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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 and extensions such as localized adjoint-weighted fluxes, more sophisticated kinetics models, higher-order perturbation theory, and temperature coefficients.

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 paper gives overview of the theory of the adjoint function and the IFP method as implemented 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 also discussed.

II. Theory & Method

The static, or k-eigenvalue form of the neutron transport equation is

$$H\psi = \frac{1}{k}F\psi, \tag{1}$$

where ψ is the neutron flux, H is the operator containing the physics for streaming, collisions, and scattering, F is the operator for fission, and k is the system eigenvalue. This equation has, for a general system, infinitely many solutions k and ψ. The solution corresponding to the highest value of k_0 (called the effective multiplication factor) is the fundamental mode ψ_0 corresponding to the steady state neutron distribution in the system.

Many representative quantities about a system may be derived from the neutron transport equation, such as the point kinetics parameters, that involve integrating over the problem domain. The resulting expression can often be simplified by finding a special weighting function ζ satisfying

$$\langle \zeta, Af \rangle = \langle f, B\zeta \rangle, \tag{2}$$

where f is an arbitary function and A and B are generic linear operators and the brackets denote integration over all phase space. This property can be satisfied if B is chosen such that it is the adjoint of A, or $A^\dagger$ and the weighting function ζ is the solution to the adjoint form of the equation involving operator A, or, in this case, $\psi^\dagger$. Such reactor physics quantities therefore involve an integral of the form

$$\left\langle \psi^\dagger, A\psi \right\rangle \tag{3}$$

that is to be solved by Monte Carlo.

The adjoint function $\psi^\dagger$ is obtained by solving the adjoint neutron transport equation

$$H^\dagger\psi^\dagger = \frac{1}{k}F^\dagger\psi^\dagger. \tag{4}$$

The adjoint of the operator H reverses the direction of streaming and changes the scattering kernel such that the velocity transfers "backwards" in collisions, and the adjoint operator of F reverses the roles of the fission multiplicty $\nu\Sigma_f$ and emission spectrum χ. Note that the eigenvalue k can be proven to be equivalent to the adjoint eigenvalue $k^\dagger$.

The often given physical interpretation of the adjoint function is that it can be thought of as the equation for describing a quantity that is transported "backwards" from normal transport. This quantity can be shown to the expected response resulting from a unit neutron injected into a system at that point in phase space along with all its secondary particles. Therefore, the adjoint function is often called importance. For the k-eigenvalue problem, the response can be thought of as the self sustaining fission process, and the importance as the propensity of a unit neutron at that point in phase space to sustain that chain reaction.

A thought experiment to further explain the adjoint function or importance is as follows: Consider a critical assembly—if the assembly is not critical in the real word, a mathematical factor $1/k_0$ is magically applied to make it so as it would be in a simulation—devoid of neutrons. An experimentalist takes a neutron and places it at some location in the assembly, points it in a certain direction, and sets it along at a particular energy. The experimentalist then leaves and returns after an effectively

infinite time and records a count of the number of neutrons in the assembly. She then flushes all the neutrons out of the assembly and then proceeds to repeats the exact same process a large number of times, always taking care to record the neutron count, which will vary because neutron transport is an inherently stochastic process subject to quantum mechanical effects. The average of the recorded counts is then taken, and this count (relative to those obtained at different phase space locations) corresponds to the importance at that point.

This thought experiment forms the basis for the IFP method implemented in MCNP. An iteration (often called a cycle or batch depending on the parlance of a particular code) in the power iteration process used to solve the k-eigenvalue neutron transport equation typically corresponds to a single fission generation—alternative definitions of an iteration involving multiple fission generations are sometimes used, but are not of concern here. Suppose the iterations are grouped into *blocks* containing N consecutive iterations; the block physically corresponds to a fission chain with the number of progeny adjusted by a factor of $1/k_0$ each fission event. The number of iterations per block N is chosen such that the fission chain is long enough that effectively an infinite amount of time has passed and the asymptotic neutron population has reached its stationary state; exactly how large N should be is problem dependent, but a choice of $N = 10$ seems to work well empirically.

