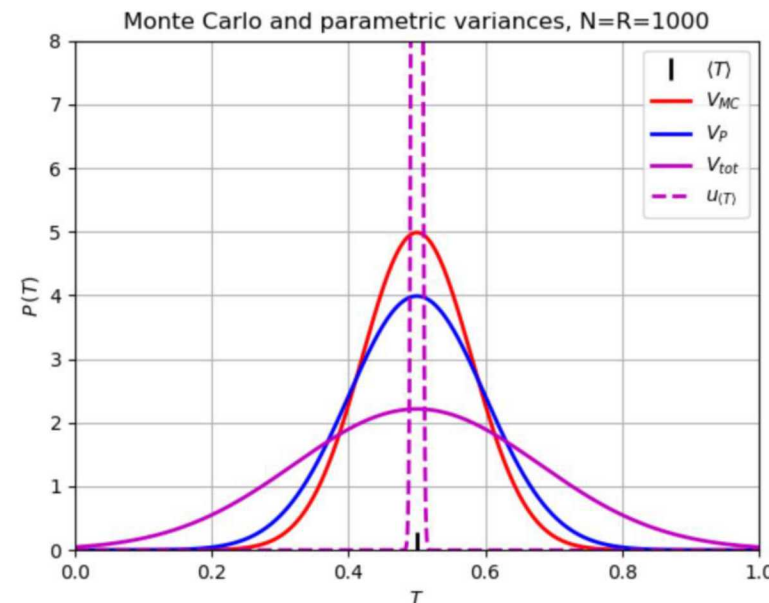


Diagram of V_P , V_{MC} , V_{tot} , and u_{tot}

Related Work (Stochastic Media Applications)



Adams et. al, JQSRT, 1989 (**deterministic solver**)

- Computed u_{tot} ($u_{tot} = u_P$ since deterministic solver)
- Computed V_P ($V_{tot} = V_P$ since deterministic solver)
- Crude estimate for u_{V_P}

Donovan et. al, NSE, 2003 (MC solver, $N = 1$)

- Computed V_{tot} and u_{tot} (straightforward since $N = 1$)

Donovan et. al, M&C, 2003 (MC solver, $N \gg 1$)

- Computed u_{tot} using $u_{tot}^2 = u_{MC}^2 + u_P^2$
- To estimate u_P , assumed $V_P \gg u_{MC}$ (good if $N \gg 1$)
- Computed, **but didn't report** values for V_{MC} and V_P

Larmier et. al, JQSRT, 2018 (MC solver)

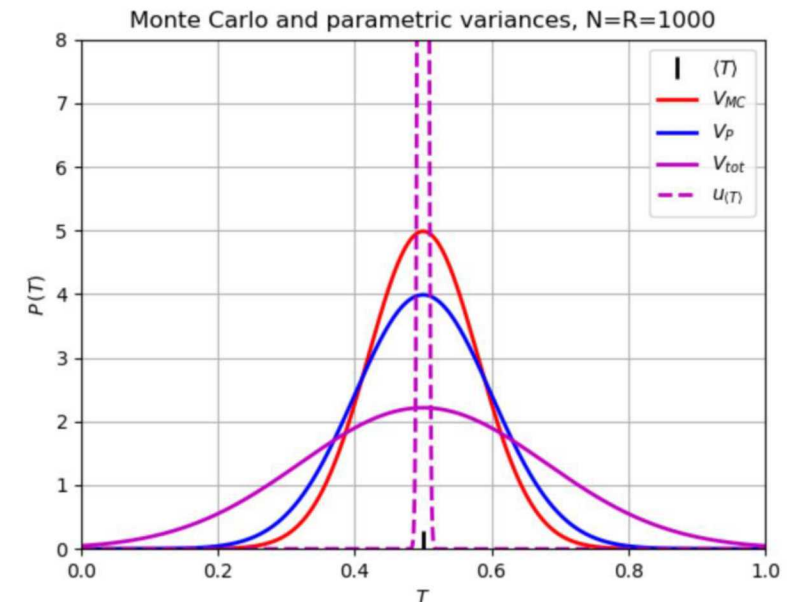
- Approaches same as Donovan's

What we want:

- $\langle T \rangle \pm u_{tot}$
- $V_P \pm u_{V_P}$

New:

- Compute V_P w/ MC, no assumption, small N
- Rigorously compute u_{tot} and u_{V_P}

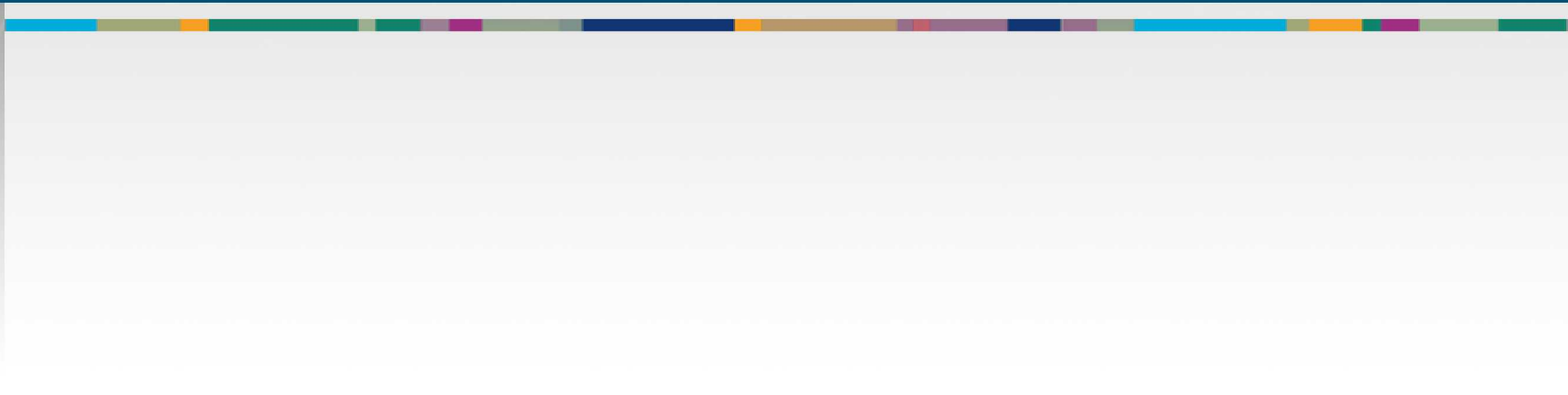


Goal: Improved methods for uncertainty quantification and stochastic media with Monte Carlo transport

