Reprinted from JAI, Vol. 9, No. 3
doi:10.1520/JAI104115
Available online at www.astm.org/JAI

Roberto Capote,[1] *Donald L. Smith,*[2] *Andrej Trkov,*[3] *and Mehdi Meghzifene*[4]

A New Formulation of the Unified Monte Carlo Approach (UMC-B) and Cross-Section Evaluation for the Dosimetry Reaction ^{55}Mn(n,γ)^{56}Mn

ABSTRACT: Two relatively new approaches to neutron cross section data evaluation are described. They are known collectively as Unified Monte Carlo (versions UMC-G and UMC-B). Comparisons are made between these two methods, as well as with the well-known generalized least-squares (GLSQ) technique, through the use of simple, hypothetical (toy) examples. These new Monte Carlo methods are based on stochastic sampling of probability functions that are constructed with the use of theoretical and experimental data by applying the principle of maximum entropy. No further assumptions are involved in either UMC-G or UMC-B. However, the GLSQ procedure requires the linearization of non-linear terms, such as those that occur when cross section ratio data are included in an evaluation. It is shown that these two stochastic techniques yield results that agree well with each other, and with the GLSQ method, when linear data are involved, or when the perturbations due to data discrepancies and nonlinearity effects are small. Otherwise, there can be noticeable differences. The present investigation also demonstrates, as observed in earlier work, that the least-squares approach breaks

Manuscript received June 7, 2011; accepted for publication November 28, 2011; published online March 2012.

[1] NAPC-Nuclear Data Section, International Atomic Energy Agency, P.O. Box 100, Vienna International Centre, A-1400 Vienna, Austria (Corresponding author), e-mail: r.capotenoy@iaea.org
[2] Argonne National Laboratory, 1710 Avenida del Mundo, #1506, Coronado, CA 92118.
[3] Jozef Stefan Institute, 1000 Ljubljana, Slovenia.
[4] NAPC-Nuclear Data Section, International Atomic Energy Agency, P.O. Box 100, Vienna International Centre, A-1400 Vienna, Austria.

Cite as: Capote, R., Smith, D. L., Trkov, A. and Meghzifene, M., "A New Formulation of the Unified Monte Carlo Approach (UMC-B) and Cross-Section Evaluation for the Dosimetry Reaction ^{55}Mn(n,γ)^{56}Mn," *J. ASTM Intl.*, Vol. 9, No. 3. doi:10.1520/JAI104115.

down when these conditions are not satisfied. This paper also presents an actual evaluation of the ^{55}Mn(n,γ)^{56}Mn neutron dosimetry reaction cross section in the energy range from 100 keV to 20 MeV, which was performed using both GLSQ and UMC-G approaches.

KEYWORDS: evaluation methods, Unified Monte Carlo, generalized least-squares, nuclear data

Introduction

Accurate knowledge of the differential cross sections and their correlations and uncertainties for a diverse collection of neutron reactions, as a function of neutron energy, is essential for effective neutron spectrum adjustment applications in neutron dosimetry. The selection of these reactions and steady improvements in the knowledge of their cross sections and corresponding reduction of their uncertainties have been a work in progress for many years. Advances in nuclear models and the codes that implement them, along with growth in the content and improvement in the quality of the experimental cross-section databases, have enabled evaluators to produce evaluations that very likely approach the true cross section values within the limits of the assumed uncertainties. The use of theory allows threshold-reaction cross sections to be extrapolated reliably to energies near threshold for which the values are very small and experimental data are either lacking or unreliable. Also, theory can be used for interpolation elsewhere, particularly in certain neutron energy regions, such as between 10 and 14 MeV and above 14 MeV, where measurements are difficult and for which experimental data are sparse. However, nuclear models alone usually cannot provide adequate knowledge of the normalization of these cross sections, at least not with sufficient accuracy to satisfy the stringent requirements for neutron dosimetry applications. Also, fine features in the shapes of these cross sections as a function of energy generally cannot be reproduced sufficiently well using nuclear models. Therefore, experimental data are essential. The two approaches to nuclear data development—modeling and experimentation—clearly complement each other in many ways.

An important aspect of nuclear data evaluation is the application of objective methods to merge theoretical results (calculated using the nuclear models) and experimental information. Early evaluation methods based on qualitative comparisons of experimental and theoretical data were generally superseded in the late 1970s by more objective approaches based mainly on the least-squares concept [1]. When extensive experimental data are available to define the cross sections, the simple least-squares method can be applied. In other situations in which experimental data are somewhat sparse and reliance on theory is greater, the generalized least-squares method (GLSQ) is usually used. Both techniques are widely employed by data evaluators, but there are limitations to their applicability. One important limitation is that these two methodologies are essentially linear in nature. That is, the equations used to implement least-squares analyses are derived via the linearization of more complicated (and generally non-linear) expressions. Often this does not cause any problems in actual evaluations, but in certain circumstances the neglect of non-linear terms can lead to excessive

biases when high accuracy is sought. In particular, problems might be encountered when ratio data and data with large uncertainties or discrepant data are considered in the evaluation process.

With these limitations in mind, a new approach to nuclear reaction cross section data evaluation was suggested a few years ago by Smith [2]. It is generally referred to as the Unified Monte Carlo (UMC) method; in this paper it is denoted by UMC-G. This method involves constructing a multi-parameter joint probability density function using data generated from nuclear modeling, in addition to available experimental data. This probability distribution is then sampled stochastically to generate a Markov chain of statistically distributed random cross section values and other observable physical quantities that can be used subsequently to calculate mean values and covariances, i.e., the elements of a typical Evaluated Nuclear Data File (ENDF)-type evaluation [3]. This approach was first demonstrated by means of a very simple hypothetical example ("Toy Story 1") [2]. It was discovered quite early that this method yields results comparable to those of the established GLSQ under conditions consistent with the assumptions of this venerable approach. However, in addition it offers the opportunity to deal properly with evaluation situations that involve more complicated types of experimental data (e.g., ratios) that cannot be dealt with as rigorously when using GLSQ. The advantages and possible limitations of UMC have been explored extensively during the intervening years since it was first proposed, and the results of this work have been reported in two more recent publications [4,5]. Again, this work involved using simple hypothetical examples ("Toy Story 2" and "Toy Story 3").

