A UNIFIED MONTE CARLO APPROACH TO FAST NEUTRON CROSS SECTION DATA EVALUATION

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A new "Unified Monte Carlo" (UMC) approach to fast neutron cross section data evaluation that incorporates both model-calculated and experimental information in a consistent manner, and offers significant advantages compared to other contemporary methods, is described. The technique is based on applications of Bayes Theorem and the Principle of Maximum Entropy as well as on fundamental definitions from probability theory. This paper describes the mathematical formalism, discusses various related practical considerations, provides a numerical example to illustrate the method, and offers some conclusions about the viability as well as benefits of the method in realistic evaluation applications.

I. INTRODUCTION

Nuclear data, such as neutron cross sections, that are required for applications in nuclear science are rarely obtained directly from experiments or theoretical calculations. Instead, cross section values extracted from formal evaluated nuclear data libraries are utilized. These evaluated results amount to best estimate determinations of the physical parameters that are generally based on evaluator examination of all the pertinent information, including that derived from both measurements and theoretical modeling. Over the years, nuclear data evaluation methodology has evolved from largely subjective approaches to relatively rigorous analytical procedures that combine all the available information to produce the recommended values. Most of the more recent approaches strive to minimize subjective biases while at the same time making optimal use of all pertinent information. Descriptions of various contemporary analytical techniques employed for nuclear data evaluation can be found in the extensive literature on this subject (e.g., Ref. 1).

This paper describes a new approach to generating evaluated cross sections in the fast neutron region (above the resolved resonances) that is based entirely on Monte Carlo simulation rather than on deterministic analysis as is the case with other contemporary methods. It is referred to as the Unified Monte Carlo (UMC) approach because it is capable of incorporating both experimental and theoretical information in a consistent (unified) manner within the framework of Monte Carlo simulation.

Section II describes the mathematical formalism upon which the UMC approach is based. Section III discusses various practical considerations associated with applying this method. Section IV provides a detailed example to illustrate the method. Finally, Section V offers some conclusions about the viability of this method in realistic situations, based on experience acquired from the investigation that led to its development, and points out some important advantages of this approach compared with other contemporary evaluation methods.

II. FORMALISM

The present method, like various others, finds its origins in Bayes Theorem. This theorem is non-controversial and can be derived easily from the basic postulates of probability theory following some simple steps involving the algebra of probabilities (e.g., Refs. 1 and 2). Bayes Theorem provides a rigorous procedure for learning from experience by establishing a simple formula that relates prior and posterior information. For present purposes, we will express Bayes theorem in terms of probability density functions rather than actual probabilities. In the following discussion, items expressed in bold font represent vectors and matrices while those in ordinary font are scalars. The symbol "•" is used to represent vector (or matrix) multiplication. The symbol "x" signifies scalar multiplication; it is used only in situations where it is needed for clarity.

Let $\mathbf{y}_E$ represent a collection of measured (experimental) quantities with a corresponding covariance matrix $\mathbf{V}_E$ that expresses their uncertainties as well as correlations. Let us suppose that there are "n" elements in the vector $\mathbf{y}_E$ and n^2 elements in the "n x 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 quantities representing the prior information available before considering the experimental data.

Usually, these prior results are calculated by means of nuclear modeling. The uncertainties and their correlations corresponding to these prior values are represented by a covariance matrix $\mathbf{V}_C$. We assume that there are "m" calculated quantities and that the corresponding covariance matrix has dimensions "m x m". It must also be symmetric and positive definite. For convenience, we use the symbol "σ" to signify all the quantities being evaluated even though this collection might include not just cross sections but other observables as well (e.g., angular distributions). A method for generating $\mathbf{V}_C$ by Monte Carlo simulation when the prior is based on nuclear modeling has been suggested by this author and is discussed in considerable detail in Ref. 3. Basically, this approach involves use of Monte Carlo simulation to propagate uncertainties of the nuclear model parameters through to the computed physical observable quantities. We will not dwell on the matter of how nuclear model parameters and their uncertainties and correlations are chosen to provide the most reasonable values for $\boldsymbol{\sigma}_C$ and $\mathbf{V}_C$. Thus, an evaluator generates prior estimates of the physical quantities by means of nuclear modeling and then "refines" the evaluation by incorporating experimental data in the evaluation procedure through a merging process to be described in this paper. If no relevant experimental data exist, then the evaluation will be based on nuclear modeling alone and the evaluator's job is finished.