With this model in mind, the algorithm to perform an adjoint-weighted integral via Monte Carlo is as follows: In the first iteration in the block, the quantity $A\psi$ is tabulated at various events in the simulation. The neutrons causing these events are given a tag that is associated with the events where $A\psi$ is tallied, and these tags are inherited by subsequent progeny neutrons. These tags persist throughout the fission chain until the final generation in the block, at which point a "measurement" of the neutron population caused by that chain is made by way of a Monte Carlo tally. The value of this measurement is multiplied by the corresponding $A\psi$ contributions made many iterations ago and this product is the score of the adjoint-weighted tally. This process is repeated in subsequent blocks and the mean value of the products of asymptotic population and $A\psi$ contributions is the Monte Carlo estimate of the adjoint-weighted integral.

III. Current MCNP Applications

There are three applications of adjoint-weighted tallies in MCNP6.1, the current version as of the time of this writing. These are: point kinetics parameters,[3] perturbations from material substitutions,[4] and nuclear data sensitivities.[5]

1. Point Kinetics

The point kinetics model is often used as a simple approximation of time behavior of the neutron population in a reactor. This is done by assuming that the time behavior is separable from the rest of the phase space,

$$\psi(\mathbf{r}, \mathbf{v}, t) = n(t)\varphi(\mathbf{r}, \mathbf{v}). \tag{5}$$

Substituting this expression into the neutron transport equation, multiplying by the adjoint function $\psi^\dagger$, and some rearrangement yields the classic point kinetics equations:

$$\frac{dn}{dt} = \frac{\rho - \beta_{\text{eff}}}{\Lambda} n(t) + \sum_{i=1}^{M} \lambda_i C_i(t), \tag{6}$$

$$\frac{dC_i}{dt} = \frac{\beta_{i,\text{eff}}}{\Lambda} n(t) - \lambda_i C_i(t), \quad (i = 1 \ldots M). \tag{7}$$

$n(t)$ is the neutron population and $C_i(t)$ is the delayed neutron precursor concentration of species i at time t. The rest of the terms are the kinetics parameters, which must be obtained via simulation or measurement. ρ is the reactivity, which is usually defined as $(k - 1)/k$, λ_i is the radioactive decay constant for species i, which is usually a fission-weighted average of the measured decay constants for each precursor species for each isotope, and the other kinetic parameters are ratios of adjoint-weighted integrals:

$$\Lambda = \frac{\left\langle \psi^\dagger, v^{-1}\psi \right\rangle}{\left\langle \psi^\dagger, F\psi \right\rangle}, \tag{8}$$

is the effective neutron reproduction time representing the time a representative neutron driving the chain reaction takes to replace itself (v is the neutron speed);

$$\beta_{\text{eff}} = \frac{\left\langle \psi^\dagger, B\psi \right\rangle}{\left\langle \psi^\dagger, F\psi \right\rangle}, \tag{9}$$

is the effective delayed neutron fraction, representing the fraction of the neutrons that are delayed, regardless of species, accounting for the relative effectiveness of delayed and prompt neutrons toward driving the chain reaction (B is the operator for fissions that eventually lead to delayed neutron emission);

$$\beta_{i,\text{eff}} = \frac{\left\langle \psi^\dagger, B_i\psi \right\rangle}{\left\langle \psi^\dagger, F\psi \right\rangle}, \tag{10}$$

is the effective delayed neutron fraction specifically for species i (B_i is the operator for fissions that eventually lead to delayed neutron emission of just species i), which is needed to account for the fact different species emit delayed neutrons at slightly different energies.

