Annals of Nuclear Energy 112 (2018) 9–16

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Generalized equivalence methods for 3D multi-group neutron transport

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ARTICLE INFO

Article history:
Received 19 June 2017
Received in revised form 14 September 2017
Accepted 15 September 2017

Keywords:
Neutron transport
Self-shielding
Equivalence
Condensation
Discontinuity factors
Jump conditions

ABSTRACT

The process of generating multi-group cross section data to be used in full core 3D transport models requires not only accurate resonance self-shielding methods, but also some form of equivalence method in order to precisely preserve reaction rates of spectral geometry calculations. This paper presents extensions of the traditional concepts of local reaction rate preservation (common in discontinuity factor, SPH, and BBH methods), to derive a new state-of-the-art transport equivalence method that incorporates angular flux jump conditions that provide polar angle neutron current preservation. This method is tested on numerous fixed-source pin-cell problems by condensing fine energy resonance fluxes and cross sections. The method is demonstrated to precisely preserve all spectral geometry multi-group reaction rates as well as polar angle neutron currents for a wide range of cross section resonance heights, fuel pin diameters, coolant densities, and group energy widths.

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1. Introduction

Neutron transport calculations of nuclear reactor cores require accurate methods for treating the complexities in space and energy that arise from the resolved resonances in nuclear cross sections of reactor fuel and structural materials. Treatment of resolved resonance effects is implicit in continuous-energy Monte Carlo methods that represent resonances with hundreds of thousands of energy points. Unfortunately, full-core, steady state reactor calculations with Monte Carlo require tens of billions of neutron histories (Miao et al., 2016) to converge local fluxes and pin power distributions for cores that have near-unity dominance ratios, which is common in commercial light water reactors (LWRs). In addition, Monte Carlo methods are not easily extendable to transient reactor safety analysis where transients must be followed for 100 s or 1000 s of seconds.

For these reasons, deterministic neutron transport (or diffusion) methods are likely to be used for performing the bulk of nuclear reactor analysis for years into the future. In deterministic neutron transport methods, the fine-energy detail of Monte Carlo is not practical because of the overwhelming amount of data needed to represent group-to-group transfer cross sections. Instead, deterministic neutron transport models employ some form of approximate resonance treatment that enables direct computation of multi-group cross sections for core analysis using only 50 to 500 neutron energy groups.

Historically, multi-group cross sections for core analysis have been generated for representative spectral geometries (e.g., 1D pin cells or 2D fuel assemblies). In recent years, even full-core spectral geometries have been used in some core analysis systems. However, the common trend among all deterministic methods is that simplified resonance approximations (e.g., equivalence theory, sub-group, equivalent self-shielding method, etc.) are made in the process of producing multi-group cross sections for core transport models. In order to avoid such simplifying assumptions, some researchers have recently employed direct full-core Monte Carlo calculations and massive cross section tallies to directly compute multi-group cross sections for downstream deterministic transport calculations (Boyd, 2017; Gunow et al., 2017). Such approaches are feasible because Monte Carlo cross section tallies converge much more rapidly than local fluxes and power distributions and because cross section tallies can be agglomerated across many spatial regions through use of sophisticated clustering or machine-learning algorithms (Boyd, 2017).

However, none of these methods for generating multi-group cross sections, including Monte Carlo, are capable of directly producing multi-group cross sections that preserve local reaction rates and pin power distributions in 3D core transport models. Even formally exact multi-group cross sections lead to errors in downstream core models (Boyd, 2017; Boyd et al., 2017) unless additional equivalence parameters are introduced to force conservation of local reaction rates.

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https://doi.org/10.1016/j.anucene.2017.09.024
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2. Equivalence methods

The starting point for all equivalence methods is the concept of preservation of reaction rates. If one assumes that a very fine spatial, angular, and energy mesh solution to the neutron transport equation, Eq. (1), is known for the spectral geometry of interest (from either Monte Carlo or from some approximate resonance model), then one can simply define the multi-group transport equation and its corresponding multi-group cross sections as shown in Eqs. (2) and (3).

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

The first term on the left is the streaming of the neutrons, the second the sink rate by absorption and scattering. On the right, $Q(\vec{r},\Omega,E)$ includes the creation of neutrons by fission, the scattering source and fixed sources. Each term of the neutron transport equation can be integrated over energy groups.

$$\vec{\Omega}\cdot\vec{\nabla}\psi_g(\vec{r},\vec{\Omega})+\Sigma_{tg}(\vec{r},\vec{\Omega})\psi_g(\vec{r},\vec{\Omega})=Q_g(\vec{r},\Omega) \tag{2}$$

$$\Sigma_{tg}(\vec{r},\vec{\Omega})=\frac{\int_{E_1}^{E_2}\mathrm{d}E'\Sigma_t(\vec{r},E')\psi(\vec{r},\vec{\Omega},E')}{\int_{E_1}^{E_2}\mathrm{d}E'\psi(\vec{r},\vec{\Omega},E')} \tag{3}$$

Each multi-group cross section is then a function of angle. Since hundreds of discrete angles are typically used in reactor core calculations, there is a massive data explosion associated with using multi-group cross sections with a full angular dependency, even if it can be partially mitigated by using polynomial expansions. Consequently, it is common to define cross sections that are angle independent, as shown in Eq. (4), and to use these cross sections in conjunction with Eq. (2) for downstream core analysis.