In the present context, Bayes theorem is embodied in the following formula (e.g., Refs. 1 and 2):

$$p(\boldsymbol{\sigma}) = C \times \mathcal{L}(\mathbf{y}_E,\mathbf{V}_E \mid \boldsymbol{\sigma}) \times p_0(\boldsymbol{\sigma} \mid \boldsymbol{\sigma}_C,\mathbf{V}_C). \qquad (1)$$

In this equation, "p" is the *a posteriori* (posterior) probability density function, p_0 is the *a priori* (prior) probability density function, "$\mathcal{L}$" is a likelihood function (also a probability density function), and "C" is a normalization constant. This constant is chosen so that the following normalization condition is satisfied:

$$\int_{\mathbb{S}} p(\boldsymbol{\sigma})\, d\boldsymbol{\sigma} = 1 , \qquad (2)$$

where $d\boldsymbol{\sigma}$ is a volume element (voxel) in the m-dimensional space of possible values for $\boldsymbol{\sigma}$ and $\mathbb{S}$ is the region of that space over which one must integrate in order to achieve convergence. By convergence it is meant that increasing the size of $\mathbb{S}$ would not change the value of the integral in Eq. (2) significantly. In practice it is not necessary to know the value of "C" since it cancels in the formulas that are used for the Monte Carlo analysis.

It is important to understand that while the components of $\boldsymbol{\sigma}$ are random variable arguments of the indicated functions, $\mathbf{y}_E$, $\mathbf{V}_E$, $\boldsymbol{\sigma}_C$, and $\mathbf{V}_C$ are simply collections of fixed numbers insofar as the present evaluation procedure is concerned. Since $\boldsymbol{\sigma}$ is a vector, it has the following m components: $\sigma_1, \sigma_2, \ldots, \sigma_i, \ldots, \sigma_m$. 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, e.g., 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,

$$< \sigma_i > = \int_{\mathbb{S}} \sigma_i\, p(\boldsymbol{\sigma})\, d\boldsymbol{\sigma} \quad (i = 1,m) \qquad (3)$$

is the evaluated value that is sought for the variable σ_i.

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

$$\mathrm{Cov}(\sigma_i,\sigma_j) = (\mathbf{V}_\sigma)_{ij} = \\ < \sigma_i\, \sigma_j > - < \sigma_i > \times < \sigma_j > \quad (i,j = 1,m) , \qquad (4)$$

where <…> represents multivariate integration of the indicated quantities in the same manner as shown for σ_i in Eq. (3). Note that when i = j we obtain the variances from Eq. (4) while the off-diagonal elements (often referred to as "covariances") are obtained when $i \neq j$.

Eqs. (1) - (4) provide all that is needed – at least conceptually – to perform an evaluation of the components of $\boldsymbol{\sigma}$ and determine the covariance matrix $\mathbf{V}_\sigma$.

It is crucial to know exactly what forms the functions p_0 and $\mathcal{L}$ should assume since without this knowledge numerical analysis is impossible. Bayes formula, i.e., Eq. (1), offers no specific guidance in this matter. Fortunately, a rigorous solution to this problem can be found in the pioneering work on information entropy by Shannon (in the 1940's), Jaynes (in the 1960's), and other statisticians of this period (e.g., Ref. 1). The Principle of Maximum (Information) Entropy states that if all we know about a collection of random variables can be summarized by giving their mean values and associated covariance matrix, then the best estimate for the form of the appropriate probability density function is a multivariate normal function (Gaussian). Thus, in our case we have the following expression for p_0:

$$p_0(\boldsymbol{\sigma} \mid \boldsymbol{\sigma}_C,\mathbf{V}_C) \\ \sim \exp\{-(\tfrac{1}{2})[(\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)^T \bullet \mathbf{V}_C^{-1} \bullet (\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)]\} . \qquad (5)$$

By the same reasoning one obtains the following expression for $\mathcal{L}$:

$$\mathcal{L}(\mathbf{y}_E, \mathbf{V}_E \mid \boldsymbol{\sigma}) \sim \exp\{-(\tfrac{1}{2})[(\mathbf{y} - \mathbf{y}_E)^T \bullet \mathbf{V}_E^{-1} \bullet (\mathbf{y} - \mathbf{y}_E)]\} \ . \quad (6)$$