A quantity that is often measured in experiments is the delayed critical Rossi-α, which is approximately

$$\alpha_R \approx -\frac{\beta_{\text{eff}}}{\Lambda} = -\frac{\left\langle \psi^\dagger, B\psi \right\rangle}{\left\langle \psi^\dagger, v^{-1}\psi \right\rangle}. \tag{11}$$

Once the parameters are known, the point kinetics equations can be solved (usually with some feedback model) to obtain the neutron population as a function of time $n(t)$.

To validate the method as implemented in MCNP6, calculation results of α_R are compared with experimental measurements in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook.[6] These comparisons are shown in Table 1, and the calculations tend to overpredict this set of benchmarks by a few percent, but overall the agreement should be good enough considering the approximations of the point kinetics model.

Benchmark	Measured	Calculated	C/E
Godiva	-111(2)	-113(2)	1.02
Flattop	-38.2(2)	-39.7(2)	1.04
Big-Ten	-11.7(1)	-11.8(1)	1.01
Jezebel	-64(1)	-65(1)	1.02
Thor	-19(1)	-20(1)	1.05
STACY-30	-0.0127(3)	-0.0133(3)	1.05

Table 1: Comparison of delayed critical Rossi-α (10^4 s^{-1}) measurements and MCNP6.1 calculations.

2. First-Order Material Substitution Perturbations

As part of reactor design, it is often desirable to know the change in reactivity $\Delta\rho$, magnitude and sign, for various small changes to a system. Many of these can be cast in the form of a material substitution, e.g., enrichment or composition changes, moderator density changes, control rod movement, etc.

The need for adjoint weighting arises for similar reasons to the point kinetics equations. To see, first expand the terms in the neutron transport equation as $x \rightarrow x + \Delta x$,

$$(H + \Delta H)(\psi + \Delta\psi) = \left[\frac{1}{k} + \Delta\left(\frac{1}{k}\right)\right](F + \Delta F)(\psi + \Delta\psi). \quad (12)$$

The desired unknown is $\Delta(1/k) = -\Delta\rho$; however, the change in the flux $\Delta\psi$ is unknown as well. By multiplying out the terms and assume all higher-order terms are negligible (e.g., $\Delta H\Delta\psi \approx 0$), the expression can be simplified, but still involves $\Delta\psi$. If, however, the resulting equation is multiplied by $\psi^\dagger$ and integrated over all phase space, the adjoint property $\left\langle \psi^\dagger, A\psi \right\rangle = \left\langle \psi, A^\dagger\psi^\dagger \right\rangle$ can be employed to eliminate the $\Delta\psi$ terms. This leads to a tractable form that does not require knowing the change in the flux:

$$\Delta\rho = -\frac{\left\langle \psi^\dagger, \left(\Delta\Sigma_t - \Delta S - k^{-1}\Delta F\right)\psi \right\rangle}{\langle \psi^\dagger, (F + \Delta F)\psi \rangle}, \quad (13)$$

where Σ_t is the total interaction cross section, and S is the integral operator for scattering. All the Δ terms are assumed to be known because they are defined by the perturbation, an input to the calculation. Note that the because of the denominator, this equation is a non-linear perturbation, even though it is still technically first order. Often this expression is further linearized where the denominator is written as the unperturbed fission source.

To demonstrate the method's capability, two perturbations are shown: the buildup of ^{135}Xe and control rod worth. In both cases, the predicted perturbed eigenvalue k' is found both with perturbation theory and directly from an MCNP6 calculation where the materials have been substituted.

For the xenon worth calculation, a detailed 2-D Pressurized Water Reactor (PWR) model is used, where the base case has no xenon. The perturbation involves adding some small amount of ^{135}Xe to the fuel uniformly (not a terrible assumption because the flux in this system is fairly flat across the core). Figure 1 shows the perturbed k for various concentrations of ^{135}Xe (in ppb). The results show good agreement for additions less than 20 ppb, but the results begin to diverge as the concentration increases; there is about a 1.4% relative error for the 50 ppb case.

