An Analytical Solution to Sensitivity/Uncertainty Equations at Different Enrichments for Criticality Code Validation

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Abstract

This paper reviews current Sensitivity/Uncertainty (S/U) methodology as applied to code validation for criticality safety and shows how the method may be used to analyze the correlation of a single parameter through the application of suitable approximations. S/U methodology based upon perturbation theory has been used to develop special parameters called sensitivity coefficients which may be used to determine the applicability of benchmarks. Uncertainty analysis uses the sensitivity coefficients to determine the propagated error in k_{eff} due to the experimental uncertainties in the underlying cross sections, which are major contributors to the bias. An overview of S/U methodology is provided to highlight the principle assumptions and components of the method and show drawbacks of the method due to complexity. An analytical approximation is then developed for a single parameter, enrichment, to show how the method may be used to demonstrate correlation when all but one parameter is constant. The correlation parameters determined for this special case are graphically displayed. Enrichment was chosen as the trending parameter because validation of criticality code calculations for enrichments >5wt% ^{235}U is currently of interest and because the effect on the combined cross section of changing the enrichment is easily predicted and expressed in equation form.

Introduction

Sensitivity/Uncertainty (S/U) methodology has recently been applied to the problem of criticality code validation, in particular to the rigorous determination of the area of applicability. These methods are especially useful for establishing the applicability of benchmark experiments to particular situations. Draft NUREG/CR-5593, Vol.1[1], discusses the use of first-order perturbation theory to determine the sensitivity of calculated k_{eff}'s to small changes or uncertainties in the underlying cross section data. The method allows the contributions of various cross section uncertainties in the bias to be evaluated, providing a more rigorous understanding of trends in the bias and allowing for applicability determinations of benchmarks to specific applications. Following a brief review of S/U methodology, we demonstrate an approximate analytical method of evaluating the area of applicability for cases differing only in enrichment.

Overview of S/U Methodology

The S/U methods discussed in draft NUREG/CR-5593 are based on first-order perturbation theory to derive an approximation to the change in k_{eff} due to a small change in the Boltzmann transport equation linear operators.[2345] The transport equation may be written in eigenvalue form $\{A-\lambda B\}|\Phi\rangle=0$, where Φ represents the neutron flux, A consists of the neutron transport, scattering, and absorption terms, and B represents the neutron fission term. λ is therefore k_{eff}^{-1}, the proportionality constant of the fission source term. There is a similar adjoint equation $\langle\Phi^*|\{A^* -\lambda B^*\}=0$ that must be satisfied. The perturbed operators,

eigenvalue, and flux $A'=A+\delta A$, $B'=B+\delta B$, and $\lambda'=\lambda+\delta\lambda$ and Φ' may be substituted into this equation. This is an exact equation, and can in principle be solved for the new eigenvalue and eigenfunctions. Due to the practical difficulty in determining the modified flux distribution, we can make the standard assumption in perturbation theory that $\Phi'=\Phi$. Thus the goal becomes to estimate the effect of small changes in the linear operators on the eigenvalue λ.

The perturbed eigenvalue equation may be left-multiplied by the adjoint flux Φ^* and the adjoint equation right-multiplied by the flux Φ, and the results subtracted.

$$\langle \Phi^* | A'\Phi \rangle - \langle \Phi^* A^* | \Phi \rangle - \langle \Phi^* | \lambda' B' \Phi \rangle + \langle \Phi^* \lambda B^* | \Phi \rangle = 0. \qquad \text{(Eq.1)}$$

Substituting the values of A', B', and λ', and making use of the adjoint properties $\langle \Phi^* | A\Phi \rangle = \langle \Phi^* A^* | \Phi \rangle$ and $\langle \Phi^* | B\Phi \rangle = \langle \Phi^* B^* | \Phi \rangle$, the terms in A,A^* and B,B^* cancel out. Dropping the term in $\delta B\delta\lambda$, as a second-order perturbation, the following expression is derived:

$$\langle \Phi^* | \delta A\Phi \rangle - \langle \Phi^* | \{\lambda(\delta B) + (\delta\lambda)B\}\Phi \rangle = 0. \qquad \text{(Eq.2)}$$

Rearranging terms to solve for $\delta\lambda$ yields:

$$\delta\lambda = \lambda' - \lambda = -(k'-k)/kk' = \langle \Phi^* | (\delta A - \lambda\delta B)\Phi \rangle \div \langle \Phi^* | B\Phi \rangle \qquad \text{(Eq.3)}$$

