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Inverse Sensitivity/Uncertainty Methods Development for Nuclear Fuel Cycle Applications

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The Standardized Computer Analyses for Licensing Evaluation (SCALE) software package developed at the Oak Ridge National Laboratory includes codes that propagate uncertainties available in the nuclear data libraries to compute uncertainties in nuclear application performance parameters. We report on our recent efforts to extend this capability to develop an *inverse* sensitivity/uncertainty (IS/U) methodology that identifies the improvements in nuclear data that are needed to compute application responses within prescribed tolerances, while minimizing the cost of such data improvements. We report on our progress to date and present a simple test case for our method. Our methodology is directly applicable to thermal and intermediate neutron energy systems because it addresses the implicit neutron resonance self-shielding effects that are essential to accurate modeling of thermal and intermediate systems. This methodology is likely to increase the efficiency of nuclear data efforts.

I. INTRODUCTION

Measurements of nuclear cross sections incur operating costs of facilities, scientific and support personnel, target preparation, detectors, data analysis, and evaluation, and can add up to more than $400,000/measurement. Therefore, there is a need to minimize the overall cost of the nuclear data program by suggesting an optimal sequence of nuclear data measurements, sorted by their respective quantified impact on a nuclear application of interest. The prioritization of measurements ought to be specified in terms of nuclides, the nuclear reactions to be measured, and the required accuracy of the measurements. The prioritization ought to take into account evaluated nuclear databases, both of differential and integral benchmark data, to leverage the vast prior investment into nuclear data.

IS/U analysis has been used previously to project required nuclear differential data needs to meet target accuracies on fast reactor performance parameters such as criticality, reaction rates, and depletion metrics [1]. However the earlier work has focused exclusively on future fast reactor designs rather than the current light water reactor (LWR) fleet. Thermal reactors such as LWR's have very different neutron physics characteristics from fast reactors. For example, fast reactors are mainly sensitive to nuclear data above 50,000 eV where cross sections tend to have smoother variations, while LWR behavior is sensitive to reaction cross sections in the resolved resonance range ($\sim$1 eV to 20 keV) of actinide materials, as well as moderator thermal scattering kernels below $\sim$1 eV. In the low- to intermediate-energy range ($\sim$1 keV to 1-2 MeV region), the resonance self-shielding effects are important to model the neutron slowing down through the resonance region. Therefore we use problem-dependent self-shielding calculations to obtain a robust solution to the neutron slowing down equation and provide self-shielded cross sections for the forward and adjoint transport calculations that are used in the IS/U calculations. Consequently, the proposed IS/U method will be uniquely applicable to thermal, intermediate, and fast reactor systems, including fast reactor core analyses and various aspects of the fuel cycle such as spent nuclear fuel (SNF) reprocessing, transportation, storage, and waste disposal. These various applications can have neutron sensitivities that span the thermal, intermediate, and fast neutron energy regions. One of the long-term goals for our IS/U methodology is to include the capability to determine required accuracies in input data other than differential nuclear data. For example, what tolerances should be imposed on design parameters such as dimensions, material impurities, etc., has not been considered in previous IS/U methods.

II. FORMALISM AND IMPLEMENTATION

In this section, we define a cost function that is to be minimized, and constraints that are to be satisfied. All expressions are to the first-order perturbation approximation that we assume to be reasonably accurate on the

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scale of the uncertainties in nuclear data. This first-order expansion is also consistent with the approximation that is used in the SCALE module TSURFER that we use to implement the IS/U. Nevertheless, we are aware of the well known potential problems and limitations associated with first-order analytical approaches, such as Peelle's Pertinent Puzzle (PPP) effect and potential biases due to ignored non-linear terms. The formalism is at first presented without using integral benchmark experiments, but these are incorporated later in Sect. II B.

