Resonance Parameter Adjustment using Continuous-energy Monte Carlo Perturbation Calculation

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1. Introduction

Nowadays, Monte Carlo neutron transport calculation have been utilized in data assimilation field, nuclear data adjustment with integral experiments [1, 2]. The advantage of using Monte Carlo (MC) transport code in the data assimilation is that it has far less modeling and methodological bias as it treats the particle's energy, spatial, angular domain continuously with no discretization. It is an important asset in the data assimilation where the bias from the code can be accounted for the uncertainty of adjusted data. In addition to that, the straightforward methodology in handling the nuclear data helps to make a more robust adjustment framework whereas it should be carefully addressed in the deterministic counterpart, which is varied from code to code.

Recently, the resonance parameter adjustment with Monte Carlo code has been studied to propose a new general adjustment framework [1]. Considering that the resonance parameter in Evaluated Nuclear Data File (ENDF) is one of the most basic data for cross section representation, it is expected that it can be a fundamental approach for nuclear data adjustment. A bottleneck mentioned in the previous study is that they adopted the direct subtraction method for sensitivity calculation. The direct subtraction requires one independent MC transport calculation for each sensitivity evaluation, so it becomes impractically time-consuming when there are hundreds of resonance parameters to adjust. Fortunately, much more efficient sensitivity evaluation is now available with the help of the MC perturbation technique [3-5], one of the recent advancements in modern MC transport codes. The multiple sensitivities can be obtained at once in a single MC calculation with the perturbation method. Moreover, the evaluation of sensitivity to resonance parameter by MC perturbation calculation has been already presented [6], which was originally developed for MC continuous-energy sensitivity and uncertainty analysis.

In this study, a preliminary study for resonance parameter adjustment using MC perturbation calculation has been conducted. One major difference from the previous study is that Monte Carlo perturbation technique is utilized for more efficient sensitivity evaluation, thus more extended adjustment is available. The developed feature is implemented in McCARD [7], a Monte Carlo code developed in Seoul National University.

2. Methods

2.1 Asymptotic Generalized Linear Least-Squares

For the adjustment, Asymptotic Generalized Linear Least-Squares (AGLLS) methodology equation [1] is adopted as follows,

$$X_{i+1} = X_i + M_0 G_i^T (G_i M_0 G_i^T)^{-1}(E - C_i), \quad (1)$$

where X_i is the resonance parameters to adjust, G_i is the sensitivity coefficient of *k* eigenvalue to the resonance parameter, and M_0 is the covariance matrix of X_0. The components of vector E and C_i are eigenvalues from experiments and calculations, respectively. The index *i* refers the iteration number.

2.2 Calculation of sensitivity to Resonance Parameter by MC perturbation

The calculation method for resonance parameter sensitivity by MC perturbation theory [6] is briefly described in this section. The *k* eigenvalue sensitivity to resonance parameter can be expressed as follows,

$$\frac{\partial k_i}{\partial \Gamma_i^{j,m}} = \sum_r \int \frac{\partial \sigma_i^{j,r}\left(E \middle| \boldsymbol{\Gamma}_i^j\right)}{\partial \Gamma_i^{j,m}} \frac{\partial k_i}{\partial \sigma_i^{j,r}\left(E\right)} dE, \quad (2)$$

where k_i denotes a *k* eigenvalue at adjustment iteration *i*. $\boldsymbol{\Gamma}_i^j$ is a vector whose elements are the resonance parameters of nuclide *j* at adjustment iteration *i*, and $\Gamma_i^{j,m}$ is *m*-th element of the vector. Note that $\boldsymbol{\Gamma}_i^j$ is a subset of X_i. $\sigma_i^{j,r}(E)$ is a point-energy cross section of nuclide *j* and reaction *r* at energy *E* in *i*-th adjustment iteration. The sensitivity coefficient, the element of G_i, is defined as $(\partial k_i / k) / (\partial \Gamma_i^{j,m} / \Gamma_i^{j,m})$.

