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Estimating Reactivity Changes from Material Substitutions with Continuous Energy Monte Carlo

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1. INTRODUCTION

Monte Carlo codes such as the MCNP (Monte Carlo N-Particle) code use the differential operator method to estimate changes in a response due to a perturbation [1]. This has been shown to work well for fixed source problems, but does not capture the perturbation in the fission source and therefore cannot adequately estimate eigenvalue perturbations [2].

An alternative for estimating reactivity changes to the differential operator method is to use linear perturbation theory. This uses a ratio of inner-products of weighted functions. The typical weighting function used is the adjoint flux [3]. Unfortunately, calculating adjoint fluxes with continuous energy Monte Carlo is difficult.

The iterated fission probability interpretation of the adjoint flux [4] offers a more tractable way to estimate adjoint functions in critical systems. Promising results have been obtained for similar calculations of point reactor kinetics parameters [5, 6]. These methods have been extended to calculate changes in reactivity.

2. THEORY & METHOD DEVELOPMENT

The change in reactivity due to perturbation **P** can be estimated by

$$\Delta\rho = -\frac{\left\langle \psi^{\dagger}, \mathbf{P}\psi \right\rangle}{\left\langle \psi^{\dagger}, \mathbf{F}'\psi \right\rangle}. \tag{1}$$

Here the flux and adjoint for the original problem are given by ψ and $\psi^{\dagger}$, and $\mathbf{F}'$ denotes the perturbed fission source. The inner-product is taken as an integral over all phase space. The perturbation operator **P** is given by

$$\mathbf{P} = \Delta\Sigma_t - \Delta\mathbf{S} - \frac{1}{k}\Delta\mathbf{F}\,. \tag{2}$$

The first term represents the change in the total collision rate, the second is the change in the scattering source, and the third is the change in the fission source. Σ_t is the total cross section and k denotes the multiplication factor for the system.

2.1. Monte Carlo Adjoint-Weighting

In the Monte Carlo simulation, each tally score must be weighted by an estimate of the adjoint flux. In a critical system, the adjoint flux (via the iterated fission probability) at a point in phase space is proportional to the expected steady state population of neutrons caused by a neutron introduced into the system at that point.

Neutrons are "introduced" at some specified point in the random walk in the "zeroth" or original generation. At each point of introduction, the neutron random walk is assigned a progenitor index p. This index is inherited by any progeny.

After many generations, the asymptotic population can be estimated by a track length estimator for neutron production:

$$\pi_p = \sum_{\tau \in p} \nu\Sigma_f w d\,. \tag{3}$$

$\nu\Sigma_f$ is the average neutron emission per fission times the macroscopic fission cross section, w is the particle weight, d is the track length, and the summation is over only tracks τ caused by progeny of neutron p.

This asymptotic population is multiplied by whatever tally score stored in the original generation that needs to be weighted by its importance.

2.2. Perturbation Tallies

The numerator of equation (1) consists of three terms: total collision perturbation, scattering source perturbation, and fission source perturbation. Each of these must be stored in the original generation separately.

The progenitor index p is assigned at each fission source event in the original generation. For each track in the original generation τ, the perturbation in the collision rate is estimated and later weighted by the asymptotic population:

$$\left\langle \psi^\dagger, \Delta\Sigma_t \psi \right\rangle = \frac{1}{W}\frac{1}{V}\sum_p \pi_p \sum_{\tau \in p} \Delta\Sigma_t w_0 d \ . \qquad (4)$$

$\Delta\Sigma_t$ is the change in the total cross section from the perturbation, w_0 is the source weight of the neutron, V is the volume of the system, and W is the total source weight of all progenitors.

The perturbation in the scattering source is tallied at every scatter event s in the original generation. The tally for the perturbed scattering source is

$$\left\langle \psi^\dagger, \Delta\mathbf{S} \psi \right\rangle = \frac{1}{W}\frac{1}{V}\sum_p \pi_p \sum_{s \in p} \frac{\Delta\Sigma_s}{\Sigma_s} w_0 \ . \qquad (5)$$

The ratio in the inner summation is the ratio of the perturbation of the scattering cross section to the actual scattering cross section of the neutron at the incident energy.

The fission source is tallied similarly at each fission event f:

$$\left\langle \psi^\dagger, \frac{1}{k}\Delta\mathbf{F} \psi \right\rangle = \frac{1}{W}\frac{1}{V}\sum_p \pi_p \sum_{f \in p} \frac{\Delta\Sigma_f}{\Sigma_f} w_0 \ . \qquad (6)$$

Like the scattering source tally, the ratio in the inner summation is the ratio of the fission cross section perturbation to the actual fission cross section at the energy of the neutron that caused the fission. The factor of $1/k$ comes from the population normalization each generation.

The denominator requires the perturbed fission source. This is calculated by

$$\left\langle \psi^\dagger, \mathbf{F}' \psi \right\rangle = \frac{k}{W}\frac{1}{V}\sum_p \pi_p \sum_{f \in p} \frac{\Sigma_f + \Delta\Sigma_f}{\Sigma_f} w_0 \ . \qquad (7)$$

To compute the reactivity change, the sum of (4), (5), and (6) is divided by (7).