The present paper reports on the recent development and subsequent testing of an alternative formulation of UMC (UMC-B). Although closely related to the original approach (UMC-G), this variant is conceptually somewhat simpler to understand, and it would appear to offer some advantages in certain situations relative to the earlier version of UMC. The idea of this new approach is that nuclear model parameters are randomly sampled as in UMC-G, but in addition weighting factors are calculated on the fly, one for each sampling history. The weighting factors are based on the quality of agreement between available experimental data and the corresponding observable quantities calculated using individual samples of theoretical cross section values generated from the randomly selected model parameters. These weighting factors are retained as additional components of the above-mentioned Markov chain of stochastic values for use in calculating weighted mean values and covariances, as well as other statistical quantities that might be desired. UMC-B has been tested using simple hypothetical examples ("Toy Story 4"), and the results are compared to corresponding ones obtained using both the GLSQ and UMC-G approaches. The present work describes the new UMC-B approach, indicates the differences between it and UMC-G, and provides results from the various numerical examples selected to demonstrate it. Finally, this paper documents applications of the GLSQ and UMC-G approaches to a realistic nuclear data evaluation exercise: the evaluation of ^{55}Mn(n,γ)^{56}Mn dosimetry reaction cross sections in the fast-neutron energy region from 100 keV to 20 MeV.

Formalism

All of the methods described in this paper have their origins in a common probabilistic approach to the merging of data based on the Bayes theorem [1] and a fundamental principle of information theory known as the principle of maximum entropy, as first introduced by Shannon [6] and later expanded by Jaynes [7]. For the reader's convenience it is worthwhile to summarize these concepts and elucidate the steps leading up to the specific formulas applied in various manifestations of the techniques mentioned in the Introduction. For the present purposes, the Bayes theorem is expressed in terms of probability density functions rather than actual probabilities. Quantities expressed in bold font represent vectors and matrices, and those in regular font are scalars. The symbol "•" is used to represent vector (or matrix) multiplication, and the symbol "×" represents scalar multiplication. The latter symbol is used only when needed for clarity. The following discussion describes the UMC-G method that was first proposed by Smith [2] in some detail, so that differences between this approach and UMC-B can be better understood.

Let $\mathbf{y}_E$ represent a collection of measured (experimental) quantities with a corresponding covariance matrix $\mathbf{V}_E$ that expresses their uncertainties and correlations. Let us suppose that there are n elements in the vector $\mathbf{y}_E$ and n^2 elements in the $n \times n$ matrix $\mathbf{V}_E$. $\mathbf{V}_E$ must be a symmetric matrix, so the actual number of distinct elements in this matrix is $n(n+1)/2$. It must also be a positive definite matrix. Furthermore, let $\boldsymbol{\sigma}_C$ represent a collection of m quantities calculated from a nuclear model with a corresponding $m \times m$ covariance matrix $\mathbf{V}_C$ that expresses their uncertainties and correlations. There are both deterministic and stochastic procedures for generating this information. We assume that a stochastic approach first proposed by Smith can be used for this purpose [8]. A collection of K nuclear model parameter sets $\{\boldsymbol{\rho}_k\}$ is produced at random by sampling within ranges of the individual parameters corresponding to their uncertainties. It is usually assumed that each individual nuclear model parameter of the collection $\boldsymbol{\rho}$ is independent of all the other parameters, but parameters' correlations could be taken into account if desired. The parameter sampling generates a corresponding collection of K derived cross section vectors $\{\boldsymbol{\sigma}_{Ck} = \mathcal{M}[\boldsymbol{\rho}_k]\}$, where $\mathcal{M}$ represents the nuclear-model computational algorithm that generates $\boldsymbol{\sigma}_{Ck}$ from $\boldsymbol{\rho}_k$. From this analysis, one can obtain the mean-value vector and corresponding covariance matrix, denoted by $\boldsymbol{\sigma}_C$ and $\mathbf{V}_C$, respectively, by applying formulas mentioned in the report from Smith [8]. Even though the nuclear model parameters are usually treated as independent, the components of $\boldsymbol{\sigma}_C$ will not be independent, owing to the effects of the nuclear modeling algorithm $\mathcal{M}$, and as a consequence $\mathbf{V}_C$ will not be diagonal. However, this matrix should be symmetric and positive definite as a consequence of the manner in which it is produced. These values for $\boldsymbol{\sigma}_C$ and $\mathbf{V}_C$ serve as the "priors" in the following discussion. In other words, we assume that the evaluator begins the evaluation process by generating prior results from nuclear modeling and then "refines" the evaluation by incorporating experimental data in the evaluation procedure. The prior information (based on modeling) and experimental information are treated as independent. When no relevant experimental data exist, the evaluation relies solely on nuclear theory, i.e., on the

evaluator's best estimates of the model parameter values and their uncertainties propagated through to the cross sections via the model.

For the present purposes, the Bayes theorem is embodied in the following formula

$$p(\boldsymbol{\sigma}) = \mathcal{C} \times \mathcal{L}\left(\mathbf{y}_{\mathrm{E}}, \mathbf{V}_{\mathrm{E}} | \boldsymbol{\sigma}\right) \times p_0(\boldsymbol{\sigma} | \boldsymbol{\sigma}_{\mathrm{C}}, \mathbf{V}_{\mathrm{C}}\right). \tag{1}$$

where:

p = a posteriori (posterior solution) probability density function,

p_0 = a priori (prior) probability density function,

$\mathcal{L}$ = likelihood function (also a probability density function), and

$\mathcal{C}$ = normalization constant chosen so that the following normalization condition is satisfied

$$\int_{\mathcal{S}} p(\boldsymbol{\sigma}) \mathrm{d}\boldsymbol{\sigma} = 1$$

where:

$\mathrm{d}\boldsymbol{\sigma}$ = volume element (voxel) in the m-dimensional space of possible values for $\boldsymbol{\sigma}$, and

$\mathcal{S}$ = region of that space over which one must integrate in order to achieve convergence.

It is also important to realize that whereas the components of $\boldsymbol{\sigma}$ are random variable arguments of the indicated functions, the quantities $\mathbf{y}_{\mathrm{E}}$, $\mathbf{V}_{\mathrm{E}}$, $\boldsymbol{\sigma}_{\mathrm{C}}$, and $\mathbf{V}_{\mathrm{C}}$ are simply collections of fixed numbers.

