Monte Carlo Calculation of Sensitivities to Secondary Angular Distributions – Theory and Validation

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Introduction.

The basic methods for solution of the transport equation that are in practical use today are the discrete ordinates (S_N) method, and the Monte Carlo (Monte Carlo) method. While the S_N method is typically less computation time consuming, the Monte Carlo method is often preferred for detailed and general description of three-dimensional geometries, and for calculations using cross sections that are point-wise energy dependent. For analysis of experimental and calculated results, sensitivities are needed. Sensitivities to material parameters in general, and to the angular distribution of the secondary (scattered) neutrons in particular, can be calculated by well known S_N methods, using the fluxes obtained from solution of the direct and the adjoint transport equations. Algorithms to calculate sensitivities to cross-sections with Monte Carlo methods have been known for quite a time. However, only just recently we have developed a general Monte Carlo algorithm for the calculation of sensitivities to the angular distribution of the secondary neutrons [1].

Monte Carlo Calculation of Sensitivity to Secondaries' Angular Distribution (SAD)

M.C. Hall [2] formulated the differential operator method for Monte Carlo sensitivity calculations. This approach was extended to the calculation of sensitivities for point detectors [3]. Using the terminology of that work, the sensitivity of any response to a cross section is essentially obtained as a properly performed sum of two kinds of terms, the response term, and the flux term. Between the time when a neutron emerges from the source, and the time when the neutron makes its contribution to the response, it typically moves – and possibly collides – through various material zones. The material parameters can influence both, the neutron's movement (and therefore the probability with which the contribution to the response is made) and the actual contribution to the response. The response term deals with the latter's sensitivity to the material parameters of that specific contribution, while the flux term quantifies the influence of the material parameters on the neutron's movement through the material.

Given a neutron that collides at a given energy E with a given isotope and reaction x, the sensitivity to the cross section of this reaction is a qualitatively different entity than the sensitivity to the angular distribution with which the neutron emerges from the collision. The secondaries' angular distribution is a (normalized) function of the scattering angle, while the cross section is a number. In order to discretisize the secondaries' angular distribution and keep it normalized, we represent it as a Legendre series. The sensitivity calculated is the sensitivity to the various Legendre coefficients. The algorithm we developed allows calculation of these sensitivities, which have clear physical significance, even in cases when the actual description of the secondaries' angular distribution in the cross section library is not given as

Legendre series, but in another form, e.g. as angular histogram or as Kalbach-Mann distribution.

The sensitivity to the Legendre moments f_l – using the notations of refs. [1] and [3] – is shown to be

$$s_{xi} = \frac{\partial(\bar{r}_i P_i)}{\partial f_{x,l}(E)} = \sum_{j=1}^{J_i} \left\{ \frac{\partial \bar{r}_{ij}}{\partial f_{x,l}(E)} \prod_{k=0}^{j-1} P_{ik} + \bar{r}_{ij} \frac{\partial}{\partial f_{x,l}(E)} \left(\prod_{k=0}^{j-1} P_{ik} \right) \right\}$$

$$= \sum_{j=1}^{J_i} \frac{\partial}{\partial f_{x,l}(E)} \left(\ell n \bar{r}_{ij} + \sum_{k=0}^{j-1} \ell n P_{ik} \right) \bar{r}_{ij} \prod_{k=0}^{j-1} P_{ik} \qquad (1)$$

The first term in the summation is the response term, and the second is the flux term. The explicit expressions for the response term is

$$\frac{\partial \ell n \bar{r}_{ij}}{\partial f_{x,l}(E)} = \frac{\partial S_{x_{j-1}}(E_d, E_{j-1}, \mu_{d,j-1})}{\partial f_{x,l}(E)} \frac{1}{S_{x_{j-1}}(E_d, E_{j-1}, \mu_{d,j-1})}$$
$$= \frac{(2l+1) P_l(\mu_{d,j-1})}{2 f_x(\mu_{d,j-1}, E)} \delta_{x, x_{j-1}} \delta(E - E_{j-1}) \qquad (2)$$

and the flux term is given by

$$\frac{\partial \ell n P_{ik}}{\partial f_{x,l}(E)} = \frac{\partial S_{x_{k-1}}(E_k, E_{k-1}, \mu_{k,k-1})}{\partial f_{x,l}(E)} \frac{1}{S_{x_{k-1}}(E_k, E_{k-1}, \mu_{k,k-1})}$$
$$= \frac{(2l+1) P_l(\mu_{k,k-1})}{2 f_x(\mu_{k,k-1}, E)} \delta_{x, x_{k-1}} \delta(E - E_{k-1}) \qquad (3)$$

