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MONTE CARLO CALCULATIONS OF EIGENVALUE SENSITIVITIES TO SYSTEM DIMENSIONS

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ABSTRACT

A Monte Carlo method is developed that computes sensitivities or derivatives of the k-eigenvalue with respect to interface boundary locations for uniform expansions or contractions. The method is implemented in a research version of MCNP6 and its results are compared with reference solutions obtained from equivalent multigroup calculations with PARTISN (discrete ordinates) and direct Monte Carlo perturbations. The test problems involve finding the sensitivity of the radius of bare uranium sphere, the interface location of a reflected uranium sphere, and the radii of plates in the Zeus benchmark. The results match within 5% except for the radii of the thin uranium plates, which agrees within about 10%.

Key Words: Adjoint, Perturbation, Geometric Tolerances, Verification, Discrete Ordinates

1. INTRODUCTION

The location of interfaces between components in a critical system is not known exactly and therefore is a source of uncertainty that propagates to an uncertainty for the system multiplication factor or eigenvalue k. Certain interface locations have greater effects than others on the system eigenvalue, and these relative impacts may be characterized if the sensitivity coefficients are known. For example, in the design or evaluation of a critical experiment, it may be useful to understand which geometric tolerances have the greatest impact and therefore require the most attention to accurate representation.

Rahnema [1] has developed expressions to compute eigenvalue perturbations with respect to interface boundaries based on adjoint-based perturbation methods. More recently, Favorite and Bledsoe [2,3] derived similar expressions for derivatives of k with respect to interfaces based upon treating the perturbation as a material substitution and demonstrated calculations of these derivatives with a discrete ordinates method using PARTISN [4]. Earlier developments by Rearden [5] have demonstrated the calculation of sensitivity coefficients to k with respect to neutron cross sections in multigroup Monte Carlo, and this was later extended by Kiedrowski, Brown, and Wilson [6,7] to continuous-energy physics.

Herein, the continuous-energy Monte Carlo methods for sensitivities of nuclear cross sections are extended to calculate sensitivities to interface boundaries or system dimensions. For reasons to be discussed, a different approach for computing the derivatives to scattering and fission sources has to be implemented - this, unfortunately, results in significant reductions in efficiency. The implementation in MCNP [8] is discussed. Verification of these calculations is performed by comparing with the discrete ordinates results of Ref. 2 as well as direct Monte Carlo calculations.

2. THEORETICAL DEVELOPMENT & METHOD

The interface between two zones within a geometry is defined by a surface contour B with an outgoing surface normal $\hat{\mathbf{n}}$ as shown in Fig. 1. The zone on the positive side of the surface normal is defined to be the positive zone with respect to the surface, whereas the zone on the negative side is defined as the negative zone. The positive and negative zones have generic macroscopic cross sections Σ^+ and Σ^- respectively. With these definitions, it is possible to derive [2] an expression for the derivative of k with respect to interface location b located on surface contour B.

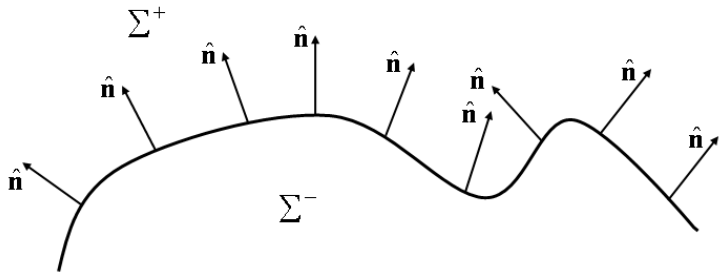

Figure 1. Illustration of surface defined by contour B with corresponding cross sections.

