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ADJOINT-WEIGHTED KINETICS PARAMETERS WITH CONTINUOUS ENERGY MONTE CARLO

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ABSTRACT

A method is developed and implemented in MCNP5-1.51 to calculate adjoint-weighted quantities for continuous energy Monte Carlo criticality calculations. The method is based on the iterated fission probability and uses only the existing random walks resulting in only a small CPU time increase. Reactor kinetics parameters such as the neutron generation time Λ and effective delayed neutron fraction β_{eff} are defined by ratios of integrals of adjoint-weighted quantities. Using this method, these adjoint-weighted quantities are estimated with MCNP and results are compared to various experiments. The non-adjoint-weighted prompt fission lifespan l_f in MCNP is compared to the adjoint-weighted Λ and non-negligible differences are observed in some cases.

1. Introduction

Monte Carlo methods have not been able to calculate continuous energy adjoint fluxes for reactor criticality problems. Many important parameters in nuclear reactor engineering, however, require them. An example is the effective delayed neutron fraction β_{eff} and neutron generation time Λ in one of the point-reactor kinetics equations [1,2]:

$$\frac{dn}{dt} = \frac{\rho - \beta_{\text{eff}}}{\Lambda} n(t) + \sum_i \lambda_i C_i(t) . \quad (1)$$

A method is developed and implemented in MCNP5-1.51 [3,4] that computes β_{eff} and Λ using only the existing random walks. The adjoint-weighting is done by estimating a proportional quantity called the iterated fission probability. Results are given for various test cases.

2. Theory

The parameters are defined [1,2] as inner-products of the adjoint flux and some operator on the flux as follows:

$$\beta_{\text{eff}} = \frac{\langle \psi^\dagger, \mathbf{B}\psi \rangle}{\langle \psi^\dagger, \mathbf{F}\psi \rangle} , \quad (2)$$

$$\Lambda = \frac{\langle \psi^\dagger, \frac{1}{v}\psi \rangle}{\langle \psi^\dagger, \mathbf{F}\psi \rangle} . \quad (3)$$

Here the flux is given by ψ , v is the neutron speed, and \mathbf{F} and \mathbf{B} are the operators for total and delayed fission. The inner-product is taken as an integral over all phase space.

In theory, Monte Carlo can compute any integral quantity. However, estimating the adjoint flux is not easy with this approach. However, in a reactor at critical, the adjoint flux is directly proportional to the iterated fission probability (IFP) defined as follows [5]: A neutron (call it a progenitor) introduced at a point in phase space may produce more neutrons via fission. These progeny neutrons may produce more neutrons in successive generations. After a sufficient number of generations, the neutron population from this progenitor will reach an asymptotic value. This value is the IFP and is proportional to the adjoint flux at the introduction site.

3. Method Development

Computing β_{eff} and Λ requires the calculation of the three integrals found in equations (2) and (3). Three tallies will need to be performed in the simulation.

First consider the adjoint-weighted fission source. Neutrons are sampled from an estimate of the fission source every cycle in a criticality calculation. Suppose these source neutrons (index p) are followed through several generations (cycles) with a memory of where each started. After many generations the asymptotic population of each neutron π_p is estimated by a track length estimator,

$$\pi_p = \sum_{\tau \in p} v \Sigma_f w d . \quad (4)$$

$v\Sigma_f$ is the neutrons 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 with a progenitor index p .

Suppose the estimates are tallied with some space-energy discretization for positions of the source neutrons. The resulting scores are proportional to both the asymptotic population (adjoint flux) and the fission density in the regions. This insight shows this tally gives a fission density weighted by its adjoint.

To formulate a tally, both the effect of the importance and the fission density must be taken into account. The fission density distribution as a function of space and energy can be sampled by the fission source weight, and the importance weighting can be done by multiplying the source weight by the asymptotic population many cycles later.

If the arbitrarily small regions are joined into one that covers the entire reactor (effectively an integration over phase space), this tally defines one of the kinetics integrals:

$$\langle \psi^\dagger, \mathbf{F}\psi \rangle = \frac{1}{W} \frac{1}{V} \sum_p \pi_p w_{0,p}. \quad (5)$$

Here $w_{0,p}$ is the weight of the fission source neutron, W is the total source weight of the progenitors, and V is the reactor volume.

The tally for the adjoint-weighted delayed fission source is very similar except only neutrons from delayed emission score. All other parameters, including W , are unchanged.

$$\langle \psi^\dagger, \mathbf{B}\psi \rangle = \frac{1}{W} \frac{1}{V} \sum_{p \in \beta} \pi_p w_{0,p}. \quad (6)$$

The use of the fission source is completely arbitrary. In fact, any starting distribution may be used. This opens up the possibility of calculating all sorts of adjoint-weighted quantities. However, one relevant distribution is the flux, which can be obtained from the track lengths of the random walks.

Progenitors can be introduced, mathematically-speaking, along each track and tallied. Further, each track can be weighted by a multiplier, namely one over the neutron speed. This allows the calculation of the adjoint-weighted neutron density:

$$\left\langle \psi^\dagger, \frac{1}{v}\psi \right\rangle = \frac{1}{W} \frac{1}{V} \sum_p \pi_p \sum_{\tau \in p} \frac{1}{v_\tau} \frac{w_{0,p}}{w} w d_\tau. \quad (7)$$

The extra weighting factor of the fission source weight over the particle weight arises from the need to start each progenitor in the IFP calculation with an equal weight. Also note that implicit capture leads to many fission neutrons produced at different points within the same history (branching) and everything must be summed carefully to preserve causality.

