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Monte Carlo perturbation methods using "virtual density" theory for calculating reactivity due to geometry change

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ABSTRACT

The "virtual density" theory in the field of neutronics is a method to quantify reactivity of a reactor core due to geometry changes by altering the material density or nuclear cross section instead of explicitly changing the geometry. The Monte Carlo perturbation methods—differential-operator sampling (DOS) and correlated sampling (CS)—can efficiently yield accurate small reactivity for cross section changes. However, Monte Carlo perturbation methods have weakness in their inability to deal with geometry changes. This study incorporates the virtual-density theory into the Monte Carlo perturbation methods. When an entire core expands or swells uniformly, k_{eff} of the perturbed core can be calculated by simply changing the material density without changing the geometry. Regarding uniform expansion or swelling, conventional Monte Carlo perturbation methods—where cross sections change proportionally to the material density—can predict the altered k_{eff}. According to the virtual-density theory, k_{eff} perturbed due to a uniform anisotropic expansion or swelling can be predicted by stretching or shrinking the mean free path of neutrons in only one direction without changing the geometry. A new Monte Carlo algorithm is developed to incorporate the path length-stretching or -shrinking in only one direction into a random-walk process in a Monte Carlo k_{eff}-eigenvalue calculation. The new Monte Carlo algorithm provides accurate k_{eff} values for uniform anisotropic expansion and swelling regardless of the perturbation degree. New formulations of the Monte Carlo perturbation methods are derived to predict the change in k_{eff} due to a uniform anisotropic expansion or swelling. Both Monte Carlo perturbation methods can accurately and efficiently predict changes in k_{eff} for a small uniform anisotropic expansion or swelling.

1. Introduction

So far, perturbation methods using Monte Carlo calculations to determine changes in the k_{eff} eigenvalue or general responses of neutrons have been developed. In many cases, the perturbation is caused by a change in the neutron cross sections. Perturbations caused by a change in geometry have long been known as "boundary perturbation theory" or "geometry perturbation" (Larsen and Pomraning, 1981; Rahnema and Pomraning, 1983; Rahnema, 1996; Yamamoto, 1996; McKinley and Rahnema, 2002; Favorite and Bledsoe, 2010; Favorite and Gonzalez, 2017). The boundary perturbation theory has been mainly applied within deterministic approaches because it requires estimating the adjoint flux. The development of the boundary or geometry perturbation method in the Monte Carlo method has not been as widely studied as perturbations due to cross section changes. This is partly due to the difficulty of estimating the adjoint flux using the Monte Carlo method. Few examples of Monte Carlo perturbation approaches for geometry perturbations are published in (Takahashi, 1970; Kiedrowski et al., 2011; Wang et al., 2017; Burke and Kiedrowski, 2018). The most recent one (Burke and Kiedrowski, 2018) uses the adjoint-based perturbation theory and the differential-operator sampling (DOS) method to compute the sensitivities of the k_{eff} eigenvalue to the system dimension. This paper introduces kernel density estimators to circumvent the difficulty in estimating adjoint-weighted scattering and fission sources at the material interfaces.

Recently, the "virtual density" theory has been proposed for estimating reactivity caused by geometry changes (Reed et al., 2012, 2018a,b; Zheng et al., 2017). The theory does not require an estimation of the adjoint flux. A reactivity caused by a geometry deformation can be obtained by virtually changing the material density instead of explicitly changing the geometry. The virtual-density theory argues that the reactivity can be exactly estimated by changing the material density when the geometry *swells* or *expands uniformly* and *isotropically*. In the virtual-density theory, *swell*, *expand*, *isotropic* (or *anisotropic*), and *uniform* (or *nonuniform*) have specific meanings. The definitions of these terms are provided later in this paper.

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By using the virtual-density theory for a uniform isotropic swelling or expansion, the effect of a light geometry change on the reactivity change can be easily and accurately estimated using conventional Monte Carlo perturbation methods because they easily handle density changes. Although the reactivity before and after the perturbation can be obtained from two independent k_{eff}-eigenvalue calculations, it takes more computation time to obtain the reactivity with a small statistical uncertainty. Monte Carlo perturbation methods can yield accurate reactivities for small perturbations with much less computational effort. So far, two Monte Carlo perturbation methods, the correlated-sampling (CS) method (Spanier and Gelbard, 1969; Bernnat, 1974; Nakagawa and Asaoka, 1978; Rief, 1984; Kitada et al., 1996) and the DOS method (Olhoeft, 1962; Takahashi, 1970; Rief, 1984), have been developed. These methods have been widely investigated and their unique advantages and drawbacks have been identified in many publications (e.g., McKinney and Iverson, 1996; Densmore et al., 1997; Morillon, 1998; Favorite and Parsons, 2001; Favorite, 2002; Nagaya and Mori, 2005; Nagaya and Mori, 2011; He and Su, 2010; He and Su, 2011; Raskach, 2009; Raskach, 2010; Jinaphanh et al., 2016; Sakamoto and Yamamoto, 2017; Kiedrowski, 2017; Yamamoto, 2018). This study applies the two Monte Carlo perturbation methods (CS and DOS) to uniform isotropic expansion and swelling. It is investigated how the Monte Carlo perturbation methods behave for the virtual-density theory.