2.1. Interface Sensitivity Derivation

Adjoint-based perturbation theory yields the following relationship for the change in k (define $\lambda = 1/k$, where k is that of the unperturbed system, so $d\lambda = -\lambda^2 dk$) with respect to some cross section perturbation:

$$dk = -\frac{1}{M} \left\langle \psi^\dagger, \left(d\Sigma_t - dS - \lambda dF \right) \psi \right\rangle , \tag{1}$$

where the brackets $\langle ., . \rangle$ indicate an integration over all phase space (position $\mathbf{r}$, direction $\hat{\mathbf{\Omega}}$, and energy E), ψ is the forward angular flux, $\psi^\dagger$ is the corresponding adjoint function, Σ_t is the total macroscopic cross section, S is the scattering operator given by

$$S = \iint dE' \, d\mathbf{\Omega}' \, \Sigma_s(\mathbf{r}, E' \rightarrow E, \hat{\mathbf{\Omega}}' \rightarrow \hat{\mathbf{\Omega}}) \tag{2}$$

with Σ_s as the double-differential scattering cross section, F is the fission operator given by

$$F = \frac{1}{4\pi} \iint dE' \, d\mathbf{\Omega}' \, \chi(E' \rightarrow E) \nu \Sigma_f(\mathbf{r}, E') \tag{3}$$

with χ as the fission emission spectrum, ν as the mean number of neutrons produced per fission, Σ_f as the macroscopic fission cross section, and the quantity M is the adjoint-weighted fission source times λ^2 or

$$M = \left\langle \psi^\dagger, \lambda^2 F \psi \right\rangle . \tag{4}$$

Both the forward and adjoint flux correspond to the unperturbed system.

The functional form of a generic cross section in the vicinity of the surface boundary at b along some ray r crossing the surface at B in the positive direction is

$$\Sigma(\mathbf{r}) = \Sigma^- + \Theta(r-b)(\Sigma^+ - \Sigma^-), \tag{5}$$

where Θ is the Heaviside step function. Differentiating the cross section with respect to b, the location of the surface crossing, yields

$$\frac{d\Sigma}{db} = -\delta(r-b)(\Sigma^+ - \Sigma^-), \tag{6}$$

where δ is the Dirac delta function. By substituting Eq. (6) into Eq. (1) and rearranging, the following convenient form is obtained:

$$\frac{dk}{db} = \frac{1}{M}\Bigg[\left\langle \psi^\dagger, \left(\Sigma_t^+ - \Sigma_t^-\right)\psi\right\rangle_B + \left\langle \psi^\dagger, S^-\psi\right\rangle_B - \left\langle \psi^\dagger, S^+\psi\right\rangle_B + \left\langle \psi^\dagger, \lambda F^-\psi\right\rangle_B - \left\langle \psi^\dagger, \lambda F^+\psi\right\rangle_B\Bigg]. \tag{7}$$

Subscript B denotes that the volume in the inner product is now a surface integral on contour B. The operators with the $+$ and $-$ superscripts are identical to the corresponding definitions except that their constituent cross sections have inherited the corresponding superscript. Recall that the superscripts denote which side the surface the material is on, not the direction that the neutron is traveling. The reason for the particular form chosen in Eq. (7) is seen in the Monte Carlo methodology.

2.2. Monte Carlo Computation

Each inner product of Eq. (7) constitutes an adjoint-weighted tally computed during a random walk simulation. The numerator has five such terms, and accumulation of information for each occurs each time a neutron crosses the surface for which the sensitivity is desired. The essential component for all these tallies is an estimate of the flux at the surface, which is done by the traditional estimator of

$$\tilde{\psi}_B = \frac{w}{|\mu|}, \tag{8}$$

where $\tilde{\psi}_B$ denotes an individual contribution to the flux estimate at the surface, w is the numerical particle weight, and μ is the cosine of the angle between the particle trajectory and the surface normal. Note that the traditional approximation of constant flux is used for small values of μ to keep the variance of the tally finite [9].

Each contribution $\tilde{\psi}_B$ must then be multiplied by an estimate of the adjoint function of that particle after having undergone a process representing the differential change in the interface location. For reasons of efficiency and necessity, this is done differently for the collision rate derivative term and the derivatives of the scattering and fission sources. Each of these will be discussed separately.