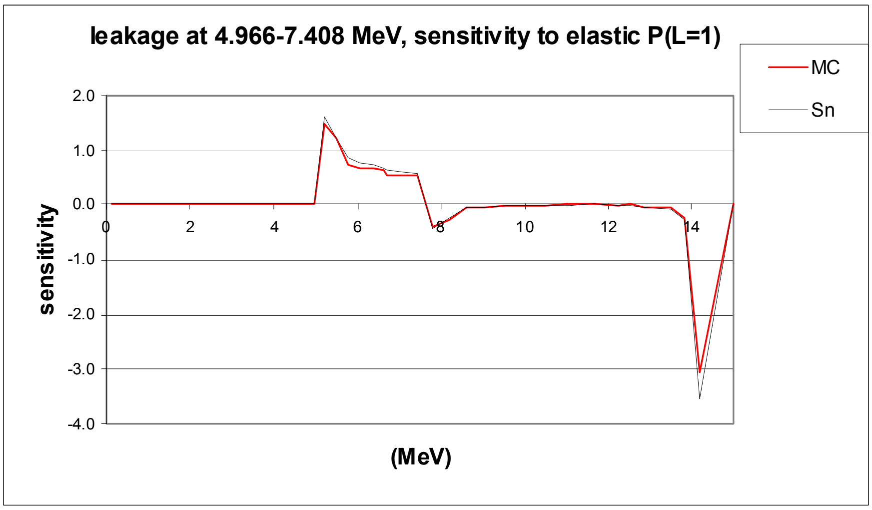
The algorithm allows also to calculate sensitivities to parameters corresponding to specific models, such as the Kalbach-Mann parameters “r” and “a”.

Implementation and Benchmarking

The algorithm was implemented in a local update to the MCNP code. For verification of the algorithm and its implementation, sensitivities to various Legendre coefficients were calculated for suitable sample problems; these sensitivities were found to agree well with the sensitivities obtained “by brute force”, i.e. by comparing the responses obtained in a regular Monte Carlo calculation and in a Monte Carlo calculation with selectively perturbed Legendre coefficients.

A comparison of sensitivities calculated with different basic methods (S_N versus Monte Carlo) has been performed as well [4]. A benchmark relevant to fusion research was defined, and the sensitivities to secondaries’ angular distributions were calculated with those two basic methods, using the specific sensitivity algorithms for each method on one hand, and calculating the sensitivity based on regular transport calculations with perturbed and un-perturbed Legendre coefficients in the cross section data. The benchmark consists of a spherical iron shell (pure Fe^{56}) with an inner radius of 4.5 cm and an outer radius of 12 cm, containing a "14 MeV" (13.84 - 14.19 MeV) neutron point source at its center. The flux at a distance of 680 cm from the center is calculated in 175 fine groups, as well as the flux spectral integrals in 7 wide groups. The sensitivity of these flux integrals to various cross sections and Legendre moments for selected neutron reactions with Fe^{56} was calculated. As illustration, the sensitivity - of the detector flux between 4.966 - 7.408 MeV - to the first (L = 1) Legendre coefficient of elastic scattering of Fe^{56} at the source energy (13.84 - 14.19 MeV), is presented in Fig. 1.

Fig. 1:



Also direct ("brute force") calculations with perturbed and unperturbed cross section files validated the methods and codes.

Conclusions

A Monte Carlo algorithm for calculation of sensitivities to secondaries' angular distributions has recently been developed and implemented. It has been verified with suitable benchmark calculations. It is a powerful and reliable tool for analysis of relevant experiments and calculations.

References:

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