In these formulas $\mathbf{V}_C^{-1}$ and $\mathbf{V}_E^{-1}$ are inverse matrices, "T" denotes the transpose of the indicated vector, and the symbol "~" indicates that the respective normalization constants are not shown explicitly. They are actually not needed as is shown below. It is clear why $\mathbf{V}_C$ and $\mathbf{V}_E$ must be square, symmetric, positive definite matrices; they have to be inverted. The reason why "$\mathbf{y}$" and "$\mathbf{y}_E$" appear in Eq. (6) rather than "σ"-type variables is that the relationship between the experimental data $\mathbf{y}_E$ and the variables $\boldsymbol{\sigma}$ to be evaluated may be indirect. For example, the experimental data may represent ratios of the variables to be evaluated or they may 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 m scalar functions $f_1, f_2, \ldots, f_i, \ldots, f_m$ each of whose variables are one or more of the elements of $\boldsymbol{\sigma}$.

While the conditions that lead to a multivariate normal probability density function for both the prior and likelihood distributions are relatively common ones, it should be noted that other functions may be more appropriate in applications where alternative information is available (Ref. 1). For example, if there are estimates of the mean values but no uncertainty information, then an exponential function should be used. Another example might be that both central values and covariance matrices are available but the uncertainties are very large. Under these conditions, lognormal distributions should be used rather than normal distributions (Ref. 4). Lastly, if the experimental information is based entirely on raw detectors counts, then a Poisson distribution could be used for the likelihood function.

When Eqs. (1), (5), and (6) are combined, one obtains the expression

$$p(\boldsymbol{\sigma}) \sim \exp\{-(\tfrac{1}{2}) \left[\{(\mathbf{y} - \mathbf{y}_E)^T \bullet \mathbf{V}_E^{-1} \bullet (\mathbf{y} - \mathbf{y}_E)\} + \{(\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)^T \bullet \mathbf{V}_C^{-1} \bullet (\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)\} \right] \} \ . \quad (7)$$

Once again, the implied normalization constant is omitted for the reason mentioned above. Although it is not relevant to the present derivation, it is interesting to note that if we were to assume that the best solution for the evaluation corresponds to values of the components of $\boldsymbol{\sigma}$ that maximize $p(\boldsymbol{\sigma})$, then we would require that

$$[(\mathbf{y} - \mathbf{y}_E)^T \bullet \mathbf{V}_E^{-1} \bullet (\mathbf{y} - \mathbf{y}_E)] + [(\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)^T \bullet \mathbf{V}_C^{-1} \bullet (\boldsymbol{\sigma} - \boldsymbol{\sigma}_C)] = \text{minimum} \ . \quad (8)$$

However, this would be an appropriate assumption only if $p(\boldsymbol{\sigma})$ is a multivariate normal distribution with respect to the variables $\boldsymbol{\sigma}$ (e.g., Ref. 1). Acceptance of this assumption leads directly to the well-known generalized least-squares (GLS) formalism (e.g., Refs. 1 and 2).

Eq. (7), combined with Eqs. (2), (3), and (4), provides a way to carry out the numerical analysis required to produce an evaluation based on a direct consideration of the underlying probability density function. The difficulty in applying this approach lies in the need to compute multi-dimensional integrals. This is a formidable challenge to deterministic numerical computation when even a few variables are involved and impractical when many have to be considered as is the case for a typical evaluation. However, such calculations should be amenable to analysis by Monte Carlo simulation, at least to precisions which, in principle, are limited only by the number of traced histories. This is one of the premises upon which the present method is based.

Let us imagine pursuing K Monte Carlo histories. For each history a potential solution vector $\boldsymbol{\sigma}_k$ (k = 1,K) is generated. Each component of this vector is selected at random from its associated uniform distribution independently from all the others. A typical sampling range would be defined by:

$$\sigma_{i\text{-}min} \le \sigma_{ik} \le \sigma_{i\text{-}max} \qquad (i = 1,m \ ; \ k = 1,K) \quad (9)$$

Expressed another way, σ_{ik} is generated using the following formula:

$$\sigma_{ik} = \sigma_{i\text{-}min} + (\sigma_{i\text{-}max} - \sigma_{i\text{-}min}) \times (RN)_{ik} \quad (10)$$

where $(RN)_{ik}$ represents a real random number uniformly selected from the interval (0,1). The indicated intervals define a unique "rectangular" region $\mathcal{S}$ in m-dimensional space with volume $\mathcal{V}(\mathcal{S})$ given by the formula

$$\mathcal{V}(\mathcal{S}) = \Pi_{i=1,m} (\sigma_{i\text{-}max} - \sigma_{i\text{-}min}) \ . \quad (11)$$