Here, $\boldsymbol{\sigma}$ is a vector that has the following m components: σ_1, σ_2, …, σ_{i}, …, σ_{m}. The dimension and interpretation of $\boldsymbol{\sigma}$ is comparable to that of $\boldsymbol{\sigma}_{\mathrm{C}}$. The solution to the evaluation problem is completely embodied in the probability density function $p(\boldsymbol{\sigma})$. In probability theory, the "best estimate" value for a random variable, in this case for σ_{i}, is defined as its expectation value (better known as "mean value") with respect to the associated probability density function. Therefore

$$\langle \sigma_{\mathrm{i}} \rangle = \int_{\mathcal{S}} \sigma_{\mathrm{i}} p(\boldsymbol{\sigma}) \mathrm{d}\boldsymbol{\sigma}, \quad \mathrm{i} = 1, \mathrm{m} \tag{2}$$

The same reasoning can be applied in order to generate a formula for determining elements of the evaluation solution covariance matrix $\mathbf{V}_{\sigma}$

$$\mathrm{cov}(\sigma_{\mathrm{i}}, \sigma_{\mathrm{j}}) = (\mathbf{V}_{\sigma})_{\mathrm{ij}} = \langle \sigma_{\mathrm{i}} \sigma_{\mathrm{j}} \rangle - \langle \sigma_{\mathrm{i}} \rangle \langle \sigma_{\mathrm{j}} \rangle, \quad \mathrm{i}, \mathrm{j} = 1, \mathrm{m} \tag{3}$$

where $\langle ... \rangle$ represents the multivariate integration of the indicated quantities in the same manner as shown for σ_{i} in Eq 2. When $\mathrm{i} = \mathrm{j}$ we obtain the variances from Eq 3, and the off diagonal elements (often referred to as "covariances") are obtained when $\mathrm{i} \neq \mathrm{j}$. Equations 1 through 3 provide all that is needed—at least conceptually—in order to perform an evaluation of the components of the

solution vector $\boldsymbol{\sigma}$ and determine the covariance matrix $\mathbf{V}_\sigma$. Obviously, we cannot proceed further unless we actually have knowledge of the probability density function p_0 and the likelihood function $\mathcal{L}$. Fortunately, a rigorous solution to this problem emerged from the pioneering work on information entropy by Shannon (in the 1940s) [6] and Jaynes (in the 1960s) [7]. The principle of maximum (information) entropy tells us that if all we know about a collection of random variables can be summarized by their mean values and associated covariance matrix, then the best estimate for the form of the prior probability density function is a multivariate normal function (Gaussian). In our case we have

$$p_0(\boldsymbol{\sigma}|\boldsymbol{\sigma}_C, \mathbf{V}_C) \sim \exp\left\{ -\frac{1}{2}[(\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)^T \bullet \mathbf{V}_C^{-1} \bullet (\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)]\right\} \tag{4}$$

$$\mathcal{L}(\mathbf{y}_E, \mathbf{V}_E|\boldsymbol{\sigma}) \sim \exp\left\{ -\frac{1}{2}[(\mathbf{y} - \mathbf{y}_E)^T \bullet \mathbf{V}_E^{-1} \bullet (\mathbf{y} - \mathbf{y}_E)]\right\} \tag{5}$$

where:

$\mathbf{V}_C{}^{-1}$ and $\mathbf{V}_E{}^{-1}$ = inverse matrices,

T = transpose of the indicated vector, and

$\sim$ = indication that normalization constants are required but are not shown explicitly.

$\mathbf{V}_C$ and $\mathbf{V}_E$ must be square, symmetric, positive definite matrices because they have to be inverted. The reason $\mathbf{y}$ and $\mathbf{y}_E$ appear in Eq 5, rather than "σ"-type variables, is that the relationship between the experimental data $\mathbf{y}_E$ and the variables $\boldsymbol{\sigma}$ to be evaluated might be indirect. For example, the experimental data might represent ratios of the variables to be evaluated, or they might be integral quantities. In fact, it is appropriate to define $\mathbf{y}$ by the expression $\mathbf{y} = \mathbf{f}(\boldsymbol{\sigma})$, where $\mathbf{f}$ represents a vector collection of n scalar functions f_1, f_2, …, f_i, …, f_n, with the variables of each being one or more of the elements of $\boldsymbol{\sigma}$. Combining Eqs 1, 4, and 5 leads to the expression

$$p_{(\boldsymbol{\sigma})} \sim \exp\left\{ -\frac{1}{2}[\{(\mathbf{y} - \mathbf{y}_E)^T \bullet \mathbf{V}_E^{-1} \bullet (\mathbf{y} - \mathbf{y}_E)\} + \{(\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)^T \bullet \mathbf{V}_C^{-1} \bullet (\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)\}]\right\} \tag{6}$$

Again, the required normalization constant is omitted from this formula. Application of the maximum entropy principle also leads to the conclusion that the best solution for the evaluation should correspond to values of the components of $\boldsymbol{\sigma}$ that maximize $p(\boldsymbol{\sigma})$, and therefore that

$$[\{(\mathbf{y} - \mathbf{y}_E)^T \bullet \mathbf{V}_E^{-1} \bullet (\mathbf{y} - \mathbf{y}_E)\} + \{(\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)^T \bullet \mathbf{V}_C^{-1} \bullet (\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)\}] = \text{minimum} \tag{7}$$

This, in turn, leads directly to the well-known GLSQ [9]. Finally, if we assume that there is no prior information available (comparable to the exceedingly large uncertainties manifested in $\mathbf{V}_C$), then the second term in Eq 7 in the brackets after the "+" sign can be neglected. The remaining term in Eq 7 then leads to the

simple least-squares method [9]. In both cases, the formulas yielding the solution of $\boldsymbol{\sigma}$ that satisfies Eq 7 involve the linearization of the mathematical problem, as mentioned above [9].

The UMC method, as originally formulated (UMC-G), involves calculating the integrals shown in Eqs 2 and 3 to obtain the solution vector $\boldsymbol{\sigma}$ and its covariance matrix $\mathbf{V}_\sigma$. The posterior probability density function p that is given in Eq 6 is used for this purpose, subject to the normalization requirement mentioned above. Although this approach is conceptually simple, it is mathematically very difficult to implement. In fact, these integrals can rarely, if ever, be determined in closed form. Also, deterministic numerical integration is usually impractical. However, it was demonstrated in earlier papers that these integrals can be computed stochastically to any desired degree of accuracy by pursuing a suitably large number of Monte Carlo histories [2,4,5]. Two different sampling methods were considered in earlier works: an easy to visualize "brute force" approach, UMC-G (BF), in which possible values of $\boldsymbol{\sigma}$ are sampled in the whole space $\mathcal{S}$ with no conditions imposed, and the more efficient but less transparent "Metropolis" scheme, UMC-G (METR), described in one of the papers documenting these studies [4], in which sampling occurs preferentially in regions of $\mathcal{S}$ corresponding to the highest values of $p(\boldsymbol{\sigma})$. Both of these methods yield essentially the same results, to statistical precision, but many more histories need to be followed in the BF approach in order to achieve adequate convergence comparable to that of the METR scheme. The METR method is vastly more efficient because minimal computational effort is expended in regions of low probability. The details of these two sampling schemes are extensively discussed in the earlier papers, and various simple "toy" examples are given to illustrate UMC-G ("Toy Stories" 1, 2, and 3) [2,4,5]. We do not mention these results here, but the following summarizes the key points that were learned from this earlier work:

- UMC-G and GLSQ yield the same converged results for both the mean values and the corresponding uncertainties for all situations that involve linear relationships between the experimental data and the cross sections to be evaluated. This would include consideration of integral experimental data as well as of differential data.
- Significant differences between the UMC-G and GLSQ solutions are observed in certain situations involving ratio data, large uncertainties, and discrepant experimental data.
- Transformation of variables to logarithm form can eliminate non-linear effects in the case of simple ratio data, but the evaluated results will always differ from the solutions in untransformed space (to a greater or lesser extent, depending on the details of the problem); i.e., a biased solution is obtained.

