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Variance Reduction Factor of Nuclear Data for Integral Neutronics Parameters

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We propose a new quantity, a variance reduction factor, to identify nuclear data for which further improvements are required to reduce uncertainties of target integral neutronics parameters. Important energy ranges can be also identified with this variance reduction factor. Variance reduction factors are calculated for several integral neutronics parameters. The usefulness of the variance reduction factors is demonstrated.

I. INTRODUCTION

Nuclear data uncertainty is becoming a dominant component of uncertainty in fission reactor integral neutronics parameters since accurate and precise numerical simulations for particle transport and fission chain reactions are being realized nowadays. Even though the quality of evaluated nuclear data files also has been significantly improved, their accuracy is not yet sufficient in some fields of nuclear engineering application, such as reactor core designs of advanced and future nuclear systems [1, 2].

When a 'target' reactor core design is provided, one would quantify nuclear data-induced uncertainties of integral parameters of this design. If the estimated uncertainties are larger than the target accuracy, further efforts should be made. One reasonable and well-known approach is to utilize measurement data of integral neutronics parameters obtained (or planned to be obtained) at mock-up nuclear facilities. This approach was initially proposed by Usachev *et al.* [3], and it has been applied by Palmiotti and Salvatores [4].

If reduced uncertainties do not satisfy the target even when integral measurement data are effectively utilized, one would attempt to know which nuclear data should be further improved. Lately, the Oak Ridge group has proposed the inverse sensitivity/uncertainty quantification (IS/UQ) method to quantify the required accuracy for the nuclear data to achieve the target accuracy of the integral parameters [5]. In this method, variance reduction required to achieve the target accuracy are uniquely determined by the optimization process assuming cost functions for all the nuclear data, which quantify how much the microscopic nuclear data improvement costs.

Although the IS/UQ method is quite a beneficial tool to know the target accuracy of the microscopic nuclear data, there is one defect; it assumes that correlations between nuclear data are invariant. It is natural to consider that covariance matrices including correlations are altered when new measurement data are obtained, so the assumption of invariant correlations would be unrealistic.

In the present paper, we propose a new quantity to identify which nuclear data should be further improved to reduce the variance of the target integral parameters. With the proposed quantity we cannot quantify the target accuracy for the microscopic nuclear data like the IS/UQ method, but this quantity properly considers correlations between the nuclear data. Thus, the proposed method would be complementary to the IS/UQ method.

II. THEORY

Here, let us consider a nuclear data vector $\mathbf{T}$ and its covariance matrix $\mathbf{M}$. In the cross section adjustment procedure with integral measurement data [6],one considers several dozens/hundreds of integral data and prepares numerically-predicted values for these integral data using $\mathbf{T}$. Through the cross section adjustment, we get a posterior nuclear data vector $\mathbf{T}'$ and its covariance matrix $\mathbf{M}'$ which is given as

$$\mathbf{M}' = \mathbf{M} - \mathbf{M}\mathbf{G}^{\mathrm{T}} \left[\mathbf{G}\mathbf{M}\mathbf{G}^{\mathrm{T}} + \mathbf{V}_e + \mathbf{V}_m\right]^{-1} \mathbf{G}\mathbf{M}, \tag{1}$$

where $\mathbf{G}$ is the sensitivity matrix of integral data with respect to $\mathbf{T}$, and the matrices $\mathbf{V}_e$ and $\mathbf{V}_m$ are covariance matrices of integral measurement data and the numerically-predicted values, respectively. The uncertainty considered in $\mathbf{V}_m$ comes only from uncertainties due to employed numerical methods: statistical uncertainties in Monte Carlo calculations, for example.

Next, let us suppose that new experimental data for the kth microscopic nuclear data with measurement uncertainty (variance) V_k is obtained, and $\mathbf{T}$ is adjusted with

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this new data. In this case, $\mathbf{V}_m$ is zero since the integral parameter is the microscopic nuclear data itself, and the sensitivity matrix $\mathbf{G}$ becomes a vector $\mathbf{e}_k$ in which the kth entry is unity and others are zero. Thus, the posterior covariance matrix $\mathbf{M}^{(k)}$ for the adjusted nuclear data $\mathbf{T}^{(k)}$ is written as follows:

$$\mathbf{M}^{(k)} = \mathbf{M} - \mathbf{M}_{*k}\left[M_{kk} + V_k\right]^{-1}\mathbf{M}_{k*} = \mathbf{M} - \bar{\mathbf{M}}^{(k)}. \tag{2}$$

Here, we express the uncertainty of the new measurement V_k as

$$V_k = \alpha M_{kk}. \tag{3}$$

If the measurement is done with the same degree of uncertainty as the prior cross section uncertainty, α is unity. Using Eq. (3), the entry of $\bar{\mathbf{M}}^{(k)}$ can be written as

$$\begin{aligned}\bar{M}_{ij}^{(k)} &= \frac{M_{ik}M_{kj}}{M_{kk}+V_k} = \frac{C_{ik}C_{kj}\sigma_i\sigma_j M_{kk}}{(1+\alpha)M_{kk}} \\ &= \frac{C_{ik}C_{kj}\sigma_i\sigma_j}{1+\alpha} = \frac{\hat{M}_{ij}^{(k)}}{1+\alpha},\end{aligned} \tag{4}$$

where σ_i is the standard deviation of T_i and C_{ik} is the correlation between T_i and T_k. Using this equation, it is easily shown that the correlation matrix for $\boldsymbol{T}^{(k)}$ is not identical to that for $\boldsymbol{T}$.