$$\Sigma_g(\vec{r})=\frac{\int_{E_1}^{E_2}\mathrm{d}E'\Sigma(\vec{r},E')\Phi(\vec{r},E')}{\int_{E_1}^{E_2}\mathrm{d}E'\Phi(\vec{r},E')}=\frac{R_g}{\Phi_g} \tag{4}$$

This angular independence of cross section is an approximation, and as a consequence, even a fully converged (in phase space) multi-group calculation will not preserve the desired reaction rates. Equivalence parameters are introduced in order to force this desired preservation of reaction rates. In this process, it is also common to integrate over space in addition to energy and angle over finite spatial volumes (e.g., individual pins, or cladding, or coolant channels), as shown in Eq. (5), and the desired equivalence parameters are now sought to implicitly correct for angular-integration, energy-condensation, and spatial-homogenization.

$$\Sigma_g(\vec{r})=\frac{\int_V\int_{E_1}^{E_2}\mathrm{d}r'\mathrm{d}E'\Sigma_t(\vec{r}',E')\Phi(\vec{r}',E')}{\int_V\int_{E_1}^{E_2}\mathrm{d}r'\mathrm{d}E'\Phi(\vec{r}',E')}=\frac{R_g}{\Phi_g} \tag{5}$$

The need for practical equivalence parameters has been understood for more than 50 years, and numerous schemes have been proposed and utilized. Bell et al. (1967) proposed a method of introducing artificial anisotropic scattering cross sections (the BHS model) to treat multi-group cross sections with low-order Legendre expansions as the equivalence parameters. While feasible, this method has not been widely adapted in any practical reactor analysis system.

For systems that utilize the diffusion approximation for 3D core analysis, Koebke's heterogeneity factors (Koebke, 1978) and Smith's extension, discontinuity factors (Smith, 1984) have been widely used equivalence methods for nodal diffusion reactor analysis of commercial LWRs. Discontinuity factors are simply jump conditions on the scalar flux that are applied when the diffusion equations are solved, and the appropriate values of the discontinuity factors are defined to preserve the surface-integrated net neutron current between spatially homogenized and/or energy collapsed regions. Discontinuity factors are computed directly from lattice spectral geometries used in nodal diffusion core models. In addition, discontinuity factors can be computed for pin-cell spatial regions and used in pin-cell-based 2D or 3D full core reactor models. Discontinuity factors must be saved for each surface of each homogenized/collapsed region, in each of the neutron energy groups. Unfortunately, discontinuity factors are only directly applicable to diffusion theory and not to transport theory equivalence. They have however been derived for simplified P3 equivalence (Kozlowski et al., 2011) and transport acceleration (Grassi, 2007).

The most widely used of the transport equivalence methods is Kavenoky's (Kavenoky, 1978) super-homogenization and its later generalization by Hebert and Benoist (1991), often referred to as the SPH method. The SPH method introduces a factor, f_ig, multiplying the multi-group cross sections, and this factor is chosen to conserve the reaction rates in a spatial region i and energy group g. As shown in Eq. (6), the flux computed by the transport solver, Φ_{ig}^{SPH}, is not the same as the group flux from condensation of the reference flux, but rather, it is the flux that is obtained when the transport equation is solved when employing $f_{ig}\Sigma_{ig}$ rather than Σ_{ig} as the group cross section.

$$(f_{ig}\Sigma_{ig})\Phi_{SPH}=\Sigma_{ig}\Phi_{ig} \tag{6}$$

In the SPH method, f_{ig} is iteratively determined by solving the multi-group problem over and over again until converged values of f_{ig} are obtained for each spatial region of the spectral geometry. Because the same SPH factor is used on all cross sections within group g, this method preserves up- and down-scatter rates, as well as total reaction rates. In practice, the larger the correction, f_{ig}, the more the SPH flux changes from the reference group flux, and iterative convergence is not guaranteed. The SPH method is very general and it can be used for condensation, for spatial homogenization, or even for employing lower-order transport models. The SPH method is transport-solver-agnostic, and has virtually no memory-cost, since equivalence factors can be absorbed directly into the multi-group cross sections.

In an extension to SPH and Discontinuity factors, Sanchez (2009) has defined a class of methods he refers to as black box homogenization (BBH), in which two discontinuity factors are used on each surface of each homogenized/condensation region in order to preserve the neutron partial currents. Sanchez's implementation of BBH for pin-cell homogenization involves determining the transmission matrix of the system and the escape vector of the internal source, for each pin in the assembly, for each neuron energy group. The BBH class of methods is very general, and it allows preservation of reaction rates in any arbitrary spatial region and energy group of the spectral geometry.

In this paper we introduce a new method, which uses an extension of the discontinuity factor concept by applying jump conditions on the angular flux. Jump conditions are explicitly treated as a function of the polar angle neutron fluxes. These equivalence parameters are defined to preserve neutron flow in the polar direction something that neither SPH nor BBH currently provides. The new equivalence methods preserves 3D transport effects, which are anticipated to enable more accurate full-core deterministic transport calculations. These new equivalence methods are, in principle, applicable to any deterministic resonance cross section method or core transport model, but the methods will be demonstrated here using a simple Single Level Breit-Wigner (SLBW) resonance models, in the low temperature approximation, and 2D Step Characteristic pin-cell transport calculations.

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