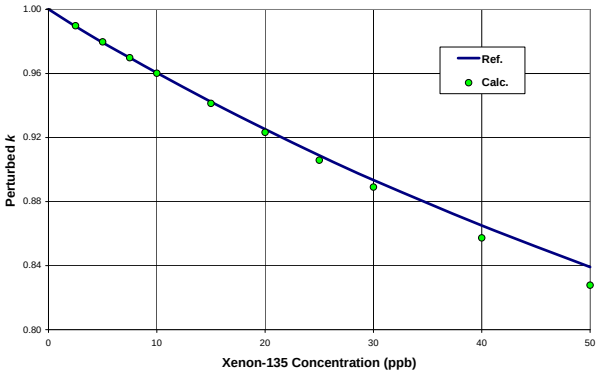

Figure 1: Perturbation theory and direct calculation estimates of perturbed k for varying ^{135}Xe concentration.

The second test examines control rod worth. A reflected, homogeneous cylindrical reactor is used. The cylinder has a height of 200 cm with an inner region of radius 100 cm and an outer region with radius of 150 cm. The inner region (atomic density of 9.02878 x 10^{-2} atoms per barn-cm) is a homogeneous mixture of water, uranium oxide (UO_2 at 4% enrichment), and iron-56 in atomic fractions of 63.3%, 31.7%, and 5.0% respectively. The outer region is simply a water blanket surrounding the inner core region with atomic density of 2.3024 x 10^{-2} atoms per barn-cm.

The inner region is subdivided axially into three zones. The top zone contains a relative boron-10 concentration of 1.0 x 10^{-4} to simulate the addition of control rods from the top of the core. The bottom zone is the area where no control material has been inserted. The middle zone is 1 cm in length; it takes the property of the bottom zone in the unperturbed case, and has the material of the top zone in the perturbed case.

The differential rod worth, $d\rho/dz$, is approximated by the ratio of the change in reactivity $\Delta\rho$ to the change in rod height Δz. The control rod bank height is given an unperturbed insertion starting from z = 10 cm and going in 10 cm increments to z = 190 cm. The perturbation is moving the entire control rod bank (represented by a homogeneous axial zone) downward by 1 cm. The differential rod worth estimates along with the reference values (obtained from subtracting $1/k$ obtained from two independent Monte Carlo calculations) are given in Fig. 2. Figure 3 displays k estimated from an integral worth curve obtained from trapezoidal integration of the differential rod

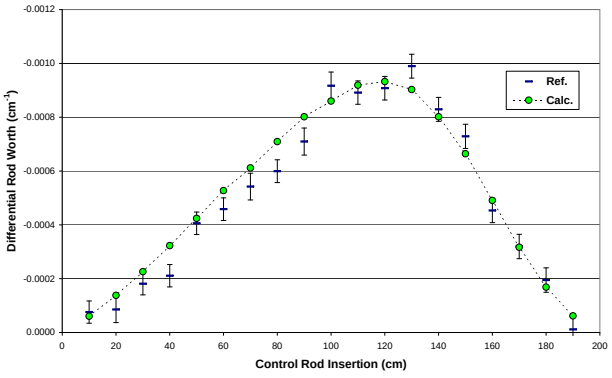

Figure 2: Perturbation theory and direct calculation estimates of differential rod worth.

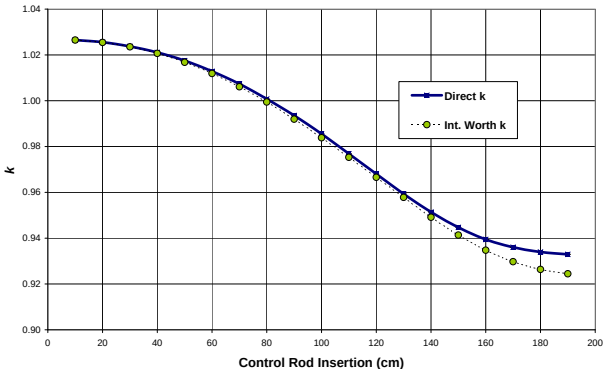

Figure 3: Perturbation theory and direct calculation estimates of integral rod worth.

