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Code development for eigenvalue total sensitivity analysis and total uncertainty analysis

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ABSTRACT

The uncertainties of multigroup cross sections notably impact eigenvalue of neutron-transport equation. We report on a total sensitivity analysis and total uncertainty analysis code named UNICORN that has been developed by applying the direct numerical perturbation method and statistical sampling method. In order to consider the contributions of various basic cross sections and the implicit effects which are indirect results of multigroup cross sections through resonance self-shielding calculation, an improved multigroup cross-section perturbation model is developed. The DRAGON 4.0 code, with application of WIMSD-4 format library, is used by UNICORN to carry out the resonance self-shielding and neutron-transport calculations. In addition, the bootstrap technique has been applied to the statistical sampling method in UNICORN to obtain much steadier and more reliable uncertainty results. The UNICORN code has been verified against TSUNAMI-1D by analyzing the case of TMI-1 pin-cell. The numerical results show that the total uncertainty of eigenvalue caused by cross sections can reach up to be about 0.72%. Therefore the contributions of the basic cross sections and their implicit effects are not negligible.

1. Introduction

In recent years, there has been an increasing demand for best estimate predictions to be provided with their confidence bounds in many domains, including nuclear research, industry, safety and regulation (Ivanov et al., 2013). Uncertainty analysis is a proper way to determine the appropriate design margins. The neutronics calculations are prerequisite for the predictions of reactor system, and the uncertainties introduced by neutronics calculations would be propagated to the subsequent calculations, such as thermal/hydraulics, neutron kinetics and safety analysis. Therefore, uncertainty analysis for neutronics calculations is the basic analysis in reactor design. Recently, the imprecision of cross sections, which would introduce uncertainties to responses of neutronics calculations, has been treated as one of the most significant sources of uncertainty (Pusa, 2012). According to the previous researches, the relative standard deviations of the eigenvalue caused by cross-section uncertainties are significant and non-ignorable (Wieselquist et al., 2012; Yankov et al., 2012). In this context, it's necessary to perform uncertainty analysis for neutronics calculations to obtain much more confident and appropriate safety margins introduced by cross-section uncertainties.

In order to perform the uncertainty propagations from nuclear cross sections to the responses of neutronics calculations, two categories of methodologies have been widely applied: the deterministic method and the statistical sampling method. For the deterministic method, sensitivity analysis is implemented firstly to obtain the sensitivity coefficients of responses with respect to cross sections. Perturbation theory (PT) (Weisbin et al., 1976; Pusa, 2012) and direct numerical perturbation (DNP) (Rearden, 2009) method are widely used to perform the sensitivity analysis. After the sensitivity coefficients are obtained, uncertainties of responses can be calculated by applying the "sandwich rule" (Rearden et al., 2009) combining sensitivity coefficients with corresponding covariance matrix of the cross sections. For the statistical sampling method, samples of cross sections are generated from their distributions regions firstly. The cross-section samples are then used as input parameters to carry out the neutronics calculations to obtain the responses of interest with respect to corresponding cross-section samples. Finally, the statistical calculation is applied to calculate the uncertainties of responses.

There are two important problems which should be considered when performing sensitivity and uncertainty analysis for responses with respect to cross sections. Firstly, in neutronics

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calculations, only the integral cross sections, such as the total cross section σ_t and scattering cross section σ_s are required, while the basic cross sections like $\sigma_{(n,\text{elas})}$, $\sigma_{(n,2n)}$, $\sigma_{(n,\gamma)}$ and so forth are not directly used. However, the uncertainties of these basic cross sections can also cause uncertainties to the responses. Therefore, the analysis should be performed not only to the integral cross sections, including σ_t, σ_s and σ_a, but also to the basic cross sections, including $\sigma_{(n,\text{elas})}$, $\sigma_{(n,\text{inel})}$, $\sigma_{(n,2n)}$, $\sigma_{(n,3n)}$, $\sigma_{(n,f)}$, $\sigma_{(n,\gamma)}$, $\sigma_{(n,p)}$, $\sigma_{(n,D)}$, $\sigma_{(n,T)}$, $\sigma_{(n,\text{He})}$, $\sigma_{(n,\alpha)}$ and ν.

Secondly, the effects of cross sections on the responses can be divided into two parts: the explicit portion and the implicit portion. This phenomenon is due to the fact that in deterministic method for neutronics calculation, both resonance self-shielding and neutron-transport calculations are required. The explicit portion is defined as the direct contributions of effective self-shielding cross sections on the responses through neutron-transport calculation. The implicit portions are the contributions of cross sections on responses through resonance self-shielding calculation. And the total effect is defined as summation of the explicit portion and implicit portion. It has been observed that the implicit portions are important and non-ignorable (Rearden et al., 2005). There are two categories of methodologies having been applied to consider the implicit portions. The first one focuses on resonance self-shielding calculation model, such as works done by Liu et al. (2015), Rearden et al. (2009), Foad and Takeda (2015) and Dion and Marleau (2013). The other one focuses on the multigroup cross-section library and cross-section perturbation models have been established, such as works done by Ball et al. (2013) and Kinoshita et al. (2014).

