Generating Nonnegative Multigroup Scattering Cross Sections with Monte Carlo Simulation

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1. Introduction

In conventional discrete ordinates transport calculation, the truncated Legendre expansion is used to represent scattering cross sections. In case of highly anisotropic scattering problems, the truncated scattering gives unphysical negative cross sections in some value of μ. As a result of this, negative scattering source and negative angular flux can occur. In this paper, we use $\sigma_{0,g'g}$ from the conventional cross section data and Monte Carlo simulation to make up the weakness of the currently existing data (negative in some values of μ and sometimes inaccurate angular distribution in the truncated Legendre expansion).

2. New Method

2.1 Description of New Method

The method in this paper is similar to that of DelGrande and Mathews[2] in that we use Monte Carlo simulation. However, it is different from theirs in that we use $\sigma_{0,g'g}$ from the conventional cross section data.

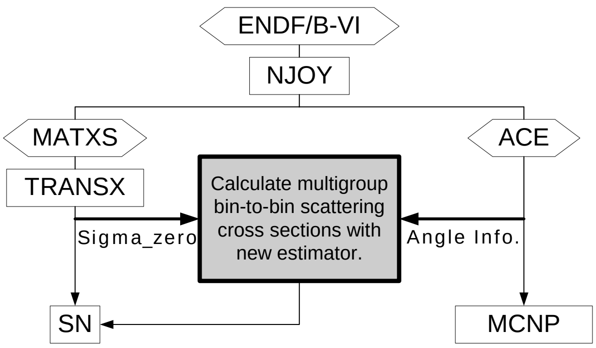

Figure 1. Schematic view of the new method

We use two basic data ($\sigma_{0,g'g}$ from the multigroup cross section data and the angular distribution data from ACE file[1] that is used for MCNP[4] calculation) to generate nonnegative scattering cross section for discrete ordinates calculation. One dimensional discrete ordinates equation is

$$\mu_n \frac{d}{dz}\Psi_{g,n}(z) + \sigma_g(z)\Psi_{g,n}(z) = S_{g,n} + \frac{1}{k_{eff}}\chi_g \sum_{g'=1}^{G} \nu\sigma_{fg'}(z)\Phi_{g'}(z),$$

where (1)

$$S_{g,n} = \sum_{\ell=0}^{L} (2\ell+1)P_\ell(\mu_n)\sum_{g'=1}^{G} \sigma_{\ell gg'}(z)\Phi_{\ell g'}(z), \qquad (2)$$

$$\Phi_{\ell g'}(z) = \frac{1}{2}\sum_{n'=1}^{N} w_{n'}P_\ell(\mu_{n'})\Psi_{g',n'}(z), \qquad (3)$$

$$\Phi_g(z) = \frac{1}{2}\sum_{n=1}^{N} w_n\Psi_{g,n}(z), \quad \sum_{n=1}^{N} w_n = 2. \qquad (4)$$

In this method, we use the following instead of Eqs. (2), (3), and (4):

$$S_{g,n} = \sum_{g'=1}^{G}\sum_{n'=1}^{N} \Delta\Omega_{n'}\ \bar{\sigma}_{g'g}^{n'n}(z)\ \Psi_{g',n'}(z), \qquad (5)$$

$$\Phi_g(z) = \frac{1}{4\pi}\sum_{n=1}^{N} \Delta\Omega_n\Psi_{g,n}(z), \qquad (6)$$

$$\sum_{n=1}^{N} \Delta\Omega_n = 4\pi, \qquad (7)$$

where $\bar{\sigma}_{g'g}^{n'n}$ is nonnegative multigroup, average bin-to-bin scattering cross section and this will be generated with $\sigma_{0,g'g}$ and Monte Carlo simulation.

Let us consider

$$\bar{\sigma}_{g'g}^{n'n} = \int_{\Delta\Omega_{n'}} \frac{d\Omega'}{\Delta\Omega_{n'}} \int_{\Delta\Omega_n} \frac{d\Omega}{\Delta\Omega_n}\ \sigma_{g'g}(\hat{\Omega}'\cdot\hat{\Omega}), \qquad (8)$$

and separate $\sigma_{g'g}(\hat{\Omega}'\cdot\hat{\Omega})$ in Eq. (8) as

$$\sigma_{g'g}(\hat{\Omega}'\cdot\hat{\Omega}) = \sigma_{0,g'g}\ \mathrm{F}(\mathrm{g}'\to \mathrm{g},\hat{\Omega}'\cdot\hat{\Omega}), \qquad (9)$$

where $\sigma_{0,g'g}$ is obtained from TRANSX[3] data and $\mathrm{F}(\mathrm{g}'\to \mathrm{g},\hat{\Omega}'\cdot\hat{\Omega})$ is the conditional probability density function for the distribution of the scattered neutron in $\hat{\Omega}'\cdot\hat{\Omega}$ and energy group g given that the incident neutron energy group was g'. Substituting Eq. (9) into Eq. (8) and rearranging Eq. (8) gives

$$\bar{\sigma}_{g'g}^{n'n} = \sigma_{0,g'g} \int_{\Delta\Omega_{n'}} \frac{d\Omega'}{\Delta\Omega_{n'}} \int_{\Delta\Omega_n} \frac{d\Omega}{\Delta\Omega_n}\ \mathrm{F}(\mathrm{g}'\to \mathrm{g},\hat{\Omega}'\cdot\hat{\Omega}). \qquad (10)$$