Acronyms		Random Variables (r.v.)/ Stochastic Media (s.m.)		Takeaway(s)
Olson, ANS, 2017		r.v.	(s.m.)	<ul style="list-style-type: none"> Characterize MC/parametric convergence Analytic benchmark
Olson, ANS, 2018	Optimal-Cost Monte Carlo (OCMC)	(r.v.)	s.m.	<ul style="list-style-type: none"> Optimize MC convergence for mean
Vu, ANS, 2019	Conditional Point Sampling (CoPS)		s.m.	<ul style="list-style-type: none"> New algorithm accurate in 1D
Olson, ANS, 2019	Embedded Variance Deconvolution (EVADE)	r.v.	(s.m.)	<ul style="list-style-type: none"> Method for computing parametric variance Expand benchmarks
Vu, M&C, 2019			s.m.	<ul style="list-style-type: none"> CoPS can use EVADE to compute parametric variance
Olson, M&C, 2019			s.m.	<ul style="list-style-type: none"> CoPS accurate for mean in multi-D



Variance Deconvolution Implementations



Computing Total Variance



Use (or only tally) one history per realization ($N = 1$)

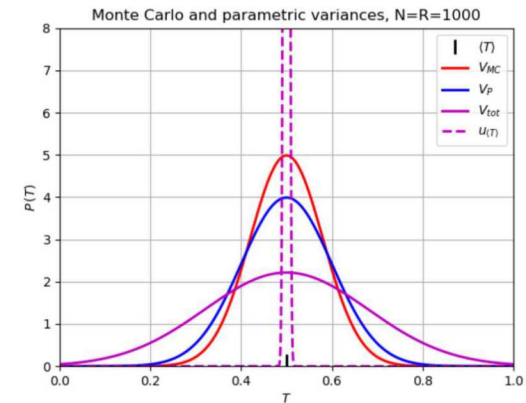
This convolves the effect of random variables and the Monte Carlo transport process

Compute (sample) **total variance** on results:

$$V_{tot} \approx \frac{R_{tot}}{R_{tot} - 1} (\langle T^2 \rangle - \langle T \rangle^2)$$

Mathematical justification:

- Propagation of parametric and Monte Carlo uncertainties on mean: $u_{tot}^2 = u_p^2 + u_{MC}^2$
- Relationship of parametric and Monte Carlo variances: $V_{tot} = V_p + V_{MC}$
- Combine to derive $u_{tot}^2 = \left(V_{tot} - \left(1 - \frac{1}{N} \right) V_{MC} \right) / R$
- When one history per realization ($N = 1$), $u_{tot}^2 = V_{tot} / R$
- Therefore V_{tot} is leading coefficient of uncertainty estimate that can be computed with moments of $N = 1$ transport computations



Computing Monte Carlo Variance

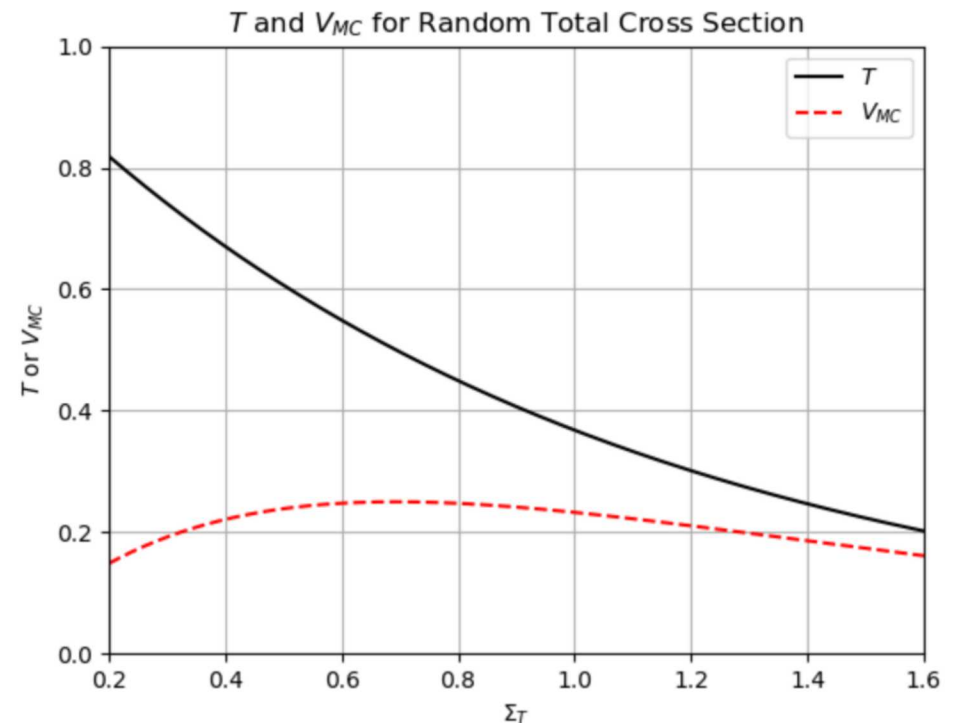
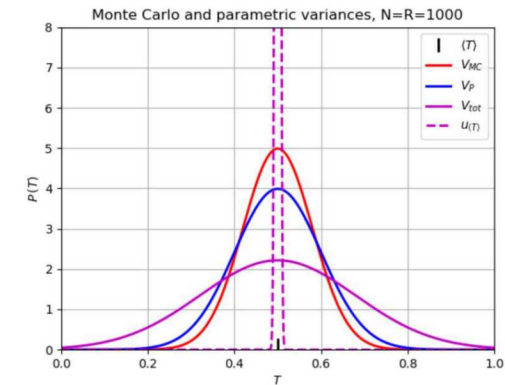
Monte Carlo variance for a realization r computed

$$V_{MC,r} \approx \frac{N_{MC}}{N_{MC} - 1} \left(\langle T^2 \rangle_{N_{MC,r}} - \langle T \rangle_{N_{MC,r}}^2 \right)$$

Monte Carlo variance is different for different problems, i.e., for different values of the random variables (see figure to right)

Must compute the average Monte Carlo variance over the uncertainty space:

$$V_{MC} \approx \frac{1}{R_{MC}} \sum_{r=1}^{R_{MC}} V_{MC,r}$$

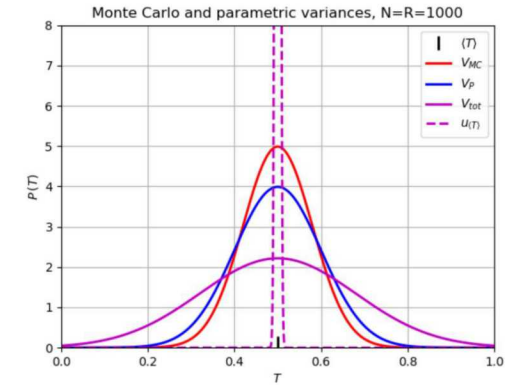


Transmittance and Monte Carlo variance of transmittance (analytically solved) as a function of random total cross section for a single-material attenuation problem. Demonstrates V_{MC} varying as a function of random variable.