In order to consider the two aspects of works above, a new code named UNICORN, performing the total sensitivity analysis and total uncertainty analysis for eigenvalue with respect to cross sections, has been developed in this paper. To consider the implicit effects of cross sections to eigenvalue, the method applied in the UNICORN code is chosen focusing on the multigroup cross-section library. This method has the advantage of convenient practice and a multigroup cross-section perturbation model is required. Ball et al. (2013) has proposed a multigroup cross-section perturbation model, with which total sensitivity analysis can be performed for eigenvalue to the cross sections stored in the WIMSD-4 format library. However, total sensitivity analysis to various basic cross sections which are important to sensitivity and uncertainty analysis, are beyond the capability of this model. Therefore, the improvements, including the perturbation propagations and consistency rules for various basic cross sections, have been accomplished to the multigroup cross-section perturbation model. With the improved cross-section perturbation model, the UNICORN code has the capability of performing total sensitivity analysis and total uncertainty analysis for the eigenvalue with respect to all types of integral and basic cross sections mentioned above. Moreover, some conclusions about detailed origins of the implicit effects, which haven't been published before, are laid out in this work from the neutron physics point of view.

The statistical sampling method and DNP method have been chosen and accomplished in the UNICORN code to perform sensitivity and uncertainty analysis. For uncertainty analysis, the statistical sampling method has the obvious advantages including convenience, no approximation and no limit to the number of responses, compared with the deterministic method. However, the sensitivity coefficients, which are essential elements for sensitivity analysis, can't be obtained by the statistical sampling method. However, the sensitivity coefficients are important and essential for similarity analysis (Rearden and Jessee, 2009), and cross-section adjustment (Broadhead et al., 2004). Therefore, in order to perform sensitivity analysis, the DNP method has been selected and accomplished in the UNICORN code. In the context, the desirable features of DNP method and statistical sampling method have been incorporated in the UNICORN code to perform total sensitivity analysis and total uncertainty analysis respectively. In addition, the lattice code DRAGON 4.0 (Marleau et al., 2014) is used to carry out the resonance self-shielding calculation and neutron-transport calculation with application of the WIMSD-4 format multigroup cross-section library.

An overview of the UNICORN code is given in Section 2. In sequences, Section 3–5 describe the multigroup cross-section perturbation model, statistical sampling method and direct numerical perturbation method, respectively. In Section 6, verification of the UNICORN code is given and the corresponding numerical results and analysis are presented.

2. Overview of the UNICORN code

In this paper, the UNICORN code has been developed to perform total sensitivity analysis and total uncertainty analysis for the eigenvalue of neutronics calculations with respect to the multigroup cross sections. The flowchart of the UNICORN code is shown in Fig. 1.

In the UNICORN code, the basic models include these three parts: the multigroup cross-section perturbation model (described in Section 3), the statistical sampling method (described in Section 4) and the direct numerical perturbation method (described in Section 5). The nuclear data which is necessary, including all types of integral and basic cross sections, are obtained by incorporating the WIMSD-4 format library and the output of NJOY (Macfarlane et al., 2012). Based on the nuclear data and basic models, the UNICORN code has the capability of detailed sensitivity and uncertainty analysis for various kinds of cross sections.

3. Multigroup cross-section perturbation model

In order to consider the basic cross sections and implicit effects mentioned above, the multigroup cross-section perturbation model proposed by Ball et al. (2013) has been improved in this paper. This section will describe the improved multigroup cross-section perturbation model in detail. This section consists of three parts: firstly, the generations of multigroup cross sections and resonance integrals from point-wise cross sections are introduced as the basic theory for the multigroup cross-section perturbation model; secondly, the perturbation propagations from the point-wise cross sections to the multigroup ones and resonance integrals are introduced; finally, the consistency rules between the integral and basic cross sections are explained.

3.1. Multigroup cross sections and resonance integrals

The cross sections in ENDF files should be processed to specific multigroup format, e.g. the WIMSD-4 format, before they can be utilized by the deterministic lattice code, such as DRAGON. The energy- and temperature-dependent point-wise cross sections are converted into specific multigroup format using weighting flux $\phi(E,\sigma_0)$ shown as the following formula:

$$\sigma_{x,g}(T,\sigma_0) = \frac{\int_{\Delta E_g} \sigma_x(E,T)\phi(E,\sigma_0)dE}{\int_{\Delta E_g} \phi(E,\sigma_0)dE} \tag{1}$$

where T, E and σ_0 represent the temperature, energy and background cross section respectively. And $\sigma_x(E,T)$ stands for the energy- and temperature-dependent point-wise cross sections. For the non-resonance cross sections, the weighting flux is the function of energy (formulated as $\phi(E)$), and for the cross sections with resonances, the weighting flux is relative to both energy and