2.2.1. Collision rate derivative term

The change in the collision rate from the differential surface perturbation is computed by multiplying $\tilde{\psi}_B$ by $\tilde{\psi}_B^\dagger(\Sigma_t^+ - \Sigma_t^-)/w$, where $\tilde{\psi}_B^\dagger$ is the estimate of the adjoint function for the particle that just crossed the surface. This adjoint function estimate is computed by following the neutron and its progeny through many successive fission generations and then tallying the number of progeny in some distant generation. The details for doing this and the reasons for dividing by the particle weight w are discussed extensively in Ref. 5. The factor $(\Sigma_t^+ - \Sigma_t^-)$ arises from the differential change in the collision rate that would have occurred had the surface been moved uniformly an infinitesimal amount at every point in the direction of the surface normal.

2.2.2. Scatter source rate derivative terms

The scatter (and fission) source rate derivative terms are computed in a different, and far less efficient, manner. As with the collision rate derivative term, $\tilde{\psi}_B$ is multiplied by $\tilde{\psi}_B^\dagger \Sigma_s^\pm/(\Sigma_s^+ + \Sigma_t^-)$, but in this case $\tilde{\psi}_B^\dagger$ is the importance of a neutron that would have undergone a scattering process on both sides of the interface had it undergone a differential, uniform perturbation along the surface normal.

Unfortunately, unless from happenstance, such a neutron will not exist in the simulation to follow and estimate its adjoint function. This is unlike the collision rate derivative term, where the importance is with respect to the existing neutron that will be followed in the course of the normal random walk. Also consider that the adjoint function poses a "what if" question about a neutron's expected future – the neutron need not actually exist or even be possible to appear in the problem, but it may still have a non-zero importance function. Since this "what if" question is being asked about a neutron that does not normally exist in the random walk, one must be created with unit weight and followed for the sole purpose of making an estimate of its importance, and this must be done in a way that does not influence the results since it is not an actual neutron in the system.

To produce this so-called *pseudoneutron*, the simulated (physical) neutron must undergo an artificial scattering event (a *pseudoscatter*) and the resulting secondary, the pseudoneutron, from that is treated separate from the physical particles. Pseudoneutrons undergo all interactions that a physical neutron would and produce progeny (also pseudoneutrons) from fission, but they do not contribute to any tallies in the problem except for making a single estimate of the adjoint function $\tilde{\psi}_B^\dagger$. Pseudoneutrons do not interact with the boundary sensitivity tallies that produced them and therefore their surface crossings do not result in the production of more pseudoneutrons. The main drawback to the pseudoneutron approach is that it adds additional random walks and therefore necessitates increases in computational time that in practice are quite significant. Unfortunately, because this "what if" question must be answered for a neutron that would not normally exist, this computationally expensive operation must be carried out.

Since perturbing the surface results in a gain in the size and material of the negative zone and in a corresponding loss to the positive zone, both the gain (positively weighted collision) and loss (negatively weighted collision) must be accounted for by an individual pseudoneutron. In the case where one of the materials is vacuum, no pseudoneutron for that zone (whether positive or negative) is generated since no collision may occur there. Also, in the case where the materials

and densities of the zones are identical, no pseudoneutrons are generated for reasons of efficiency since, on average, the two scatter terms will sum to zero.

2.2.3. Fission source rate derivative terms

In most respects, the fission source rate derivative terms are computed similarly to the scatter source rate derivative terms. At each surface crossing, the contribution $\tilde{\psi}_B$ is multiplied by $\tilde{\psi}_B^\dagger \nu\Sigma_f^\pm/(\nu\Sigma_f^+ + \nu\Sigma_f^-)$ and $\tilde{\psi}_B^\dagger$ is the importance for a neutron that would be produced from a hypothetical fission event from the differential perturbation of the surface boundary. As with the scattering terms, this interaction will not happen in the normal course of the random walk, and therefore a similar introduction of pseudoneutrons must occur, except this time via a process of *pseudofission*. Otherwise, these pseudoneutrons behave exactly like those for the scattering source rate derivative terms. Should either or both materials between the perturbed interface not be able to cause fission, no pseudoneutron(s) will be created for the material.

