

LA-UR-19-28572

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Intended for: MC2019, 2019-08-25/2019-08-29 (Portland, Oregon, United States)

Issued: 2019-09-12 (rev.1)

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Predicting Monte Carlo Tally Variance and Calculation Time when Using Forced-flight Variance Reduction—Verification

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American Nuclear Society

International Conference on Mathematics and Computational Methods applied
to Nuclear Science and Engineering (M&C 2019)

August 25–29, 2019

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

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Implementation

- Software Overview

- Monte Carlo Time Profiling

Test Case Descriptions & Results

- 1-D, Monoenergetic, Heterogeneous, Surface Source, Leakage-current Tally

- 1-D, Two-group, Heterogeneous, Distributed Source, Track-length Tally

- 2-D, Right-angle Duct, Leakage-current Tally, Configuration A

- 2-D, Right-angle Duct, Leakage-current Tally, Configuration B

- 2-D Results Additional Discussion

Summary & Future Work

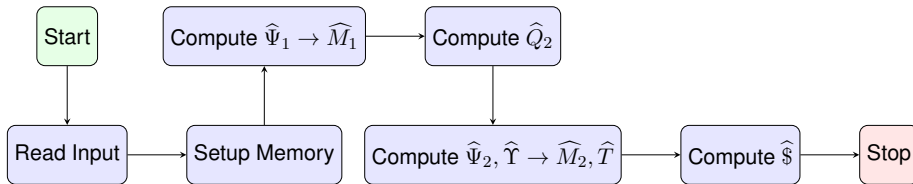
Objective: Numerically solve the forced-flight history-score moment and future-time equations

- ▶ Previously derived the forced-flight HSMEs and FTE
- ▶ This work builds upon the COVRT software (Solomon, 2010)
- ▶ COVRT originally solved:
 - ▶ Cell-based importance splitting and rouletting
 - ▶ Implicit capture & weight cutoff (rouletting)
 - ▶ Weight windows
- ▶ New work:
 - ▶ Modified transport sweep to account for forced-flight particle creation
 - ▶ Python-based interface to optimization (generally out of scope)

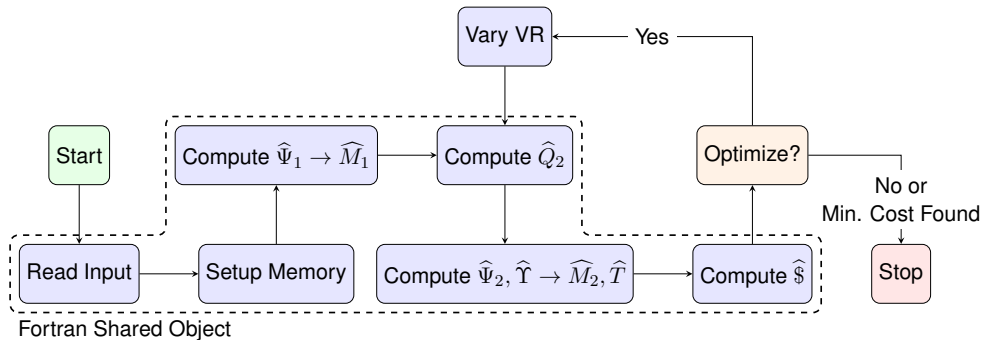
Implementation Overview

- ▶ Forced-flight HSMEs and FTE added to COVRT
 - ▶ COVRT: **C**ost-**O**ptimized **V**ariance **R**eduction **T**echnique
 - ▶ Cartesian multi-group discrete ordinates HSME & FTE solver
- ▶ Two approaches to solving the HSMEs and FTE
 - ▶ Explicitly separated and truncated moment
 - ▶ Combined moments and implicitly truncated moments
 - ▶ Eases combination with other variance reduction techniques
- ▶ COVRT is also bound to a Python driver via ctypes
 - ▶ Permits Python-based optimization
 - ▶ This work uses MADS-based optimization from NOMAD
 - ▶ (Audet et al., 2009; Le Digabel, 2011)
 - ▶ Tested other optimization algorithms
 - ▶ SLSQP, COBLYA, Basinhopping, Differential Evolution
 - ▶ Particle Swarm
 - ▶ Markov-chain Monte Carlo (MCMC)

