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Monte Carlo current-based diffusion coefficients: Application to few-group constants generation in Serpent

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ABSTRACT

Criticality eigenvalue and power distributions of a medium-sized sodium-cooled fast reactor core were studied by combined diffusion theory and Monte Carlo methods. Few-group XS data sets generated by the Monte Carlo code Serpent for both normal and sodium-voided cells were used in the multi-group diffusion code TRIZ. Two different approaches were adopted in order to account for neutron leakage at fuel assembly level: a radially-reflected and axially-heterogeneous model with vacuum boundary conditions at the bottom and the top; and a more typical infinite cell calculation, followed by criticality spectrum corrections. In addition to the standard diffusion coefficients calculated by Serpent, a novel method for the calculation of directional diffusion coefficients was implemented and tested, yielding satisfactory results for normal and sodium-voided conditions, using Monte Carlo results as a reference. The feasibility of using the B_1 criticality spectrum as a weighting function for these diffusion coefficients was also tested, and slightly better estimates of *k-eff* were obtained when compared to the direct use of diffusion coefficients arising from the solution of the B_1 equations.

1. Introduction

The Gen-IV International Forum (NERAC and GIF, 2002) has identified liquid metal fast reactor (LMFR) designs as a promising path towards the achievement of the goals of sustainability, safety, reliability, proliferation resistance and economic competitiveness. Amongst LMFRs, sodium-cooled fast reactors (SFRs) have supplied vast operational experience and lessons learnt (International Atomic Energy Agency, 2007). One of the main safety aspects of SFRs under study is the reactivity insertion caused by a reduction in the sodium density in some regions of the core, and how to minimize or eliminate it by design. As means of an example, the ASTRID design (Chenaud et al., 2013) favors an axially-heterogeneous layout and the presence of an upper sodium plenum, in addition to a large pin concept.

The use of sophisticated tools is mandatory for an adequate neutronic and thermal–hydraulic characterization of the sodium void worth. Pertaining neutronics, modern Monte Carlo codes offer highly realistic geometric modeling capabilities, as well as the use of continuous energy cross-section (XS) data. The implementation of the best available physical models and the introduction of virtually no approximations in the neutron energy dependence confer the character of reference solutions to those results obtained by Monte Carlo codes, provided that convergence is properly assessed. Uncertainty in the basic nuclear and model data cannot be overcome by the use of Monte Carlo codes.

Advances in computer architecture and parallelization render whole core calculations with Monte Carlo possible. Nevertheless, computational burden hinders the use of this method for routine reactor analysis (Martin, 2012). A two-step approach, where Monte Carlo is used for few-group XS data generation at sub-assembly level, followed by a multi-group diffusion calculation at core level is an efficient way of circumventing the aforementioned computational burden. The Serpent code (Leppänen, 2007) has been successfully applied to this task. Amongst others, Fridman and Leppänen (2011) and Fridman and Shwageraus (2013) demonstrate the successful application of the sequence Serpent-DYN3D for both a Pressurized Water Reactor (PWR) and a SFR, respectively.

In the case of SFRs, core designs may differ substantially from one another. Consequently, the successful generation of XS data by a Monte Carlo code for one specific core does not necessarily validate the use of such code for all possible configurations. In an attempt to broaden the examples of use of the Serpent code, we chose a core design with increased axial leakage, which is achieved by means of a long gas plenum directly above the active core.

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The presence of this type of gas plenum poses difficulties due to the directional dependence of the diffusion coefficients. Previous work on the generation of direction-dependent diffusion coefficients by Monte Carlo methods through various approaches may be found, for example in Milgram (1997), Gelbard and Pego (1979) and Yamamoto (2012). Recently, one of the authors of this work proposed another method for the estimation of anisotropic diffusion coefficients (Dorval, 2014). An extended version of this proposal has been implemented in Serpent in order to test its performance in a more realistic environment.

Multi-group diffusion calculations were conducted reading XS data generated by Serpent for a coarse 7-group and a finer 24-group energy structures. Neutron leakage was accounted for in two different ways, as will be described later. This allowed direct comparison not only against the use of standard diffusion coefficients calculated by Serpent, but also against those obtained when B_1 corrections are applied.

2. Derivation

The original derivation of the proposed method may be found in Dorval (2014), but it will be reproduced here for completeness. Also, it must be mentioned that the final way of estimating diffusion coefficients differs from the original work. This modification followed thorough testing of three-dimensional cases.

Throughout this paper, variables have their usual meanings, unless otherwise stated. The main idea of this method is to estimate a diffusion coefficient that satisfies the relationship:

$$\vec{J}(\vec{r},E) \equiv -D(\vec{r},E)\nabla\phi(\vec{r},E) \tag{1}$$

Moreover, in this work we enforce that the sought solution is constrained to the following functional form, in order to be consistent with one-group diffusion theory in a homogeneous medium:

$$D(\vec{r},E) = \frac{1}{3\Sigma_{tr}(\vec{r},E)} \tag{2}$$

with

$$\Sigma_{tr}(\vec{r},E) = \Sigma_t(\vec{r},E) - \overline{\mu}_0\Sigma_s(\vec{r},E) \tag{3}$$

Clearly, the problem at hand resides in finding the appropriate transport cross section (Σ_{tr}) in Eq. (2) such that Eq. (1) holds. Milgram (1997) clarifies that Eq. (1) is not the embodiment of Fick's Law applied to neutron transport. Fick's Law holds when the variations in $D(\vec{r},E)$ may only be attributed to material composition changes or spectral effects. Our method aims at determining $D(\vec{r})$ in Eq. (2) by tallying a special score upon surface crossings. In what follows, the energy variable E will be dropped to ease the syntax.