The only other exception is the factor of λ multiplying these two terms. Some estimate must be made upon scoring the tally, and, in the MCNP implementation, this is the inverse of the geometric mean of collision estimates of k for the cycles over which the neutrons for this estimate were being followed. This is not the only possible choice, but it is convenient to implement.

2.2.4. Denominator term

The normalization on the perturbation tally in Eq. (7) is the factor $1/M$. Every cycle an estimate of $\langle 1, \lambda F\psi\rangle$ is made by the power iteration method, and renormalization always results in the sum of particle weights being the initial source weight. The denominator term can be calculated similarly by weighting by the adjoint function estimates rather than the implicit unity factor. This can be done by the same process of tagging each fission source neutron, following it and its progeny, and finding the response in some distant generation. As with the fission source rate derivative terms, another estimate of λ must be made in the same way and multiplied with the adjoint-weighted fission source estimate.

2.3. Implementation

The Monte Carlo method for computing sensitivity coefficients is implemented in a research version of MCNP for possible inclusion into the mainline production version should results be promising and performance adequate.

The algorithms [6] in MCNP for performing adjoint-weighted tallies such as the point kinetics parameters are extended for computing boundary sensitivities. A brief description is as follows: The active iterations (cycles) are divided into blocks of generations. Original contributions to the tallies (without the adjoint weight $\tilde{\psi}_B^\dagger$) are accumulated in the first iteration in the block, and those neutrons are tagged such that memory is preserved about which neutrons caused which contributions. Pseudoneutrons are also produced in this iteration within the block. In the last cycle of the block (after a “large number” of fission generations), a track-length estimator of fission neutron production is made for all progeny and multiplied by their corresponding original contributions to form the final tally score. More detail can be found in Ref. 5.

The adjoint weighting routines are modified to perform computations and accounting at each relevant surface crossing. Within MCNP, cross sections and pseudoneutrons are produced and stored before and after the software fetches and interpolates cross section data for the new cell. Having all cross sections available allows use of MCNP routines for performing collision mechanics – certain global variables that are unfortunately modified within the collision mechanics routines must be copied and restored to preserve random walks.

The pseudoneutrons are tagged with a "scoring particle" flag that, if zero, indicates the neutron is not to contribute to any tallies. This tag is also placed into the fission source bank so that all progeny of pseudoneutrons are also pseudoneutrons and do not contribute. MCNP6 also has the capability to use a different random number sequence for different particles. All pseudoneutrons use a sequence distinct from the main random number sequence, and therefore results of other tallies are unaffected.

3. VERIFICATION

Comparisons with deterministic calculations or direct Monte Carlo central differences are the two means of verifying this feature. For the former, angular forward and adjoint fluxes at interfaces may be obtained from a deterministic calculation – in this case a discrete ordinates solver, PARTISN – that may be postprocessed by integrating them with appropriate cross sections to compute dk/db. The latter approach obtains an approximate derivative from a central difference by subtracting the obtained values of k from two perturbed cases where the interface is moved small distances $\pm\Delta b$ and dividing by $2\Delta b$. This approach suffers from the limitation that Monte Carlo results must have high statistical precision for a small Δb to ensure the subtraction is statistically meaningful. Indeed, the motivation for this paper is to produce a more computationally efficient scheme so as to avoid the direct Monte Carlo approach, but both should yield the same result in the limit of very small Δb.

For the purposes of verification, both external and internal boundary sensitivities must be calculated correctly. For an external boundary, a simple, yet illustrative, case is finding the sensitivity to the radius of Godiva, a bare, highly-enriched uranium sphere. A simple case for an internal boundary is finding the sensitivity to the interface between a modified (smaller) version of Godiva and a spherical graphite reflector shell. Finally, a more complicated reference calculation is various plate radii of the Zeus benchmark. Detailed specifications for the Godiva and Zeus benchmarks may be obtained in the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP Handbook) [10].

3.1. External Interface – Godiva

The Godiva benchmark (ICSBEP identifier heu-met-fast-001) is a bare sphere (radius of 8.7407 cm) of highly-enriched uranium (about 93.8% uranium-235) at a density of 18.74 g/cc. The sensitivity to the radius R, dk/dR, is desired. An example where this might be useful is for designing such an experiment to understand how precisely the sphere radius must be known such that the impact on k is small.