Once-through COVRT Calculation Process

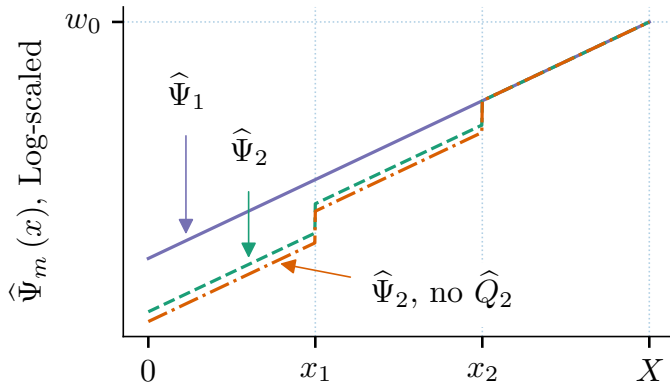


Python-driven Optimization Calculation Process



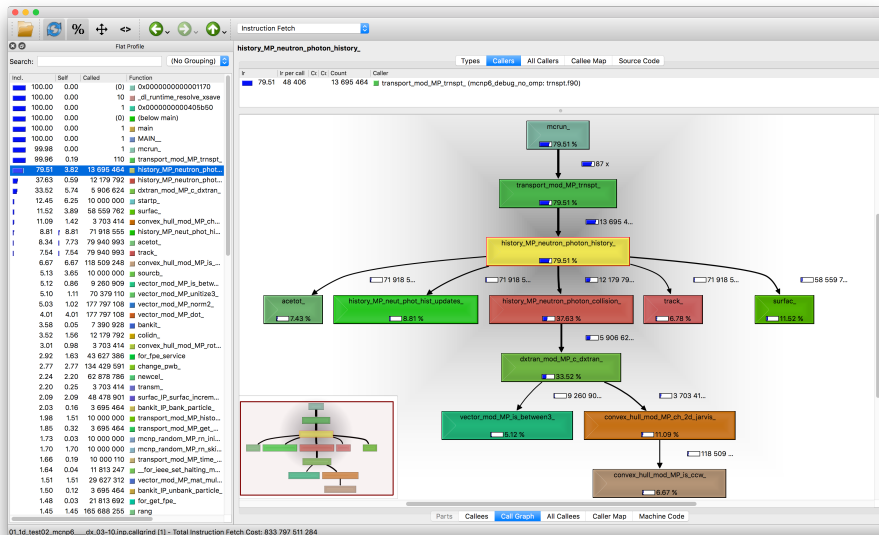
Solving for Moments

- ▶ The integral equations are recast into integro-differential form
- ▶ Solver for the HSMEs and FTE uses unaccelerated source iteration
- ▶ Complications can arise when computing \widehat{Q}_2 : the $\widehat{\Psi}_2$ source term
 - ▶ Detecting incorrect \widehat{Q}_2 can be difficult; differences can be subtle



Monte Carlo Time Profiling

- ▶ Future-time Equations require computational event times τ_{XS} , τ_{ff} , etc.
 - ▶ Specific to Monte Carlo code and problem definition
- ▶ Overall timing function somewhat insensitive to times
 - ▶ Relative trends are important to capture, accurate values less so
- ▶ The MCNP code is used for this work
 - ▶ Representative problems are used to compute event times
- ▶ Times are obtained with Valgrind's Callgrind (Weidendorfer et al., 2004; Nethercote and Seward, 2007)
 - ▶ The MCNP code is compiled with debugging symbols
 - ▶ Obtain: the total time to run the calculation and the number of instructions for each computational event
 - ▶ Assume: each instruction takes the same amount of time
 - ▶ Calculate: time per instruction for each computational event
 - ▶ Validate: compare Monte Carlo and deterministic cost-surfaces

