Multigroup Cross Section Generation with Spatial and Angular Adjoint Weighting

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Introduction

The multigroup discretization is the most common technique used to treat the energy variable in deterministic transport methods. In contrast, most Monte Carlo simulations are able to use the piecewise linear continuous, or pointwise, energy discretization. Monte Carlo simulations may thus be used to benchmark approximations made in multigroup calculations. Several such benchmarks and other studies [e.g. 1,2] have been applied to the problem of light water reactor pressure vessel fluence determination and reduction at Penn State. These studies indicate that a significant portion of the discrepancy between Monte Carlo and deterministic calculations may be attributed to the techniques used to generate multigroup constants.

The general procedure used to generate multigroup cross section libraries has been developed over many years of trial and experience and promulgated in the ANSI/ANS-6.1.2 standard [3, 4, 5]. The first step in the procedure is to generate a fine-group library from continous energy cross sections using an empirical approximation. The fine-group library may then be used in a simplified calculation to collapse the fine-group cross section library to the final broad-group form. We have developed/analyzed three techniques that are or may be used to perform the collapse. These techniques are the scalar flux approximation, the consistent P_n approximation [6], and a new method which we call the adjoint approximation [7].

Adjoint/Flux Weighting

Exact expressions for group constants may easily be derived by integrating the transport equation over each energy subdomain, E_k. This yields expressions for the exact total and scattering cross sections

$$\sigma_k(\mathbf{r},\hat{\mathbf{\Omega}}) = \frac{\int\limits_k dE\sigma(\mathbf{r},E)\varphi(\mathbf{r},E,\hat{\mathbf{\Omega}})}{\int\limits_k dE\varphi(\mathbf{r},E,\hat{\mathbf{\Omega}})} \ ,$$

$$\sigma_{j\to k}(\mathbf{r},\mu_0,\hat{\mathbf{\Omega}}') = \frac{\int\limits_k dE\int\limits_j dE'\sigma(\mathbf{r},E'\to E,\mu_0)\varphi(\mathbf{r},E',\hat{\mathbf{\Omega}}')}{\int\limits_j dE'\varphi(\mathbf{r},E,'\hat{\mathbf{\Omega}}')} \ , \tag{1}$$

where the notation is standard [8]. Note that the multigroup discretization imposes additional spatial and angular dependency into the group constants due to the spatial and angular dependency of the flux. This additional dependency is undesirable in the discretization and is not representable in most deterministic transport codes [e.g. 8]. We thus need to approximate the spatial and angular dependency of the flux in the multigroup constant expressions. The most commonly used method is simply to use the scalar flux in Eqs. 1, which we call the scalar flux approximation. The spatial integration may be performed over materially uniform (or otherwise chosen) subregions, D_s, of the spatial domain as a spatial zone average. The method used in the well known cross section libraries SAILOR [3] and BUGLE-93 [4] is an even more approximate form of the scalar flux approximation. In these libraries, a single scalar flux spectra is selected on an *ad hoc* basis from the fine-group calculation to collapse each spatial region.

The scalar flux approximation may lead to significant errors in problems with high spatial and angular dependencies. To incorporate the spatial and angular variation of the flux into the flux weighting of the group constants, we have developed a new way of using the adjoint in these integrals; we use it as a spatial and angular weighting function. This means that we give weight to the spatial and angular variation of the flux if it is important to the response we are attempting to calculate. Our adjoint approximation in terms of spherical harmonic moments on each materially uniform subdomain, D_s, is

$$\sigma_k = \frac{\int\limits_k dE\sigma(E)\int\limits_{D_s} d\mathbf{r}\left(\sum\limits_{l=0}^{\infty}\frac{2l+1}{4\pi}\sum\limits_{m=-l}^{l}\varphi_l^m(\mathbf{r},E)\varphi_l^{m,\dagger\prime\prime}(\mathbf{r})\right)}{\int\limits_k dE\int\limits_{D_s} d\mathbf{r}\left(\sum\limits_{l=0}^{\infty}\frac{2l+1}{4\pi}\sum\limits_{m=-l}^{l}\varphi_l^m(\mathbf{r},E)\varphi_l^{m,\dagger\prime\prime}(\mathbf{r})\right)} \ ,$$

$$\sigma_{l,j\to k} = \frac{\int\limits_k dE \int\limits_j dE' \sigma_l(E' \to E) \int\limits_{D_s} d\mathbf{r} \left(\sum\limits_{m=-l}^{l} \varphi_l^m(\mathbf{r},E) \varphi_l^{m,\dagger\prime\prime}(\mathbf{r}) \right)}{\int\limits_j dE' \int\limits_{D_s} d\mathbf{r} \left(\sum\limits_{m=-l}^{l} \varphi_l^m(\mathbf{r},E) \varphi_l^{m,\dagger\prime\prime}(\mathbf{r}) \right)} , \qquad (2)$$

where

$$\varphi^{\dagger\prime\prime}(\mathbf{r},\hat{\mathbf{\Omega}}) = \int\limits_k dE \varphi^\dagger(\mathbf{r},E,\hat{\mathbf{\Omega}}) \ .$$

