Journal of Computational Physics 345 (2017) 245–259

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Improvement and performance evaluation of the perturbation source method for an exact Monte Carlo perturbation calculation in fixed source problems

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ARTICLE INFO

Article history:
Received 26 September 2016
Received in revised form 24 January 2017
Accepted 5 May 2017
Available online 17 May 2017

Keywords:
Monte Carlo
Perturbation
Fixed source problem
Transport equation

ABSTRACT

This paper presents improvement and performance evaluation of the "perturbation source method", which is one of the Monte Carlo perturbation techniques. The formerly proposed perturbation source method was first-order accurate, although it is known that the method can be easily extended to an exact perturbation method. A transport equation for calculating an exact flux difference caused by a perturbation is solved. A perturbation particle representing a flux difference is explicitly transported in the perturbed system, instead of in the unperturbed system. The source term of the transport equation is defined by the unperturbed flux and the cross section (or optical parameter) changes. The unperturbed flux is provided by an "on-the-fly" technique during the course of the ordinary fixed source calculation for the unperturbed system. A set of perturbation particle is started at the collision point in the perturbed region and tracked until death. For a perturbation in a smaller portion of the whole domain, the efficiency of the perturbation source method can be improved by using a virtual scattering coefficient or cross section in the perturbed region, forcing collisions. Performance is evaluated by comparing the proposed method to other Monte Carlo perturbation methods. Numerical tests performed for a particle transport in a two-dimensional geometry reveal that the perturbation source method is less effective than the correlated sampling method for a perturbation in a larger portion of the whole domain. However, for a perturbation in a smaller portion, the perturbation source method outperforms the correlated sampling method. The efficiency depends strongly on the adjustment of the new virtual scattering coefficient or cross section.

1. Introduction

Monte Carlo methods have difficulties in calculating the effect of a small perturbation in the system parameters. The effect of a perturbation, of course, can be obtained by performing two independent Monte Carlo calculations and subtracting the estimates of the unperturbed system from those of the perturbed system. A prohibitively huge computational cost would however be required to obtain statistically significant estimates for a small perturbation. The statistical uncertainty of the difference between two independent runs is sometimes comparable with the change of the estimates if the perturbation is small and the computation time short. Thus far, two perturbation calculation methods, the correlated sampling method

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http://dx.doi.org/10.1016/j.jcp.2017.05.004
0021-9991/

[1–5] and the differential operator sampling method [4,6,7], have been developed to overcome difficulties in the Monte Carlo perturbation calculations. These methods have been widely investigated; their unique advantages and drawbacks have been identified in many publications (e.g., [8–12]).

In the correlated sampling method, the perturbed history is forced to follow the unperturbed one along the same tracks in phase space. It has been found that the correlated sampling method suffers from a large or unbounded variance when the perturbation exceeds a certain limit [4].

The differential operator sampling method accumulates a sum of products combining cross section, path segment probabilities, and associated partial derivatives (first order and higher) for all trajectories. The divergence of the variance, which frequently occurs in the correlated sampling method for a larger perturbation, can be circumvented in the differential operator method. However, the differential operator sampling method uses up to the second-order terms in a widely used Monte Carlo code, MCNP [12], and the higher-order terms, beyond the third order, are truncated. A localized and large perturbation would require higher-order terms, truncated in commonly-used differential operator sampling method. As the order becomes higher, the mathematical formulation of the higher-order terms becomes more involved. In addition, many quantities need to be scored during the course of the particle's random walk, making the calculation less efficient. In the Monte Carlo code, MVP, the order of the differential operator method is uniquely expanded to the 8th order [9]. However higher the order is, the differential operator sampling method remains essentially approximate and may be occasionally insufficient for large and localized perturbations.