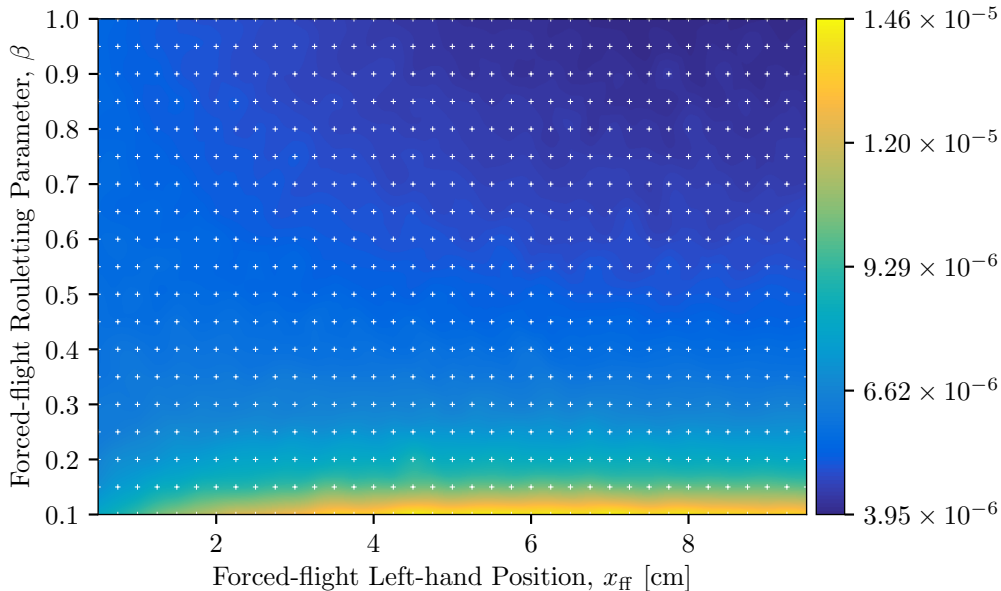


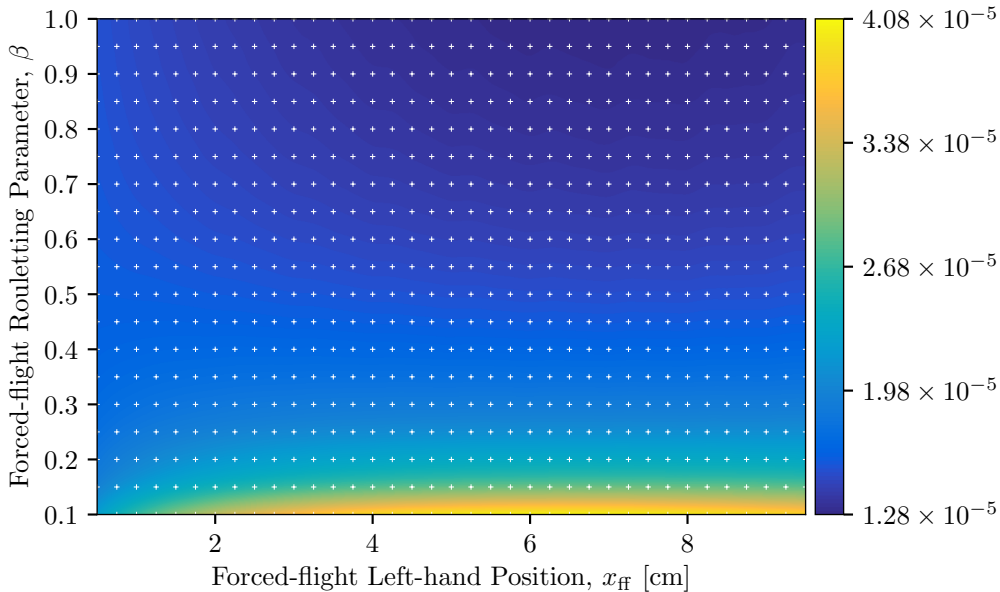
01_16_test02_mcnrp6_dx_03-10.np.callgrind [1] - Total Instruction Fetch Count: 833 797 511 284