Non-intrusive Implementation: VADE

Variance DEconvolution (VADE) – non-intrusive implementation

- (Can be implemented with existing transport solver and external scripting)



Task 1: Compute V_{MC}

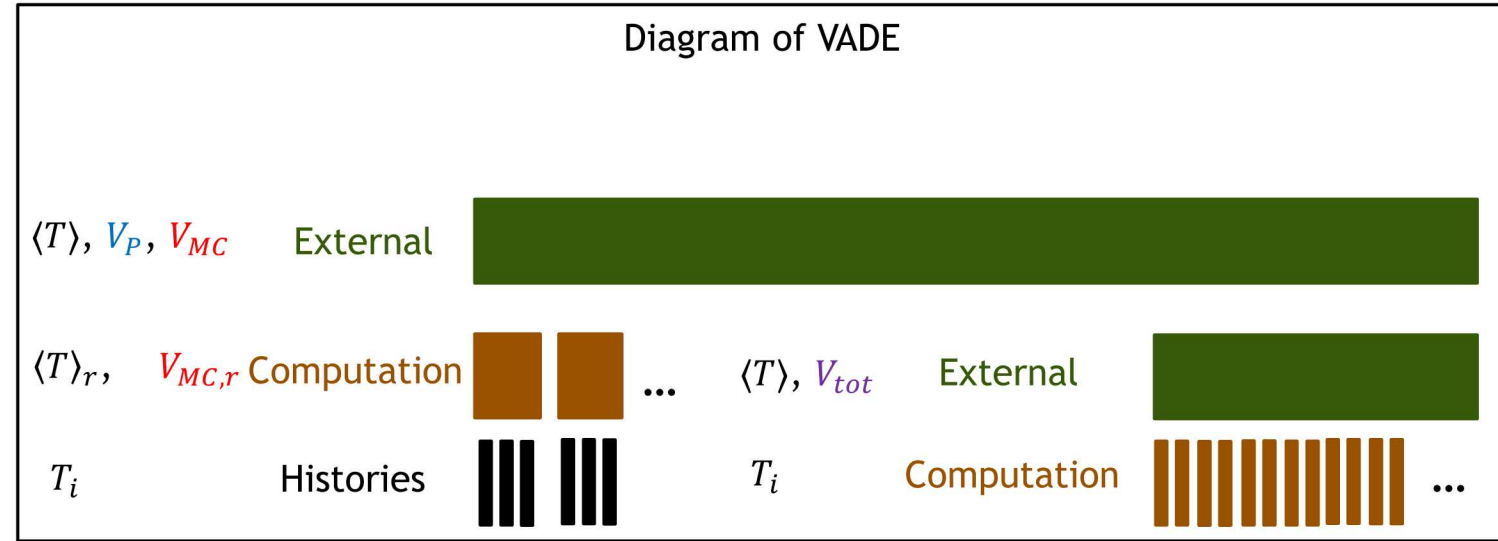
- Compute $V_{MC,r}$ on each of a collection of realizations with $N > 1$
- Take average of $V_{MC,r}$ for V_{MC}

Task 2: Compute V_{tot}

- Compute T_i on each of a collection of realizations with $N=1$
- Use these results to compute V_{tot}

Task 3: Compute V_P

- Use variance deconvolution to get V_P



Intrusive Implementation with Batches: EVADE

Embedded Variance DEconvolution (EVADE) – intrusive implementation

Compute u_{V_P} (and u_{tot}) using batches of realizations:

$$u_{V_P} = \frac{1}{B-1} \left(\langle V_P^2 \rangle_B - \langle V_P \rangle_B^2 \right); \quad u_{tot} = \frac{1}{B-1} \left(\langle \langle T \rangle^2 \rangle_B - \langle \langle T \rangle \rangle_B^2 \right)$$

Practically:

- Compute V_{tot} for batch tallying one history per realization in batch
- Compute V_{MC} and $\langle T \rangle$ for batch by averaging estimates from each realization in batch
- Compute V_P for that batch ($V_P = V_{tot} - V_{MC}$)
- Estimate $\langle V_P \rangle$ and $\langle T \rangle$ (and $\langle V_{tot} \rangle$ and $\langle V_{MC} \rangle$ if desired) and uncertainties over batches

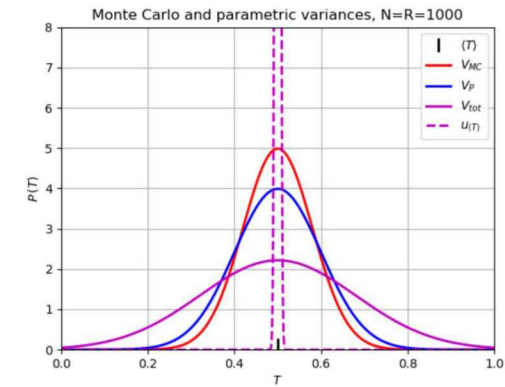


Diagram of EVADE

$\langle T \rangle, \langle V_P \rangle, \langle V_{tot} \rangle, \langle V_{MC} \rangle$
 $u_{tot}, u_{V_P}, u_{V_{tot}}, u_{V_{MC}}$

Computation



$\langle T \rangle, V_P, V_{tot}, V_{MC}$

Batches



$\langle T \rangle_r, V_{MC,r}$

Realization



T_i

Histories



Special Case Possible Values

If:

- Analog MC
- Leakage tally
- # Hist/realization = 2
- # Realization/batch = 2

Then:

$$\langle T \rangle \in [0,1], \langle V_P \rangle \in [-0.5,0.5], \langle V_{tot} \rangle \in [0,0.5], \langle V_{MC} \rangle \in [0,0.5]$$

Note: If $\langle V_{tot} \rangle \geq \langle V_{MC} \rangle : \langle V_P \rangle \in [0,0.5]$

$$\langle T \rangle \in \{0,0.25,0.5,0.75,1\}, \quad V_P \in \{-0.5, -0.25, 0, 0.25, 0.5\}, \\ V_{tot} \in \{0,0.5\}, \quad V_{MC} \in \{0,0.25,0.5\}$$

$$\langle T \rangle_r \in \{0,0.5,1\}, \quad V_{MC,r} \in \{0,0.5\}$$

$$T_i \in \{0,1\}$$



Expand Analytic/Semi-Analytic Benchmarks



Problem Description



Stochastic Transport Equation (attenuation physics only)

