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Sensitivity Analysis in Coupled Radiation Transport Simulations

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INTRODUCTION

Sensitivity coefficients have found extensive use in nuclear criticality safety applications; for example, by allowing analysts to propagate the impact of uncertainty in evaluated neutron data, by determining the degree of similarity between benchmark experiments and a target validation application, and by using the results of integral benchmark measurements to calibrate neutron cross section data. The goal of this work was to explore whether recently developed generalized perturbation theory (GPT) reaction rate sensitivity methods can be extended to coupled photon-electron Monte Carlo radiation transport simulations.

As shown in Eq. (1), sensitivity coefficients predict the impact of changes to or uncertainties in the nuclear data parameter Σ_x on some integral response of interest, R.

$$S_{R,\Sigma_x} = \frac{\delta R/R}{\delta\Sigma_x/\Sigma_x}. \tag{1}$$

Sensitivity coefficients for eigenvalue responses (i.e. $R = k_{eff}$) have historically been computed using first-order perturbation theory, which relies on determining some representation of the adjoint flux, or "importance". The derivation of first-order perturbation theory is well-documented by various sources, and it has recently been applied to compute sensitivity coefficients in continuous-energy, eigenvalue simulations.

Recent work by Perfetti [1, 2] has developed a methodology for estimating sensitivity coefficients for responses that are ratios of reaction rates using continuous-energy Monte Carlo neutron transport methods, i.e.:

$$R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle} \tag{2}$$

Algorithms for computing these GPT sensitivity estimates use a combination of the CLUTCH methodology [3] and a modified version of the IFP method [4] (which is only needed for sensitivity analysis of eigenvalue problems).

This work has demonstrated proof of principle for extending these GPT sensitivity analysis methods to coupled photon-electron Monte Carlo radiation transport simulations. Theoretical developments provide a methodology for extending these methods in these coupled simulations, and a simple 1-D Monte Carlo test code was developed to achieve proof-of-principle for the new methodology.

CONTRIBUTON THEORY FOR COUPLED RADIATION TRANSPORT SIMULATIONS

Consider a photon flux, Φ, and an electron flux, ψ. A response, R_{tot}, is a combination of response functionals generated by the photon and electron fluxes integrated over some phase space:

$$\mathrm{R}_{tot} = \langle \mathrm{R}\Phi \rangle + \langle \mathrm{r}\,\psi \rangle \tag{4}$$

These response operators are arbitrary, but are here considered to be linear functionals, i.e. the product of a flux and some cross section Σ_R:

$$\mathrm{R}_{pho.} = \langle \mathrm{R}\Phi \rangle = \langle \Sigma_{R,pho.}\Phi \rangle \tag{5a}$$

$$\mathrm{R}_{ele.} = \langle \mathrm{r}\,\psi \rangle = \langle \Sigma_{R,ele.}\psi \rangle \tag{5b}$$

The change in the total response that occurs in response to perturbations or uncertainties in system parameters (typically nuclear data) is given by:

$$\delta\mathrm{R}_{tot} = \langle \delta\mathrm{R}\,\Phi \rangle + \langle \delta\mathrm{r}\,\psi \rangle + \langle \mathrm{R}\,\delta\Phi \rangle + \langle \mathrm{r}\,\delta\psi \rangle \tag{6}$$

The $\langle \delta\mathrm{R}\,\Phi \rangle$ and $\langle \delta\mathrm{r}\,\psi \rangle$ terms in Eq. (6) represent the "direct effect" of data perturbations on the response, i.e. the impact of perturbating the nuclear data that is directly contained in the responses of interest from Eq. (5). The terms containing the flux perturbations in Eq. (6) represent the "indirect effect" that the data perturbations will have on the response by changing the flux encountered by the response [2]. In Eq. (7), the direct effect terms from Eq. (6) are combined into a single term, and all perturbations are recast as derivatives with respect to an arbitrary nuclear data parameter, Σ_X:

$$\begin{aligned}\frac{\delta\mathrm{R}_{tot}}{\mathrm{R}_{tot}} = \langle \frac{1}{\mathrm{R}_{tot}}\frac{\partial\mathrm{R}_{tot}}{\partial\Sigma_X}\delta\Sigma_X \rangle \\ + \langle \frac{1}{\mathrm{R}_{tot}}\frac{\partial\mathrm{R}_{tot}}{\partial\Phi}\frac{\partial\Phi}{\partial\Sigma_X}\delta\Sigma_X \rangle \\ + \langle \frac{1}{\mathrm{R}_{tot}}\frac{\partial\mathrm{R}_{tot}}{\partial\psi}\frac{\partial\psi}{\partial\Sigma_X}\delta\Sigma_X \rangle\end{aligned} \tag{7}$$

The direct effect sensitivity terms are generally simple to calculate, and this work will focus on developing expressions to estimate the indirect effect sensitivities.