| MCNP Routine | # Instructions | Time In Routine | Calls | Time Per Call |
|---------------------------------|----------------|-----------------------|----------|-----------------------|
| surfac | 87353373653 | 5.59 | 58559762 | 9.54×10^{-8} |
| bankit | 29833481748 | 1.91 | 7390928 | 2.58×10^{-7} |
| acetot | 69569700257 | 4.45 | 79940993 | 5.57×10^{-8} |
| transm | 18370101431 | 1.18 | 3703414 | 3.17×10^{-7} |
| track | 62894992419 | 4.02 | 79940993 | 5.03×10^{-8} |
| startp | 103766122730 | 6.64 | 10000000 | 6.64×10^{-7} |
| tally | 8718657535 | 5.58×10^{-1} | 2850356 | 1.96×10^{-7} |
| colidn | 29370590911 | 1.88 | 12179792 | 1.54×10^{-7} |
| mcnp_random_mp_rn_init_particle | 14418536758 | 9.23×10^{-1} | 10000000 | 9.23×10^{-8} |
| dxtran_mod_MP_c_dxtran | 261080123457 | 1.67×10^1 | 5906624 | 2.83×10^{-6} |
| cell_properties_MP_acetot_embed | 8264243712 | 5.29×10^{-1} | 8022438 | 6.59×10^{-8} |

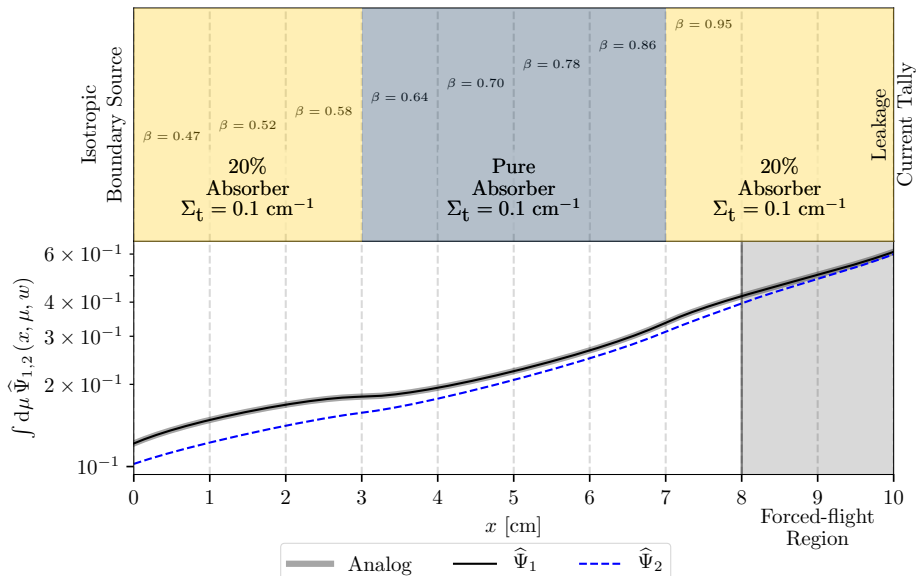
Obtained from a total of 833797511284 instructions in a 53.35 minute run.

| FTE Term | COVRT Input Variable | Value [min] | Note |
|-----------------------|----------------------|--------------------------|------------------------------|
| τ_{tally} | tally | 4.31506×10^{-7} | Reused from (Solomon, 2010). |
| τ_{col} | colidn | 1.52900×10^{-7} | Reused from (Solomon, 2010). |
| τ_{xs} | acetot | 8.45004×10^{-8} | — |
| τ_{geom} | track | 1.05709×10^{-7} | — |
| τ_{rt} | transm | 9.55000×10^{-8} | — |
| τ_{ff} | dxtran | 5.88000×10^{-7} | — |
| τ_{surf} | surfac | 4.39085×10^{-7} | — |
| τ_{bank} | bankit | 2.24612×10^{-7} | — |
| τ_{src} | startp | 1.34064×10^{-6} | — |