Referring to Fig. 1, let $\mathcal{S}$ be an arbitrary surface, and assume that every neutron that crosses that surface has been emitted by an *isotropic* point source located at $\vec{r}'$, with strength equal to the neutron's weight (w). $\vec{r}'$ denotes the position where the last collision or source event took place. The *deterministic* contribution to the scalar flux at $\vec{r}$, located on the surface $\mathcal{S}$ at a distance $R = |\vec{R}| = |\vec{r} - \vec{r}'|$ from the source, may be written as:

$$\phi(\vec{r}) = \frac{w\ \exp\left(-\int_0^R \Sigma_t(s)ds\right)}{4\pi R^2} \tag{4}$$

In Eq. (4), the variable s indicates that integration occurs along the flight path. Further assuming that attenuation happens only along this path, the gradient of flux is:

$$\nabla\phi(\vec{r}) = \frac{\partial\phi(\vec{r})}{\partial s}\hat{\Omega} \tag{5}$$

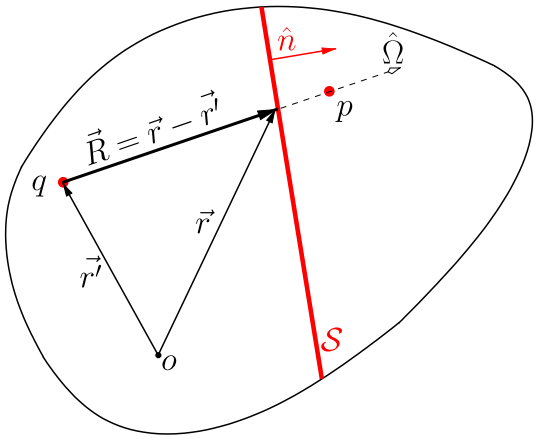

Fig. 1. Surface crossing variables: the neutron flying from point q to point p intersects the surface $\mathcal{S}$ at the coordinate $\vec{r}$.

Noticing that $\frac{\partial R}{\partial s} = 1$ and applying Leibniz's Integral Rule, the derivative of Eq. (4) along the flight path yields:

$$\nabla\phi(\vec{r}) = -\frac{w\ \exp\left(-\int_0^R \Sigma_t(s)ds\right)}{4\pi R^2}\left(\Sigma_t|_R + \frac{2}{R}\right)\hat{\Omega} \tag{6}$$

In Eq. (6), the notation $\Sigma_t|_R$ refers to the total cross section evaluated at the surface crossing point. For the same event, the contribution to the *angular current* is:

$$\vec{J}(\vec{r}) = \frac{w\ \exp\left(-\int_0^R \Sigma_t(s)ds\right)}{4\pi R^2}\hat{\Omega} \tag{7}$$

Eqs. (6) and (7) can be projected along the surface normal $\hat{n}$ in order to calculate, respectively, the gradient of flux normal to $\mathcal{S}$:

$$\frac{\partial\phi(\vec{r})}{\partial n} = -\phi(\vec{r})\left(\Sigma_t|_R + \frac{2}{R}\right)\hat{\Omega}\bullet\hat{n} \tag{8}$$

and the *net current* crossing[1] the same surface:

$$J_n(\vec{r}) = \phi(\vec{r})\hat{\Omega}\bullet\hat{n} \tag{9}$$

Taking the ratio of the two,[2] one readily finds:

$$D_n(\vec{r}) = -\frac{J_n(\vec{r})}{\partial\phi(\vec{r})/\partial n} = \frac{R}{2 + R\Sigma_t|_R} \tag{10}$$

The estimator $D_n(\vec{r})$ in Eq. (10) is unnormalized, due to the fact that the net current was estimated based on a single event. Since the current is the result of a collective contribution from all neutrons crossing the surface, and since such information is unavailable at the time of scoring, a means of relating the average value of the estimator $D_n(\vec{r})$ with other parameters is needed.

2.1. Normalization

By assuming isotropic angular flux in an infinite homogeneous medium, it can be shown (Dorval, 2014) that the space- and angle-integrated estimator D_n takes the form:

$$\langle D_n\rangle = \frac{2e^2\mathrm{Ei}(-2)+1}{\Sigma_t} \simeq \frac{0.2773427662}{\Sigma_t} = \frac{\alpha}{\Sigma_t} \tag{11}$$

[1] It is important to highlight that in this case the net current is estimated *for this event only*.

[2] The possible divergence corresponding to $\hat{\Omega}\bullet\hat{n} = 0$ is avoided, because in such a case there would be no contribution to the net current, and the score would not be computed.