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Overview of methodology for spatial homogenization in the Serpent 2 Monte Carlo code

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ABSTRACT

This paper describes the methods used in the Serpent 2 Monte Carlo code for producing homogenized group constants for nodal diffusion and other deterministic reactor simulator calculations. The methodology covers few-group reaction cross sections, scattering matrices, diffusion coefficients and poison cross sections condensed in infinite and B_1 leakage-corrected critical spectra, as well as the calculation of discontinuity factors, pin-power form factors, delayed neutron parameters and total and partial albedos. Also included is a description of an automated burnup sequence, which was recently implemented for the handling of restart calculations with branch variations. This capability enables covering the full range of local operating conditions required for the parameterization of group constants within a single run. The purpose of this paper is to bring the methodological description provided in earlier publications up to date, and provide insight into the developed methods and capabilities, including their limitations and known flaws.

1. Introduction

The use of the continuous-energy Monte Carlo method for producing homogenized group constants for nodal diffusion and other deterministic reactor simulator calculations has gained considerable interest during the past ten years, even though the practical applications are still limited by the high computational cost of the transport simulation. Covering all assembly types and reactor operating conditions over multiple core cycles requires solving the local heterogeneous transport problem thousands of times, which poses a major challenge for any calculation code. The long running time, however, is thought to be outweighed by the inherent advantages of the Monte Carlo method – the capability to handle interaction physics without major approximations and three-dimensional geometries at an arbitrary level of spatial detail.

Another significant advantage is that Monte Carlo lattice physics codes not only allow performing spatial homogenization at the fuel assembly level, but also running transport simulations for the full-scale heterogeneous system. This provides ideal reference solutions for the validation of the calculation scheme, since all additional discrepancies resulting from evaluated nuclear data libraries and methodological differences can be eliminated. The differences between the homogeneous and the heterogeneous reference solution instead reflect on how well the physics of the transport process is preserved over the calculation chain, which can be extremely valuable for the development of new methods for core calculations.

The Serpent code (Leppänen et al., 2015) has been developed at VTT Technical Research Center of Finland since 2004, and the current user basis includes more than 500 users in 155 universities and research organizations in 37 countries around the world. The code is used for a multitude of applications in reactor physics, but spatial homogenization based on the Monte Carlo method was, in fact, the original incentive for starting the work. The progress has been steady over the years, but so far the use of Serpent for group constant generation has mostly been limited to preliminary studies with simplified core models.[1] This is in part because of the complexity and computational cost of producing the full set of group constants for realistic fuel cycle and transient simulator calculations, but no doubt also because of the insufficient documentation of methods and procedures used in the code.

In an effort to correct this deficiency, work on a comprehensive User's Manual in the form of an on-line Wiki[2] was started in late 2015. The purpose of this paper, on the other hand, is to bring the

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[1] See (Leppänen et al., 2014b and Leppänen et al., 2015) for a review of examples.
[2] See: serpent.vtt.fi/mediawiki.

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methodological description provided in some earlier publications (Leppänen, 2007; Fridman and Leppänen, 2011, 2012; Leppänen et al., 2014b, 2015) up to date. This part is covered in Section 2, and the description corresponds to code version 2.1.26, distributed to users in April 2016. Recent development includes also an automated burnup sequence capable of performing branch variations, which considerably simplifies setting up the inputs for group constant generation and the management of output data. The procedure is described in Section 3. Since Serpent is still a developing code, there are a number of flaws and limitations in the methodology, as discussed in Section 4. Some future plans are outlined along with the conclusions in Section 5.

This paper covers the theory of homogenization and nodal diffusion methods only as far as is considered necessary for understanding the methods used in the Serpent code. The fundamentals can be found in Koebke (1978) and Smith (1980), as well as most text books on reactor theory (Bell and Glasstone, 1970; Duderstadt and Hamilton, 1976; Stamm'ler and Abbate, 1983). Practical issues, such as the input and output formats are addressed at the Serpent on-line Wiki.

2. Methods used for spatial homogenization

The purpose of spatial homogenization is to preserve the local reaction balance when group constants obtained from the solution of the local heterogeneous transport problem (assembly-level calculation) are used as the building blocks for the global homogeneous system (core-level calculation). Formally, the homogenization of reaction cross section Σ_g can be written as:

$$\Sigma_g = \frac{\int_{E_g}^{E_{g-1}} dE \int_V d^3r\, \Sigma(\mathbf{r},E)\phi(\mathbf{r},E)}{\int_{E_g}^{E_{g-1}} dE \int_V d^3r\, \phi(\mathbf{r},E)}, \tag{1}$$

where ϕ is the scalar flux and the integration is carried over the volume of the homogenized region and energy group g. The spatial dependence of Σ reflects the fact that the geometry is heterogeneous, albeit typically composed of discrete uniform material zones. In other words, spatial homogenization implies averaging the physical continuous-energy cross sections over volume and the spatial and energy distribution of neutron flux. This paper is primarily focused on the generation of macroscopic interaction parameters, but the same procedures generally apply to microscopic cross sections, which are used in modern nodal diffusion codes to employ micro-depletion in fuel cycle simulations. This topic is briefly discussed in Section 4.1.

