Title: Applications of Adjoint-Based Techniques in Continuous-Energy Monte Carlo Criticality Calculations

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Applications of Adjoint-Based Techniques in Continuous-Energy Monte Carlo Criticality Calculations

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The method for performing adjoint-weighted tallies in MCNP is discussed along with the applications of point kinetics, perturbation theory, and nuclear data sensitivities. Future applications are also discussed.

KEYWORDS: MCNP, kinetics, perturbation, sensitivity

I. Introduction

Many quantities in reactor physics and criticality safety are expressible as ratios of integrals of adjoint-weighted quantities. Examples of these are point kinetics parameters, reactivity changes from material substitutions, etc. The Monte Carlo code MCNP(1) has recently implemented the Iterated Fission Probability (IFP) method for computing adjoint-weighted tallies(2), allowing for the calculation of many of these reactor physics quantities.

This summary gives a brief overview of the IFP method in MCNP. The various applications and how the specific tallies are performed are discussed, and results are given for benchmarks or other systems. The current status of the research and near-term future efforts are discussed.

II. Method

The IFP method uses the physical interpretation of the adjoint function in an eigenvalue transport problem: the expected number of neutrons in a system, after a very long time, as a result of a hypothetical neutron introduced into the system at a point in phase space.

This is done in MCNP by grouping the active iterations of an eigenvalue calculation into contiguous blocks of about 10 iterations. In the first iteration of the block, neutrons are tagged and contributions to tallies to be adjoint weighted are made, the tags are passed to progeny in subsequent generations, and in the last iteration, estimates of neutron production are made and multiplied by the original scores, and the products are used to tally adjoint-weighted quantities of interest.

III. Current Applications

Currently, MCNP6 supports three adjoint-weighted quantities: point kinetics parameters, adjoint-based reactivity changes from material substitutions, and nuclear data sensitivity coefficients.

1. Point Kinetics

The point kinetics model is important for doing analysis of transients with feedback models. While MCNP does not do feedback, it can compute the parameters needed for the point kinetics model. These are Λ the neutron generation time, and β the effective delayed neutron fraction. The ratio is called delayed critical Rossi-α. For example, the equation for calculating the neutron generation time is

$$\Lambda = \frac{\left\langle \psi^{+}, F\psi \right\rangle}{\left\langle \psi^{+}, v^{-1}\psi \right\rangle}, \tag{1}$$

where F is the linear operator for fission, v is the neutron speed, and the brackets denote integration over all phase space.

This capability was implemented in MCNP5-1.60 and released in the Fall of 2010. Validation was performed by comparing to Rossi-α measurements of critical benchmarks(3). These are given in Table 1 using MCNP5-1.60 with ENDF/B-VII.0 data.

Benchmark	Measured	Calculated
Godiva	-111(2)	-113(2)
Flattop	-38.2(2)	-39.7(2)
Big-Ten	-11.7(1)	-11.8(1)
Jezebel	-64(1)	-65(1)
Thor	-19(1)	-20(1)
STACY-30	-0.0127(3)	-0.0133(3)

Table 1: **Calculated versus Measured Rossi-**α (10^4 s^{-1})

2. Reactivity Changes

A common problem in reactor analysis is the estimation of the change in reactivity from a small perturbation to the system, which is often a material substitution (e.g., small changes in control rod position, additions of boron to coolant). Using perturbation theory, the expression for the change in reactivity is

$$\Delta\rho = -\frac{\left\langle \psi^{+}, \Delta H\psi \right\rangle}{\left\langle \psi^{+}, (F + \Delta F)\psi \right\rangle}, \tag{2}$$

where ΔH is the change in the transport operator from the material substitution, and the denominator is the perturbed fission source (for linear-perturbation theory, this is unperturbed).

This capability was released in MCNP6-beta2 in the Spring of 2012. An example calculation of a differential control rod worth calculation is given in Fig. 1, where the reference results are obtained from a Δk of two MCNP calculations.