An alternative approach to UMC (UMC-B) was suggested by two of the present authors (Capote and Trkov). Subsequently, it has been tested through comparisons to GLSQ and UMC-G for some simple problems. This method is described and the results from its testing are reported for the first time in this paper. The concept of UMC-B evolved from the perceived need to overcome a limitation in analyses of the performance of complex nuclear systems based on the powerful Total Monte Carlo (TMC) approach developed by Koning and

Rochman [10], i.e., its excessive reliance on nuclear modeling and inadequate consideration of experimental nuclear data.

There are strong similarities between UMC-B and UMC-G in terms of the underlying mathematical assumptions. In both cases, stochastic methods are applied and the inherent properties of the probability distributions associated with the model-calculated and experimental data are taken into consideration, as discussed in detail above. The main difference lies in the manner in which the mathematical problem is formulated and stochastic analysis is carried out. As is the case for UMC-G, the UMC-B approach involves generating a collection of K calculated cross section sets $\{\boldsymbol{\sigma}_{Ck} = \mathcal{M}[\boldsymbol{\rho}_k]\}$ based on K randomly chosen model parameter vectors $\{\boldsymbol{\rho}_k\}$. However, the mean values $\boldsymbol{\sigma}_C$ and the covariance matrix $\mathbf{V}_C$ are not explicitly calculated at the outset, as is the case for UMC-G. Instead, a collection of K scalar weighting parameters $\{\omega_k\}$ is generated. Individual ω_k values are calculated on the fly during each sampling history, where

$$\omega_k = \exp\left\{ -\frac{1}{2}[(\mathbf{y}_k - \mathbf{y}_E)^T \bullet \mathbf{V}_E^{-1} \bullet (\mathbf{y}_k - \mathbf{y}_E)] \right\} \tag{8}$$

Here, $\mathbf{y}_k = \mathbf{f}(\boldsymbol{\sigma}_{Ck})$, as indicated above. The resemblance of the term on the right-hand side of Eq 8 to the expression for the function $\mathcal{L}$ in Eq 5 is not coincidental. The weighting parameter ω_k provides a measure of the deviation of the calculated vector $\mathbf{y}_k$ from the experimental one $\mathbf{y}_E$ for the kth Monte Carlo history. If the deviation is large, ω_k will be small (or even zero, for all practical purposes), and this particular history will have little or no influence on the outcome.

The procedure of UMC-B yields the Markov chain of pairs of quantities $\{\boldsymbol{\sigma}_{Ck}, \omega_k\}$ for k = 1,K. From this information one can obtain the solution mean values $\boldsymbol{\sigma}$ and covariance matrix $\mathbf{V}_\sigma$ for an evaluation by using the following formulas (for i,j = 1,m)

$$\sigma_i \approx \left[\sum_{k=1,K} \omega_k \sigma_{Cik} \right] \Big/ \left[\sum_{k=1,K} \omega_k \right], \quad i = 1, m \tag{9}$$

$$(\mathbf{V}_\sigma)_{ij} \approx \left[\sum_{k=1,K} \omega_k \sigma_{Cik} \sigma_{Cjk} \right] \Big/ \left[\sum_{k=1,K} \omega_k \right] - \sigma_i \sigma_j, \quad i, j = 1, m \tag{10}$$

Notice that we have dropped the use of $\langle ... \rangle$ to represent averages. One could also retain the collection $\{\boldsymbol{\sigma}_{Ck}, \omega_k\}$ of values for a variety of further analyses, e.g., for use in an augmented version of the TMC approach mentioned above [10]. In UMC-B, the results obtained from each sampling history need to be taken into consideration, because the mean values and covariances are calculated after the sampling process is complete. The computational effort required for histories involving small values of the weight factor ω_k is identical to that for heavily weighted histories, and can be substantial for complicated nuclear models and an extensive range of data. Also, the sampling range for the nuclear model parameters must be sufficiently large to ensure that no histories involving

significant values of ω_k are overlooked, because biases will result if they are neglected. Although this procedure is conceptually straightforward, and thus appealing, just as it is in the case of the UMC-G (BF) method [2,4,5], and although it should give reasonable results if applied carefully, it is not very efficient. There is no obvious way to invoke the METR sampling scheme in UMC-B as is the case for UMC-G. The UMC-B approach clearly takes into account both the prior and likelihood probability functions, but the manner in which this is done is obviously quite different from that in the UMC-G approach, with which the posterior joint probability function (inclusive of both theoretical and experimental information) is constructed (either deterministically or stochastically) before the second stage in the analysis commences. If no experimental data are involved, then the UMC-B and UMC-G methods degenerate to a common approach. In UMC-B, all the weighting factors ω_k can be treated as a common constant (unity for convenience) in Eqs 9 and 10. These equations then also apply directly in the UMC-G method. Although we offer no formal proof that this is the case, it is intuitively reasonable to assume that UMC-B and UMC-G should yield essentially the same results, within statistical accuracy, provided that a comprehensive sampling of parameter spaces takes place (please note that the employed parameter space is identical in both methods). In the next section we examine two simple "toy" examples, using three distinct methods (GLSQ, UMC-G, and UMC-B) to explore the equivalences (or differences) in these distinct methods.

The reader might wonder why "B" and "G" are used to identify these two UMC approaches. The reason is a historical one and involves three authors of the current work. The UMC-G approach was conceived when Smith was getting his automobile repaired (thus "G" for "garage"). The UMC-B approach was conceived when Capote and Trkov were having breakfast one morning at a Port Jefferson covariance workshop (thus "B" for "breakfast").