Since the evaluation process is based on Eqs. (2), (3), (4), and (7), we proceed next to specify forms for these equations that are amenable to Monte Carlo analysis. The equivalent of Eq. (3) is

$$< \sigma_i >_K = [\Sigma_{k=1,K} \ \sigma_{ik} \ p(\boldsymbol{\sigma}_k)] \ / \ [\Sigma_{k=1,K} \ p(\boldsymbol{\sigma}_k)] \ , \qquad (i = 1,m) \quad (12)$$

while in the same fashion the equivalent to Eq. (4) is

$$\{\text{Cov}(\sigma_i,\sigma_j)\}_K = \{(\mathbf{V}_\sigma)_{ij}\}_K = \quad (13)$$

$$< \sigma_i \sigma_j >_K - < \sigma_i >_K \mathbf{x} < \sigma_j >_K \quad (i,j = 1,m) .$$

To avoid confusion, we note that

$$< \sigma_i \sigma_j >_K = [\Sigma_{k=1,K} \sigma_{ik} \sigma_{jk} p(\boldsymbol{\sigma}_k)] / [\Sigma_{k=1,K} p(\boldsymbol{\sigma}_k)] . \quad (i,j = 1,m) \tag{14}$$

The sums appearing in the denominators of Eqs. (12) and (14) are there to insure proper normalization. The index "K" which appears as a subscript in Eqs. (12) - (14) suggests that the values determined using these equations will depend quite strongly on the number of histories K, at least for relatively small K. In fact, for small K the results are essentially meaningless. However, as K becomes large it is anticipated that these quantities should converge toward the values that would be obtained if the corresponding integrations were actually performed as originally indicated in Eqs. (2) - (4). How large does K have to be to achieve acceptable convergence? This can be determined only from experience. The Monte Carlo approach has been demonstrated to work very well in the analysis of complex nuclear systems with many variables so it seems reasonable to apply it to the evaluation of nuclear data.

Thus, we see that the UMC evaluation method amounts to employing Bayes Theorem and the Principle of Maximum Entropy, along with the given prior and measured values and their covariance matrix elements as constants, to generate a posterior probability density function p for the random variables $\boldsymbol{\sigma}$ that correspond to the evaluation in question. The evaluated values $< \boldsymbol{\sigma} >$ are the first moments (or mean values) of the probability density function p while the elements of the solution covariance matrix $\mathbf{V}_\sigma$ are derived from the second moments of p. The integrals required to determine the mean values and the covariance matrix elements are estimated by Monte Carlo simulation rather than by deterministic numerical computations.

III. PRACTICAL CONSIDERATIONS

The following issues must be considered in practical applications of the UMC method: convergence, the compatibility of prior and experimental information, the independence of prior and experimental data, appropriate preparation of the measured data, and the consistency of prior and experimental information.

The UMC method will not succeed unless the quantities computed by Monte Carlo simulation using Eqs. (12) - (14) actually converge to stable values as K becomes large. Therefore, it is essential to test convergence by examining the trend of all expressions of the form $<\ldots>_K$ (or ratios of these quantities) as K becomes large. Rather than using sophisticated tests, simple plots of $<\ldots>_K$ versus K may suffice in many instances. Another convergence issue involves insuring that these sums converge to values close to the true value of the multivariable integrals that are being estimated. This requires that the "volume" $\mathcal{V}(\mathbb{S})$ of the sampling space $\mathbb{S}$ be sufficiently large. In particular, one needs to be certain that it is large enough so that outside region $\mathbb{S}$ the magnitude of the posterior probability density function p is vanishingly small. More precisely, if a sampled vector $\boldsymbol{\sigma}_k$ is not contained in $\mathbb{S}$, then $p(\boldsymbol{\sigma}_k) \approx 0$. Of course, one could insure this by choosing $\mathbb{S}$ to be very large. However, the penalty to pay for such a conservative choice is that K would also need to be extremely large in order to achieve acceptable convergence. This, in turn, would lead to excessively long computation times. Clearly, a tradeoff between the sizes of $\mathbb{S}$ and K is needed. Experience will have to be the guide in dealing with this issue. Finally, it is certain that a wide dynamic range of real number values will be encountered in computations of the $p(\boldsymbol{\sigma}_k)$ weighting factors. Therefore, a high degree of numerical precision is essential when performing realistic evaluations if one aims to achieve accurate results that are not afflicted by numerical round-off effects.

