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Computing eigenvalue sensitivity coefficients to nuclear data based on the CLUTCH method with RMC code

Yishu Qiu [a,*], Ding She [b], Xiao Tang [a], Kan Wang [a], Jingang Liang [a]

[a] Department of Engineering Physics, Tsinghua University, Beijing 100084, China
[b] Institute of Nuclear and New Energy Technology, Tsinghua University, Beijing 100084, China

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ABSTRACT

Recently, there is a need to develop advanced methods of computing eigenvalue sensitivity coefficients to nuclear data in the continuous-energy Monte Carlo codes. One of these methods is the iterated fission probability (IFP) method, which is adopted by most of Monte Carlo codes of having the capabilities of computing sensitivity coefficients, including the Reactor Monte Carlo code RMC. Though it is accurate theoretically, the IFP method faces the challenge of huge memory consumption. Therefore, it may sometimes produce poor sensitivity coefficients since the number of particles in each active cycle is not sufficient enough due to the limitation of computer memory capacity. In this work, two algorithms of the Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization (CLUTCH) method, namely, the collision-event-based algorithm (C-CLUTCH) which is also implemented in SCALE and the fission-event-based algorithm (F-CLUTCH) which is put forward in this work, are investigated and implemented in RMC to reduce memory requirements for computing eigenvalue sensitivity coefficients. While the C-CLUTCH algorithm requires to store concerning reaction rates of every collision, the F-CLUTCH algorithm only stores concerning reaction rates of every fission point. In addition, the fission matrix method is put forward to generate the adjoint fission source distribution for the CLUTCH method to compute sensitivity coefficients. These newly proposed approaches implemented in RMC code are verified by a SF96 lattice model and the MIT BEAVRS benchmark problem. The numerical results indicate the accuracy of the F-CLUTCH algorithm is the same as the C-CLUTCH algorithm while the F-CLUTCH algorithm requires less memory and has higher computational efficiency.

1. Introduction

Several years ago, "Benchmarks for Uncertainty Analysis in Modelling (UAM) for the Design, Operation and Safety Analysis of LWRs" was put forward by the Expert Group on Uncertainty Analysis method in Modelling (EGUAM) of OECD/NEA Nuclear Science Committee (NSC) (Ivanov et al., 2013). In these benchmarks, the uncertainties of nuclear data are treated as an important source of uncertainties. As a tool for analyzing nuclear data sensitivity and uncertainties, the TSUNAMI-3D code (Rearden, 2004) within the SCALE code package (Oak Ridge National Laboratory, 2011) has been widely used for more than a decade. By applying the sensitivity/uncertainty analysis method, TSUNAMI-3D computes sensitivity coefficients firstly and then performs uncertainty analysis through sandwich rules. According to the linear perturbation theory, TSUNAMI-3D performs a separate adjoint transport calculation in addition to a forward transport calculation so as to compute the adjoint weighting functions which are necessary to compute sensitivity coefficients. What is more, since TSUNAMI-3D (Rearden, 2004) uses multi-group cross sections, the implicit sensitivity coefficients should be calculated to consider the impact of resonance calculation. To pursue higher fidelity in sensitivity coefficients with a simpler work flow and analyze simulations of advanced reactors including high-temperature gas-cooled reactors, sodium-cooled fast reactors and other new-concept reactors, there is a need to use continuous-energy Monte Carlo codes to generate sensitivity coefficients. Therefore, several continuous-energy Monte Carlo codes, including McCARD (Shim and Kim, 2011), MONK (ANSWERS, 2008), MCNP6 (Kiedrowski and Brown, 2013), and the continuous-energy version of TSUNAMI-3D (Perfetti and Rearden, 2013), have developed capabilities of computing eigenvalue sensitivity coefficients to nuclear data.

In our previous work, the Rector Monte Carlo RMC (Wang et al., 2015) has also developed such a capability based on the iterated fission probability (IFP) method and the data decomposition strat-

* Corresponding author. Tel.: +861 369 364 8694; fax.: +8610 62782658.
E-mail address: qys12@mails.tsinghua.edu.cn (Y. Qiu).

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egy has been suggested to distribute memory requirements averagely on parallel processors (Qiu et al., 2015). Since the number of parallel processors should be increased in accordance with the complexity of problems, the number of sensitivity coefficients is restricted if there are not sufficient parallel processors are put into used. Therefore, the Contribution-Linked eigenvalue sensitivity/Uncertainty estimation via Tracklength importance CHaracterization (CLUTCH) method (Perfetti and Rearden, 2013) which requires a small and manageable memory, is implemented in RMC in this work. Two algorithms based on the CLUTCH method, namely, the collision-event-based algorithm (C-CLUTCH) which is previously implemented in SCALE and the fission-event-based algorithm (F-CLUTCH) which is put forward in this work, are investigated in terms of, accuracy, computational efficiency and memory requirements. Additionally, the fission matrix method (Carney et al., 2014) is proposed to generate the adjoint fission source distributions for the CLUTCH method.