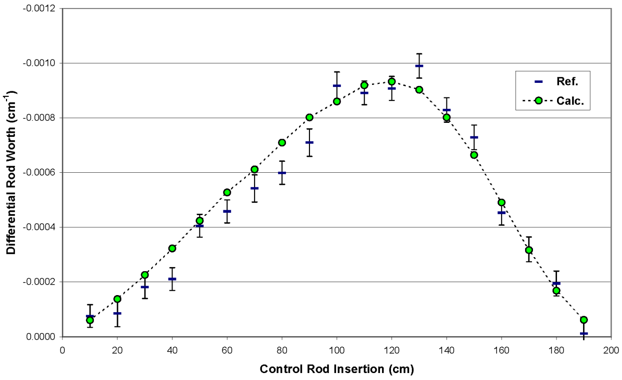

Figure 1: **Differential Rod Worth Curve**

3. Nuclear Data Sensitivities

Sensitivity coefficients to nuclear data are useful for uncertainty quantification, benchmark assessment, critical experiment design, etc. The sensitivity coefficient of k with respect to some data x is

$$S_{k,x} = \frac{x}{k}\frac{dk}{dx} = -\frac{\left\langle \psi^{+}, H_x \psi \right\rangle}{\left\langle \psi^{+}, k^{-1} F \psi \right\rangle}, \qquad (2)$$

where H_x is the transport operator, but only for interactions by nuclear data x.

This capability was released in MCNP6-beta3 in the Winter of 2012/2013[4]. This has been used for the preparation of a new benchmark specification for the Jezebel critical experiment. An example sensitivity profile is given in Fig. 2 for the Cu-63 elastic cross section in the copper-reflected Zeus experiment[5]. The energy resolution is 100 equal lethargy bins each lethargy decade. Note that the spikes in the plot are not from statistical noise, but a result of resonances of copper reflector and other structural components (mainly aluminum) in the experiment.

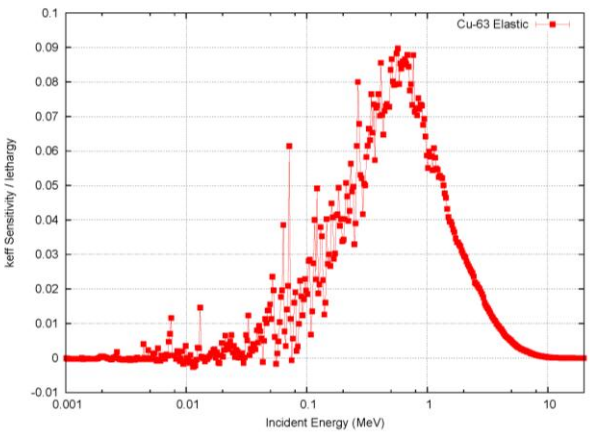

Figure 2: **Cu-63 Elastic Scattering Sensitivity Profile**

III. Summary and Future Applications

MCNP is currently capable of computing adjoint-weighted tallies for point kinetics parameters, reactivity changes from material substitutions, and nuclear data sensitivities. All of these have been verified and/or validated and used successfully for various applications.

Development continues in this area. In the near term, efforts will focus on sensitivity analysis. The next application of the nuclear data sensitivities is to compute sensitivities to material compositions or enrichments. This is a straightforward extension, and is already possible to compute manually from total cross section sensitivities. In fact, this has already been used for uncertainty quantification of the revised Jezebel specification.

Similar techniques can be used to estimate the derivatives of k with respect to interface locations. This is important for uncertainty quantification from uncertainties in experiment dimensions or considering manufacturing tolerances. A prototype of this has already been developed in MCNP, and results show generally good agreement. Further work will need to be done to integrate this into a production version of MCNP6.

Research is also being performed on Doppler temperature coefficients, which are important for reactor safety calculations. These can also be formulated as adjoint-weighted integrals using perturbation theory, and, in principle, these should be possible to compute using continuous-energy Monte Carlo. Other future developments include more general responses than k such as foil activations or leakage, and this should be possible using similar techniques.

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