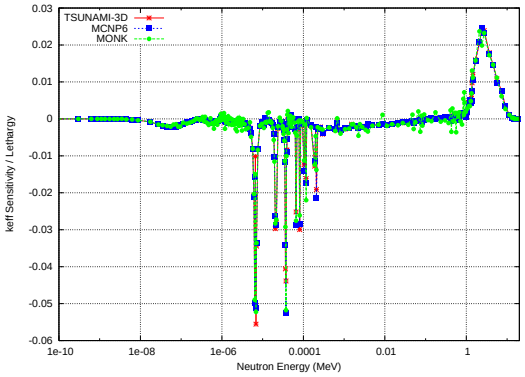

Figure 4: Code comparison of ^{238}U total cross section sensitivity in OECD/NEA UACSA Benchmark Phase III.1.

worth curve.

The first-order perturbation results produce curves representative of what is expected. However, as seen in Fig. 3, the predicted values of k from the differential worths do not match the corresponding directly computed values. This is especially so when the control rods are deep into the core. This is likely because a first-order approximation is inadequate; as the control rods near the bottom of the core, the flux becomes quite peaked.

3. Nuclear Data Sensitivities

Closely related to material substitutions is the application of nuclear data sensitivities. In this case, the motivation is to understand which nuclear data are the most important driver toward determining a system's k. This is particularly important in the area of validation and uncertainty analysis. Assessing the predictive capability of a particular transport software package and nuclear data library requires to see how well the calculations perform on similar established benchmarks. Establishing commonality between a calculation model and benchmarks can be done by comparing their sensitivity coefficients $s_{k,x}$; two systems that have similar sensitivities can be said to be alike from a validation point of view.

The sensitivity coefficient of the eigenvalue k with respect to nuclear data x (e.g., fission cross section, etc.) is defined as

$$s_{k,x} = \frac{dk/k}{dx/x}, \tag{14}$$

or the ratio of the relative differential change in k as a result of a relative differential change in x. The derivation of the sensitivity coefficient in terms of adjoint-weighted integrals is very similar to that of perturbation theory. The final result is

$$s_{k,x} = -\frac{\left\langle \psi^\dagger, \left(\Sigma_x - S_x - k^{-1}F_x\right)\psi \right\rangle}{\langle \psi^\dagger, F\psi \rangle}. \tag{15}$$

The form is very similar to that of estimating $\Delta\rho$ from a material substitution. Σ_x is the cross section for nuclear data x; or zero if x is not a cross section (e.g., fission ν). S_x is the scattering operator for just nuclear data x; e.g., if x was elastic scattering off ^{238}U, S_x would be the partition of the scattering integral for just elastic scattering involving 238U. Likewise, F_x is the fission operator for just nuclear data x.

The sensitivity coefficients can be applied to estimate the uncertainty in k. Given a covariance matrix $\mathbf{C}$ of the nuclear data and a corresponding sensitivity vector $\mathbf{S}$ the uncertainty in the eigenvalue δk may be found via the so-called sandwich rule:

$$(\delta k)^2 = \mathbf{SCS}^T. \tag{16}$$

To assess the applicability of the IFP method for computing sensitivity coefficients, comparisons with other software packages, TSUNAMI-3D[7] and MONK,[8] are done. The problem used for comparison is the OECD/NEA UACSA Benchmark Phase III.1 benchmark,[9] which is an array of MOX fuel pins immersed in light water, simulating a criticality accident where a lattice of MOX fuel in a storage or shipping cask is flooded. This is based on the benchmark within the ICSBEP Handbook having the identifier MIX-COMP-THERM-001-001. The detailed 3-D model is a square lattice with a pitch of 0.9525 cm. The lattice is 28×22, except for the top row, which has only 17 pins, for a total of 605 pins. The fuel pins have a diameter of 0.5842 cm and a height of 91.44 cm. The areas axially above and below are buffers that are treated as homogenized mixtures of water and pin materials. A light-water scattering kernel is used for thermal scattering with hydrogen in the water. ENDF/B-VII.0 data is used for the calculations.