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

$$0 \leq x \leq L; \quad -1 \leq \mu \leq 1, \\ \psi(0, \mu) = \delta(1 - \mu), \mu > 0; \psi(L, \mu) = 0, \mu < 0$$

- x, μ, ω – spatial, angular, and stochastic dependence
- $\Sigma_t(x, \omega)$ – total cross section, source of uncertainty
- $\psi(x, \mu, \omega)$ – angular flux, response
- Beam source on “left” boundary, otherwise vacuum BCs
- Quantity of interest: Transmittance

Sources of parametric uncertainty (described on next slides)

- Random total cross sections
- Random material boundaries

Analytic Benchmark Random Cross Section Problem



Uniformly distributed random cross sections:

$$\Sigma_{t,m}(\omega) = \langle \Sigma_{t,m} \rangle + \widehat{\Sigma_{t,m}} \xi_m(\omega),$$

$$\xi_m(\omega) \in U[-1,1] \quad \forall m \in \{1,2, \dots, M\}$$

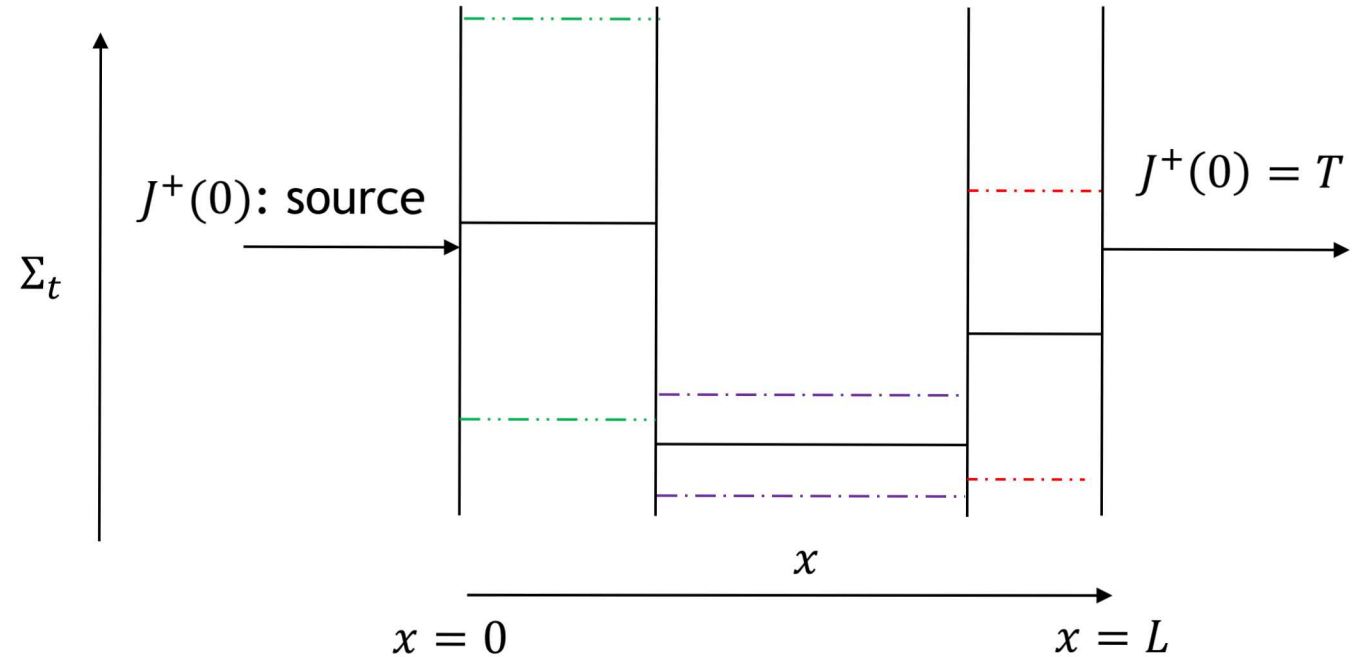
Analytic Transmittance (T) for realization ω :

$$T(\omega) = \exp[-\tau(\omega)]; \quad \tau(\omega) = \sum_{m=1}^M \Sigma_{t,m}(\omega) \Delta x_m$$

Analytic Moment of Expectation of Transmittance:

$$\mathbb{E}[T^p] = \int_{-1}^1 \dots \int_{-1}^1 T^p(\omega) \left(\frac{1}{2}\right)^M d\xi_1 \dots d\xi_M \Rightarrow$$

$$\mathbb{E}[T^p] = \prod_{m=1}^M \exp[-p \langle \Sigma_{t,m} \rangle \Delta x_m] \frac{\sinh[p \widehat{\Sigma_{t,m}} \Delta x_m]}{p \widehat{\Sigma_{t,m}} \Delta x_m}$$