The input experimental and model-calculated information must be compatible. In setting up an evaluation exercise an evaluator needs to establish grid points (or node points) that define the scope of the evaluation. These grid points are characterized by such parameters as incident neutron energy, particle emission angle, etc. The situation is unambiguous for model-calculated prior results since they can be generated in a straightforward manner for all selected node points. For experimental results the situation is murkier. There are two issues involved. As indicated above, there is a reason why prior and posterior (solution) quantities are labeled "σ" while "y" is used to designate experimental results. The experimental results may be more complicated than simple cross sections. Consider a particular example. Among the experimental data included in vector $\mathbf{y}_E$, suppose one particular component, say y_{E7}, corresponds to a measured differential cross section ratio involving cross sections associated with grid points 6 and 18. We then require that $y_7 = f_7(\boldsymbol{\sigma}) = (\sigma_6/\sigma_{18})$. This must be reflected in the explicit expression for $p(\boldsymbol{\sigma})$. Another issue to consider is that to be perfectly compatible all input experimental information must be adjusted to correspond to the selected grid points. An example will clarify this point. Referring to the discussion above, let us suppose that the neutron energy corresponding to grid point 6 is 5 MeV while that for grid point 18 is 14 MeV. Then y_7, as defined above, is meant to represent a ratio corresponding exactly to these two energies. However, let us suppose that the measured value y_{E7} actually corresponds to a ratio involving

experimental energies 4.9 MeV and 14.1 MeV. Then, it is necessary to adjust the measured value y_{E7} as needed so that it is compatible with y_7. These details are not unique to the present method. In principle, they need to be considered in order to apply correctly any of the more commonly used evaluation techniques, including the generalized least-squares (GLS) method.

The formalism for the UMC method described in Section II requires that the prior information and the experimental information that are to be merged to generate an evaluation be independent. Therefore, it is important that the selection of nuclear model parameters and their uncertainties be influenced as little as possible by experimental data relevant to the specific nucleus for which the evaluation in question is being carried out. A reasonable way to achieve an adequate degree of independence is for the choice of nuclear model parameters used to generate the prior to be guided by global considerations, e.g., by knowledge gained from consideration of a wide range of nuclei across the Periodic Table rather than strictly by narrow regional or local nuclear model behavior.

The need to adjust experimental data so that they will correspond to calculated values at the selected grid points has been mentioned above. It is also necessary to be concerned with the actual quality of the experimental data used in an evaluation, regardless of the method used to perform the evaluation. Poor quality experimental data and incomplete or improperly constructed covariance matrices can thwart the evaluation process and lead to erroneous results. The need for weeding out bad data, applying adjustments for changes in measurement standards, possibly enhancing some unrealistically small uncertainties assigned by original authors, and other routine data "adjustment" steps is widely acknowledged by evaluators as absolutely necessary if one is to obtain reasonable evaluated results.

The last practical issue to be discussed is that of data consistency. By examining the data "consistency", we are studying the relative scatter of the results that are to be used in an evaluation. In the generalized least-squares (GLS) formalism it is well known that there exists a chi-square test of input data consistency that can be applied before the GLS analysis is performed (e.g., Refs. 1 and 2). Since this test involves only the input data it seems reasonable to consider applying it in the present UMC methodology as well. The formula used in this test of consistency is as follows:

$$\chi^2/(\text{d.o.f.}) = [(\mathbf{y}_E - \mathbf{q})^T \bullet (\mathbf{V}_q + \mathbf{V}_E)^{-1} \bullet (\mathbf{y}_E - \mathbf{q})] / n \, . \quad (15)$$