Eq. (2) can be seen as a integration of *k* sensitivity to cross section, $\partial k_i / \partial \sigma_i^{j,r}\left(E\right)$, with a weighting function called cross section sensitivity to resonance parameter, $\partial \sigma_i^{j,r}\left(E \middle| \boldsymbol{\Gamma}_i^j\right) / \partial \Gamma_i^{j,m}$. Considering that the conventional MC perturbation theory have already calculated the *k* sensitivity to cross section, the only

thing one should do to calculate Eq. (2) is just multiplying the weighting function to k sensitivity to cross section during the perturbation calculation. The cross section sensitivity to resonance parameter, $\partial\sigma_i^{j,r}\left(E\middle|\boldsymbol{\Gamma}_i^j\right)/\partial\Gamma_i^{j,m}$, can be obtained by direct subraction as follows,

$$\frac{\partial\sigma_i^{j,r}(E)}{\partial\Gamma_m^i}=\frac{\sigma_i^{j,r}\left(E|\ldots,\Gamma_i^{j,m}+\Delta\Gamma_i^{j,m},\ldots\right)-\sigma_i^{j,r}\left(E|\ldots,\Gamma_m^i,\ldots\right)}{\Delta\Gamma_m^i} \tag{3}$$

where $\Delta\Gamma_m^i$ is set to 0.0001 Γ_m^i in this study. To obtain the perturbed crosss section in Eq. (3), a single resonance parameter in ENDF is pertubed, then nuclear data processing code NJOY [8] generates a perturbed ACE-formated cross section file from the perturbed ENDF.

It should be noted that MC code can not hold the whole perturbed ACE-formatted cross section files, because a memory issue can be raised if there are thousands of resonance parameters to adjust. Fortunately, most cross section deviation by perturbation of resonance parameter is observed near the resonance energy, so the file size of the sensitivity coefficient can be reduced by linearization. For example, the sensitivity coefficient file for the gamma width at 6.674 eV of ENDF/B-VIII.0 can be linearized to a 200 KB file if 0.1% tolerance is applied while the whole ACE formatted-file requires 130 MB

3. Numerical Results

3.1 Integral Experiments and Resonance Parameters for Adjustment

Three ICSBEP (International Criticality Safety Benchmark Evaluation Project) [9] problems, LEU-SOL-THERM-001, LEU-SOL-THERM-002-001, LEU-SOL-THERM-002-002, are selected as integral experiments for adjusting the resolved resonance parameters of U-235 and U-238. It is reported [1] that strong sensitivities are observed in those three problems for the resolved resonance parameters of U-235 and U-238. The k_{eff} of the calculated (C_0) and experimental (E) values for the target integral experiments are given in Table I. The calculated values are obtained using unadjusted ENDF/B-VIII.0 by McCARD. The standard deviations of all k_{eff} values in the table are less than 40 pcm.

Table I: k_{eff} of the integral experiments

Experiment	C_0	E
LEU-SOL-THERM-001	1.0122	0.9991
LEU-SOL-THERM-002-001	0.9996	1.0038
LEU-SOL-THERM-003-001	0.9970	0.9997

The resonance parameters to adjust are 4 resonance widths (Γ_n, Γ_γ, Γ_{fA}, Γ_{fB}) of 100 resonance energies for U-235, and 2 resonance widths (Γ_n, Γ_γ) of 100 resonance energies for U-238, 600 parameters in total, in ENDF/B-VIII.0 [10] library.

3.2 Sensitivity Coefficients to Resonance Parameters

The sensitivity coefficients to resonance parameters are evaluated for the three benchmark problems by MC perturbation calculation. The MC perturbation calculation is performed by McCARD with 100 active cycles of 50,000 neutrons each.

Fig. 1 and Fig. 2 show some examples for the calculated sensitivity coefficients to resonance parameters, fission widths of U-235 and neutron widths of U-238 from unadjusted ENDF/B-VIII.0, respectively. It is observed that resonance parameters in negative energy range, determining 1/v dependence of the low-energy cross section, are sensitive to k_{eff} estimation of the target benchmark problems.