The geometry is defined such that the surface normal $\hat{\mathbf{n}}$ points away from the center of the sphere

such that escaping particles are traveling in the positive direction with respect to the sphere. This sign convention leads to finding the dk that would result if the spherical radius is increased by dR. From physical considerations, dk should be positive.

The result from PARTISN obtained in Ref. 2 for dk/dR is 0.09488 cm^{-1} using multigroup MENDF6 (30 group) cross-section data [11], which has no upscattering. For comparison, a direct Monte Carlo result using continuous-energy ENDF/B-VII.0 nuclear data [12] yields 0.09445 ± 0.0042 cm^{-1}.

The final result from the MCNP6 boundary sensitivity routine is 0.09491 ± 0.0039 cm^{-1}. This is within two standard deviations of both the multigroup PARTISN and direct Monte Carlo results and gives some confidence MCNP6 can accurately predict the sensitivity with respect to an external boundary. Also, suppose that the uncertainty in the measured radius is 0.0001, or the last decimal place. Then, the sensitivity result combined with the uncertainty asserts that the uncertainty in k from the radius is slightly less than 1 pcm (0.00001), typically below most limits of concern.

3.2. Internal Interface – Graphite Reflected Uranium Sphere

The other type of interface that is of significance is one that is internal to the geometry. A simple test case is constructed by shrinking the Godiva sphere to 6.27 cm and encasing it in a 10-cm thick graphite reflector (simply treated as natural carbon with no $S(\alpha, \beta)$ law for simplicity) with density 2.25 g/cc. As with the bare sphere case, the surface normal vectors point away from the center of the sphere.

The question posed is how much does moving the interface between the uranium and graphite layers by some distance dR impact k. The net effect of this is to add some differential amount of uranium while removing some differential amount of graphite from the overall system. In this case, the total collision rate derivative term is non-zero because neutrons can normally reach the interface and backscatter on the graphite into the uranium. Likewise, scattering can occur at the interface from either material (in Eq. (7) uranium scatter is $-$ and graphite scatter is $+$ with respect to the surface normal definition) and therefore two pseudoscatter events must be simulated. Since fission is impossible in carbon, only the $-$ term from the uranium may contribute.

A discrete ordinates calculation from PARTISN yields a sensitivity of the internal radius of 0.1200 cm^{-1}. From a central difference, direct Monte Carlo calculation, the sensitivity is 0.1212 ± 0.0008 cm^{-1}. The MCNP6 boundary/interface sensitivity capability produces a result of 0.1167 ± 0.0029 cm^{-1}, which is within two standard deviations of both reference values. This shows, at least for this simple problem, MCNP6 can compute a sensitivity to an internal interface.

3.3. Internal Interface – Zeus Plate Radii

Configuration 1 of the Zeus benchmark (ICSBEP identifier heu-met-inter-006) is used as a more complicated geometry to test the impact of various dimensional tolerances. The model used is a 2-D cylindrical approximation to the actual experiment to facilitate comparison with the discrete ordinates calculations of Ref. 2. The model consists of layered plates of highly-enriched uranium

and graphite and the purpose will be to find the sensitivity to the radii of the various plates. The surface normals of all the cylinders are defined to point away from the axis of the experiment. In Ref. 2, the calculations were performed with MENDF6 cross sections (no upscattering or self-shielding) with P_3 scattering, so exact agreement with continuous-energy/angle ENDF/B-VII.0 is not expected, but results should match approximately.

The sensitivity to the radii of all the graphite plates, the uranium plates, and both types together are calculated. The results of the PARTISN and MCNP calculations are given in Table I.