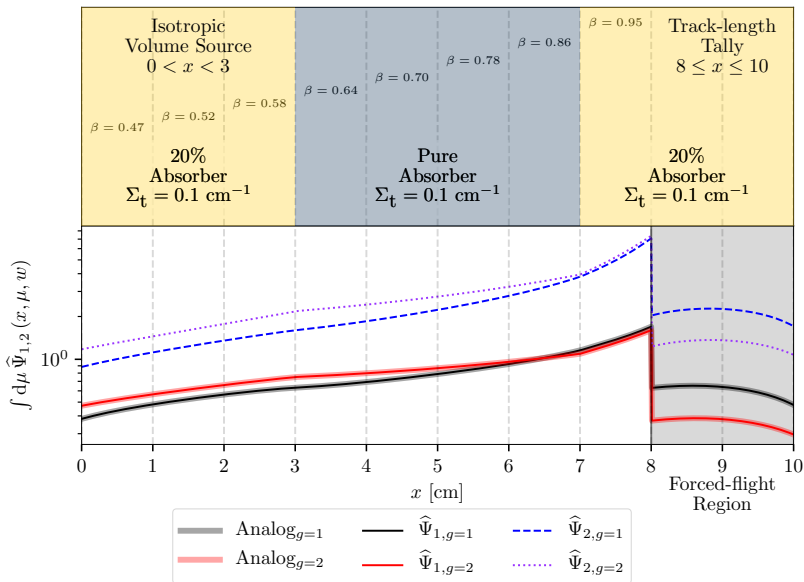
1-D, Surface Source, Leakage-current Tally



Various Forced-flight Locations

| x_{ff} [cm] | | MCNP6 | | COVRT | | MCNP6/COVRT | |
|---------------|------|------------------------|------------------------|------------------------|------------------------|-------------|----------|
| min. | max. | Mean | Variance | Mean | Variance | Mean | Variance |
| 0 | 10 | 1.216×10^{-1} | 1.068×10^{-1} | 1.215×10^{-1} | 1.067×10^{-1} | 1.00 | 1.00 |
| 1 | 10 | 1.216×10^{-1} | 9.892×10^{-2} | 1.215×10^{-1} | 9.885×10^{-2} | 1.00 | 1.00 |
| 2 | 10 | 1.216×10^{-1} | 9.471×10^{-2} | 1.215×10^{-1} | 9.463×10^{-2} | 1.00 | 1.00 |
| 3 | 10 | 1.216×10^{-1} | 9.211×10^{-2} | 1.215×10^{-1} | 9.205×10^{-2} | 1.00 | 1.00 |
| 4 | 10 | 1.216×10^{-1} | 9.139×10^{-2} | 1.215×10^{-1} | 9.135×10^{-2} | 1.00 | 1.00 |
| 5 | 10 | 1.216×10^{-1} | 9.071×10^{-2} | 1.215×10^{-1} | 9.067×10^{-2} | 1.00 | 1.00 |
| 6 | 10 | 1.216×10^{-1} | 9.013×10^{-2} | 1.215×10^{-1} | 9.007×10^{-2} | 1.00 | 1.00 |
| 7 | 10 | 1.215×10^{-1} | 8.958×10^{-2} | 1.215×10^{-1} | 8.954×10^{-2} | 1.00 | 1.00 |
| 8 | 10 | 1.216×10^{-1} | 8.757×10^{-2} | 1.215×10^{-1} | 8.750×10^{-2} | 1.00 | 1.00 |
| 9 | 10 | 1.216×10^{-1} | 8.658×10^{-2} | 1.215×10^{-1} | 8.653×10^{-2} | 1.00 | 1.00 |
| 10 | 10 | 1.216×10^{-1} | 8.651×10^{-2} | 1.215×10^{-1} | 8.648×10^{-2} | 1.00 | 1.00 |

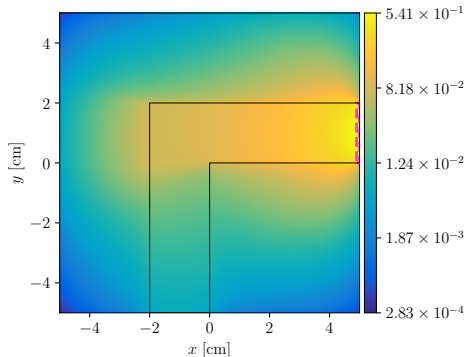
1-D, Distributed Source, Track-length Tally