This expression and some of the quantities appearing therein require some explanation. In the present formalism, the degrees of freedom (d.o.f.) are just the number of experimental data values "n". The quantities $\mathbf{y}_E$ and $\mathbf{V}_E$ require no explanation; they are defined above. The vector $\mathbf{q}$ is the collection of n calculated equivalents to the measured data based on prior values of the variables to be evaluated (not on solution values), i.e., on $\boldsymbol{\sigma}_C$ and $\mathbf{V}_C$. In other words, $\mathbf{q} = \mathbf{f}(\boldsymbol{\sigma}_C)$. Furthermore, $\mathbf{V}_q$ is an "n x n" covariance matrix which is computed by propagating the errors of $\boldsymbol{\sigma}_C$, as reflected in the covariance matrix $\mathbf{V}_C$, through to $\mathbf{V}_q$ via the functional relationships represented by $\mathbf{f}$. It is clear from Eq. (15) that the matrix $\mathbf{V}_q + \mathbf{V}_E$ needs to be inverted so it must first be tested for positive definiteness. Eq. (15) provides a means to compute the scatter of the experimental data relative to equivalent calculated values (the word "equivalent" is significant here), scaled by the combined uncertainties of the experimental and calculated results. The general rule to follow is that when $\chi^2/(\text{d.o.f.}) \leq 1$, then the uncertainties in the evaluated results generated by the UMC method ought to be accepted as they are. However, if $\chi^2/(\text{d.o.f.})$ is significantly larger than unity, one might consider enhancing all the evaluation solution uncertainties by the factor $[\chi^2/(\text{d.o.f.})]^{1/2}$ without altering the correlations (Ref. 1).

IV. AN EXAMPLE

The example presented here includes all the essential aspects of a realistic evaluation problem, but it is simplified to the point where the analysis is both straightforward and transparent. In spite of the simplicity, it serves the purpose to demonstrate the viability of the UMC method proposed in this memorandum.

The mathematical "model" chosen to determine the prior values for this example is defined by the function

$$s(E) = p_1 \text{ x } E \text{ x } \exp(-E/p_2) \, , \quad (16)$$

where p_1 and p_2 are the model "parameters" and E is a continuous variable. The mean values and errors (standard deviations) of these model parameters are chosen arbitrarily as follows: $\langle p_1 \rangle = 10$, $SD(p_1) = 1$, $\langle p_2 \rangle = 2$, and $SD(p_2) = 0.2$ ("SD" signifies standard deviation). The parameter uncertainties are obviously 10%. It is assumed that these parameters errors are uncorrelated.

To narrow the scope of this example, we choose to consider only two grid points for the present evaluation. These are defined by E = 1 and E = 3 (units are irrelevant here). Using the "model" described above, it is straightforward to determine the two calculated values which form a vector that we label $\mathbf{s}_C$. The two components

are s_{C1} and s_{C2}. To insure that there will be no confusion regarding this exercise, we have replaced "σ" by "s" (for both model-calculated and experimental results) since we are not actually dealing with cross sections in this example. Continuing with the analysis, the Monte Carlo methodology described in Ref. 3 is used to determine the prior covariance matrix $\mathbf{V}_C$. The parameters p_1 and p_2 are sampled randomly from uniform distributions whose limits are consistent with the assigned mean values and standard deviations. Values for the priors used in this example are given in Table I (shown to at most four significant figures).

TABLE I: Prior Values ($\mathbf{s}_C$ and $\mathbf{V}_C$)

$(Index)_i$	E_i	s_{Ci}	$(SD)_{Ci}$	$(Error)_{Ci}$	$\mathbf{V}_C$	
1	1	6.065	0.6790	11.19%	0.4610	0.7130
2	3	6.694	1.211	18.09%	0.7130	1.466

The covariance matrix $\mathbf{V}_C$ is positive definite so it can be inverted. The correlation for the calculated values of $\mathbf{s}_C$ is 0.8675 (shown to four significant figures), or 86.75%. This strong correlation is typical of what one generally observes for calculations based on much more complicated and realistic nuclear models.

The next step is to introduce two pseudo "experimental" data points, represented by $\mathbf{s}_E$, which are intended to be used in conjunction with the calculated prior values in this example. We choose values for these "experimental" data that are not in very good agreement (inconsistent) with the corresponding model-calculated ones. These "experimental" data, however, are entirely comparable to the model-calculated results (no ratios, no departures from grid points, etc.). In other words, the two "experimental" data points, s_{E1} and s_{E2}, correspond to E = 1 and 3, respectively, so they can be compared directly with their calculated counterparts, s_{C1} and s_{C2}. These "experimental" results can be used in the evaluation with no additional preparation required. We assume these "experimental" data to be fairly accurate (5% uncertainty for each data point) with strong error correlation (80%). This is reflected in the data covariance matrix $\mathbf{V}_E$. Table II summarizes the "experimental" input information for this example (shown to at most four significant figures).