If a core geometry does not change isotropically in all but only one or two directions, its shape changes. Such a geometry change is defined as "anisotropic" in the virtual-density theory. For example, an "anisotropic" geometry change of a cube causes it to become a rectangular parallelepiped. According to the virtual-density theory, the reactivity caused by an expansion of the box in x-direction only can be estimated by shrinking the mean free path of the neutrons in x-direction. However, the reactivity caused by a swelling of the box in x-direction can only be estimated by stretching the mean free path of the neutrons in other directions. In virtual-density parlance, *expansion* and *swelling* are not the same; these terms are defined in Section 2.1. The mean free path is changed by adjusting the macroscopic transport cross section (or diffusion coefficient) in the deformation direction. The virtual-density theory regarding anisotropic geometry changes has been theoretically proved in the context of diffusion theory (Reed et al., 2018a). This paper verifies whether an anisotropic expansion or swelling can be really attained by changing the mean free path of neutrons in the context of an exact transport theory. The change of the mean free path in only one direction in neutron transport calculations can be realized in the form of a random-walk process regarding the particle transport in the Monte Carlo method, which complies faithfully with the transport theory. This paper presents a new algorithm for random-walk processes in the Monte Carlo method regarding uniform anisotropic expansion and swelling, where the mean free path in only one direction is changed. While conventional Monte Carlo perturbation methods are available for uniform isotropic expansion or swelling, no previous study has investigated a perturbation method for mean free path changes of neutrons in only one direction. In this paper, new formulations for the Monte Carlo perturbation method regarding uniform anisotropic expansion and swelling are derived, and numerical examples are presented to validate the new method.

2. Monte Carlo perturbation for uniform isotropic expansion or swelling

2.1. Uniform expansion and swelling in the virtual-density theory

Uniform expansion or swelling is depicted in Fig. 1. The expansion or swelling is deemed as *isotropic* if the core shape retains its shape during enlargement. The aspect ratio in a rectangular geometry remains unchanged when it enlarges *isotropically*. *Swelling* comprises a dimension change with corresponding density change while mass is conserved, e.g., the thermal expansion of a solid. *Expansion* comprises a geometry change without a density change. Thus, an expansion of the geometry results in an increased mass. It is assumed that a reactor core expands isotropically by a factor f. The virtual-density theory precisely predicts the reactivity caused by the isotropic expansion by including the increasing material density of the core via the factor f and without altering the core geometry. When the reactor core isotropically swells by a factor f, the reactivity is predicted by decreasing the material density by f^{n-1}, where n is the dimension. Therefore, swelling produces no reactivity in an infinite one-dimensional slab with $n = 1$. In conclusion, reactivity can be predicted by changing the material density according to an expansion or swelling.

2.2. The correlated-sampling (CS) method

The Monte Carlo algorithm of CS for perturbations caused due to a material density change (Rief, 1984; Nagaya, 2012; Zhu and Liu, 2013) is shown in this section. In the CS method, the perturbed history is forced to follow the same track as the unperturbed history. It is assumed that a particle flies in an unperturbed material whose total macroscopic cross section is Σ_t. The flight distance, s, is determined with $s = -\ell n\xi/\Sigma_t$, where ξ is a uniform pseudorandom number from (0, 1). When a particle with weight W flies a distance s and undergoes a collision, the weights of unperturbed and perturbed histories after the collision are:

$$\textit{Unperturbed} : W \Rightarrow W\frac{\Sigma_s}{\Sigma_t}, \tag{1}$$

$$\textit{Perturbed} : W \Rightarrow W\frac{\Sigma_t' e^{-\Sigma_t' s}}{\Sigma_t e^{-\Sigma_t s}} \cdot \frac{\Sigma_s'/\Sigma_t'}{\Sigma_s/\Sigma_t} \cdot \frac{\Sigma_s}{\Sigma_t} = We^{-\Delta\Sigma_t s}\frac{\Sigma_s'}{\Sigma_t}, \tag{2}$$

respectively, where the prime symbol denotes the perturbed cross section, $\Sigma_s =$ macroscopic scattering cross section, and $\Delta\Sigma_t = \Sigma_t' - \Sigma_t$ (Zhu and Liu, 2013). For simplicity, the variables of the energy are omitted. Throughout this study, it is assumed that macroscopic cross sections change proportionally to their material densities. Further, changes in microscopic cross sections caused

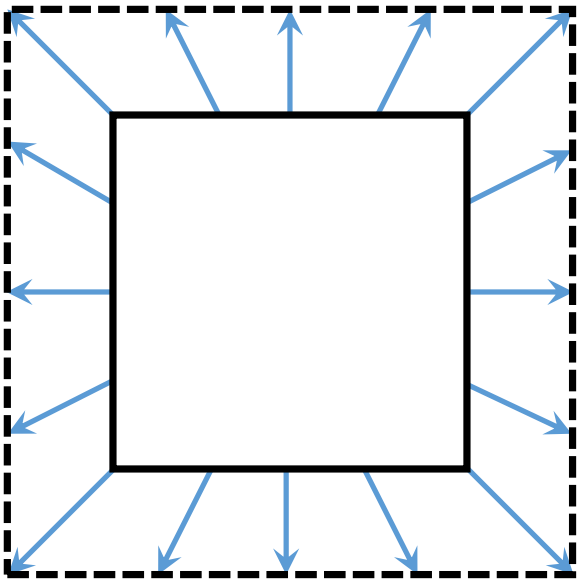

Fig. 1. Illustration of uniform isotropic expansion or swelling.