2. Theory

2.1. Linear perturbation theory

The eigenvalue sensitivity coefficients are calculated using the linear perturbation theory (Rearden, 2004), from which the differential change in effective multiplication factor causing by a differential change in nuclear data can be expressed as

$$dk = \frac{\langle \Psi^* dM\Psi\rangle - \langle k\Psi^* dA\Psi\rangle}{\langle \frac{1}{k}\Psi^* M\Psi\rangle}, \tag{1}$$

where

k is the effective multiplication factor,
Ψ is the neutron flux,
Ψ^* is the adjoint neutron flux,
$A\Psi = \Omega\cdot\nabla\Psi(r,\Omega,E) + \sum_t(r,E)\Psi(r,\Omega,E) - \int_0^\infty\int_{4\pi}\sum_s(r,\Omega'\to\Omega, E'\to E)\Psi(r,\Omega',E')d\Omega' dE'$ is the transport-collision term in the Boltzmann equation,
$M\Psi = \frac{\chi(r,E)}{4\pi}\int_0^\infty\int_0^{4\pi}\bar{\nu}\sum_f(r,E')\Psi(r,\Omega',E')d\Omega' dE'$ is the fission production term in the Boltzmann equation,
r is some position, and
E is some energy range.

The relationship of $A\Psi$ and $M\Psi$ is,

$$A\Psi = \frac{1}{k}M\Psi, \tag{2}$$

which is the Boltzmann equation.

The eigenvalue sensitivity coefficient to some nuclear data $x(r,E)$ (it could be a cross section, nubar, fission energy transfer function, etc.), $S_{k,x(r,E)}$ is defined as

$$S_{k,x(r,E)} = \frac{x(r,E)}{k}\frac{dk}{dx(r,E)}, \tag{3}$$

Substituting Eq. (1) into Eq. (3), sensitivity coefficients can be expressed as

$$S_{k,x(r,E)} = \frac{\left\langle \Psi^*\frac{1}{k}\frac{x\partial M}{\partial x}\Psi\right\rangle - \left\langle \Psi^*\frac{x\partial A}{\partial x}\Psi\right\rangle}{\left\langle \Psi^*\frac{1}{k}M\Psi\right\rangle}. \tag{4}$$

According to Eq. (4), determining sensitivity coefficients requires computing the adjoint-weighted fission production term in the denominator and three different terms in the numerator, i.e., the total interaction term, the scattering term, and the fission production term (Qiu et al., 2015).

The total interaction term in the numerator can be expressed as

$$N_t(r,E) = \delta_{x,t}\int_0^{4\pi}\Psi^*(r,\Omega,E)\Sigma_x(r,E)\Psi(r,\Omega,E)d\Omega, \tag{5}$$

where $\delta_{x,t}$ = one if x is a cross section and zero otherwise.

The scattering term in the numerator can be expressed as

$$N_s(r,E'\to E) = \delta_{x,s}\int_0^{4\pi}\int_0^{4\pi}\Psi^*(r,\Omega,E)\Sigma_s(r,\Omega'\to\Omega,E'\to E) \times\Psi(r,\Omega',E')d\Omega' d\Omega, \tag{6}$$

where $\delta_{x,s}$ = one if x is a scattering cross section and zero otherwise.

The fission production term in the numerator can be expressed as

$$N_f(r,E'\to E) = \delta_{xf}\int_0^{4\pi}\frac{1}{k}\frac{\chi(r,E)}{4\pi}\Psi^*(r,\Omega,E)d\Omega \times\int_0^{4\pi}\bar{\nu}\Sigma_f(r,E')\Psi(r,\Omega',E')d\Omega', \tag{7}$$

where $\delta_{x,f}$ = one if x is a fission cross section, nubar or a fission energy transfer function and zero otherwise.

The adjoint-weighted fission production term in the denominator can be expressed as

$$\left\langle \Psi^*\frac{1}{k}M\Psi\right\rangle = \int_0^\infty\int_v\int_{4\pi}\Psi^*(r,\Omega,E)\frac{1}{k}\frac{\chi(r,E)}{4\pi} \times\int_0^\infty\int_0^{4\pi}\bar{\nu}\sum_f(r,E')\Psi(r,\Omega',E')d\Omega' dE' d\Omega dV dE. \tag{8}$$

As can be seen from Eqs. (5)–(8), the key to calculate sensitivity coefficients is to obtain adjoint flux or adjoint-weighted reactions in the form of inner product $\Sigma_x\Psi^*\Psi$. Different from the multi-group TSUNAMI-3D method (Rearden, 2004), methods developed for the continuous-energy Monte Carlo codes compute eigenvalue sensitivity coefficients within a single forward transport calculation. One of these method is the IFP method, which calculates the adjoint weighting function by counting the expected fission neutrons produced in some future time after a neutron is introduced into the system (Kiedrowski and Brown, 2013). Though accurate, it faces the challenge of huge memory consumption. To reduce memory requirements, the CLUTCH method is developed by Perfetti (2012). The concept of the CLUTCH method is similar to the Contribution method (Williams, 1977).

2.2. Contributon method

Assume that there is a neutron source, S, which is equal to the fission source of a system

$$S = \frac{1}{k}M\Psi. \tag{9}$$

Multiplying Eq. (9) by adjoint flux Ψ^* and integrating over all phase space yields

$$\langle\Psi^* S\rangle = \left\langle \Psi^*\frac{1}{k}M\Psi\right\rangle. \tag{10}$$

Assume there is a neutron originating at phase space P_0 and its strength is S_0, then this neutron source can be expressed as

$$S = S_0\delta(P - P_0). \tag{11}$$

Substituting Eq. (11) into Eq. (10) produces an expression for the adjoint function at phase space P_0,