Library Generation and Analysis

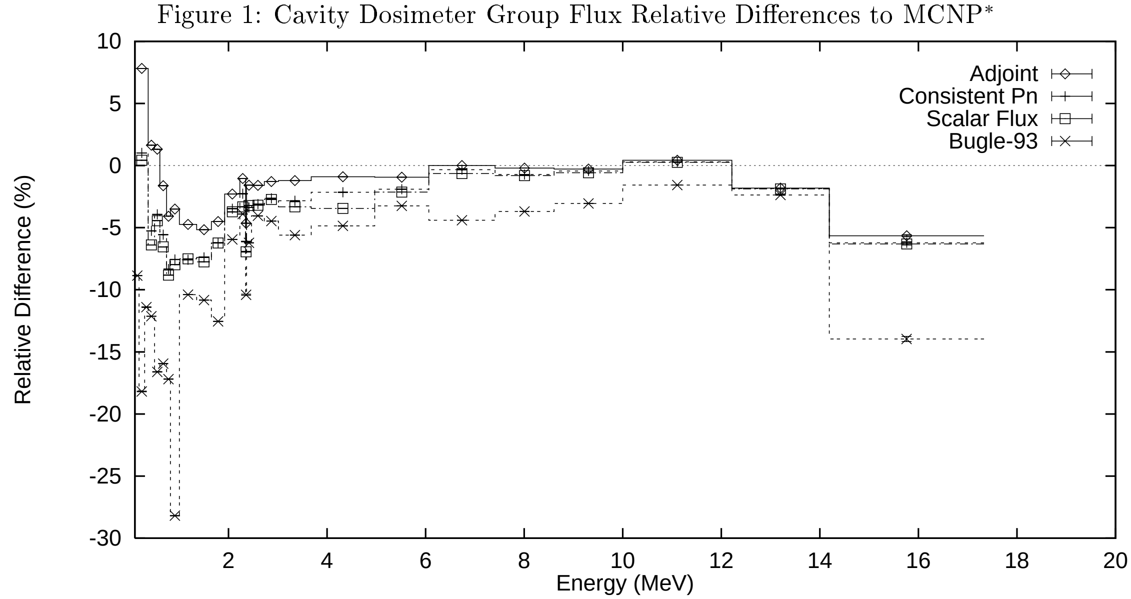
We have used the scalar flux and adjoint approximations as well as an approximate implementation of the consistent P_n method to generate broad-group libraries for cavity dosimetry calculations in pressure vessel fluence estimation [7]. Our fine-group forward and adjoint calculations are based on the Penn State models of the TMI-1 Pressurized Water Reactor [2]. Our adjoint source is the normalized sum of six commonly used response cross sections at the cavity dosimeter. The fine-group library is based on a 492-group structure developed at Penn State for these calculations [7]. Our broad-group structure is a 25-group subset of the 492-group structure similar (for comparison) to the ($>$ 0.1 MeV) 47-group structure of SAILOR and BUGLE-93. We use the transport code DORT [9] for multigroup deterministic calculations and the MCNP code [10] for pointwise Monte Carlo calculations using the same 1-D model and fine-group source that are used in the deterministic calculation. The ratios of the 25-group calculated responses to the 492-group calculated responses using the different collapsing techniques are shown in Table 1. We also show the ratios of BUGLE-93 responses to the 199-group responses; note that BUGLE-93 is collapsed from 199-groups with the *ad hoc* spatial approximation. It can be seen that the adjoint approximation is significantly more accurate than the other approximations. We compare the group fluxes yielded by the broad-group calculations to those yielded by the same calculation using continuous energy Monte Carlo [7]. The relative differences in group fluxes at the cavity dosimeter are shown in Figure 1. Note that the group fluxes calculated using the adjoint approximation library are significantly closer ($<$ 6% instead of as much as 30%) to the Monte Carlo group fluxes than are the group fluxes yielded by any of the other collapsed library calculations.

Table 1: Ratios of Broad-Group to Fine-Group Responses

Response Function	492-Group	Scalar Flux	Consistent P_n	Adjoint
Sum	1.0	0.957	0.962	0.997
^{63}Cu	1.0	0.987	0.989	0.992
^{46}Ti	1.0	0.985	0.988	0.994
^{58}Ni	1.0	0.978	0.982	0.994
^{54}Fe	1.0	0.980	0.985	0.995
^{237}Np	1.0	0.953	0.958	0.997
^{238}U	1.0	0.971	0.974	0.991

Response Function	199-Group	BUGLE-93
Sum	1.0	0.929
^{63}Cu	1.0	0.973
^{46}Ti	1.0	0.974
^{58}Ni	1.0	0.969
^{54}Fe	1.0	0.973
^{237}Np	1.0	0.919
^{238}U	1.0	0.957

Figure 1: Cavity Dosimeter Group Flux Relative Differences to MCNP*



* Errorbars are MCNP 1σ standard deviations.

Conclusions

It is evident that the approximations which may be used to collapse a fine-group to a broad-group library improve in accuracy in direct correspondence to the amount of fine-group information that they include. The adjoint approximation uses all of the forward and adjoint angular dependent fine-group information available, and it is the most accurate of the techniques that we have considered for collapsing. The *ad hoc* approximation used to generate SAILOR and BUGLE-93 uses only a fraction of the information that is available, and the accuracy of these libraries is as *ad hoc* as is their generation, although in none of the cases we have considered are these libraries as accurate as the library generated with the adjoint approximation.

We have developed/analyzed three techniques that may be used to collapse a fine-group cross section library to a broad-group library. We have developed a new way of using the adjoint as a bilinear spatial and angular, but not energy, weighting function. The adjoint weighted library we have generated improves the broad-group calculation accuracy by a factor of 2 over that obtained using the scalar flux approximation library and by as much as a factor of 10 over that obtained using the BUGLE-93 library. For future work, we are developing better methods of generating and using cross sections in multigroup deterministic transport calculations. This includes study of group structure (fine and broad), self-shielding techniques, and problem dependency in multigroup libraries.

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