## 5. Comparison of Sensitivity Analysis Techniques in Monte Carlo Codes for Multi-Region Criticality Calculations, *Bradley T. Rearden, Douglas E. Peplow (ORNL)*

### INTRODUCTION

Recently, sensitivity and uncertainty (S/U) techniques have been used to determine the area of applicability (AOA) of critical experiments used for code and data validation [1]. These techniques require the computation of energy-dependent sensitivity coefficients for multiple reaction types for every nuclide in each system included in the validation. The sensitivity coefficients, as used for this application, predict the relative change in the system multiplication factor due to a relative change in a given cross-section data component or material number density. Thus, a sensitivity coefficient, $S$, for some macroscopic cross section, $\Sigma$, is expressed as

$$S = \frac{\Sigma}{k}\frac{\partial k}{\partial \Sigma} ,$$

where $k$ is the effective neutron multiplication factor for the system. The sensitivity coefficient for the density of a material is equivalent to that of the total macroscopic cross section.

Two distinct techniques have been employed in Monte Carlo radiation transport codes for the computation of sensitivity coefficients. The first, and most commonly employed, is the differential sampling technique. The second is the adjoint-based perturbation theory approach. This paper briefly describes each technique and presents the results of a simple test case, pointing out discrepancies in the computed results and proposing a remedy to these discrepancies.

### DESCRIPTION

Differential sampling is an advanced Monte Carlo method that calculates the derivatives of the response with respect to some parameter at the same time that the response is calculated. First, second, third, etc., and cross derivatives can all be found by adding a few variables that follow the particles and adding a few more accumulators to the problem. Once found, the derivatives can be used to find the sensitivities of the response to the parameter, compute the total uncertainty in the response (stochastic plus uncertainties in parameters), and find the values of the response for different values of the parameters using a simple Taylor series expansion.

Differential sampling with respect to material parameters (e.g., individual cross sections and material density) is available in MCNP [2]. It can be used with criticality problems, but the manual gives the following warning: "The track length estimate of $k_{eff}$ in KCODE criticality calculations assumes the fundamen-

TABLE I

Comparison of GODIVA Sensitivity Coefficients for Fuel Density

| | Whole System | Outer 2-cm Thick Shell |
|---|---|---|
| MCNP | 0.7987 ± 0.0019 | 0.3968 ± 0.0012 |
| MCNP direct recalculation | 0.8312 ± 0.0045 | 0.2788 ± 0.0042 |
| SEN3 | 0.8179 ± 0.0042 | 0.2749 ± 0.0030 |
| KENO V.a direct recalculation | 0.8260 ± 0.0071 | 0.2714 ± 0.0072 |

tal eigenvector (fission distribution) is unchanged in the perturbed configuration." This means that the source dependence on the parameter of interest is not taken into account by the differential sampling, which could lead to incorrect values of the derivatives if that source dependence is large.

The perturbation theory approach uses two independent multigroup transport calculations for the same system, one in the forward mode and one in the adjoint mode [3]. The scalar fluxes and their moments from these calculations are folded together with the multigroup cross-section data and the calculated $k_{eff}$ to produce the sensitivity coefficients. This technique is only valid for linear perturbations and does not predict higher order terms. Also, a primary assumption of this technique is that the perturbations are small enough that the flux solution does not change because of the perturbation.

Recently, this methodology has been updated and implemented in SEN3 [4], a sensitivity analysis sequence using the KENO V.a multigroup Monte Carlo code within the SCALE code system [5]. A publicly available version of SEN3 is expected to be released with version 5 of SCALE in 2002.

## RESULTS

To compare the two methods, the GODIVA [6] highly enriched uranium metal spherical critical experiment was modeled with both MCNP and SEN3. The specifications for the models are as follows: radius, 8.7414 cm; density, 18.74 g/cm$^3$; uranium composition, 1.02% $^{234}$U, 93.71% $^{235}$U, and 5.27% $^{238}$U. ENDF/B-V data were used in both codes to ensure consistency. The MCNP calculations were performed with continuous energy, and the SEN3 calculations were performed with the SCALE 44-group energy structure. First, the sensitivity of $k_{eff}$ to the material density of the entire system was computed through the sensitivity options of MCNP and SEN3. Next, the actual effect of density perturbations was found by varying the input material density and recalculating $k_{eff}$ though independent Monte Carlo runs. A 10% density variation was used in MCNP, and 5% was used in KENO V.a. Good agreement between the direct perturbations and sensitivity results was obtained from both MCNP and SEN3 for this calculation. These are shown in the "Whole System" column of Table I.

The next set of calculations was performed to determine the sensitivity coefficients for only the outer 2-cm shell of the GODIVA sphere. This accounts for more than half of the volume of the system and is used as a demonstration of sensitivity coefficients from a multi-region system. These results are shown in the "Outer 2-cm Thick Shell" column of Table I. Here, the MCNP differential operator results are about 40% higher than those produced by direct recalculation, where the SEN3 results are consistent with those produced by direction recalculation.

The source of the discrepancy in the MCNP results appears to be the lack of consideration of the changing source distribution. When perturbing the density of the entire system, the source distribution changes only slightly because the perturbation is uniform and the value calculated by differential sampling is fairly reasonable. For the harder problem of only perturbing the density of the outer 2-cm thick shell of the sphere, the source distribution change is too great to be ignored by differential sampling, and an incorrect value results. For the SEN3 results, perturbation theory accounts for the importance of the neutrons through the adjoint calculation in the inner and outer region and computes the correct result in both cases.

When the results are interpreted on an energy-dependent basis (not shown), the most significant differences between the MCNP and SEN3 results are seen in the energy ranges where $k_{eff}$ is the most sensitive. Thus, if these results were used with the AOA techniques, erroneous code and data validations would result.

For a fixed source problem, where the source is a function of material density (e.g., uranium gas in an enrichment plant or xenon-133 for a lung scan) the source dependence on material density can be added to the differential sampling scheme [7]. Here, an accumulator that follows the particle of history $i$ keeps track of the sum of the relative derivatives of the interaction probabilities, $P_{ij}$ (where the interactions $j$ are transports or collisions). The accumulator value for derivatives with respect to parameter $a$ after the $J$'th interaction is

$$t_a^i = \sum_{j=1}^{J} \frac{1}{P_{ij}} \frac{\partial}{\partial a} P_{ij} \ .$$

To include the effect of a source that was proportional to material density ($S = c\rho$), one would start this accumulator with the relative derivative of the source with respect to density

$$\frac{1}{S}\frac{\partial}{\partial \rho} S = \frac{1}{\rho}$$

instead of zero. The second derivative of the source probability for the corresponding second order accumulator would be zero.

For a criticality problem, something like the above extended from one cycle to the next may be able to correctly account for the source dependence on density. When fission occurs in one cycle and the location is stored, information about the neutron's accumulated derivatives may also be needed when that location is picked as a source particle in the next cycle. Similar accumulators would need to be created for each parameter (e.g., energy-dependent cross sections) for which sensitivity results are desired.

## SUMMARY

Differential sampling, as currently applied in MCNP, may be able to be extended to account for the dependence of the source on the parameter of interest so that the perturbation feature gives more accurate estimates. This would allow the calculation of sensitivities (of first, second, etc., order) to be done within one Monte Carlo run, providing a very powerful tool to researchers.

The perturbation theory approach, as currently implemented in SEN3, produces accurate results for multi-region systems. Although this approach is limited to first-order, linear perturbations, it is adequate for systems typically encountered in criticality validation studies. However, the availability of a more general differential sampling tool would prove useful for comparison studies and for the computation of the higher-order terms of the sensitivity coefficients.


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