Next, let us consider how much uncertainty of an integral parameter is reduced when we use the adjusted cross section set $\mathbf{T}^{(k)}$, *i.e.*, when we obtain new measurement data for the kth nuclear data. If we write a sensitivity vector of the target integral parameter as $\mathbf{G}_t$, variances of the integral parameter obtained using $\mathbf{T}$ and $\mathbf{T}^{(k)}$ can be written as $\mathbf{G}_t\mathbf{M}\mathbf{G}_t^{\mathrm{T}}$ and $\mathbf{G}_t\mathbf{M}^{(k)}\mathbf{G}_t^{\mathrm{T}}$, respectively. Thus, the variance reduction of the target integral parameter ΔV_t is written as

$$\begin{aligned}\Delta V_t &= \mathbf{G}_t\left(\mathbf{M} - \mathbf{M}^{(k)}\right)\mathbf{G}_t^{\mathrm{T}} = \mathbf{G}_t\bar{\mathbf{M}}^{(k)}\mathbf{G}_t^{\mathrm{T}} \\ &= \frac{1}{1+\alpha}\mathbf{G}_t\hat{\mathbf{M}}^{(k)}\mathbf{G}_t^{\mathrm{T}}.\end{aligned} \tag{5}$$

In the present paper, we define a *variance reduction factor* (VRF) of the kth nuclear data, f_k, as

$$f_k = \frac{\mathbf{G}_t\hat{\mathbf{M}}^k\mathbf{G}_t^{\mathrm{T}}}{\mathbf{G}_t\mathbf{M}\mathbf{G}_t^{\mathrm{T}}}. \tag{6}$$

With this VRF, we can know which nuclear data require further accuracy improvement in order to reduce the variance of the target integral parameter. It should be also emphasized that calculations of the proposed VRFs are quite easy; one needs sensitivity profiles for target neutronics parameters and covariance matrices of nuclear data. The proposed method can provide us useful information on microscopic nuclear data measurements.

If correlations among different cross sections are ignored in the adjustment process, $\hat{M}_{ij}^{(k)}$ is written as $\hat{M}_{ij}^{(k)} = M_{kk}\delta_{ik}\delta_{jk}$, where δ is Kronecker's delta, and the numerator of the VRF is written as $\mathbf{G}_t\hat{\mathbf{M}}^k\mathbf{G}_t^T = M_{kk}\left(G_{t,k}\right)^2$, where $G_{t,k}$ is the kth entry of $\mathbf{G}_t$.

It should be noted that a similar method for determining the contribution of each nuclear data to target integral parameters has been already proposed by Muir [7]. The basis of the theories of Muir's method and ours is almost identical except for the uncertainty treatment for new measurement. In Muir's method, the new measurement is done in an ideal condition and measurement uncertainty is assumed to be zero while in our method the measurement uncertainty is expressed by Eq. (3). It should be emphasized that the present study presents rich numerical examples in the following section to show performance of our method, whereas Muir's study has not shown any application results of his method.

III. RESULTS AND ANALYSES

In order to demonstrate the performance of our method, we calculate VRFs for several integral parameters. Some of them are measurement data obtained in previous critical experiments. In the actual application, such existing integral data would be used for the cross section adjustment,and then our method is used with the covariance data of the adjusted nuclear data for integral parameter of a target reactor core design such as an innovative fast reactor or an accelerator-driven subcritical system. In future study, we will apply the proposed method into such future nuclear systems.

A. Numerical Procedure

All the sensitivities of integral neutronics parameters to nuclear data are calculated with a general-purpose reactor physics calculation code system CBZ [8], which is being developed at Hokkaido university. Sensitivities of criticality and reactivity worth are calculated with the classical perturbation theory, and those of burnup-related integral parameters (nuclide number densities after burnup) are calculated with the generalized perturbation theory. Forward and (generalized) adjoint neutron fluxes are obtained from neutron transport calculations with the discrete ordinates method or the collision probability method. 70-group and 107-group energy-averaged cross sections based on JENDL-4.0 [9] are used for fast neutron systems and thermal neutron systems respectively. The covariance data given in JENDL-4.0 are also processed to those in a multi-group form. Note that correlations between different nuclides are ignored in the present study. Inter-energy and inter-reaction correlations are taken into account.