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Directional diffusion coefficients and leakage-corrected discontinuity factors: Implementation in Serpent and tests

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ABSTRACT

A recently proposed method has been extended to treat the generation of radial directional diffusion coefficients with the Monte Carlo code Serpent. In addition to a previous implementation for the axial direction, the new method was applied to the study of a sodium-cooled fast reactor by combined Monte Carlo and diffusion theory. The performance of anisotropic diffusion coefficients was found to be superior to that one of standard diffusion coefficients already available in Serpent. A diffusion solver was also implemented in Serpent in order to compute leakage-corrected discontinuity factors in hexagonal-Z geometry for multiplicative and non-multiplicative multi-group problems. The use of face discontinuity factors improved the agreement among results achieved by diffusion theory and by full-core Monte Carlo calculations. The performance of anisotropic diffusion and discontinuity factors is compared in terms of sensitivity to the micro-energy group structure used in Serpent, core eigenvalue, power distribution, sodium void reactivity worth and control rod worth. Anisotropic diffusion coefficients furnished a better overall agreement. Means of improving the performance of both modeling approaches are proposed.

1. Introduction

For over a decade, sodium-cooled fast reactor (SFR) designs have been studied with renewed interest, given their potential to meet the goals of sustainability, economics, safety and reliability, proliferation resistance and physical protection set for Generation IV nuclear energy systems (U.S. DOE Nuclear Energy Research Advisory Committee, 2002).

Several fuel options are considered for SFRs, ranging from metal alloys to mixed oxides (Kim et al., 2009). The type of fuel has a direct impact on, for instance, the power density, fuel temperature, fissile conversion ratio, discharge burnup, sodium void reactivity worth and Minor Actinide (MA) transmutation ratio.

The characterization of the aforementioned performance parameters can be achieved by deterministic or stochastic methods. Among the deterministic suites of codes used for neutronic calculations, the ERANOS system (Rimpault et al., 2002) can be mentioned. With regard to stochastic neutronic codes, we would like to focus our attention on the Monte Carlo (MC) code Serpent (Leppänen et al., 2007).

Serpent has been applied to the modeling of full-core SFRs (see, for example, Korkmaz and Agar (2014)). However, a more versatile approach that uses Serpent as a cell code for the generation of SFR multi-group cross section data for diffusion codes has been demonstrated (Fridman and Shwageraus, 2013; Rachamin et al., 2013).

In Dorval and Leppänen (2015), a new method for the calculation of directional diffusion coefficients was implemented in Serpent and tested with certain limitations pertaining the treatment of the radial dependence of these coefficients. Thanks to the insights gained during that work, it is now possible to ponder upon the possibility of performing a finer treatment of the radial diffusion coefficients.

Given that the development of more refined methods is aimed at improving the accuracy of diffusion calculations, it is of interest to study a realistic system in order to compare the performance of such methods against the ones already available in Serpent. Any realistic reactor system relies on strong neutron absorbers for control purposes. We will study a few alternatives to treat these absorbers in diffusion theory.

The anterior work highlighted the need for axial discontinuity factors in Serpent. This work describes the implementation of that feature and tests its performance.

The rest of the work is structured as follows: Section 2 introduces some concepts necessary for the analysis proposed in this work, as well as the system to be studied. In Section 3, the main results are presented and discussed. Finally, Section 4 summarizes the conclusions of this work.

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It is worthwhile to mention that all the code modifications made to Serpent are for the sake of this work only, and do not constitute a part of Serpent's standard distribution package.

2. Materials and methods

2.1. Energy grids and XS generation in Serpent

The Serpent Monte Carlo code can be used either as a three-dimensional (3-D) reactor physics burnup code, primarily aimed at the calculation of benchmark-quality reference solutions, or as a few-group cross section (XS) data generation code. When few-group data generation is enabled, four different energy structures can be identified.

Serpent reads linearly-interpolable, continuous-energy XS data contained in ACE format files, generally processed by the NJOY code (MacFarlane et al., 2012) from ENDF-formatted (Cross Sections Evaluation Working Group, 2010) library data.

In addition to the Woodcock delta-tracking method (Leppänen, 2010), the adoption of a unionized energy grid (Leppänen, 2009) for all point-wise cross sections provides a substantial reduction in computation times without loss of accuracy.

The generation of few-group XS constants requires two additional energy grids: the *micro-group* structure and the *macro-* or *few-group* structure itself, whose energy bounds need be a subset of those from the micro-group structure. The latter can be either arbitrarily defined by the user or selected from a set of predefined grids.

During the course of Monte Carlo random walks, partial quantities (such as collision-based scalar flux estimates, or the product of these estimates times reaction cross sections, for the final computation of scalar fluxes or cross sections, respectively) are accumulated on arrays of size equal to the number of bins in the micro-group grid. After a certain number of cycles, the contents of each array are mapped onto their corresponding counterparts in the few-group structure and normalized to convert reaction rates to cross sections. At this stage, statistics are updated. At the end of this stage, the contents of micro-group arrays are erased, thus making them ready for a new data accumulation.