3. RESULTS

The method was implemented in the production MCNP5-1.5.1 code [7].

Two case studies are performed to verify the method. The first uses artificial multigroup cross section data in MCNP with a direct comparison with a discrete ordinates code Partisn [8]. The second looks at changing the cross section library (ENDF/B-VII.0 to ENDF/B-VI.5) for uranium in the Godiva [9] problem.

3.1. Multigroup Slab Perturbations

A 4-group slab problem was constructed in both MCNP and Partisn with fictitious cross section data (see Appendix). The bare slab (half-thickness of 7.75 cm) of fissile material was approximately at critical and the following perturbations (Table I) were made to the lowest energy group.

Table I. Cross section perturbations for group 4 for the bare slab problems.

Case	Perturbation
1	capture +0.05 b
2	fission +0.05 b
3	capture +0.05 b, fission +0.05 b
4	nubar +0.01
5	capture +0.05 b, fission +0.05 b, nubar +0.01
6	scatter (4-4) +0.05 b

The change in reactivity was computed with the linear perturbation scheme in MCNP and compared to the exact calculated change in reactivity from two separate Partisn calculations. Table II gives the reactivity changes are given in percent-million (pcm).

Table II. Change in reactivity (pcm) for the various perturbations in the bare slab problems.

Case	MCNP	Partisn
1	-32.748 +/- 0.152	-32.839
2	+49.506 +/- 0.308	+49.517
3	+16.758 +/- 0.406	+16.644
4	+32.901 +/- 0.107	+33.098
5	+49.988 +/- 0.484	+49.767
6	+2.192 +/- 0.283	+2.166

The results for perturbing the cross sections are consistent between the multigroup MCNP and exact Partisn.

As a further test, a reflected slab problem was run. The core region has a half thickness of 4.5 cm and a total half-thickness of 50 cm. The perturbation is shrinking the core region by 0.05 cm and filling that region with the reflector material. This simulates a differential control rod worth calculation.

The reactivity change from linear perturbation in MCNP was measured as -476.664 +/- 9.131 pcm. The exact reactivity calculated in Partisn is -489.238 pcm. While the results are outside of the error bounds, recall that the two calculations are between first order (MCNP) versus exact (Partisn).

3.2. Cross Section Library Perturbation

The Godiva sphere problem was run with continuous energy physics in MCNP. A question an engineer may want to know is the difference in *k*-effective from using different cross section data sets.

To see if the new method can answer this question, MCNP calculated *k* for Godiva with both ENDF/B-VI.5 and ENDF/B-VII.0 with separate calculations. The results were used to calculate an exact Δk. Next, a separate calculation was run where the material was perturbed from one library to the other and the reactivity change $\Delta\rho$ was estimated. From this, a predicted value of Δk is made. The results of the calculations are given in Table III.

Table III. Validation of ability for method to estimate change in *k* due to perturbed cross sections.

	***k*-Eigenvalue/Reactivity**
k (ENDF/B-VI.5)	0.99644 +/- 0.00004
k (ENDF/B-VII.0)	0.99988 +/- 0.00004
Δk (exact)	**+0.00344 +/- 0.00006**
$\Delta\rho$ (predicted)	-0.0031925 +/- 0.00015232
Δk (predicted)	**+0.00318 +/- 0.00016**

The predicted change in the multiplication factor lines up fairly well with the exact results computed by taking the difference of two separate calculations. In principle it should now be possible to estimate the reactivity change with only one calculation rather than two or more.

4. CONCLUSIONS & FUTURE WORK

A method has been developed for estimating the change in reactivity (using adjoint-weighting in linear perturbation theory) caused by changing cross section or material definitions. The results have been benchmarked for both multigroup and continuous energy cases.

Further validation of both cases will be required using more complicated and diverse problems. Nonetheless, the early results seem promising.

Future applications involve doing multiple perturbations in the same calculation for practical applications such as boron or control rod worth calculations. Also, this may be extendable to calculating sensitivity coefficients for various nuclear cross sections.

APPENDIX

Table A.I. Fissile cross section data (barns).

g	σ_a	$\nu\sigma_f$	σ_t	σ_{sg1}	σ_{sg2}	σ_{sg3}	σ_{sg4}
1	2.0	4.5	4.0	0.5	0.5	0.5	0.5
2	3.5	7.125	6.0	0.0	1.0	1.0	0.5
3	5.0	10.0	8.0	0.0	0.0	2.0	1.0
4	8.0	12.5	10.0	0.0	0.0	0.0	2.0

Table A.II. Reflector cross section data (barns).

g	σ_a	$\nu\sigma_f$	σ_t	σ_{sg1}	σ_{sg2}	σ_{sg3}	σ_{sg4}
1	0.1	0.0	2.0	0.3	0.4	0.6	0.6
2	0.2	0.0	3.0	0.0	0.6	1.0	1.2
3	0.4	0.0	4.0	0.0	0.0	1.6	2.0
4	1.0	0.0	5.0	0.0	0.0	0.0	4.0

For both materials, the atomic density is 0.01 atoms/b-cm. All fission neutrons are born in group 1.

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