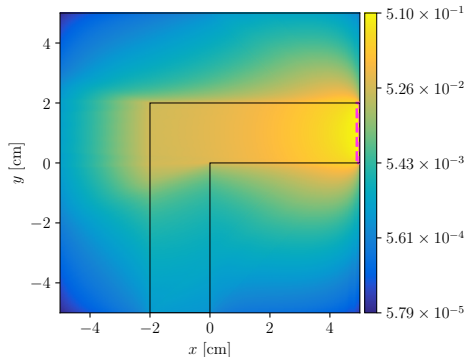
Various Forced-flight Locations

| x_{ff} [cm] | | MCNP6 | | COVRT | | MCNP6/COVRT | |
|---------------|------|------------------------|------------------------|------------------------|------------------------|-------------|----------|
| min. | max. | Mean | Variance | Mean | Variance | Mean | Variance |
| 0 | 10 | 5.210×10^{-1} | 1.400×10^0 | 5.198×10^{-1} | 1.382×10^0 | 1.00 | 1.01 |
| 1 | 10 | 5.210×10^{-1} | 1.316×10^0 | 5.198×10^{-1} | 1.300×10^0 | 1.00 | 1.01 |
| 2 | 10 | 5.211×10^{-1} | 1.223×10^0 | 5.198×10^{-1} | 1.209×10^0 | 1.00 | 1.01 |
| 3 | 10 | 5.212×10^{-1} | 1.138×10^0 | 5.198×10^{-1} | 1.126×10^0 | 1.00 | 1.01 |
| 4 | 10 | 5.211×10^{-1} | 1.114×10^0 | 5.198×10^{-1} | 1.104×10^0 | 1.00 | 1.01 |
| 5 | 10 | 5.210×10^{-1} | 1.092×10^0 | 5.198×10^{-1} | 1.084×10^0 | 1.00 | 1.01 |
| 6 | 10 | 5.210×10^{-1} | 1.073×10^0 | 5.198×10^{-1} | 1.066×10^0 | 1.00 | 1.01 |
| 7 | 10 | 5.209×10^{-1} | 1.052×10^0 | 5.198×10^{-1} | 1.046×10^0 | 1.00 | 1.01 |
| 8 | 10 | 5.212×10^{-1} | 9.798×10^{-1} | 5.198×10^{-1} | 9.688×10^{-1} | 1.00 | 1.01 |

2-D, Right-angle Duct, Configuration A



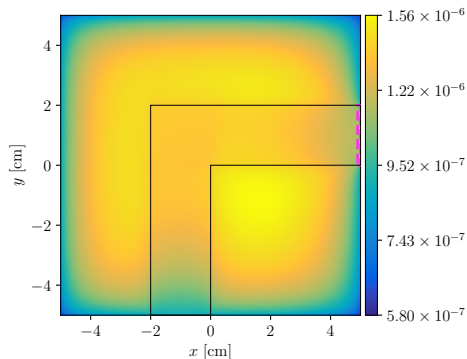
First HSME, $\hat{\Psi}_1$



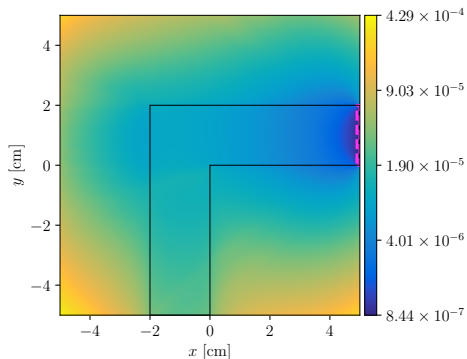
Second HSME, $\hat{\Psi}_2$

| MCNP6 | | COVRT | | MCNP6/COVRT | |
|------------------------|------------------------|------------------------|------------------------|-------------|----------|
| Mean | Variance | Mean | Variance | Mean | Variance |
| 5.418×10^{-3} | 5.388×10^{-3} | 5.583×10^{-3} | 5.552×10^{-3} | 0.97 | 0.97 |
| 5.450×10^{-3} | 1.062×10^{-3} | 5.583×10^{-3} | 1.052×10^{-3} | 0.98 | 1.01 |

2-D, Right-angle Duct, Configuration A, cont.