The transport equations governing the balance of photon and electron fluxes in a system are given below. These equations assume that photons create electrons via the $p\Phi$ operator, that electrons create photons via the $P\psi$ operator, and that the system is subject to an external source of photons and electrons (Q and q, respectively).

$$\text{Photons: } \mathrm{T}\Phi = \mathrm{Q}_{total} = \mathrm{Q} + \mathrm{P}\psi \tag{8a}$$

$$\text{Electrons: } \mathrm{t}\,\psi = q_{total} = q + p\Phi \tag{8b}$$

Adjoint transport equations will now be defined and manipulated to calculate the indirect effect of data perturbations from Eqs. (5) and (6). The adjoint transport equations for the coupled photon and electron fluxes can be shown to be:

$$\mathrm{T}^{\dagger}\Phi^{\dagger} = \mathrm{S}^{\dagger} + p^{\dagger}\psi^{\dagger} \tag{9a}$$

$$\mathrm{t}^{\dagger}\,\psi^{\dagger} = s^{\dagger} + P^{\dagger}\Phi^{\dagger} \tag{9b}$$

The adjoint source terms, $\mathrm{S}^{\dagger}$ and $s^{\dagger}$, can be defined in a way that enables computing the indirect effect terms:

$$\mathrm{S}^{\dagger} \equiv \frac{1}{\mathrm{R}_{tot}}\frac{\partial \mathrm{R}_{tot}}{\partial \Phi} = \Sigma_{R,pho.} \tag{10a}$$

$$s^{\dagger} \equiv \frac{1}{\mathrm{R}_{tot}}\frac{\partial \mathrm{R}_{tot}}{\partial \psi} = \Sigma_{R,ele.} \tag{10b}$$

Multiplying Eqs. (9a) and (9b) by perturbations in the photon and electron flux, respectively, and integrating over all phase space gives:

$$\langle \delta\Phi\ \mathrm{T}^{\dagger}\Phi^{\dagger}\rangle = \langle \delta\Phi\ \mathrm{S}^{\dagger}\rangle + \langle \delta\Phi\ p^{\dagger}\psi^{\dagger}\rangle \tag{11a}$$

$$\langle \delta\psi\ \mathrm{t}^{\dagger}\ \psi^{\dagger}\rangle = \langle \delta\psi\ s^{\dagger}\rangle + \langle \delta\psi\ P^{\dagger}\Phi^{\dagger}\rangle \tag{11b}$$

Applying the property of the adjoint (e.g. $\langle \Phi^{\dagger}\ \mathrm{T}\ \delta\Phi\rangle = \langle \delta\Phi\ \mathrm{T}^{\dagger}\Phi^{\dagger}\ \rangle$) several times to Eq. 11 gives:

$$\langle \Phi^{\dagger}\ \mathrm{T}\ \delta\Phi\rangle = \langle \delta\Phi\ \mathrm{S}^{\dagger}\rangle + \langle \psi^{\dagger}\ p\ \delta\Phi\rangle \tag{12a}$$

$$\langle \psi^{\dagger}\ \mathrm{t}\ \delta\psi\rangle = \langle \delta\psi\ s^{\dagger}\rangle + \langle \Phi^{\dagger}\ P\ \delta\psi\rangle \tag{12b}$$