TABLE II: Pseudo Experimental Data ($\mathbf{s}_E$ and $\mathbf{V}_E$)

$(Index)_i$	E_i	S_{Ei}	$(SD)_{Ei}$	$(Error)_{Ei}$	$\mathbf{V}_E$	
1	1	6.5	0.325	5%	0.1056	0.0793
2	3	6.1	0.305	5%	0.0793	0.09303

For the purposes of this example, we choose to randomly sample s_1 uniformly in the interval (4,9) and s_2 uniformly in the interval (2,10). These intervals are generously large considering the input data as well as the solution results we are likely to obtain, so we refer to them as the "Wide Limits" condition. The first step in the treatment of this example was to solve the evaluation problem using the conventional generalized least-squares (GLS) method (Ref. 2) in order to provide a baseline for comparison with the results of the UMC procedure. Next, a single UMC simulation exercise was performed using K = 1000 histories. The progress toward convergence of $\langle s_1 \rangle_K$ (based on Eq. 12) as a function of the number of histories K is shown in Fig. 1.

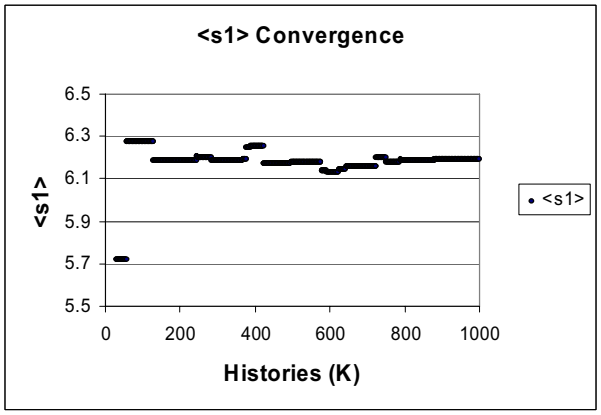

Fig. 1. Convergence of $\langle s_1 \rangle$ vs. number of histories (K)

This plot suggests that a reasonable degree of convergence is achieved for K = 1000. However, it was decided to repeat this exercise nine more times in order to examine the scatter of $\langle s_1 \rangle$ resulting from ten independent sets of 1000 random trials in more explicit terms. An average of the ten independent determinations of $\langle s_1 \rangle$ was also computed to yield the equivalent of what would have been obtained directly from K = 10,000 histories. The outcome is illustrated in Fig. 2.

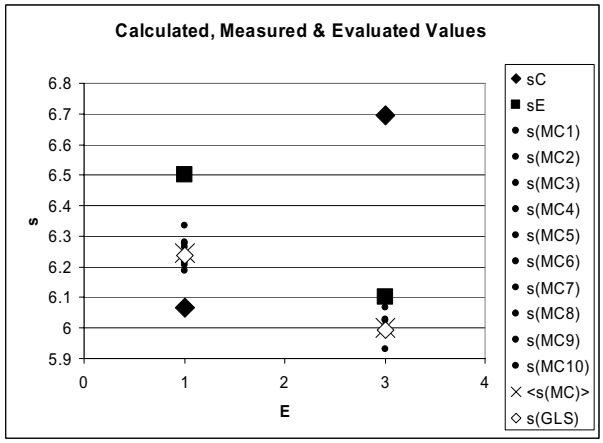

Fig. 2. Summary of results from the present exercise.

We can learn several things about this exercise and the UMC method from an inspection of Fig. 2. Although

Fig. 1 suggests that there is a measure of convergence for K = 1000 histories, it is clear from Fig. 2 that while the results from ten independent sets of these Monte Carlo simulations do clump together reasonably well, the scatter is still noticeable. On the other hand, the average of these ten results lies very close to the generalized least-squares (GLS) solution. Thus, it appears that K = 10,000 histories is quite sufficient for practical purposes to achieve convergence in this example. In this simple example where the experimental data are completely compatible with the calculated (prior) results – if not very consistent with them – it is not surprising that the UMC and GLS methods give results that are in quite good agreement as long as convergence is achieved for the UMC simulation analysis. The nature of this agreement is indicated in more quantitative terms in Table III (values are shown to at most four significant figures).