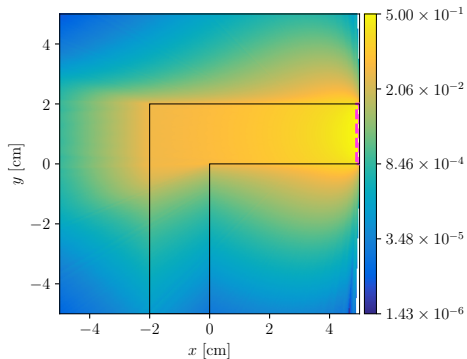
FTE, \hat{Y}



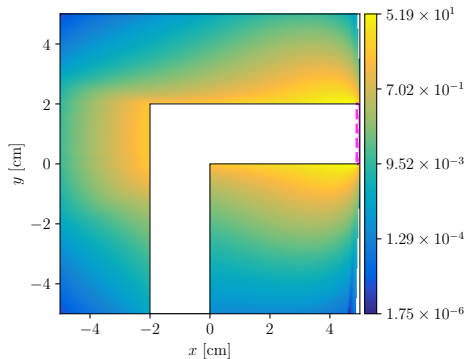
Cost, \hat{Y}

- ▶ Optimization predicted a 1% improvement; 2% degradation realized

2-D, Right-angle Duct, Configuration A, cont.