Eq. (12) will be revisited momentarily, but first we will: allow perturbations to occur to all terms in Eqs. (8a) and (8b); ignore all higher order (δ^2) terms; multiply the two equations by $\Phi^{\dagger}$ and $\psi^{\dagger}$, respectively; and take the inner product to give:

$$\begin{aligned}\langle \Phi^{\dagger}\ \delta\mathrm{T}\ \Phi\rangle + \langle \Phi^{\dagger}\ \mathrm{T}\ \delta\Phi\rangle \\ = \langle \Phi^{\dagger}\ \delta\mathrm{Q}\rangle + \langle \Phi^{\dagger}\ \delta P\ \psi\rangle \\ + \langle \Phi^{\dagger}\ P\ \delta\psi\rangle\end{aligned} \tag{13a}$$

$$\begin{aligned}\langle \psi^{\dagger}\ \delta\mathrm{t}\ \psi\rangle + \langle \psi^{\dagger}\ \mathrm{t}\ \delta\psi\rangle \\ = \langle \psi^{\dagger}\ \delta q\rangle + \langle \psi^{\dagger}\ \delta p\ \Phi\rangle \\ + \langle \psi^{\dagger}\ p\ \delta\Phi\rangle\end{aligned} \tag{13b}$$

Upon examination, one notices that Eq. (12a) contains one term in both Eq. (13a) and Eq. (13b), and that Eq. (12b) contains one term in both Eq. (13a) and Eq. (13b). These terms can be made to cancel by summing Eq. (13a) and Eq. (13b), and by then subtracting Eq. (12a) and (12b), giving:

$$\begin{aligned}\delta R_{tot}^{Indirect} &= \langle \frac{1}{\mathrm{R}_{tot}}\frac{\partial \mathrm{R}_{tot}}{\partial \Phi}\delta\Phi\rangle + \langle \frac{1}{\mathrm{R}_{tot}}\frac{\partial \mathrm{R}_{tot}}{\partial \psi}\delta\psi\rangle \\ &= \langle \delta\Phi\ \mathrm{S}^{\dagger}\rangle + \langle \delta\psi\ s^{\dagger}\rangle \\ &= \langle \Phi^{\dagger}\ \delta\mathrm{Q}\rangle - \langle \Phi^{\dagger}\ \delta\mathrm{T}\ \Phi\rangle + \langle \Phi^{\dagger}\ \delta P\ \psi\rangle \\ &+ \langle \psi^{\dagger}\ \delta q\rangle - \langle \psi^{\dagger}\ \delta\mathrm{t}\ \psi\rangle + \langle \psi^{\dagger}\ \delta p\ \Phi\rangle\end{aligned} \tag{14}$$

This expression allows for the estimation of the indirect effect if the photon and electron adjoint fluxes are known.

Contributon Equations

We will now develop a method for computing the adjoint fluxes in Eq. (14). This method is based on Contributon Theory, which was developed originally by Williams [5], and adapted to continuous-energy Monte Carlo simulations by Perfetti [3].

Consider the version of Eqs. 8a and 8b that examines the balance of particles in response to the total sources of each type of particle (Q_{total} and q_{total}). Weighting these equations by $\Phi^{\dagger}$ and $\psi^{\dagger}$, respectively, and taking the inner product gives:

$$\langle \Phi^{\dagger}\ \mathrm{T}\ \Phi\rangle = \langle \Phi^{\dagger}\ \mathrm{Q}_{total}\rangle \tag{15a}$$

$$\langle \psi^{\dagger}\ \mathrm{t}\ \psi\rangle = \langle \psi^{\dagger}\ q_{total}\rangle \tag{15b}$$

Next, the adjoint balance equations in Eqs. (9a) and (9b) are weighted by Φ and ψ, respectively, the inner product is taken, and the property of the adjoint is applied. Noting that the left-hand sides of these equations and Eqs. (15a) and (15b) are equivalent gives:

$$\langle \Phi^{\dagger}\ \mathrm{Q}_{total}\rangle = \langle \Phi\ \mathrm{S}^{\dagger}\rangle + \langle \psi^{\dagger}\ p\ \Phi\rangle \tag{16a}$$

$$\langle \psi^{\dagger}\ q_{total}\rangle = \langle \psi\ s^{\dagger}\rangle + \langle \Phi^{\dagger}\ P\ \psi\rangle \tag{16b}$$

Consider a photon or electron source that consist of one single particle traveling in phase space, i.e. $\mathrm{Q}_{total}(\tau) = Q_o\ \delta(\tau)$ or $\mathrm{q}_{total}(\tau) = q_o\ \delta(\tau)$. It should be noted that this source is either one photon or one electron, and no combination of the two. This assumption allows one to compute the adjoint flux for photons and electrons using the following Green's Function interpretation:

$$\begin{aligned}\Phi^{\dagger}(\tau) = \langle \Phi(\tau \to r)\ \mathrm{S}^{\dagger}(r)\rangle \\ + \langle \psi^{\dagger}(r)\ p(r)\ \Phi(\tau \to r)\rangle\end{aligned} \tag{17a}$$

$$\begin{aligned}\psi^{\dagger}(\tau) = \langle \psi(\tau \to r)\ s^{\dagger}(r)\rangle \\ + \langle \Phi^{\dagger}(r)\ P(\mathrm{r})\ \psi(\tau \to r)\rangle\end{aligned} \tag{17b}$$