4. Results

With these three integrals tallied, the kinetics parameters are obtained by taking the ratios given in (2) and (3). To correctly compute uncertainties, correlations between each of the three integrals are considered. Some experimental data is given in terms of Rossi- α , which is:

$$\alpha \approx -\frac{\beta_{\text{eff}}}{\Lambda} = -\frac{\langle \psi^\dagger, \mathbf{B}\psi \rangle}{\langle \psi^\dagger, \frac{1}{v}\psi \rangle}. \quad (8)$$

For many criticality benchmarks, results for either β_{eff} or $-\alpha$ are given. The calculations are done with five latent generations which appear to be sufficient for the small criticality benchmarks. The results obtained for several benchmarks are given in Table 1. The method is used to calculate β_{eff} and $-\alpha$ for the given benchmarks; results are in Table 2.

Table 1. Experimental kinetics data for various criticality benchmarks.

Benchmark	β_{eff} (pcm)	$-\alpha$ (s ⁻¹)
Godiva [6,7]	645	(1.11 +/- 0.02) x 10 ⁶
Jezebel [6,7]	190	(6.4 +/- 0.01) x 10 ⁵
Flattop-23 [6,8]	360	(2.71 +/- 0.03) x 10 ⁵
BIG TEN[6,9]	720	(1.17 +/- 0.01) x 10 ⁵
WINCO-1 [6]		(1.1093 +/- 0.0003) x 10 ³
Stacy-29 [6]		(1.227 +/- 0.0041) x 10 ²

Table 2. MCNP (ENDF/B-VI.6) calculated β_{eff} or $-\alpha$ for various criticality benchmarks.

Benchmark	β_{eff} (pcm)	$-\alpha$ (s ⁻¹)
Godiva	649.1 +/- 7.2	(1.1363 +/- 0.01271) x 10 ⁶
Jezebel	186.0 +/- 3.7	(6.4299 +/- 0.12934) x 10 ⁵
Flattop-23	375.9 +/- 6.3	(2.9615 +/- 0.05031) x 10 ⁵
BIG TEN	736.0 +/- 14.9	(1.2223 +/- 0.02496) x 10 ⁵
WINCO-1	861.0 +/- 12.6	(1.1482 +/- 0.01699) x 10 ³
Stacy-29	762.6 +/- 9.8	(1.2776 +/- 0.01563) x 10 ²

The results for the fast sphere problems appear to perform fairly well. There appears to be a trend where these results are higher than the experimental value and this requires investigation.

MCNP5 can compute the fission lifespan l_f . This is the simulated time between fissions and is a non-adjoint-weighted estimate of the neutron generation time Λ . Comparisons of the two are given in Table 3.

The results show a difference between the two estimates in MCNP.

Table 3. Comparison of l_f and Λ from MCNP (ENDF/B-VI.6). Uncertainties in l_f are $\ll 1\%$.

Benchmark	l_f	Λ
Godiva	5.9322 ns	5.7127 +/- 0.0082 ns
Jezebel	3.0649 ns	2.8924 +/- 0.0044 ns
Flattop-23	15.277 ns	12.6940 +/- 0.0417 ns
BIG TEN	63.058 ns	60.2169 +/- 0.1689 ns
WINCO-1	7.4400 μ s	7.4985 +/- 0.0142 μ s
Stacy-29	61.483 μ s	59.6897 +/- 0.0670 μ s
B&W-11-2[6]	26.623 μ s	26.3321 +/- 0.0242 μ s
APWR[10]	23.581 μ s	23.7780 +/- 0.0631 μ s

Many of the problems exhibit a non-negligible difference because Λ , unlike l_f , is weighted by importance. This is especially visible in the Flattop-23 benchmark, which is a sphere of (largely) ^{235}U surrounded by a natural uranium reflector. The prompt removal lifetime calculation treats all tracks and collisions equally regardless of their importance to the chain reaction. The tallies in the Λ calculation are weighted by their IFP that measures importance. l_f too highly weights reflector neutrons that do not have as significant a contribution to overall multiplication. The opposite is true for the inner sphere.

5. Conclusions and Future Work

A method is developed to calculate adjoint-weighted quantities in systems near critical using the iterated fission probability. The method is implemented in MCNP5-1.51 and, since it uses only the existing random walks, requires very little additional CPU time. This is applied to computing kinetics parameters and results are compared to experiments.

The results show estimates to be slightly higher than the experimental values. Further investigation will be needed, which may include studying the effect of varying the number of generations to wait until the population is considered asymptotic. Also, for many problems, the adjoint-weighting provides an improvement over MCNP's current fission lifespan calculations.

Many important quantities in reactor physics can be computed with inner-products of adjoint-weighted quantities. Examples of these involve perturbation analysis, reactivity coefficients, and sensitivity/uncertainty analysis of cross-section data. In addition, adjoint-weighted fluxes at specific regions in phase space can be computed. This method facilitates such calculations with continuous energy Monte Carlo.

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