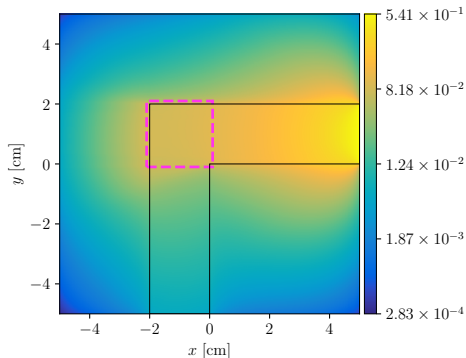


Free-flight Probability

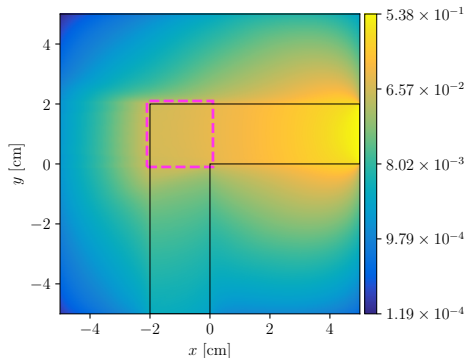


Source, \hat{Q}_2

2-D, Right-angle Duct, Configuration B



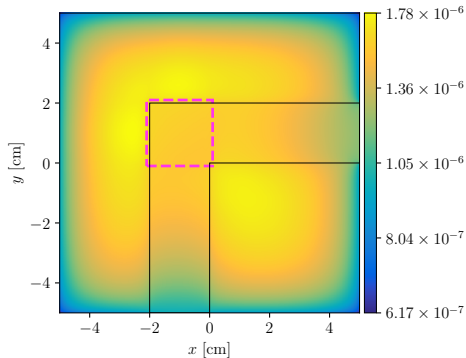
First HSME, $\hat{\Psi}_1$



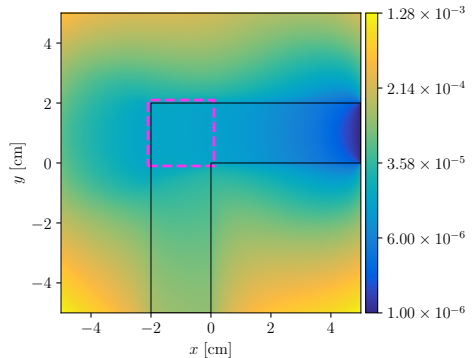
Second HSME, $\hat{\Psi}_2$

| MCNP6 | | COVRT | | MCNP6/COVRT | |
|------------------------|------------------------|------------------------|------------------------|-------------|----------|
| Mean | Variance | Mean | Variance | Mean | Variance |
| 5.418×10^{-3} | 5.388×10^{-3} | 5.583×10^{-3} | 5.552×10^{-3} | 0.97 | 0.97 |
| 5.413×10^{-3} | 3.262×10^{-3} | 5.583×10^{-3} | 3.377×10^{-3} | 0.97 | 0.97 |

2-D, Right-angle Duct, Configuration B, cont.



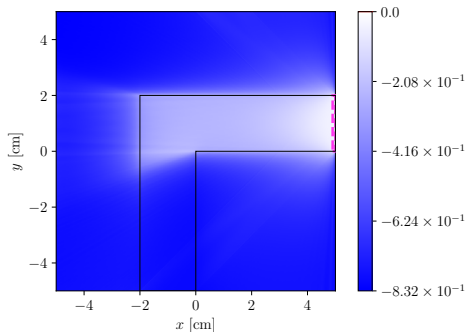
FTE, $\hat{\Upsilon}$



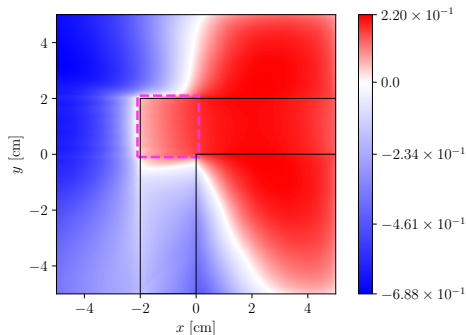
Cost, $\hat{\$}$

- ▶ Optimization predicted a 64% improvement; 954% improvement realized
 - ▶ Optimizer moves the forced-flight region to be around the tally
 - ▶ The β_c values for this case are varied across the permissible range

Biased Computational Cost Ratio (Lower is Better)



Configuration A



Configuration B

- ▶ Ratio is

$$\frac{\$_{\text{forced flight}} - \$_{\text{analog}}}{\$_{\text{analog}}}$$

- ▶ Ratio less than one provides benefit if the forward source is present there

Summary & Future Work

- ▶ History-score moment and future-time equations
 - ▶ Evidence given of correct derivation and implementation
 - ▶ Can yield effective, optimized, biasing parameters
 - ▶ Demonstrated here; shown elsewhere in detail
 - ▶ Cost field can provide useful intuition regarding biasing properties
- ▶ Future work:
 - ▶ Increase size of calculations to “engineering scale”
 - ▶ Exercise 3-D capability

Questions?

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Backup Slides

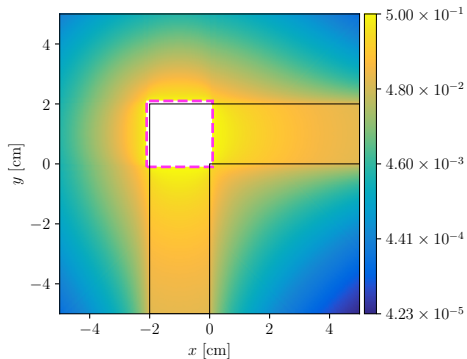
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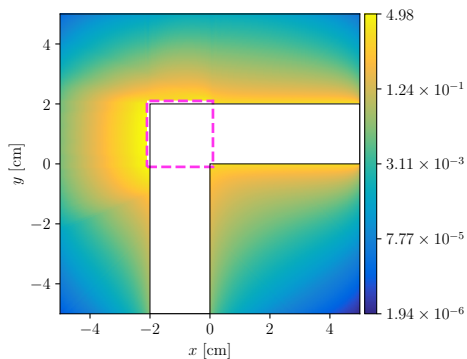
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2-D, Right-angle Duct, Configuration B, cont.



Free-flight Probability



Source, \hat{Q}_2