The definitions for $S^{\dagger}$ and $s^{\dagger}$ in Eqs. (10a) and (10b) mean that the first inner products on the right-hand side of Eqs. (17a) and (17b) can be computed by tallying the contribution of the source particle in phase space τ after it is emitted. In practice, this means that the importance of an event is equal to the response ($R_{pho.}$ or $R_{ele.}$) that is generated by the particle from the time it leaves the event until its death. The second inner products on the right-hand side of Eqs. (17a) and (17b) rely on computing the importance of any secondary electrons or photons that are created by the source photons or electrons, respectively, from the time they are emitted until their deaths. In essence, Eqs. (17a) and (17b) compute the importance of an event by tracking the cumulative response that is generated by the particle after it leaves the event and by all of its daughter secondary particles.

PROOF OF PRINCIPLE

A simple Monte Carlo test code was developed to demonstrate proof of principle for the proposed, "coupled CLUTCH" methodology of computing response sensitivity coefficients in coupled photon-electron transport simulations. The Monte Carlo code examined the sensitivity of responses in a simple 1-D slab geometry that occurred in response to an incident flux of a spectrum of photons and electrons. These particles were assumed to have an initial direction that was normal to the surface of the slab and scattered isotropically once inside the slab. These simulations assumed a three-group energy format and used artificial nuclear data for the simulation cross sections, emission probabilities, scattering kinematics, and secondary particle production probabilities. The slab in these simulations was divided into 10 1-cm-thick regions, for an overall slab thickness of 10 cm.

The CLUTCH methodology for estimating GPT response sensitivities was implemented in the test Monte Carlo code and was used to estimate the sensitivity of GPT responses to the various nuclear data in this simulation. These simulations assumed the GPT responses of interest to be particle absorption rates in each of the 10 regions, i.e.:

$$R = \langle \Sigma_{Absorb} \phi \rangle_{Cell\ i} \qquad (18)$$

Responses and response sensitivities were computed for each of the 10 cell regions for either photon or electron absorption rates: Response 1 refers to the photon absorption rate in the cell upon which the particles are incident and Response 10 refers to the photon absorption rate in the cell in the deepest part of the slab; likewise, Response 11 refers to the electron absorption rate in the cell upon which the particles are incident and Response 20 refers to the electron absorption rate in the cell in the deepest part of the slab. Figure 1 plots the photon and electron fluxes throughout the slab.

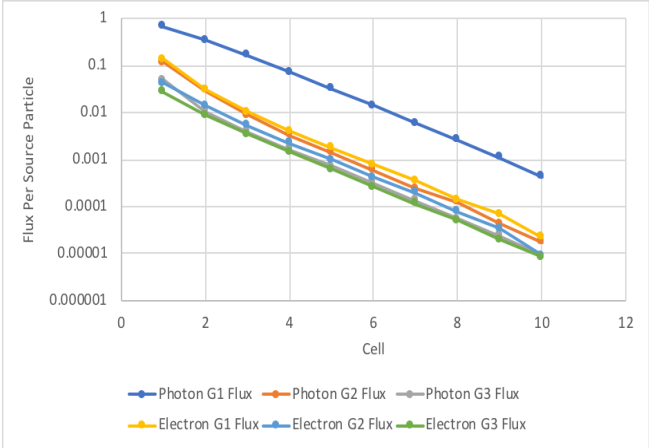

Fig. 1. Photon and electron fluxes in a sample 1-D slab.

Direct perturbation simulations were used to obtain reference sensitivity coefficient estimates. For the sake of time, these direct perturbation calculations were performed for only the photon cross section data. Select perturbations were performed for select electron data and successfully confirmed the accuracy of electron data sensitivity coefficients; however, these perturbations generally took much longer than the photon data perturbations due to the generally smaller magnitude of these electron sensitivities. The electron sensitivities share the exact same methodology and implementation as the photon sensitivities, and it is reasonable to assume that the electron sensitivities are accurate if the photon sensitivities can be shown to be accurate.