A Hypothetical Example ("Toy Story 4")

UMC analysis is computationally intensive for both UMC-G and UMC-B, as discussed earlier in this paper. Therefore, in order to compare the various approaches discussed here, i.e., GLSQ, UMC-B, and UMC-G, a simple (toy) model has been devised that incorporates several important features that are frequently encountered in realistic evaluation situations. However, the present example carries less computational overhead. This model ("Toy Story 4") involves an evaluation of energy-dependent cross section data σ_1, σ_2, and σ_3 corresponding to three distinct energies (nodes) E_1, E_2, and E_3. Three "theoretical" values (σ_{C1}, σ_{C2}, and σ_{C3}) are calculated with a model function $f(E,p_1,p_2)$ corresponding directly to these individual nodes as well as two hypothetical, related "experimental" results y_{E1} and y_{E2}. There is one node (#3) without measured data, and the goal is to "evaluate" the cross section for all three energies. The model features two parameters, p_1 and p_2. The model scheme and numerical input data utilized in the calculations are summarized in Table 1. In this table, "$\leftarrow\rightarrow$" means that the indicated quantities are comparable but not exactly equivalent.

TABLE 1—*"Toy Story 4" hypothetical model and input data.*

Model Formula and Data Scheme			
$s_C = f(E, p_1, p_2) = p_1 \times E^{1/2} \times \exp(-E/p_2)$			
Theory	Experiment (Linear)	Experiment (Ratio)	
$s_{C1} = f(E_1,p_1,p_2)$	$y_{E1} \leftarrow\!\rightarrow s_{C1}$	$y_{E1} \leftarrow\!\rightarrow s_{C1}$	
$s_{C2} = f(E_2,p_1,p_2)$	$y_{E2} \leftarrow\!\rightarrow s_{C2}$	$y_{E2} \leftarrow\!\rightarrow s_{C2}/s_{C1}$	
$s_{C3} = f(E_3,p_1,p_2)$	No data	No data	
Model Parameters: $\mathrm{cov}(p_1,p_2) = 0$ for all cases			
Non-discrepant		Discrepant	
$p_1 = 1.0$ ($\pm 25.0\%$)	$p_2 = 2.0$ ($\pm 10.0\%$)	$p_1 = 1.0$ ($\pm 28.5\%$)	$p_2 = 2.0$ ($\pm 10.0\%$)
Experimental Data: $y_{E1} = 0.5728$ ($\pm 5\%$) for all cases			
Non-discrepant		Discrepant	
Linear	Ratio	Linear	Ratio
$y_{E2} = 0.6075$ ($\pm 5\%$)	$y_{E2} = 1.1031$ ($\pm 5\%$)	$y_{E2} = 0.4050$ ($\pm 5\%$)	$y_{E2} = 0.7354$ ($\pm 5\%$)

In all, 32 separate calculations were performed using this model and data set. They encompass two parameter sampling schemes (normal and log-normal), four computational schemes [UMC-B, UMC-G (BF), UMC-G (METR), and GLSQ], and sets of both non-discrepant and discrepant linear and ratio experimental data. For simplicity, the two model parameters p_1 and p_2 employed in this exercise are assumed to be uncorrelated. Furthermore, all experimental data are also treated as uncorrelated. Strong correlations observed in the model-calculated nodal results (93% to 98%) are attributable to effects of the model itself. This situation is also typical of the more complex physical models used in nuclear data evaluations. A consequence of this is that although the uncertainties in the model-calculated nodal values are large (25% to 28%), the uncertainties in their calculated ratios are modest (about 5%) due to these strong correlations. Each Monte Carlo calculation comprised 5×10^7 sampling histories in order to ensure that stochastic variations in the final results were as small as possible, i.e., the statistical uncertainty of derived Monte Carlo values was negligible. Then, the results from the various approaches could be properly compared. Solution mean values and covariance matrices were determined for each set of calculations. For comparison purposes, ratios of the nodal mean values were calculated relative to those for UMC-G (METR). The latter were treated as the "benchmark" values for the present exercise, because it was determined in earlier work that results obtained via this method are usually relatively stable, and they might be the most reliable for a variety of evaluation situations. Results from this analysis are shown in Fig. 1.

Some general conclusions can be drawn from this work. They are summarized as follows:

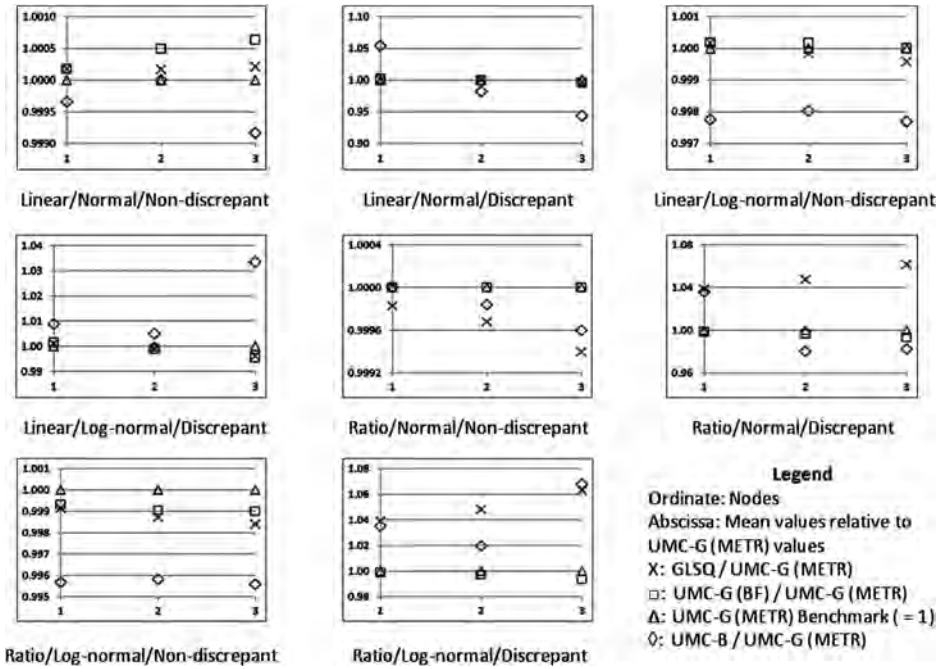

FIG. 1—*Results from 32 calculations with the "Toy Story 4" hypothetical model. The plotted values represent ratios of calculated mean values to comparable ones obtained with the UMC-G (METR) approach. Therefore, all data points with the symbol "Δ" are exactly unity. Vertical scales are very different for different plots in the figure.*