Deterministic lattice transport codes, in which the heterogeneous flux solution is obtained in space- and energy-discretized form, apply the procedure as:

$$\Sigma_g = \frac{\sum_{h\in g}\sum_i V_i \Sigma_{i,h}\Phi_{i,h}}{\sum_{h\in g}\sum_i V_i \Phi_{i,h}} \tag{2}$$

where $\Phi_{i,h}$ is the volume-averaged scalar group flux, and i refers to the spatially discretized regions and h to the multi-group structure used in the calculation. Cross section $\Sigma_{i,h}$ is obtained from spectral calculation, taking into account spatial and resonance self-shielding effects.

One of the advantages of using Monte Carlo simulations for spatial homogenization is that stochastic estimates for the integrals in Eq. (1) can be obtained directly, using continuous-energy cross sections. This means that self-shielding effects are automatically accounted for, without relying on various approximations employed by deterministic codes. Consequently, the same methods and cross section libraries can be used for modeling any fuel or reactor type, without any application-specific limitations. Another advantage typically attributed to the method is its capability to handle complicated three-dimensional structures, in which the level of spatial detail can be arbitrarily refined.

The group constant input for deterministic nodal diffusion codes typically consists of absorption ($\Sigma_{a,g}$), fission neutron production ($\nu\Sigma_{f,g}$) and group transfer ($\Sigma_{s,gg'}$) cross sections, as well as fission spectrum χ_g and diffusion coefficients (D_g). These are the constants needed for forming the group diffusion equations. Coupling between adjacent nodes is accomplished using discontinuity factors F_g, and normalization of flux with fission energy production cross sections ($\kappa\Sigma_{f,g}$). Dynamic calculations require additionally inverse neutron speeds $1/v_g$ and effective delayed neutron fractions β_{eff}, divided into a number of precursor groups. Most modern core simulators have the capability to perform pin-power reconstruction and track the concentrations of fission product poisons ^{135}Xe and ^{149}Sm separately. The group constant input then includes also pin-power form factors and production and absorption cross sections for fission product poisons and their precursors. As discussed below, the task of producing all this data becomes much more complicated than just calculating stochastic estimates for the integrals in Eq. (1) using standard reaction rate tallies.

2.1. General procedure applied in Serpent 2

For practical reasons made apparent in Section 2.4, Serpent does not evaluate the integrals in Eq. (1) directly. The procedure is instead handled in two parts:

(i) A number of multi-group homogenized reaction cross sections are calculated using standard Monte Carlo tallies and analog estimators.
(ii) The multi-group cross sections are condensed into few-group cross sections using the infinite and the B_1-leakage corrected critical spectra (see Section 2.4).

In this paper the intermediate energy group structure used internally in the calculation routines is referred to as the "multi-group structure", associated with group index h. The final group structure to be used in the simulator calculation is correspondingly referred to as the "few-group structure", with group index g. The default multi- and few-group structures used by Serpent are the WIMS 69-group structure and the conventional two-group structure with thermal and fast group separated at 0.625 eV. Both structures can be changed by input options.

Technically this two-stage approach means that instead of Eq. (1), the final energy group condensation is written as:

$$\Sigma_g = \frac{\sum_{h\in g}\Sigma_h\Phi_h}{\sum_{h\in g}\Phi_h}. \tag{3}$$

The difference to Eq. (2), applied by deterministic codes, is that Φ_h is integrated and Σ_h averaged over the volume of the homogenized geometry:

$$\Phi_h = \int_{E_h}^{E_{h-1}} dE \int_V d^3r\, \phi(\mathbf{r},E) \tag{4}$$

$$\Sigma_h = \frac{\int_{E_h}^{E_{h-1}} dE \int_V d^3r\, \Sigma(\mathbf{r},E)\phi(\mathbf{r},E)}{\int_{E_h}^{E_{h-1}} dE \int_V d^3r\, \phi(\mathbf{r},E)}. \tag{5}$$

The integrals in Eqs. (4) and (5) are obtained using standard reaction rate tallies. Since the stochastic integration is performed using continuous-energy cross sections, all self-shielding effects are automatically taken into account, so even though the calculation is divided in two parts, the most significant advantages of Monte Carlo simulation are preserved. It should also be noted that homogenization and the first energy-group condensation into the