RESULTS

Table I compares sensitivity coefficients from the coupled CLUTCH methodology with the reference direct perturbation sensitivities – the difference (**Diff.**) between the sensitivity coefficients is expressed in terms of the number of effective standard deviations of disagreement. For brevity, Table I gives only the sensitivity of the absorption responses in each Cell to the photon Group 1 total cross sections.

These results found that the coupled CLUTCH sensitivity coefficients agreed well with the direct perturbation sensitivity coefficients, generally exhibiting random disagreement of less than two standard deviations. Several sensitivities (not shown) disagreed with the reference direct perturbation sensitivities by more than three standard deviations (with a maximum disagreement of 6.21 σ), but a large majority of the sensitivities disagreed by one or fewer standard deviations.

Computing these reference sensitivities required performing a large number of simulations – in doing this it was sometimes difficult to perturb the cross sections significantly enough to overcome noise in the results while also avoiding higher-order sensitivity effects. Individual sensitivities could be resolved to a significant degree (and in

some cases, were resolved this way) by simulating more histories or by performing cross section perturbations that were tailored to that specific sensitivity, but the perturbations could not be precisely tailored to highly resolve all of the reference direct perturbation sensitivities at once. It is worth noting that during the process of debugging this code, a significant number of bugs were resolved through comparison with these reference direct perturbation sensitivities. The resolution of the direct perturbation sensitivities was always sufficient to clearly indicate when a bug was present in a given sensitivity coefficient calculation routine. Future studies could further resolve these direct perturbation reference sensitivities and remove the few instances where sensitivities disagreed by more than three standard deviations, but historical trends in sensitivity accuracy and our experience from benchmarking sensitivities in the past suggests that the coupled CLUTCH sensitivity methodology produces accurate sensitivity coefficient estimates.

TABLE I. Sensitivity of Responses to Photon Total Cross Sections

Response in Cell:	Calculated Sensitivity	Direct Pert. Sensitivity	Diff.
Photon Absorption Response Sensitivity			
1	0.368 ± 0.001	0.365 ± 0.010	0.28 σ
2	-0.023 ± 0.003	-0.025 ± 0.013	0.13 σ
3	-0.802 ± 0.006	-0.783 ± 0.033	-0.58 σ
4	-1.674 ± 0.010	-1.700 ± 0.012	1.62 σ
5	-2.583 ± 0.018	-2.549 ± 0.126	-0.27 σ
6	-3.459 ± 0.030	-3.611 ± 0.264	0.57 σ
7	-4.384 ± 0.048	-4.484 ± 0.335	0.29 σ
8	-5.332 ± 0.079	-5.176 ± 0.709	-0.22 σ
9	-6.055 ± 0.131	-6.353 ± 0.865	0.34 σ
10	-6.952 ± 0.226	-6.694 ± 1.439	-0.18 σ
Electron Absorption Response Sensitivity			
1	0.214 ± 0.001	0.211 ± 0.022	0.14 σ
2	0.002 ± 0.005	-0.043 ± 0.024	1.88 σ
3	-0.719 ± 0.010	-0.671 ± 0.053	-0.90 σ
4	-1.612 ± 0.018	-1.669 ± 0.070	0.80 σ
5	-2.544 ± 0.031	-2.338 ± 0.035	-4.42 σ
6	-3.451 ± 0.049	-3.472 ± 0.119	0.16 σ
7	-4.187 ± 0.079	-3.897 ± 0.397	-0.72 σ
8	-5.676 ± 0.136	-4.806 ± 1.113	-0.78 σ
9	-5.923 ± 0.197	-6.728 ± 1.206	0.66 σ
10	-6.924 ± 0.370	-8.258 ± 2.000	0.66 σ

CONCLUSIONS

This work has outlined an extension of Contributon theory that enables adjoint-based sensitivity coefficient calculations in coupled particle Monte Carlo transport simulations. This new sensitivity methodology was implemented into a simple 1-D test Monte Carlo code, and direct perturbation calculations were used to confirm the accuracy of the new sensitivity methodology. Future work includes implementing this methodology in a production-level coupled transport Monte Carlo code, such as the Integrated Tiger Series (ITS) code [6], and using this methodology to quantify the impact of uncertainty in photon and electron nuclear data.

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