- The computational time required for any one of the three Monte Carlo approaches considered here exceeds that required for the deterministic GLSQ approach by many orders of magnitude. Therefore, the use of stochastic methods such as UMC for evaluation purposes cannot be justified in contemporary circumstances unless the conditions suggest that GLSQ is likely to give erroneous results (e.g., for highly non-linear models, large uncertainties, ratios, and discrepant data) or new evaluation methods are employed (e.g., TMC) that explicitly require stochastic samples (instead of the closed form solution).
- When the experimental data included in the evaluation are relatively consistent (non-discrepant), regardless of whether linear values or ratio values are used or whether normal or log-normal parameter sampling is employed, all methods of analysis yield results that agree very well for the mean values and covariance matrices. Although systematic departures from unity can be seen in the various plots of the mean-value ratios appearing in Fig. 1, these are sufficiently small to be of negligible consequence.
- When the experimental data are discrepant, there are discernable and systematic differences in some of the results obtained via the various

parameter sampling and data analysis methods, as is evident from the results shown in the plots of Fig. 1. (i) For linear but discrepant data, it is observed that the UMC-B results differ from the relative consistency of the results obtained via the other three approaches (both deterministic and Monte Carlo), regardless of whether normal or log-normal parameter sampling is employed. (ii) For ratio data, only the UMC-G (BF) approach gives results that are acceptably consistent with those obtained when using the UMC-G (METR) benchmark approach. Both UMC-B and GLSQ approaches give results that deviate noticeably from the benchmark. The failure of GLSQ when discrepant ratio data are involved is well understood from earlier work [4]. The tendency of UMC-B to fail under these conditions is a new observation from the present investigation. In this particular situation, the discrepancy is likely due to an inadequacy of sampling of the nodal quantities. However, this should not be construed as a general indictment against UMC-B for all situations. Further investigation of the UMC-B is required in order to clarify this issue.

- The UMC-B advantages (and appeal) stem from the fact that theoretical sampling and experimental weighting are performed at the same time in each Monte Carlo history. However, this also implies a disadvantage, due to possible restrictions in the sampling space. Additionally, for discrepant data the low acceptance ratio of this approach is problematic, because it is then necessary to increase the number of rather time-consuming modeling calculations (especially in more realistic situations), and many of them would have to be effectively thrown away in the process because of the near-zero weighting factors obtained.

Evaluation of the $^{55}Mn(n,\gamma)^{56}Mn$ Dosimetry Reaction

We began the evaluation process by downloading the available compiled experimental data for this reaction from the Experimental Nuclear Reaction Data EXFOR website [11]. The EXFOR database is generally considered to be almost complete for neutron-induced reactions. As discussed in a recent publication [12], the need to weed out bad data and perform needed adjustments to the remaining values in order to provide consistent experimental results for an evaluation is of critical importance. All evaluation methods are very sensitive to the influences of discrepant data, as they will distort the evaluated results. The example discussed above ("Toy Story 4") provides a demonstration of how misleading evaluated results can be traced to discrepant experimental data. The procedure used to prepare the experimental database for the present evaluation of neutron capture on manganese is documented below.

Experimental Data Preparation

The retrieval of experimental data from the EXFOR database produced 24 distinct sets to be considered for this evaluation, as plotted in Fig. 2 [12]. Seventeen of these sets were retained from the retrieved collection after reviewing these

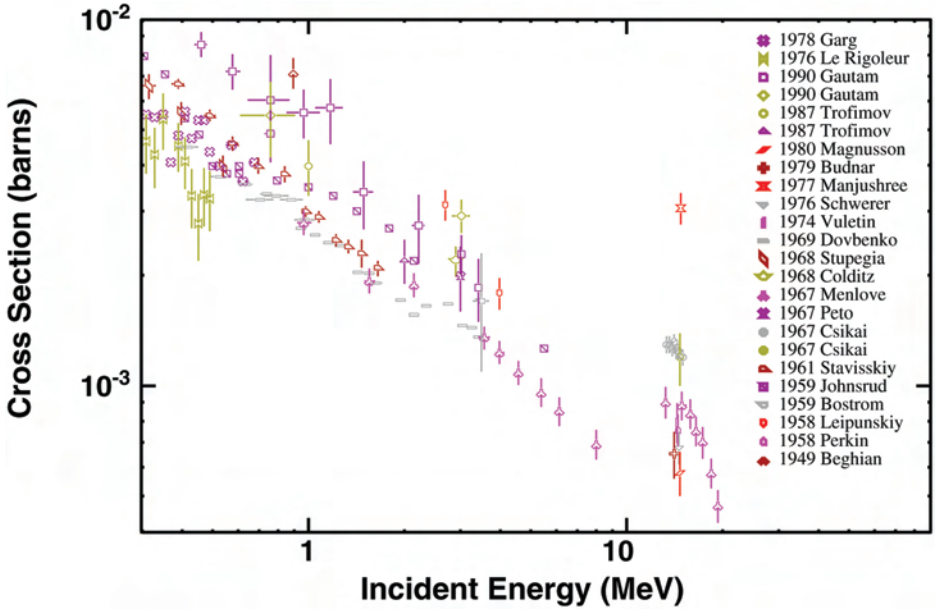

FIG. 2—*Raw experimental data as retrieved from EXFOR [11].*

data. The remaining seven sets were rejected for various reasons, including obvious discrepancies; the absence of numerical uncertainty information; and the lack, unavailability, or inadequacy of documentation. Adjustments were applied to the accepted data sets as needed in order to account for changes in standards and other factors, so as to ensure that the information from these data sets was utilized properly in the present evaluation. Some of these adjustments were rather arbitrary, but they are all based on evaluator experience.

The accepted cross section data were renormalized to reflect ENDF/B-VII.0 values for the utilized reference standards wherever possible [3]. When the reference standard cross section values originally used were provided in EXFOR, it was possible to renormalize to current reference values quite easily, and no additional uncertainty was added. If no reference was specified, an extra uncertainty of 10 % was assigned. When an acknowledged reference cross section standard was specified in EXFOR but the actual values used by the experimenters were not given, an additional uncertainty of 5 % was imposed. When a nonstandard reference cross section was used and no values for it appeared in EXFOR, an additional uncertainty of 10 % was assigned. No correlation information is available in EXFOR, so rough estimates were made of uncertainty correlations between data points within individual sets and between separate data sets. Within individual data sets, correlations were generally estimated by considering the limited descriptive information provided to EXFOR by the original authors regarding the uncertainty sources in their data. Typical values of these assumed correlations are 0, 20, 50, 80, and 100 %. Absolute data (no reference standard employed in the experiment) were assumed to be uncorrelated

(0 %) to all other data sets. This also applied when no reference standard was specified. Separate data sets involving the same reference standard were assumed to be 20 % correlated. Data measured using different reference standards were assumed to be uncorrelated. Some data sets that were judged to be widely discrepant in normalization with respect to the main body of cross section data were nevertheless retained for the useful shape information they provided. They were renormalized for evaluation purposes to the ENDF/B-VII.0 manganese capture cross section values at selected energies, and an additional uncertainty of 20 % was assigned. A strong correlation of 0.8 was imposed in order to emphasize the shape information content and de-emphasize the influence of the data normalization on the evaluation process. The adjusted experimental cross section values that were used in the present evaluation, along with their uncertainties, are plotted in Fig. 3 (points labeled with "*" are the ones that were adjusted).

