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An analysis of condensation errors in multi-group cross section generation for fine-mesh neutron transport calculations

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ABSTRACT

When collapsing multi-group cross sections, a flux separability approximation is often used. This assumes the angular variation of the flux is independent of the energy dependence, which avoids angular dependence of the total multi-group cross section. This paper investigates the impact of this approximation on fine-mesh deterministic multi-group transport methods for two PWR pin-cell benchmarks, which demonstrate errors of more than 1% in energy groups with large U-238 capture resonances and an eigenvalue bias of approximately 200 pcm between continuous energy Monte Carlo and deterministic transport methods, even when the "true" scalar flux is used to collapse cross sections. This paper also investigates two means of resolving this issue, but both are seen to have significant short-comings. First, the most direct and mathematically consistent approach is to use angularly-dependent multi-group cross sections. These cannot be easily computed for arbitrary geometries using traditional multi-group cross section generation methods, are not supported by most standard transport codes, and require significant spatial discretization. Second, SuPerHomogéneísation (SPH) factors are used to preserve reaction rates between continuous energy Monte Carlo and deterministic transport methods, but the SPH scheme requires knowledge of the reference source distribution, is dependent on the spatial discretization mesh, and is indiscriminate between various sources of approximation error.

1. Introduction

The nuclear reactor physics community has long strived for deterministic neutron transport-based tools for whole-core reactor analysis. A key challenge for whole-core multi-group transport methods is accurate reactor agnostic multi-group cross section (MGXS) generation. The MGXS generation process applies a series of approximations to produce spatially homogenized and energy condensed MGXS in each spatial zone and energy group. Many approximations related to multi-group theory, including the selection of discretized energy group structures and the truncation of the Legendre expansion of the multi-group scattering kernel, are widely studied in the literature. However, the practical impact of the flux separability approximation, which permits the use of the scalar rather than the angular neutron flux to weight the continuous energy cross sections, is less understood. This paper investigates the flux separability approximation and quantifies its significance for heterogeneous PWR problems.

In the generation of MGXS, increasingly higher-fidelity methods are becoming widespread. Most significantly, this includes Monte Carlo and ultra-fine deterministic methods, which provide a high-quality continuous-energy (or near-continuous-energy) spectrum for some reference problem. Monte Carlo methods have increasingly been used to generate few group constants for homogenized coarse mesh diffusion, most notably by the Serpent MC code Leppänen (2013), and to a much lesser extent, for high-fidelity neutron transport methods Redmond (1997), Nelson (2014), Cai (2014) and Boyd (2016).

The need to know the flux accurately to generate MGXS is the primary difficulty in generating appropriate nuclear data. However, as this work explores, the use of higher-fidelity collapsing spectra exposes other errors which are derived from approximations made in the formulation of the multi-group equations and is not sufficient for heterogeneous MGXS. This paper shows that even when the "true" scalar flux is used to generate MGXS, the flux separability approximation results in a non-negligible eigenvalue bias between continuous energy and multi-group calculations due to over-prediction of U-238 capture in resonance energy groups.

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The content in this paper is organized as follows. The flux separability approximation is introduced in Section 2. Two benchmark problems—one using simplified ultra-fine methods and a more realistic one using Monte Carlo methods—are presented and explored in Section 3 and Section 4, rigorously quantifying the impact of the approximation on PWR problems. The former demonstrates that scalar-flux-weighting of cross sections cannot preserve the reaction rate in a single resonance group. The latter investigates the flux separability approximation in the context of a fully-detailed, critical PWR fuel pin-cell. Angularly-dependent MGXS and SuPerHomogénéisation (SPH) factors are explored in Section 5 as two possible corrections to this approximation, but both methods are also noted to have significant shortcomings.

2. Flux separability approximation

The steady-state Boltzmann transport equation is an integro-differential equation solved for the neutron angular flux, $\psi(\mathbf{r},\mathbf{\Omega},E)$. It balances the rate of change of the population of neutrons in phase space to the difference between the production and loss rates of neutrons within a closed system,

$$\mathbf{\Omega}\cdot\nabla\psi(\mathbf{r},\mathbf{\Omega},E)+\Sigma_t(\mathbf{r},E)\psi(\mathbf{r},\mathbf{\Omega},E)=Q(\mathbf{r},\mathbf{\Omega},E), \tag{1}$$

where $Q(\mathbf{r},\mathbf{\Omega},E)$ is the source of neutrons from scattering, fission production, or external sources.

Monte Carlo methods typically employ a representation for the spatial, $\mathbf{r}$, angle, $\mathbf{\Omega}$, and energy, E, variables. Deterministic methods apply some form of discretization to each of these variables. For example, the multi-group approach subdivides the neutron energy into discrete bins known as energy groups g which are indexed starting at 1 for high energies and ending with G for low energies,

$$\mathbf{\Omega}\cdot\nabla\psi_g(\mathbf{r},\mathbf{\Omega})+\Sigma_{t,g}(\mathbf{r},\mathbf{\Omega})\psi_g(\mathbf{r},\mathbf{\Omega})=Q_g(\mathbf{r},\mathbf{\Omega}), \tag{2}$$

where the group-wise angular flux $\psi_g(\mathbf{r},\mathbf{\Omega})$ and source $Q_g(\mathbf{r},\mathbf{\Omega})$ are integrated across each energy group g:

$$\psi_g(\mathbf{r},\mathbf{\Omega})=\int_{E_g}^{E_{g-1}}\psi(\mathbf{r},\mathbf{\Omega},E)\,\mathrm{d}E \tag{3}$$

$$Q_g(\mathbf{r},\mathbf{\Omega})=\int_{E_g}^{E_{g-1}}Q(\mathbf{r},\mathbf{\Omega},E)\,\mathrm{d}E. \tag{4}$$