Table I. Eigenvalue Sensitivities for Plates in Zeus Benchmark

Plate Type	**MCNP6** dk/dR (cm^{-1})	**PARTISN** dk/dR (cm^{-1}) [2]	**C/E**
Graphite	0.01957 ± 0.00067	0.01895	1.033
Uranium	0.01375 ± 0.00037	0.01259	1.092
Graphite + Uranium	0.03074 ± 0.00085	0.03154	0.975

MCNP6 produces 0.01957 ± 0.0014 cm^{-1} for the graphite plate radii sensitivity, which matches the PARTISN reference value of 0.01895 cm^{-1} within one standard deviation. The uranium plates have computed sensitivities of 0.01375 ± 0.0090 cm^{-1} and 0.01259 cm^{-1} for MCNP6 and PARTISN respectively. While this is more than three standard deviations outside the MCNP uncertainty band, the result still agrees within 10%; the relatively thin nature of the uranium plates and the numerical issues of discrete ordinates is a possible factor in the discrepancy. Nonetheless, this repeats the trend, which may be non-intuitive, observed in Ref. 2 that the radii of the graphite plates are more important to k than the radii of the uranium plates where the fission actually occurs. The sensitivity of all plates should (on average) be the additive sum of the graphite and uranium plate sensitivities. The MCNP6 result for the combination is 0.03074 ± 0.00085 cm^{-1}, which agrees with the reference value of 0.03154 cm^{-1} within a few percent.

The results of the individual graphite and uranium MCNP6 calculations do not sum within three standard deviations to the result obtained for the composite calculation. There are a few possible explanations for this discrepancy. First, the uncertainties of local tallies in eigenvalue calculations are often underestimated by factors of 2-5 because positive correlation between cycles is neglected [13]. The uncertainties that should be produced may well be factors higher than the quoted value, which would make the results agree within statistics. A second possibility is that the surface flux approximations used in MCNP6 may be causing results of the thin uranium plates to be biased; it should be possible to relax this in future calculations to test this. A third source of error comes from the approximation in computing the adjoint weight. The default size of ten for the block (number of cycles) separating the tally contributions with their importance weight is used and may not be sufficient for such a localized response. Again, this would be possible to test, albeit requiring significantly more computational time than those used for these calculations. Another possibility is an error in the software.

To illustrate how this result may be useful, suppose all graphite plates in Zeus were 1 mm larger in radius than specified. In this case, a bias in k of about 200 pcm would be introduced. Likewise, an uncertainty in the plate radius of 1 mm would yield an additional uncertainty in k of the same magnitude that would need to be factored in when assessing the benchmark uncertainty values. The capability described in this paper allows a means to quantify these uncertainties.

As seen from the results, the differences are on the order of 5-10%, which is probably acceptable in this case considering the issues of comparing continuous-energy Monte Carlo with multigroup discrete ordinate and different nuclear data. These results are, however, for boundaries with fairly large neutron exposures. It would, unfortunately, be quite difficult to get such statistical precision for individual plates, and therefore further work in variance reduction techniques for these tallies will be required if Monte Carlo is to be a practical tool for boundary sensitivity calculations.

4. CONCLUSIONS

A Monte Carlo method is developed for computing the derivatives of k with respect to interface locations or system dimensions and implemented into a research version of MCNP6. The theory largely follows that developed in Refs. 1 and 2, and the convenient form of Eq. (7) is specified that allows for development of the method. Surface flux tallies are accumulated at each surface crossing and later weighted by the corresponding importance for each term. To calculate the scattering and fission source rate derivative terms, the concept of pseudoneutrons is introduced – these are artificial neutrons that undergo scattering or fission in materials on both sides of the interface and are used solely to find the importance function of those terms.

The results from the Monte Carlo implementation are compared with discrete ordinates calculations from PARTISN, and central differences obtained from two independent Monte Carlo calculations. Both system boundaries and internal interfaces are tested in simple geometries such as Godiva or a reflected version thereof and in a more complicated geometry – namely, the Zeus benchmark. All results are on the Monte Carlo tallies appear to agree (the largest discrepancy is 10% for the sensitivity of the radii of the thin Zeus plates), lending confidence that the Monte Carlo implementation matches the theory and the methods employed in Ref. 2.

The major outstanding issue is that the efficiency of these calculations may be quite low should few simulated neutrons reach surfaces. This motivates future development for variance reduction schemes of the production of pseudoneutrons, so that this may be a practical tool for criticality safety practitioners and benchmark evaluators.

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