The improvement in the consistency of the experimental results brought about by the above-mentioned deletions and adjustments is evident from a comparison of Figs. 2 and 3. There appear to be no serious discrepancies for these considered data, within the estimated experimental uncertainties.

Nuclear Reaction Modeling

The available experimental database exhibits a lack of reliable data between 4 and 13 MeV. Therefore, nuclear reaction calculations are clearly needed in

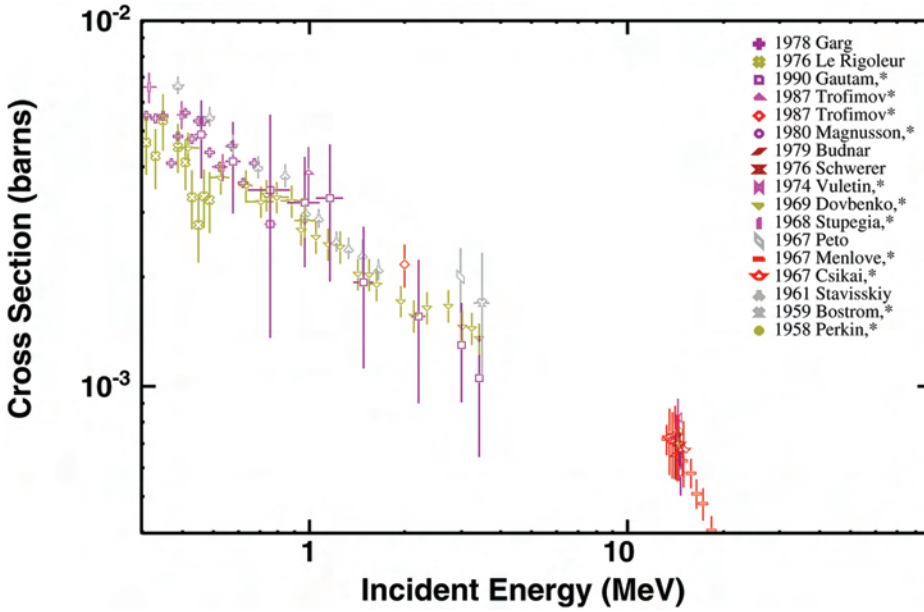

FIG. 3—*Adjusted experimental values with 1-sigma uncertainties used in the current evaluation. Data marked with "*" were modified as described in the text.*

order to provide a typically highly correlated prior for the combined evaluation process. Nuclear data modeling was undertaken using the EMPIRE code [13]. Default values for nuclear model parameters and their uncertainties were taken from the RIPL-3 collection [14]. The calculated manganese capture cross sections and corresponding theoretical (model) uncertainties are shown in Fig. 4, in which they are also compared with the accepted experimental data. No attempt was made to improve the normalization or shape of the EMPIRE calculations, because the prior was seen to be consistent with the experimental database within quoted model uncertainties from 20 % to 30 % below 1 MeV up to 60 % in the energy region of 2–10 MeV. Higher uncertainty above 3 to 4 MeV results from there being more competing channels open, with the capture contribution becoming negligible compared to competing channels at higher energies.

This evaluation was performed using both GLSQ and UMC-G (METR) methods. It should be noted that the UMC-B and UMC-G methods will yield the same results as long as both encompass the same sampling space, the experimental data are statistically consistent (non-discrepant), and a linear dependence of cross sections holds (no ratio data used). All these conditions are met in this example; therefore, the UMC-B method was not employed for this

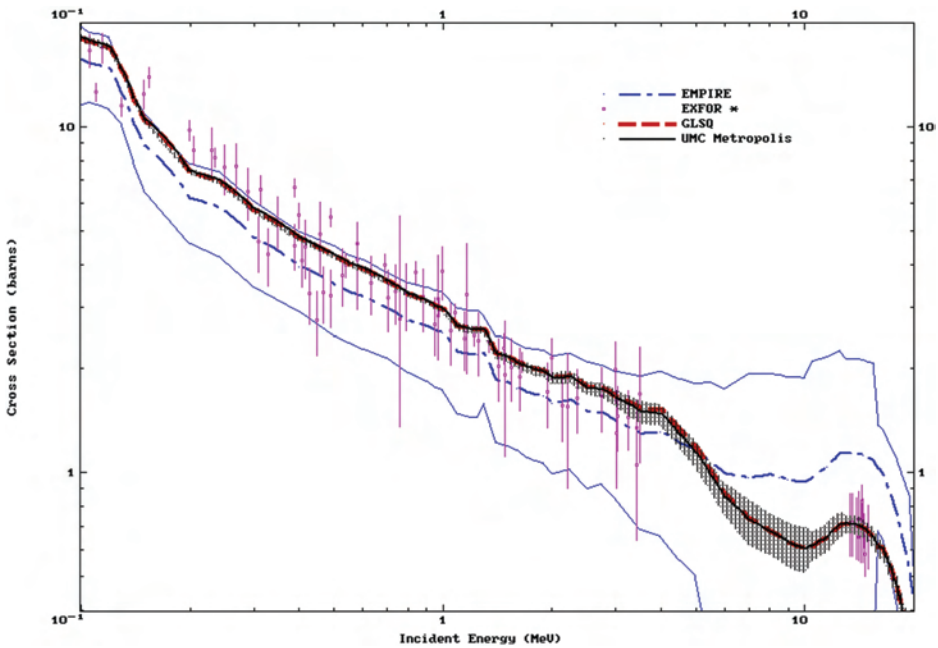

FIG. 4—*Experimental data compared to EMPIRE calculated prior (blue dashed-dotted line) with prior uncertainties (blue thin lines) versus evaluation results by GLSQ (red dashed line) and UMC-G Metropolis (black solid line) with final uncertainties (hatched area). GLSQ uncertainties are identical to UMC-G (METR) uncertainties and are not shown. All uncertainties are 1-sigma.*

evaluation. The agreement of the GLSQ and UMC-G results is excellent over the whole energy range for both posterior mean values and corresponding uncertainties. Good agreement was expected based on previous experience with the "toy" test examples, as all experimental cross sections were given directly and no ratio data were used. So, the evaluation problem was an entirely linear one. It should be noted that the inclusion of the relatively accurate experimental data in the vicinity of 200 keV resulted in an evaluated solution curve that differed considerably from the less accurate calculated model prior. These solution results, although they fall within the envelope of uncertainties for the calculated values, nevertheless lie near the upper uncertainty boundary for the theoretical results in that energy region.