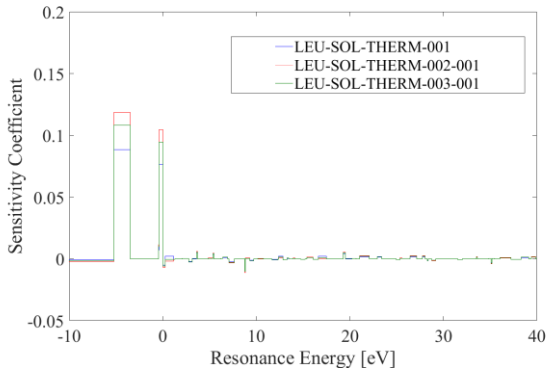

Fig. 1. Sensitivity coefficient of k_{eff} to fission width of U-235 from unadjusted ENDF/B-VIII.0

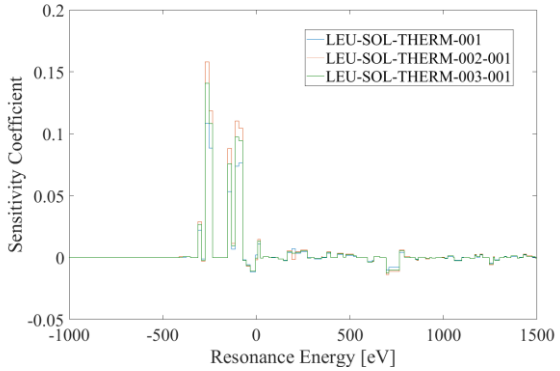

Fig. 2. Sensitivity coefficient of k_{eff} to neutron width of U-238 from unadjusted ENDF/B-VIII.0

3.2 Adjustment of Resonance Parameter

The resonance parameters of U-235 and U-238 from ENDF/B-VIII.0 are adjusted by GLLS method, the first iteration of AGLLS. Fig.3 and Fig. 4 show the ratio of adjusted U-235 fission cross section and U-238 capture cross section to unadjusted data, respectively.

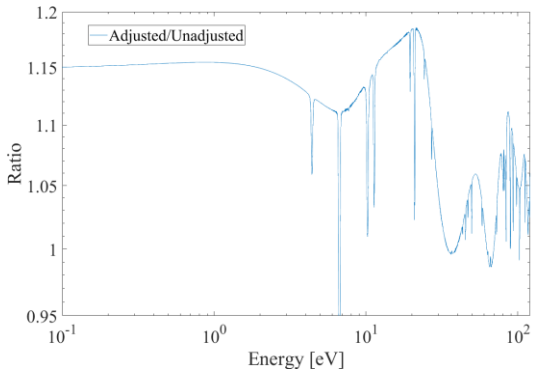

Fig. 4. Ratio of U-238 capture cross section after adjustment

The numerical results for k_{eff} estimation with adjusted data are given in Table II. C_1 in the table denotes calculated value with one adjustment iteration. χ^2 is arithmetic mean of $[C-E/\Delta E]^2$. In the three problems, χ^2 is reduced from 7.15 to 0.63 after the adjustment. It is reported in the previous study that χ^2 can be reduced to zero when more iterations are introduced, but it hasn't been conducted in this study yet.

Experiment	C_0/E	C_1/E
LEU-SOL-THERM-001	1.0119	1.0003
LEU-SOL-THERM-002-001	0.9994	0.9985
LEU-SOL-THERM-003-001	0.9963	0.9996
χ^2	7.15	0.63

3. Conclusions

The resonance parameter adjustment using Monte Carlo perturbation calculation is conducted in this study. Three ICSBEP problems are selected for integral experiments, then 600 resonance parameters in U-235 and U-238 from ENDF/B-VIII.0 are adjusted. After the adjustment, it shows reduction of χ^2 in the three problems, that is the adjustment works well. It is just preliminary study for resonance parameter adjustment, so the adjusted parameter itself is not that meaningful, but one advance in this study is that it shows the feasibility of using MC perturbation calculation in resonance parameter adjustment. Further studies about iterative adjustment using AGLLS, more extended adjustment including other integral experiments, and evaluating the adjusted parameters will be conducted and presented in the conference.

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