Equivalence between Eqs. (1) and (2) will be maintained if the $\Sigma_{t,g}(\mathbf{r},\mathbf{\Omega})$ is collapsed using the angular neutron flux,

$$\Sigma_{t,g}(\mathbf{r},\mathbf{\Omega})\equiv\frac{\int_{E_g}^{E_{g-1}}\Sigma_t(\mathbf{r},E)\psi(\mathbf{r},\mathbf{\Omega},E)\,\mathrm{d}E}{\int_{E_g}^{E_{g-1}}\psi(\mathbf{r},\mathbf{\Omega},E)\,\mathrm{d}E}, \tag{5}$$

using a weighted average to preserve reaction rates in each energy group. This expression for $\Sigma_{t,g}(\mathbf{r},\mathbf{\Omega})$ presents a complication since it is dependent on the unknown angular flux. The angular dependence of the total cross section is often treated with the flux separability approximation. Flux separability makes the simplifying assumption that the energy and angular dependence of the flux varies independently such that the angular flux can be written as the product of the scalar neutron flux $\phi(\mathbf{r},E)$ and some function $W(\mathbf{r},\mathbf{\Omega})$:

$$\psi(\mathbf{r},\mathbf{\Omega},E)\approx\phi(\mathbf{r},E)W(\mathbf{r},\mathbf{\Omega}). \tag{6}$$

The angular dependence of the $\Sigma_{t,g}$ may then be eliminated by inserting Eq. (6) into Eq. (5), factoring out $W(\mathbf{r},\mathbf{\Omega})$ and writing Σ_t in terms of the scalar flux,

$$\Sigma_{t,g}(\mathbf{r})\approx\frac{\int_{E_g}^{E_{g-1}}\Sigma_t(\mathbf{r},E)\phi(\mathbf{r},E)W(\mathbf{r},\mathbf{\Omega})\,\mathrm{d}E}{\int_{E_g}^{E_{g-1}}\phi(\mathbf{r},E)W(\mathbf{r},\mathbf{\Omega})\,\mathrm{d}E}=\frac{\int_{E_g}^{E_{g-1}}\Sigma_t(\mathbf{r},E)\phi(\mathbf{r},E)\mathrm{d}E}{\int_{E_g}^{E_{g-1}}\phi(\mathbf{r},E)\,\mathrm{d}E}. \tag{7}$$

The angular-independent total multi-group cross section is substituted into Eq. (2) to derive the equation solved by most transport codes:

$$\mathbf{\Omega}\cdot\nabla\psi_g(\mathbf{r},\mathbf{\Omega})+\Sigma_{t,g}(\mathbf{r})\psi_g(\mathbf{r},\mathbf{\Omega})=Q_g(\mathbf{r},\mathbf{\Omega}). \tag{8}$$

Although flux separability is a simple and commonly used approach to reduce the complexity of the multi-group total cross section, it is not always valid and may not preserve neutron balance. The flux separability approximation will necessarily hold in infinite homogeneous media since the flux does not vary in angle or space. However, the flux may vary greatly by angle in a heterogeneous geometry with significant spatial flux gradients.

The variation of the total cross section in angle is often neglected by deterministic transport codes which employ an isotropic multi-group total cross section $\Sigma_{t,g}(\mathbf{r})$ representation. This work seeks to isolate and quantify the impact of the flux separability approximation for PWR problems.

Two case studies were used to disaggregate the approximation errors inherent to deterministic multi-group transport methods from the component error specific to the flux separability approximation. Ultra-fine deterministic and continuous energy Monte Carlo transport methods were used to collapse multi-group cross sections and generate reference solutions for each case study as discussed in Section 3 and Section 4, respectively. Both case studies modeled a multi-region PWR fuel pin geometry with varying levels of complexity. The two analyses isolate the impact of the flux separability approximation on local reaction rates, as well as demonstrate the compounding effect of errors in each energy group on the k-eigenvalue. The following sections discuss the benchmark specifications and simulation tools used by each case study.

3. Test Case 1: Pin-cell with slowing down source

3.1. Benchmark problem

The first test case modeled a simple benchmark problem in which the reference flux could be computed precisely to demonstrate the existence of errors from approximately collapsing Eq. (1) into Eq. (8) with the flux separability approximation. The first test case problem consisted of a unit cell of an infinite array of unclad fuel pins. The fuel material contained U-238 with an atom density of 0.022 a/b · cm and a purely scattering nuclide with a constant cross section of 0.176 cm^{-1}, an analog to oxygen in UO_2. The moderator was a pure scatterer with a constant cross section of 1.23 cm^{-1}. The pin radius was 0.4 cm and the pitch was 1.26 cm. The source was given by the scatter source from the narrow resonance approximation:

$$Q(\mathbf{r},\mathbf{\Omega},E)=\frac{1}{4\pi}\frac{\Sigma_p(\mathbf{r})}{E}. \tag{9}$$

3.2. Simulation tools

A reference continuous energy flux was computed for this benchmark problem by solving Eq. (8) for each energy point using a method of characteristics solver with 32 azimuthal angles and a 0.01 cm ray spacing. The reference reaction rates in each region were obtained by integrating the flux multiplied by a cross section over an energy range of interest and over the volume of the fuel pin. The total cross section and source were collapsed using the reference flux according to Eqs. (7) and (4), respectively. Eq. (8) was solved using the same solver with the collapsed total cross section and source. The collapsed reaction rate was obtained by volume-integrating the multi-group flux multiplied by the multi-group cross section over the fuel pin. Finally, the reaction rates obtained