Conclusions

This paper discusses the underlying mathematical foundations of the generalized least-squares method (GLSQ) and two distinct Unified Monte Carlo methods (UMC-G and UMC-B), and it points out similarities and differences among them. The UMC-B approach is reported here for the first time. Through the use of various permutations of a simple example, it has been demonstrated that all three approaches yield results that are in close agreement for linear and non-discrepant data. However, the computational time required for these UMC approaches exceeds that required for the deterministic GLSQ approach by many orders of magnitude. Therefore, the use of stochastic methods such as UMC-G (METR) and UMC-B for evaluation purposes is justified for linear and non-discrepant experimental data only if new evaluation methods (e.g., TMC) that explicitly require stochastic samples are employed.

When discrepancies and/or nonlinearities (such as those arising from the use of experimental ratio data) are considered, some significant differences are seen to emerge. The UMC-G and UMC-B approaches tend to give about the same results under favorable circumstances, but noticeable differences appear for certain situations that involve unfavorable data situations. The same effect can be observed for the UMC-G approach when brute force (BF) sampling is employed and selected ranges of the sampled parameters are too limited. These differences are traced to the fact that in the UMC-B approach, it is difficult to ensure that underlying probability distributions are adequately sampled unless the experimental data and theoretical modeling are not discrepant. Therefore, for non-linear and/or discrepant experimental data, only UMC-G (METR) is recommended. The fact that the GLSQ method fails in situations involving severe non-linearity, discrepant data, and/or large uncertainties was noted in earlier work; this outcome has been reconfirmed in the present investigation.

The UMC-G (METR) and GLSQ methods were both employed to evaluate cross sections for the $^{55}Mn(n,\gamma)^{56}Mn$ neutron dosimetry reaction in the energy range of 100 keV to 20 MeV. After selection and adjustment of the available experimental data downloaded from EXFOR by the evaluator, it was observed that these selected and adjusted data were reasonably consistent with each other and with the nuclear model calculations. Under these conditions, the evaluated results provided by both UMC-G and GLSQ agreed very well, as expected.

Because stochastic approaches to data evaluation are computationally very intensive, it is difficult to justify their use in situations such as the present one in which the standard GLSQ approach is likely to give adequate results. However, in the future, when computational power is likely to be less of a concern than it is today, the more rigorous and flexible stochastic approaches might become accepted as default methods for performing nuclear reaction data evaluations.

Acknowledgments

The writers are indebted to the International Atomic Energy Agency (R.C., A.T., and M.M.) and the U.S. Department of Energy (D.L.S.) for supporting this work.

References

[1] Smith, D. L., *Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology*, American Nuclear Society, LaGrange Park, IL, 1991.

[2] Smith, D. L., "A Unified Monte Carlo Approach to Fast Neutron Cross Section Data Evaluation," *Proceedings of the 8th International Topical Meeting on Nuclear Applications and Utilities of Accelerators*, American Nuclear Society, LaGrange Park, IL, July 29–Aug 2, 2007, p. 736.

[3] Chadwick, M. B., Obložinský, P., Herman, M., Greene, N. M., McKnight, R. D., Smith, D. L., Young, P. G., MacFarlane, R. E., Hale, G. M., Frankle, S. C., Kahler, A. C., Kawano, T., Little, R. C., Madland, D. G., Moller, P., Mosteller, R. D., Page, P. R., Talou, P., Trellue, T. H., and White, M. C., "ENDF/B-VII. 0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology," *Nucl. Data Sheets*, Vol. 107, 2006, p. 2931.

[4] Capote, R. and Smith, D. L., "An Investigation of the Performance of the Unified Monte Carlo Method of Neutron Cross Section Data Evaluation," *Nucl. Data Sheets*, Vol. 109, 2008, p. 2768.

[5] Capote, R. and Smith, D. L., "Unified Monte Carlo and Mixed Probability Functions," *J. Kor. Phys. Soc.*, Vol. 59, No. 2, August 2011, pp. 1284–1287.

[6] Shannon, C. E., "A Mathematical Theory of Communication," *Bell Syst. Tech. J.*, Vol. 27, 1948, pp. 379–423, 623–656.

[7] Jaynes, E. T., "Where Do We Stand on Maximum Entropy," *The Maximum Entropy Formalism*, R. D. Legine and M. Tribus, Eds., MIT Press, Cambridge, MA, 1978.

[8] Smith, D. L., "Covariance Matrices for Nuclear Cross Sections Derived from Nuclear Model Calculations," *Report ANL/NDM-159*, Argonne National Laboratory, Argonne, IL, 2004.

[9] Smith, D. L., "A Least-Squares Computational 'Tool Kit,'" *Report ANL/NDM-128*, Argonne National Laboratory, Argonne, IL, 1993.

[10] Koning, A. and Rochman, D., "Towards Sustainable Nuclear Energy: Putting Nuclear Physics to Work," *Ann. Nucl. Energy*, Vol. 35, 2008, p. 2024.

[11] International Atomic Energy Agency, 2011, "Experimental Nuclear Reaction Data (EXFOR)," http://www-nds.iaea.org/exfor/exfor.htm (Last accessed 14 Dec 2011).

[12] Capote, R., Smith, D. L., and Trkov, A., "Nuclear Data Evaluation Methodology Including Estimates of Covariances," *EPJ Web of Conferences*, Vol. 8, 2010, p. 04001.

[13] Herman, M., Capote, R., Carlson, B. V., Obložinský, P., Sin, M., Trkov, A., Wienke, H., and Zerkin, V., "EMPIRE: Nuclear Reaction Model Code System for Data Evaluation," *Nucl. Data Sheets*, Vol. 108, 2007, pp. 2655–2715.

[14] Herman, M., Capote, R., Obložinský, P., Young, P. G., Goriely, S., Belgya, T., Ignatyuk, A. V., Koning, A. J., Hilaire, S., Plujko, V. A., Avrigeanu, M., Bersillon, O., Chadwick, M. B., Fukahori, T., Ge, Zhigang, Han, Yinlu, Kailas, S., Kopecky, J., Maslov, V. M., Reffo, G., Sin, M., Soukhovitskii, E. Sh., and Talou, P., "RIPL—Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations," *Nucl. Data Sheets*, Vol. 110, 2009, pp. 3107–3214.