Table III. Summary of Results from the Present Exercise

Quantity	<UMC>	GLS	Difference
$<s_1>$	6.245	6.237	0.14%
$<s_2>$	6.002	5.992	0.18%
$Var(s_1)$	0.07252	0.07556	-4.18%
$SD(s_1)$	0.2674	0.2749	-2.79%
% Error (s_1)	4.28%	4.41%	-2.96%
$Var(s_2)$	0.07638	0.08122	-6.33%
$SD(s_2)$	0.2751	0.2850	-3.60%
% Error (s_2)	4.58%	4.76%	-3.76%
$Cov(s_1,s_2)$	0.05802	0.06181	-6.53%
$Corr(s_1,s_2)$	0.7728	0.7890	-2.10%

Let us consider another question. What happens when the sampling limits are tightened significantly? To explore this question, the sampling limits were tightened as follows: to (5.4,7.1) for s_1 and to (5.1,6.9) for s_2. These limits are referred to as the "Tight Limits" condition. The ten sets of UMC calculations described above were repeated with these new parameter limiting conditions. The details are omitted for brevity. The main outcome is that much less scatter is observed for the ten sets of UMC results and somewhat closer agreement between the average of these individual UMC values and GLS solution is obtained. Actually, the numerical differences between the results obtained using the "Wide Limits" and "Tight Limits" conditions are not particularly significant considering the input data uncertainties. This supports the notion that adequate convergence will be obtained as long as the sampling space $\mathbb{S}$ is sufficiently large, but extending that space further will lead to minimal improvement with the requirement of a larger number of histories K to achieve convergence. Striking a practical balance between the size of the sampling space $\mathbb{S}$ and the number of Monte Carlo histories K clearly involves compromises that need to be worked out through experience gained with realistic evaluations. In the present example it was learned that a good compromise would be a sampling space defined by limits falling between the "Wide Limits" and "Tight Limits" conditions and a number of Monte Carlo histories somewhere between K = 1000 and K = 10,000.

Finally, the consistency of the input data was tested. This test is based on Eq. (15), as discussed in Section III. The result for the input information of this example is χ^2/(d.o.f.) = 1.737 (to four significant figures). Thus, in accordance with the discussion above, we are justified in multiplying the solution uncertainties by the square root of this number to compensate for the discrepancy (data inconsistency) indicated by this test. This assumes that the underlying source of the discrepancy cannot be eliminated by other means (which is the case for this example). This step leads to an increase in the errors derived by the UMC evaluation method, which should be reflected in the final evaluation, by ≈ 30 % to values on the order of 6 %.

V. CONCLUSIONS

The example given in the preceding section demonstrates that the UMC evaluation method can yield reasonable results. A comparison with the well-established GLS method for conditions that that tend to favor agreement between these two methods does indeed indicate that very reasonable agreement is obtained to within the statistical precision of this exercise.

What, then, are the advantages and disadvantages of the UMC method when compared to the GLS method? The main advantage of the UMC method is that it involves no mathematical approximations. It is completely rigorous provided that the form of the probability density function dictated by the Principle of Maximum Entropy is accepted. Of course, this same principle lies at the foundation of the GLS method as well. The approximations inherent in the GLS method, as discussed in Section II and embodied in Eq. (8), can lead to complications if the posterior probability density function is not normal with respect to the collection of solution variables $\boldsymbol{\sigma}$ (Ref. 1). When the probability density function is thus skewed, the mean values of the variables will not coincide with those yielding the peak of the function. This will be the case if some or all of the experimental data are complicated functions of these variables, e.g., ratios or certain integral quantities, or if the experimental data included in the evaluation fail to be essentially normally distributed. Under these conditions, noticeable computational biases will emerge in the GLS solution that would not be present if the UMC method were applied. A further advantage of the UMC method is that it does not require that certain expressions be linear (or approximately linear) as is the case for the GLS method. Strong non-linear effects are frequently

encountered in nuclear modeling so this can be a serious problem if the model parameter uncertainties are large. When dealing with indirect experimental data such as ratio data, in the presence of large uncertainties, similar problems can emerge.

The only clear disadvantage of the UMC method is that in realistic evaluation exercises it is likely to be quite demanding of computational resources. The prior and experimental data covariance matrices need to be inverted only once. However, extensive matrix multiplications are involved in applying the UMC method, in proportion to the number of histories traced during the simulation process. This author reached the conclusion in 1991 that any approach to nuclear data evaluation that required the evaluation of large multivariable integrals was likely to be impractical (Ref. 1). However, in the intervening 16 years available computational power has increased by several orders of magnitude with significantly reduced cost. This alters the situation dramatically from earlier times, and it has led this author to revise his opinion. Today (in 2007), it appears that evaluations that employ the UMC method should be both feasible and practical, especially when the circumstances of a particular evaluation exercise warrant adherence to rigor and avoidance of approximations that could lead to unacceptable computational biases in the evaluated solutions.

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