The two Monte Carlo perturbation methods have already been implemented into some Monte Carlo production codes [8, 9,12–16]. The two Monte Carlo perturbation methods can be applied to perturbation calculations in k_{eff}-eigenvalue problems as well as fixed source problems. In the k_{eff}-eigenvalue problems, the fission source spatial distribution is also perturbed due to the perturbation of system parameters such as cross sections and material density. To estimate the effect of the fission source perturbation, some techniques have been developed and installed into Monte Carlo codes [8,9,17]. For the fixed source problems, on the other hand, the need to consider the fission source perturbation effect can be avoided.

Besides the correlated sampling method and the differential operator method, there exists another perturbation method known as the "perturbation source" method [18–20] in which a separate random walk is performed to follow a "perturbation particle" once a perturbed region is encountered in the original random walk. The perturbation particle explicitly represents the change of the flux due to the perturbation. However, this method is less effective when a large number of collisions occurs in the perturbed region during a history, too many perturbation particles must be followed. On the other hand, if the perturbed region is very small, most of particles pass through the perturbed region without collision and too few perturbation particles are started, which make the perturbation source method less effective than other perturbation techniques. To compensate for the shortcomings of the perturbation source method, Preeg and Tsang [20] proposed a hybrid method that uses the correlated sampling method initially, and then switches to the perturbation source method for the remainder of the history. According to [18,19], the perturbation source method has been used within the first-order accuracy by neglecting higher-order terms; although it is known that the method can be easily extended to an exact perturbation method [18]. Thus, the formerly proposed perturbation source method only yields an approximate estimate of perturbation.

The present paper focuses on the Monte Carlo perturbation method for particle (light or neutron) transport in a semi-transparent material. The perturbation source method is improved to take into account higher-order terms neglected in the previous studies. This paper proposes a method for improving the effectiveness of the perturbation source method to estimate the variation of flux in problems where the perturbed region covers only a small fraction of the whole domain. The dependence of the efficiency improvement for a user-specified parameter is investigated. It is shown that the newly improved perturbation source method outperforms the correlated sampling method and the differential operator method for such problems in terms of computation efficiency. The underlying concept of this paper is applicable to other particle transport calculations. In the sections that follow, the theory and numerical examples are presented.

2. Theory of the improved perturbation source method

This section presents a theory of the perturbation method used to calculate the difference of flux variation caused by the perturbation of system parameters in a fixed source problem. The theory is already proposed [18,19] and simple, but it provides an exact perturbation method that can be performed in the Monte Carlo method. The unperturbed light transport equation with a fixed source is given by

$$\mathbf{H}\phi(\mathbf{r},\boldsymbol{\Omega},E)=S(\mathbf{r},\boldsymbol{\Omega},E), \tag{1}$$

where

$$\mathbf{H}\phi(\mathbf{r},\boldsymbol{\Omega},E)\equiv\boldsymbol{\Omega}\cdot\nabla\phi(\mathbf{r},\boldsymbol{\Omega},E)+\mu_t(\mathbf{r},E)\phi(\mathbf{r},\boldsymbol{\Omega},E)-\int_{4\pi}d\boldsymbol{\Omega}'\int dE'\mu_s\big(\mathbf{r},\boldsymbol{\Omega}'\to\boldsymbol{\Omega},E'\to E\big)\phi\big(\mathbf{r},\boldsymbol{\Omega}',E'\big), \tag{2}$$

$\phi(\mathbf{r},\boldsymbol{\Omega},E)=$ the unperturbed flux at position $\mathbf{r}$ with energy E and direction $\boldsymbol{\Omega}$, $S(\mathbf{r},\boldsymbol{\Omega},E)=$ the external light source term, $\mu_t=$ the total coefficient of absorption and scattering, $\mu_s=$ the scattering coefficient. We suppose that the coefficients in Eq. (2) are perturbed with the fixed source term being unchanged. Then, the flux is perturbed to $\phi'(\mathbf{r},\boldsymbol{\Omega},E)(\equiv\phi(\mathbf{r},\boldsymbol{\Omega},E)+$