Computational modeling is

Uncertainty quantification is \_\_ and is necessary because \_\_

Uncertainty quantification is used as part of GSA

Our research is focused on introducing stochastic solvers into UQ and GSA

A stochastic solver we’re all familiar with is Monte Carlo radiation transport (MCRT)

We propose developing a variance deconvolution method for UQ and GSA and showing its effectiveness on complex radiation transport problems.

We’ll do this by developing the var-deconv estimator and applying it to UQ with MCRT, then integrating it into GSA, then integrating it into MCDC and testing on large problems.

We start by looking at uncertainty quantification, specifically sampling-based methods with the goal is to compute variance as a function of xi. A Monte Carlo UQ sampling method is \_\_, where you calculate variance using \_\_\_.

If we include MCRT in UQ, we get a polluted QoI tilde-Q. We have developed this variance deconvolution method to separate out the two variance contributions.

We can test its accuracy using an attenuation-only radiation transport problem, which has an analytic solution.

Complex cost analysis

Now that we’ve developed and testing this estimator with UQ, we can apply it to GSA.

Global sensitivity analysis is performed using sensitivity indices. A first-order sensitivity index quantifies the sensitivity of the output to a single input. The total sensitivity index measures the first order and all of the interactions.

These are computed by comparing the total variance of the output to the conditional variances of the different inputs.

Again, the use of the MCRT solver pollutes these GSA values. We first incorporated the variance deconvolution estimator into calculating sensitivity indices for a radiation transport problem with uncertain cross-sections and stochastic media configurations. This problem also has an analytic solution to compare to. Results are good.

The existing variance-based method is the Saltelli method. This is \_\_\_. Next steps are to compare this method to var-deconv incorporated into the Saltelli method, and compare to Dakota.

We’ve tested against these attenuation-only 1D slab transport problems with analytic solutions as proof-of-concept. The third main objective is to expand these methods to be used with a more complex radiation transport problem.

CEMeNT has their challenge MCRT problem. \*Explain\*

We’ll solve a subset of those problems. \*Explain\*

has MC/DC, a MCRT solver that is efficient and solves complex problems. We will incorporate the variance deconvolution into MC/DC.

As a short-term goal, we’ll use the recently developed analytic solution to the AZUR-V1 benchmark problem which MC/DC uses as a test.

Progress toward objectives: checklist of what’s completed and what’s to come, including highlighting publications

Planned schedule

1. Title
2. Computational models
3. UQ
4. GSA
5. Stochastic solvers
6. MCRT, introduce Q-tilde
7. Proposal
8. Literature review review
   1. EVADE
   2. UQ and sensitivity for MCRT: mcnp presentation warns of only first order effects, requires user understanding and checking; scale presentation specifically points out that results come from limited sample size
9. Sampling UQ
   1. Statistics E[Q] and Var[Q]
10. With stochastic solver
11. Does the stochastic solver approximate the UQ statistics we want?
12. For E[Q], I’m skipping some math details, but the gist is that the average of an average is an average!
    1. So we look at the variance
13. UQ Methods: goal, MCRT uncertainty, law of total variance, applied
14. With some simplifications, we get the total variance broke down into this. Not only does this theoretically tell us what the total variance is broken down into, it provides us a pathway of estimating the parametric variance.
15. Attenuation-only example to compare with analytic solution
16. Both the benchmark and the deconvolved results are a single repetition of the estimator, and we can see from the histogram that it’s well distributed around the analytic solution, corroborating unbiased
17. Next step to take was to understand how the estimator was performing as a function of the number of UQ samples and number of histories per UQ sample.
18. We performed this numerical experiment over a range of costs. Found minimum, next step was to look at analytic results
19. Analytic derivations to find where the minimum of that curve is based on sample estimator statistics
20. Analytic results matched our numeric experiment, next steps will be to ensure how to run a pilot study to find the optimum cost configuration and whether that payoff is worth the effort
21. Next, look at GSA, specifically variance-based GSA
    1. Sensitivity indices
22. When we introduce a stochastic solver, we introduce complications
    1. Analyzed by incorporating variance deconvolution into sensitivity index calculations
23. GSA example with stochastic media, which uses a binomial distribution rather than uniform. The stochastic media realizations are sampling how many of the subcells are each of the two materials.
24. So if we zoom in, …, that’s what the uncertainty is.
25. Again, analytic solutions to compare to, good agreement
26. The Standard for computing sensitivity indices with sampling is the Saltelli Method
    1. Swap out matrices so that in the ith simulation, only factor “i" has been changed.
    2. Use this for Vi
    3. In our case, f is the stochastic solver
    4. Future work includes comparing the more naïve approach we used to the Saltelli method and the various efficiency improvements that have been made
27. Next, we look at the challenge problem. One component of this is considering more complex cost analysis. We’re calling it linear, but really it’s not.
    1. For example, for the stochastic media problem, a single stochastic media realization vs a single don’t have the same cost associated with them, but we’re treating them here as if they do.
28. To incorporate more complex radiation transport physics, we’ll be working with the challenge problem identified for CEMeNT. Their full challenge problem is three-dimensional, continuous energy, time-dependent neutron transport problem with moving control rods based on a NuScale-like small modular reactor (SMR). It is sectioned in time into four phases that simulate an over-withdrawal of control rods and a subsequent neutron excursion and reactor SCRAM.
29. We’ll be focusing on a smaller subset of the CEMeNT challenge problem by just looking at phase 1. The problem is physically complex with lots of tallying, which may introduce some scaling problems, but the infrastructure of the tallying will already be there because we’re just using the same tallies and variances that are already computed. Time dependence specifically will be interesting as well because there are a number of ways we could handle that.
30. How does all of this align with PhD work? The first major goal is UQ
31. The next is GSA
32. The last is the challenge problem
33. And I have my proposed schedule with what’s completed, ongoing, and future work. Of course I actually started in 2021 but that made for an ugly graph