Analytic Benchmark Random Boundary Location Problem

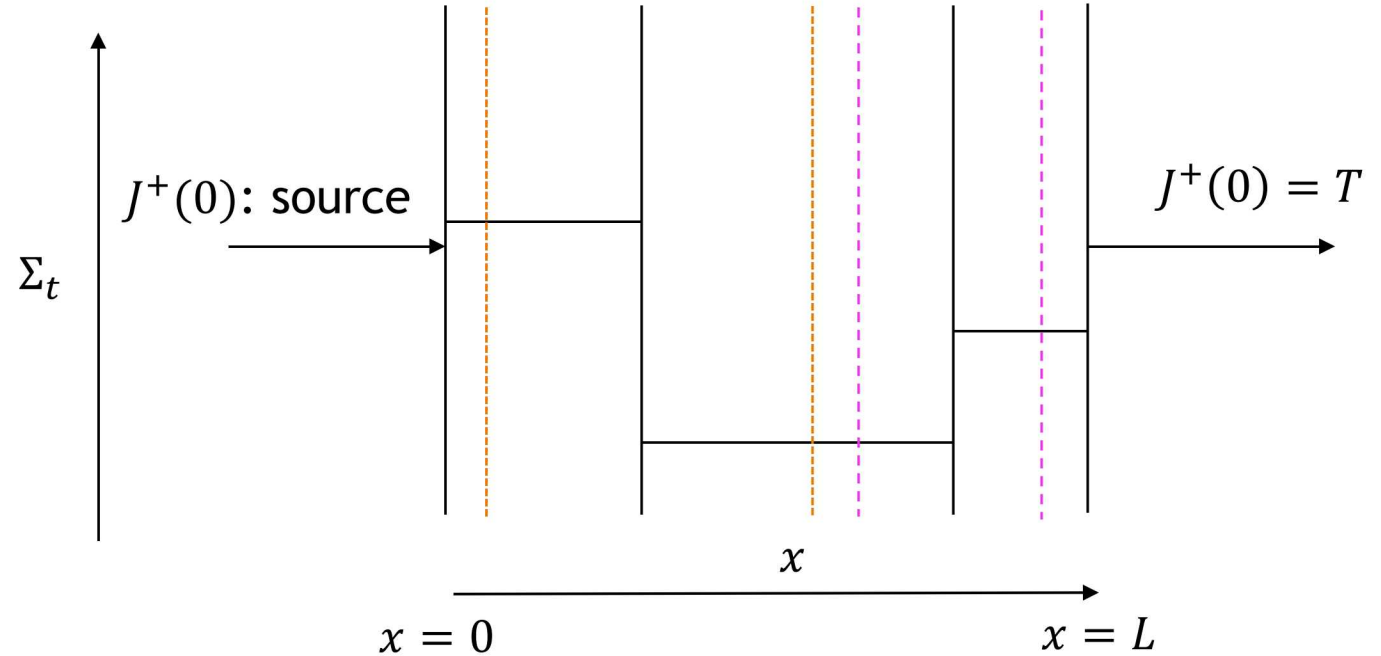


Uniformly distributed random boundary locations:

$$x_m(\omega) = \langle x_m \rangle + \widehat{x}_m \zeta_m(\omega),$$

$$\Delta x_m(\omega) = \begin{cases} x_1(\omega) & \text{if } m = 1 \\ x_m(\omega) - x_{m-1}(\omega) & \text{if } 1 < m < M \\ L - x_{M-1}(\omega) & \text{if } m = M \end{cases}$$

$$\zeta_m(\omega) \in U[-1,1] \quad \forall m \in \{1, 2, \dots, M-1\}$$



Analytic Transmittance (T) for realization ω :

$$T(\omega) = \exp[-\tau(\omega)]; \quad \tau(\omega) = \sum_{m=1}^M \Sigma_{t,m} \Delta x_m(\omega)$$

Analytic Moment of Expectation of Transmittance:

$$\mathbb{E}[T^p] = \int_{-1}^1 \dots \int_{-1}^1 T^p(\omega) \left(\frac{1}{2}\right)^M d\zeta_1 \dots d\zeta_{M-1} \Rightarrow$$

$$\mathbb{E}[T^p] = \left(\prod_{m=1}^M \exp[-p \langle \Sigma_{t,m} \rangle (\langle x_m \rangle - \langle x_{m-1} \rangle)] \right) \left(\prod_{m=1}^{M-1} \frac{\sinh[p(\langle \Sigma_{t,m-1} \rangle - \langle \Sigma_{t,m} \rangle) \widehat{x}_m]}{p(\langle \Sigma_{t,m-1} \rangle - \langle \Sigma_{t,m} \rangle) \widehat{x}_m} \right)$$

Semi-Analytic Benchmark for Problem with Both Uncertainty Sources



Uniformly distributed random cross sections and material boundary locations:

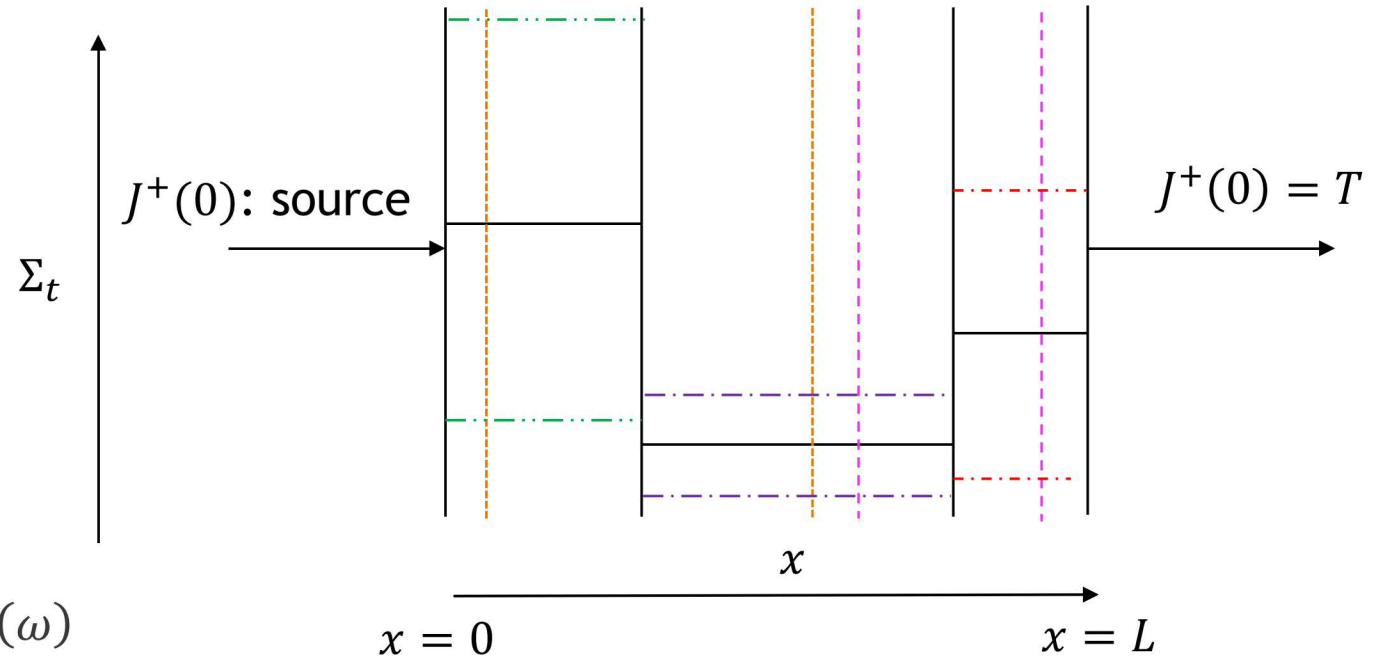
$$\Sigma_{t,m}(\omega) = \langle \Sigma_{t,m} \rangle + \widehat{\Sigma_{t,m}} \xi_m(\omega)$$

$$x_m(\omega) = \langle x_m \rangle + \widehat{x_m} \zeta_m(\omega)$$

$$\xi_m(\omega), \zeta_m(\omega) \in U[-1,1] \quad \forall m$$

Analytic Transmittance (T) for realization ω :

$$T(\omega) = \exp[-\tau(\omega)]; \quad \tau(\omega) = \sum_{m=1}^M \Sigma_{t,m}(\omega) \Delta x_m(\omega)$$