Energy-resolved sensitivities to the ^{238}U total cross section computed by MCNP6, TSUNAMI-3D, and MONK (using JEF-2.2 nuclear data) are shown in Fig. 4. All results mostly agree, with some small discrepancies between TSUNAMI-3D and the results from either MONK or MCNP6.

Reaction	Reaction	δk
elastic	elastic	462.1
elastic	inelastic	-867.5
elastic	n,2n	-3.4
elastic	fission	-82.2
elastic	n,gamma	36.0
inelastic	inelastic	859.0
inelastic	fission	1.3
n,2n	n,2n	11.1
fission	fission	331.0
fission	n,gamma	0.3
n,gamma	n,gamma	72.4
total nu	total nu	81.6
fission chi	fission chi	174.1
		587.6

Table 2: Uncertainties of k from ^{239}Pu in Jezebel.

These sensitivity results are also used to compute the uncertainty of k for the Jezebel benchmark (PU-MET-FAST-001 in the ICSBEP Handbook) using ENDF/B-VII.1 covariance data. Table 2 shows the uncertainties in k (in pcm = 1×10^{-5}) by reaction from ^{239}Pu, the dominant isotope toward determining k. The total predicted uncertainty is 587.6 pcm, which can be obtained by taking the signed sum squared of each of the individual components—the factor of two on the off-diagonal terms (e.g., elastic correlated with inelastic) is included in those values. The results show that most of the uncertainty arises from the scattering and fission cross section, with fission χ providing a significant amount as well.

IV. Potential Future Applications & Extensions

The applications of point kinetics, perturbations from material substitutions, and nuclear data sensitivities are the ones currently implemented in MCNP6.1. There are certainly ways that these can be extended, and new capabilities demanding adjoint weighting can be added as well should the need arise. Some of these possible extensions and future applications are discussed.

1. Localized Adjoint-Weighted Flux & Reaction Rates

The adjoint-weighted flux (sometimes called the contributon[10]) gives an estimate of the flow of radiation from source to response. In some respects, these can be thought of as neutron field lines analogous to those of magnetic fields. Most of the utility of such a capability is in fixed-source problems involving source and a localized detector or response to understand the most important paths neutrons take to reach a response zone. As such, these are often useful in shield design or detector placement analysis.

The usefulness of an adjoint-weighted flux (or reaction rate) is less clear in eigenvalue problems as the source and response (the fission distribution) are spatially the same. Nonetheless, there is still information to be had in systems where neutrons thermalize to cause a significant portion of the fissions driving the chain reaction. The energy-dependent adjoint-weighted flux can give information about exactly where the neutrons that most drive the chain reaction are undergoing thermalization. This information can be helpful in placement of control or poison elements to regulate reactivity in, for instance, a criticality safety application.

MCNP currently allows space- and energy-dependent flux and reaction rate tallies on structured (by way of a superimposed mesh) and unstructured meshes (by way of coupling with Computer-Aided Engineering software such as Abaqus). The quantities calculated on these meshes could be weighted by the importance function to estimate the adjoint-weighted equivalents.

2. Extensions to Kinetics

The point kinetics model represents the simplest of the kinetic models to represent dynamic behavior in nuclear systems. Two possible improvements are the multi-point kinetics model and modal kinetics.

The multi-point model is useful when the fissionable system involves multiple, not-too-tightly interacting units, such as those systems found in criticality safety analyses or some experiments. The model treats the kinetics of each unit separately and the units are connected via coupling coefficients. The kinetic parameters and coupling coefficients form a matrix equation that can be solved to better approximate the dynamic behavior of such systems. In principle, these should be calculable via Monte Carlo using existing methods.