We seek to minimize the cost of improved uncertainties contained in an improved covariance that is denoted by $\mathbf{C}'$ to distinguish it from the extant covariance matrix $\mathbf{C}$,

$$\min(\mathrm{cost}[\mathbf{C}']), \tag{1}$$

where the cost can be defined as the sum of inverse of the diagonal elements of $\mathbf{C}'$

$$\mathrm{cost}[\mathbf{C}'] = \sum_i \frac{\lambda_i}{C'_{ii}}, \tag{2}$$

where λ_i's are cost coefficients that reflect varying cost of materials, cross sections, etc. This is a fairly generic cost definition that can nevertheless be used as a guide in the sorting and prioritizing of data improvements, and it is equivalent to the cost function that has been used in the past [1]. This cost minimization is to be constrained by maximum allowed tolerances $\delta_{\mathbf{R}}$ of responses $\mathbf{R}$ of applications

$$\mathrm{diag}\left[\mathbf{S}\mathbf{C}'\mathbf{S}^T\right] \leq (\delta\mathbf{R})^2, \tag{3}$$

where $\mathbf{S}$ is a (relative) sensitivity matrix of response vector $\mathbf{R}$ with respect to a group-wise differential cross section σ_i

$$S_{ji} \equiv \frac{\sigma_i}{R_j}\frac{\partial R_j}{\partial \sigma_i}, \tag{4}$$

which is computed by the TSUNAMI module of the SCALE code. We set up this minimization problem by defining variables x_i that relate the elements of the sought-after covariance matrix $\mathbf{C}'$ to those of the available covariance matrix $\mathbf{C}$ via

$$C'_{ij} \equiv x_i C_{ij} x_j. \tag{5}$$

A composite index i consists of the energy-group index, material index, and the cross section kind index. For the applications described in this work, the covariance matrix $\mathbf{C}$ is the SCALE's 44-group relative covariance matrix that is also conventionally used by the TSURFER module. The x_i's are coefficients that are to be varied until all constraints are satisfied at a minimum cost.

One notable advantage of this definition of the covariance matrix $\mathbf{C}'$ via coefficients x_i is that it enables an intuitive set of restrictions to its values. Namely, x_i could be restricted to be less than or equal to 1 because any value larger than 1 would correspond to data uncertainties that are greater than those already present in $\mathbf{C}$. (The cost associated with the maximum value of 1 can be set to zero because it corresponds to the uncertainty of the extant data that has already been measured and evaluated.) Furthermore, if we were to allow $x > 1$, this would necessitate some other coefficients in $\mathbf{x}$ to be smaller than they would have been otherwise, and this would unnecessarily incur additional cost given by Eq. (6). So for these reasons, the upper bound for x_i is set to 1. The lower bound for x_i is determined from a condition that diagonal elements of the covariance $C'_{ii} = x_i^2 C_{ii}$ can only be as small as the smallest uncertainties presently achievable for various cross sections, as prescribed in the ENDF [2], and listed in Table I. (Since

TABLE I. Minimum relative uncertainties used for various cross sections.

Reaction	MT	Minimum relative uncertainty
Total	1	1%
Elastic	2	2%
Inelastic	4	3%
Fission	18	0.7%
Capture	102	2%
Neutron yields	452-456	0.7%
All others	*	3%

in our minimization scheme these lower limits could be viewed as input parameters, they too could be varied to estimate the benefits of improved precision.) These limits (upper and lower) on x_i are intended to make the minimization problem more tractable numerically, since the search is performed over a relatively narrow range of values. When an extant C_{ii} corresponds to an uncertainty that is already smaller than a lower limit, then its corresponding coefficient x_i is excluded from the minimization scheme since the uncertainty is already as small as it can be expected. Setting these lower bounds prevents the minimization algorithm from suggesting uncertainties that could not be achieved. (Instead we hope to use integral benchmark experiments to help satisfy the constraints, as described in Sect. II B.) With the definition in Eq. (5), the cost in Eq. (6) could be written as

$$\mathrm{cost}[\mathbf{C}'] = \sum_i \frac{\lambda_i}{C_{ii}x_i^2}. \tag{6}$$

Since the cost is obviously minimized when x_i's are at their maximum value of 1, one could initiate the minimization by setting $x_i = 1$ for all i, and the minimization would lower some x_i's in order to satisfy the constraint in Eq. 3. Setting x_i's to other initial values could be used to ensure that the minimum does not depend on the initial values of x_i's.

Our formalism and the implementation adopt the convention that covariance matrices are in the relative format, i.e., square root of its diagonal is a relative uncertainty. This convention is also used in TSURFER. Using this approach enabled a seamless reuse of the codes.