Semi-analytic Moment of Expectation of Transmittance (numerically integrate analytic cross section solution):

$$\mathbb{E}[T^p] = \int_{-1}^1 \dots \int_{-1}^1 T^p(\omega) \left(\frac{1}{2}\right)^{2M-1} d\xi_1 \dots d\xi_M d\zeta_1 \dots d\zeta_{M-1} \Rightarrow$$

$$\mathbb{E}[T^p] = \left(\frac{1}{2}\right)^{M-1} \int_{-1}^1 \dots \int_{-1}^1 d\zeta_1 \dots d\zeta_{M-1} \prod_{m=1}^M \exp[-p \langle \Sigma_{t,m} \rangle \Delta x_m(\omega)] \frac{\sinh[p \widehat{\Sigma_{t,m}} \Delta x_m(\omega)]}{p \widehat{\Sigma_{t,m}} \Delta x_m(\omega)}$$



Parametric variance

- Computed from analytic/semi-analytic moments:

$$V_p = \mathbb{E}[T^2] - \mathbb{E}^2[T]$$

Total Variance

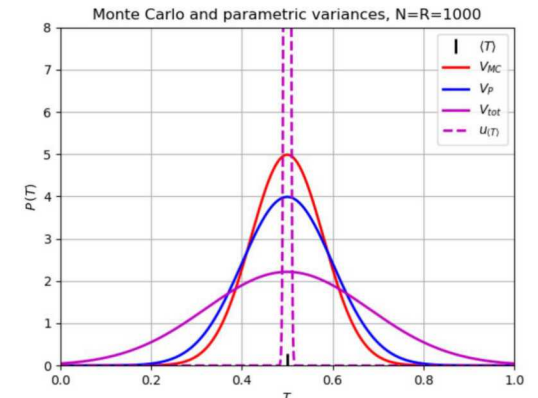
- With analog Monte Carlo and one history per realization, all tallies T_r are either 0 or 1 such that all tallied moments are the same: $\langle T \rangle_{R_{tot}} = \langle T^p \rangle_{R_{tot}} \forall p$
- In the limit of many realizations, the Monte Carlo simulation yields the expected value: $\lim_{R_{tot} \rightarrow \infty} \langle T \rangle_{R_{tot}} = \mathbb{E}[T]$
- The limit of the Monte Carlo computation thus yields an analytic solution for variance based on analytic/semi-analytic moments:

$$V_{tot} = \lim_{R_{tot} \rightarrow \infty} \frac{R_{tot}}{R_{tot} - 1} (\langle T^2 \rangle - \langle T \rangle^2) = \mathbb{E}[T] - \mathbb{E}^2[T]$$

Monte Carlo Variance

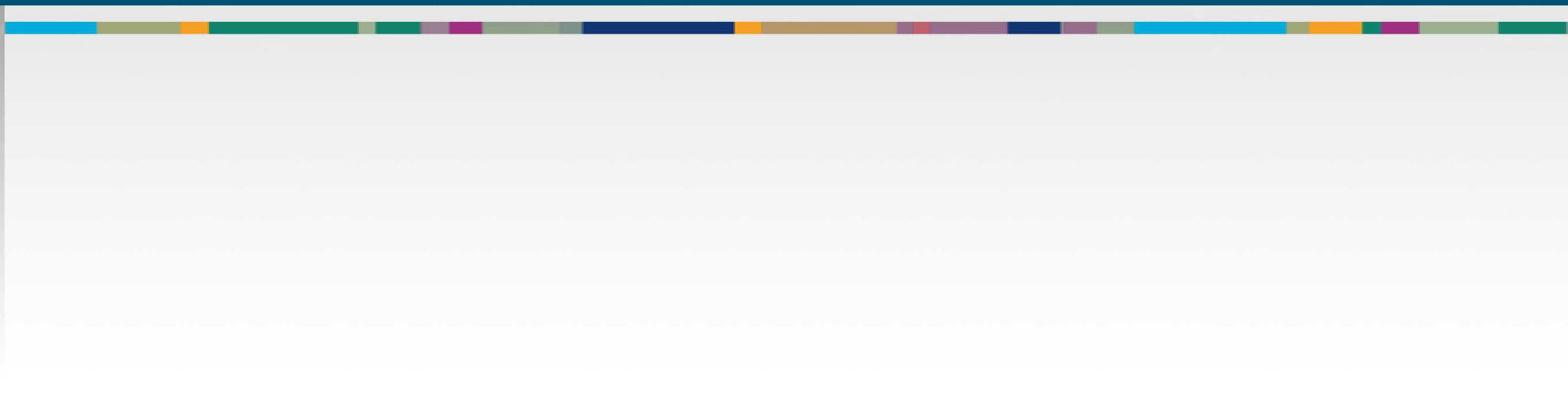
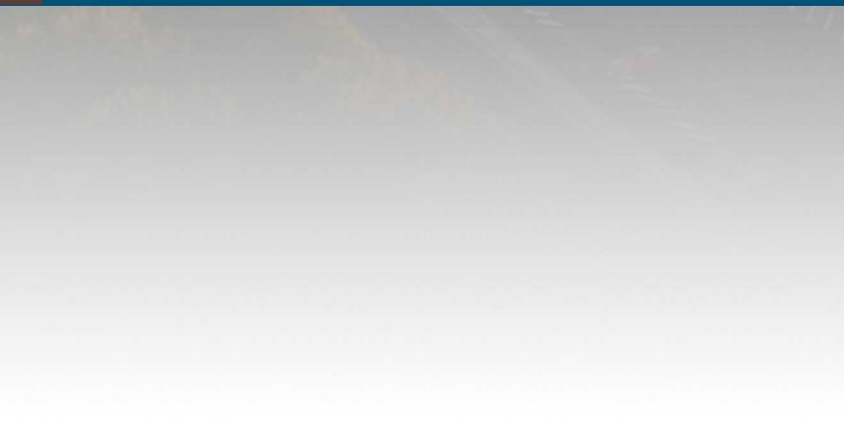
- Using variance deconvolution:

$$V_{MC} = V_{tot} - V_p = \mathbb{E}[T] - \mathbb{E}[T^2]$$





Numerical Results



Description of Problems



Problem 1: Cross Sections are Random Variables

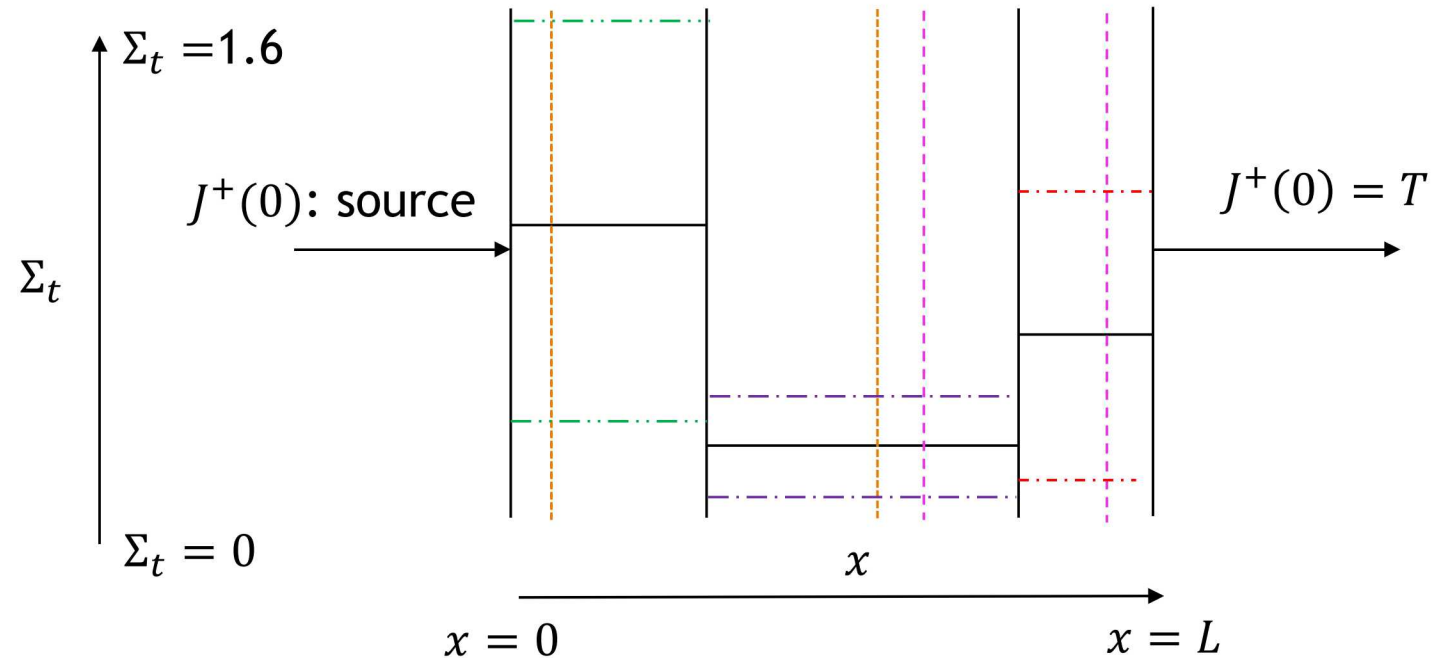
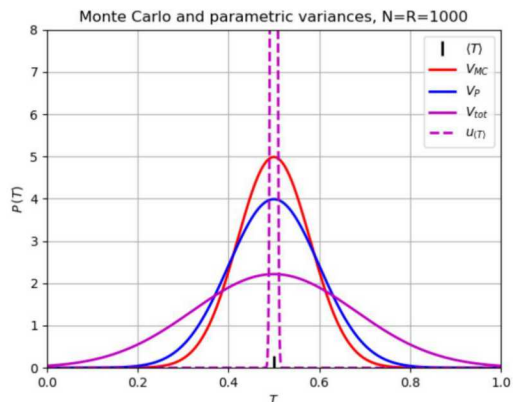
Problem 2: Boundary Locations are Random Variables

Problem 3: Both quantities are Random Variables

All problems use parameters in table

TABLE I. Stochastic Attenuation Problem Parameters

	$m = 0$	$m = 1$	$m = 2$	$m = 3$
$\langle \Sigma_{t,m} \rangle$	-	0.9	0.15	0.6
$\widehat{\Sigma}_{t,m}$	-	0.7	0.12	0.5
$\langle x_m \rangle$	0.0	2.0	5.0	6.0
\widehat{x}_m	-	1.75	0.95	-





VADE and EVADE both accurate for each quantity on each problem type

TABLE II. Higher-Fidelity Solver Parameters

VADE		EVADE	
$R_{tot} = 10^8$	$R_{MC} = 10^4$	$R_{tot} = R_{MC} = 10^8$	
$N_{tot} = 1$	$N_{MC} = 10^4$	$N_{tot} = 1$	$N_{MC} = 2$
$B = N/A$		$B = 5 \times 10^7$	
$N_{TOT} = 2 \times 10^8$		$N_{TOT} = 2 \times 10^8$	

TABLE III. Higher-Fidelity Simulation Representative Results

Random Cross Sections			
Quantity	Analytic	VADE	EVADE
$\langle T \rangle$	0.083783	0.083981	0.083773 ± 0.000020
V_P	0.005505	0.005637	0.005509 ± 0.000022
V_{tot}	0.076763	0.076749	0.076762 ± 0.000026
V_{MC}	0.071259	0.071112	0.071253 ± 0.000018
Random Boundaries			
Quantity	Analytic	VADE	EVADE
$\langle T \rangle$	0.078277	0.078828	0.078314 ± 0.000020
V_P	0.003731	0.002782	0.003734 ± 0.000021
V_{tot}	0.072150	0.072140	0.072176 ± 0.000025
V_{MC}	0.068419	0.069358	0.068442 ± 0.000017
Random Cross Sections and Boundaries			
Quantity	Semi-An.	VADE	EVADE
$\langle T \rangle$	0.104428	0.103672	0.104398 ± 0.000023
V_P	0.010069	0.011029	0.010097 ± 0.000024
V_{tot}	0.093523	0.093503	0.093532 ± 0.000028
V_{MC}	0.083454	0.082474	0.083435 ± 0.000019

EVADE uncertainty estimates accurate for each quantity ($\epsilon < u \sim 68\%$ of time)

EVADE \sim an order of magnitude more precise than VADE for three quantities (including two target quantities)

VADE $\sim 25\%$ more precise than EVADE for total variance – effect of batching?