If we denote by g and G the micro- and few-group indexes, respectively, we have that the few-group reaction XS for a reaction α is computed as:

$$\Sigma_\alpha^G = \frac{\sum_{g\in G}\Sigma_\alpha^g \phi^g}{\sum_{g\in G}\phi^g}, \tag{1}$$

where ϕ is the collision-based estimate[1] of the scalar neutron flux.

Multi-group diffusion coefficients are not calculated as the result of a single reaction rate. Instead, these quantities are calculated from the transport cross section, Σ_{tr}^G, by means of:

$$D^G = \frac{1}{3\Sigma_{tr}^G} \tag{2}$$

In Serpent, the transport cross section is estimated (Fridman et al., 2013) as:

$$\Sigma_{tr}^G = \frac{\sum_{g\in G}\phi^g}{\sum_{g\in G}\frac{\phi^g}{\Sigma_t^g - \overline{\mu}_0^g\Sigma_s^g}} \tag{3}$$

In Eq. (3), Σ_t, Σ_s and $\overline{\mu}_0$ correspond to the total XS, scattering XS, and average scattering cosine in the laboratory reference frame, respectively. In what follows, we will refer to the diffusion coefficients calculated through Eqs. (2) and (3) as **standard** diffusion coefficients.

[1] This estimate also caters for the neutron weight.

2.2. Directional diffusion coefficients in Monte Carlo

In a recent paper (Dorval and Leppänen, 2015), a novel method for the computation of directional diffusion coefficients by Monte Carlo methods was presented and tested in a sodium-cooled fast reactor system. With the exception of some elements necessary for the sake of this work, the complete derivation of the method will be omitted.

This method is based on the definition of an arbitrarily-oriented plane $\mathcal{S}$, for which a current-weighted estimate of the transport cross section is tallied. If we denote by $\Sigma_{tr}|_{\mathbb{J}}$ the current-weighted transport cross section averaged over $\mathcal{S}$, then the directional diffusion coefficient in a direction given by the normal of $\mathcal{S}$ is calculated as:

$$D_{\mathbb{J}}^G = \frac{1}{3\langle\Sigma_{tr}\rangle|_{\mathbb{J}}^G} \tag{4}$$

Further, the micro-group transport cross section is related to other quantities through:

$$\langle\Sigma_{tr}\rangle|_{\mathbb{J}}^g = (1-m)\frac{\alpha}{\langle D_n\rangle^g} + m\langle\Sigma_t\rangle|_{\mathbb{J}}^g - \overline{\mu}_0^g\langle\Sigma_s\rangle|_{\mathbb{J}}^g, \quad 0 \leqslant m \leqslant 1 \tag{5}$$

The interpolation constant m in Eq. (5) has been set to 0.85 for the system studied in Dorval and Leppänen (2015), whereas $\alpha = 0.2773427662$ is a hard-coded constant. The estimator $\langle D_n\rangle$ is the total-current-weighted value of the following score:

$$D_n = \frac{R}{2 + R\Sigma_t|_R}, \tag{6}$$

where R denotes the distance between the last source or collision point and the position where the surface $\mathcal{S}$ is traversed. $\Sigma_t|_R$ simply denotes the total cross section at that crossing point.

As described in our previous work, the quantities D_n, Σ_t and $\overline{\mu}_0\Sigma_s$ on the right-hand side of Eq. (5) are accumulated as a product of themselves times the neutron weight crossing the surface $\mathcal{S}$, which replaces the scalar flux used for standard cross section weighting. By accumulating also the total neutron weight w crossing $\mathcal{S}$, it is then possible to map between micro- and few-group arrays and compute a few-group transport XS through:

$$\langle\Sigma_{tr}\rangle|_{\mathbb{J}}^G = \frac{\sum_{g\in G}\langle\Sigma_{tr}\rangle|_{\mathbb{J}}^g w^g}{\sum_{g\in G} w^g} \tag{7}$$

The desired diffusion coefficient is obtained by substitution of $\langle\Sigma_{tr}\rangle|_{\mathbb{J}}^G$ into Eq. (4). Diffusion coefficients are treated as additional tallies with associated statistical uncertainties.

2.3. Radial treatment

The directional diffusion coefficient described so far depends on the choice of the tallying surface $\mathcal{S}$. Whereas the computation of axial coefficients could be achieved reasonably well using a single surface, as in the precedent work, the radial direction poses more challenges because different materials and, consequently, different cross sections are intersected depending on the surface under investigation. This has a direct impact on the estimators in Eq. (5).

In this work, we propose the definition of multiple parallel surfaces in the X and Y directions. For a given direction and micro-group index g, all the quantities required for the computation of $\langle\Sigma_{tr}\rangle|_{\mathbb{J}}^g$ will be accumulated on the *same* array bin whenever *any* of the surfaces normal to that direction are traversed. The rest of the data management is identical as before.

The new proposal is illustrated in Fig. 1. By defining a sufficiently large number of uniform meshes per direction, an asymptotic value of the diffusion coefficient can be attained. Moreover, the values obtained for the X and Y directions can be averaged