In evaluating Eq. (10) with Monte Carlo simulation, we consider an estimator for $\bar{\sigma}_{g'g}^{n'n}$ as follows:

$$\bar{\sigma}_{g'g}^{n'n} \approx \sigma_{0,g'g}\quad f_{g'g,n'} \frac{\dfrac{\left[\sum_{k=1}^{K}\sum_{i=1}^{I_k} \delta_{g'g,g'g_{(k,i)}}\quad \delta_{n'n,n'n_{(k,i)}}\right]}{\Delta\Omega_n}}{K}, \qquad (11)$$

where k is the index of incident particle, K is the total number of the incident particles, i is the index of secondary particle for such as $(n,2n)$, $\Delta\Omega_n$ is the solid angle of the n-th facet, $\delta_{g'g,g'g_{(k,i)}}$ and $\delta_{n'n,n'n_{(k,i)}}$ are the delta functions so that if the particle from energy g' and n'-th facet scatter into energy g and n-th facet then we count it as one:

$$\delta_{g'g,g'g_{(k,i)}} \quad \delta_{n'n,n'n_{(k,i)}} = \begin{cases} 1 & \text{if } g_{(k,i)} = g \text{ and } n_{(k,i)} = n \\ 0 & \text{otherwise} \end{cases}, \tag{12}$$

and $f_{g'g,n}$ is the normalization factor for angular distribution so that

$$\sum_{n=1}^{N} \bar{\sigma}_{g'g}^{n'n} \quad \Delta\Omega_n = \sigma_{0,g'g}. \tag{13}$$

2.2 Numerical Results

2.2.1 Cross Section Generation

We generated cross section data for ^{235}U. LANL-30 energy group, 32 facets, incident direction μ=1 and *K*=5,000,000 are used. To reduce simulation time, parallel computation system KAIST□GALAXY is used. The comparisons with P_6 truncated cross section data are shown in Fig. 2.

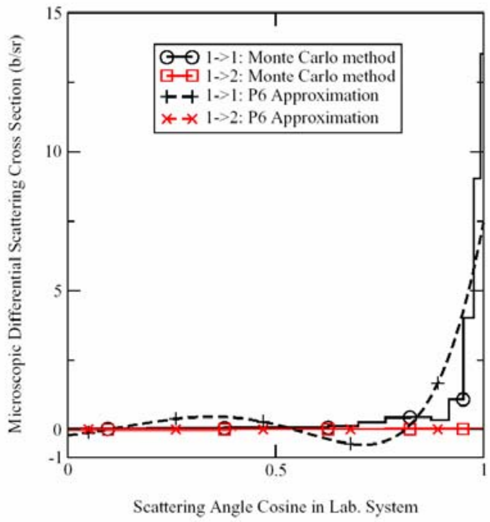

Figure 2. ^{235}U angular distribution of scattering cross sections for group 1 to 1 and 2 (32 facets for Monte Carlo simulation)

2.2.2 Test Problem

The test problem is transport calculation with the generated scattering cross section data. The neutron beam is incident on the ^{235}U slab (density: 1.0 atoms/barn-cm for arbitrary) with intensity 10 (#/cm^2-sec), average incident angle of μ=0.00351, fission source term is not considered. The comparisons with the result of S_{32}, P_6 truncated cross section data are shown in Fig. 4.

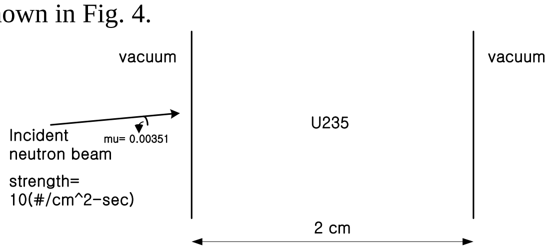

Figure 3. Configuration of test problem

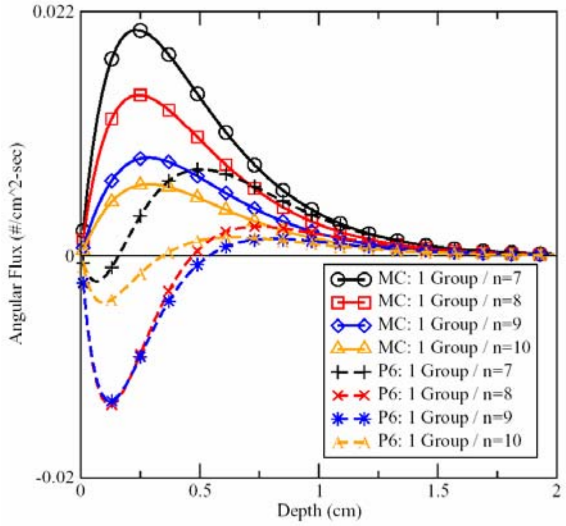

Figure 4. 1st group angular fluxes for penetration depth (7th through 10th ordinates are shown)

3. Conclusions

We use $\sigma_{0,g'g}$ and Monte Carlo simulation to generate nonnegative scattering cross section data. The generated cross section data and the results of transport calculation with this give more accurate and physical results than those with the truncated cross section. The extension to two and three dimensions is straightforward. We have applied this method to generate multigroup photon cross section as well.

ACKNOWLEDGMENT

The work was supported in part by the Ministry of Science and Technology of Korea through the National Research Laboratory (NRL) Program.

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