TABLE IV. Lower-Fidelity Solver Parameters

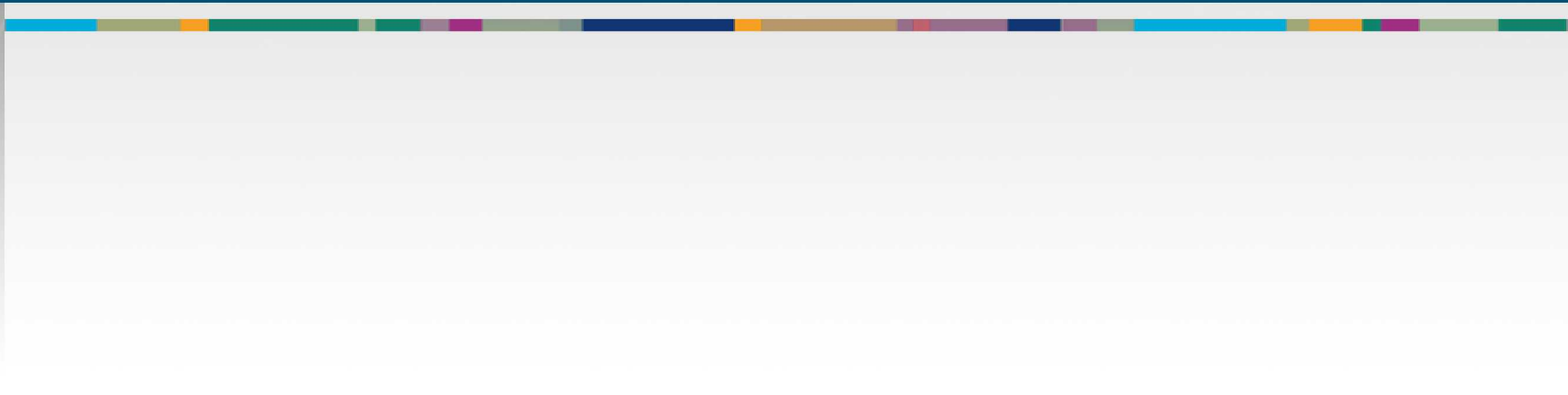
VADE		EVADE	
$R_{tot} = 10^5$	$R_{MC} = 10^2$	$R_{tot} = R_{MC} = 10^5$	
$N_{tot} = 1$	$N_{MC} = 10^3$	$N_{tot} = 1$	$N_{MC} = 2$
$B = N/A$		$B = 5 \times 10^4$	
$N_{TOT} = 2 \times 10^5$		$N_{TOT} = 2 \times 10^5$	

TABLE V. Lower-Fidelity Simulation Ensemble Results

Random Cross Sections				
Quantity	$\langle \epsilon \rangle_{VADE}$	$\langle \epsilon \rangle_{EVADE}$	$\langle u \rangle_{EVADE}$	$\epsilon < u$
$\langle T \rangle$	0.00375	0.00052	0.00064	668/1000
V_P	0.00551	0.00054	0.00068	673/1000
V_{tot}	0.00052	0.00065	0.00081	681/1000
V_{MC}	0.00550	0.00044	0.00055	681/1000
Random Boundaries				
Quantity	$\langle \epsilon \rangle_{VADE}$	$\langle \epsilon \rangle_{EVADE}$	$\langle u \rangle_{EVADE}$	$\epsilon < u$
$\langle T \rangle$	0.00333	0.00049	0.00062	658/1000
V_P	0.00525	0.00053	0.00065	674/1000
V_{tot}	0.00053	0.00065	0.00079	661/1000
V_{MC}	0.00521	0.00043	0.00054	682/1000
Random Cross Sections and Boundaries				
Quantity	$\langle \epsilon \rangle_{VADE}$	$\langle \epsilon \rangle_{EVADE}$	$\langle u \rangle_{EVADE}$	$\epsilon < u$
$\langle T \rangle$	0.00468	0.00058	0.00072	681/1000
V_P	0.00621	0.00059	0.00077	702/1000
V_{tot}	0.00057	0.00069	0.00087	707/1000
V_{MC}	0.00620	0.00047	0.00059	685/1000



Conclusions and Future Work



Deconvolution of variance to get V_P with Monte Carlo solver and no $V_P \gg u_{MC}$ assumption

- non-intrusively (VADE), intrusively (EVADE)
- for three r.v. problem types

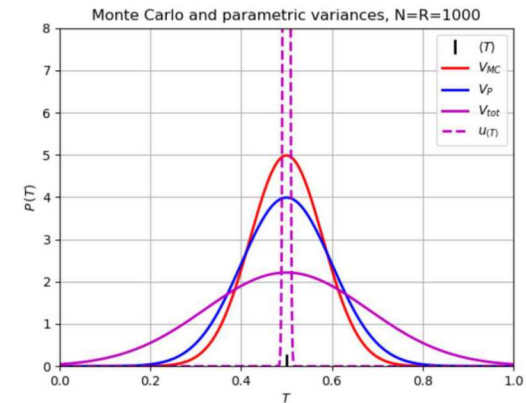
Use of batches to accurately get u_{tot} and u_{V_P} (in EVADE)

Deconvolution demonstrated w/ $N=2$ (in EVADE)

- more precise than $N>2$ (in VADE)
- $N=2$ optimized?

Analytic benchmarks expanded

- Random boundary location problem (analytic)
- Random cross section and boundary location problem (semi-analytic)
- V_P , V_{tot} , and V_{MC} (analytic)





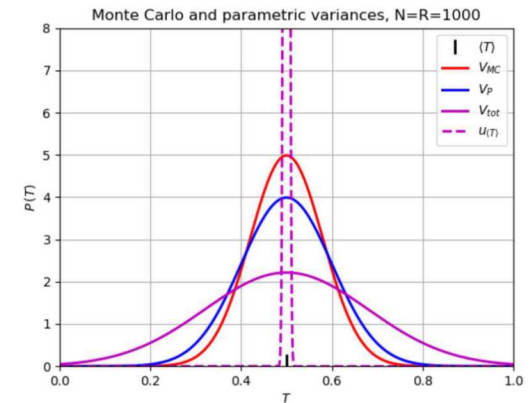
Why V_{tot} more precise in VADE than EVADE (effect of batches?)

Optimal-Cost Monte Carlo (OCMC) analysis for V_P

- $N=2$ optimal?
- $N=1$ for some realizations, $N=2$ for others?

Apply to stochastic media problems:

- EVADE with CoPS for V_P (Vu, M&C, 2019)
- Problems with both traditional r.v.s and stochastic media
- V_{tot} with one model and V_{MC} with a different one (VADE)
 - (e.g., V_{tot} using chord length sampling, V_{MC} using realizations)



Ron Kensek – for sharing with me his idea to “deconvolve” the total variance into the Monte Carlo and parametric variances ($V_{tot} = V_p + V_{MC}$)

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