Studying transients where an event occurs that causes a significant deviation in the flux shape requires modal kinetics. Recall that the k-eigenvalue neutron transport equation has infinitely many solutions, and thus far, the only solution that has been utilized is the fundamental mode. These higher modes or eigenfunctions can be used to calculate kinetics parameters for higher modes, and the transient can be described by a linear combination thereof. It is possible to compute higher eigenfunctions, adjoint-weighted higher modes, of the k-eigenvalue neutron transport equation using a hybrid of the IFP and fission matrix methods.[11–13] Such work is currently under development.

3. Higher-Order Perturbation Theory

In a similar vein, higher eigenfunctions can be used to better approximate perturbation theory. As seen in the integral worth curve in 3 first-order perturbation theory cannot capture perturbations where the flux shift is too large; i.e., the second-order terms $\Delta H \Delta\psi$ and $\Delta F \Delta\psi$ are no longer approximately zero. This can be remedied if an estimate of $\Delta\psi$ can be made, and this can be done if adjoint-weighted higher modes are used similarly to how they would for modal kinetics. Research is currently ongoing in this area.

4. Temperature Coefficients

The temperature coefficient of reactivity determines the stability of the system in the presence of increases in temperature (related to reactor power). The change in the reactivity from temperature effects arises from changes in density and Doppler broadening of the nuclear resonances. In many designs, it is vital to demonstrate that the temperature coefficient is negative in all operating and off-normal conditions. The reactivity temperature coefficient is

$$\alpha_T = \frac{d\rho}{dT}. \tag{17}$$

This can be cast into the form of adjoint-weighted integrals by way of perturbation theory:

$$\alpha_T = -\frac{\left\langle \psi^\dagger, \left(\frac{d\Sigma_t}{dT} - \frac{dS}{dT} - k^{-1}\frac{dF}{dT}\right)\psi \right\rangle}{\langle \psi^\dagger, F\psi \rangle}. \tag{18}$$

If a representation can be found for the temperature derivatives of the total cross section, scattering integral, and fission integral, an estimate of α_T can be made with the adjoint weighting techniques.

Preliminary results have been obtained that suggest this is possible for the Doppler coefficient.[14] The temperature derivatives have been obtained based on the "On-The-Fly" (OTF)

Doppler broadening method[15] implemented in MCNP6; the OTF method represents the temperature dependence of the cross sections by way of a polynomial fit in ± powers of the $\sqrt{T}$. Results show that the method can estimate the Doppler coefficient to within a few percent (reference α_T from a central difference of two calculations) for a simple problem of an infinite lattice of low-enriched uranium metal pins surrounded by hydrogen.

5. Extensions to Sensitivities

The current method in MCNP6.1 only computes sensitivities to nuclear data, and only for the response of k. This can be extended in both dimensions.

Any quantity that is uncertainty would ideally need a sensitivity to perform overall uncertainty quantification. Such quantities are, for example, geometric tolerances, locations of components, material compositions, densities, and temperatures. The latter three can probably be covered with existing methods discussed in this paper. The area of sensitivity and uncertainty analysis for geometry is an active area of research.

The expressions of perturbation theory can be extended beyond k to cover other responses such as leakages and reaction rate ratios as well. This is also an active area of development.

V. Conclusions

The IFP method allows for the computation of integrals of adjoint-weighted quantities in a continuous-energy Monte Carlo simulation. These quantities can then be used in reactor analysis. Currently, MCNP6.1 supports adjoint-weighted calculations for point kinetics, first-order perturbation theory for material substitutions, and nuclear data sensitivities. Future applications are currently being researched including the calculation of localized adjoint-weighted fluxes, higher-order kinetics and perturbation models, temperature coefficients, and various extensions to sensitivities.

Acknowledgments

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