The sensitivity coefficients S_k are defined in terms of this expression. $S_k = \delta\lambda/\lambda \div \delta\Sigma/\Sigma$, that is, the fractional change in k_{eff} as a proportion to some corresponding fractional change in one of the underlying cross sections. A total sensitivity can be derived or a sensitivity profile for each energy group and nuclear reaction (capture, absorption, fission) can be derived. The expression above becomes:

$$S_k = \Sigma/\lambda \cdot \langle \Phi^* | (\partial A/\partial\Sigma - \lambda\, \partial B/\partial\Sigma)\Phi \rangle / \langle \Phi^* | B\Phi \rangle. \qquad \text{(Eq.4)}$$

Evaluation of these sensitivity coefficients therefore requires that the forward and adjoint flux Φ and Φ^* be determined. In the sensitivity package at Oak Ridge National Laboratory, the SCALE module SEN1 (Draft NUREG/CR-5593) has been used to determine the neutron fluxes. This information currently is derived by SEN1 using a 1-D discrete ordinates approach (XSDRNPM deterministic code); the capability to extend this method to generation of 2-D sensitivities is available, but has not been fully integrated into the SCALE code package. Once the $S_k = S_{ij} \equiv \partial k_i/\partial\sigma_j$ ($i = 1,...,I$ benchmark cases; $j = 1,...,N$ cross sections) are computed for each cross section, the uncertainties in the cross section data can be propagated to produce an uncertainty matrix in k_{eff}.

If $C_{\alpha\alpha}$ is the NxN uncertainty matrix of cross section data, then these are propagated to the IxI uncertainty matrix C_{kk} by the equation:

$$C_{kk} = S_k C_{\alpha\alpha} S_k^T. \qquad \text{(Eq.5)}$$

The diagonal elements C_{ii} represent the total *variance* of the i^{th} benchmark case, due to uncertainties in the underlying cross section data. The off-diagonal elements C_{ij} represent the *covariance* between the i^{th} and j^{th} benchmark cases, representing the degree to which they contain common variance due to shared cross section contributions. The uncertainty matrix is generally formed by normalizing the off-diagonal elements by the square root of the corresponding diagonal element. If this *correlation coefficient* C_{ij} is equal to zero, the two benchmarks are considered entirely uncorrelated; if $C_{ij} = 1$, the benchmarks are fully correlated; if $C_{ij} = -1$, they are fully anti-correlated. Experience in Draft NUREG/CR-5593

demonstrates that two or more cases can be considered sufficiently correlated to be grouped together for purposes of bias determination –that is, they can be expected to have biases produced by the same cross section uncertainties and are thus in the same area of applicability– if the normalized off-diagonal elements of C_{kk} are ≥ 0.8.

The above method is useful for determining the first-order sensitivity of k_{eff} to different underlying cross section data. Drawbacks of the method include that it requires the calculation of the forward and adjoint flux and is limited to use with systems that can be reasonably represented by 1-D or 2-D models. Later in this paper, we will derive expressions that do not require the generation of this detailed flux information, though these are more limited in scope.

Uncertainty analysis uses the sensitivity coefficients S_k to determine the propagated error of k_{eff} due to the experimental uncertainties in the underlying cross sections, which are major contributors to the bias. This technique also determines the degree of shared covariance (that is, correlation) between different sets of benchmark experiments. This is useful because the degree to which covariance is shared between two benchmarks, or sets of benchmarks, provides information about the degree to which the behavior of the bias can be expected to be related between the two cases.

Analytical Approximation

The main disadvantage of the above method is the determination of the forward and adjoint flux for the systems of interest, which are generally calculated using a 1-D or 2-D Discrete Ordinates Code such as XSDRNPM. This requires that the system be readily reduced to a simple geometrical model, and also requires generation of a large amount of nuclear data from the calculations.

Presented below is an analytical approximation to the sensitivity and uncertainty coefficients derived in their general form in the previous section. This type of analysis can be generalized to any parameter of the system of which k_{eff} is a function. Enrichment is chosen here for two reasons: (1) validation of criticality code calculations for enrichments >5wt% ^{235}U is currently of interest to the NRC and its licensees, and (2) total cross section can be expressed easily as a function of the underlying ^{235}U and ^{238}U cross sections in terms of the enrichment.

We express the total cross section of two systems in the following manner:

$$\sigma_1^i = \sigma_A^i \varepsilon_1 + \sigma_B^i (1-\varepsilon_1) \qquad \text{(Eq.6)}$$
$$\sigma_2^i = \sigma_A^i \varepsilon_2 + \sigma_B^i (1-\varepsilon_2),$$

where σ_A^i, σ_B^i are the i^{th} ^{235}U and ^{238}U cross sections, where i can range over the set of energy groups of the system and/or nuclear processes (capture, scattering, and fission). This can be done using total cross sections or, by setting up similar equations for each neutron energy group, as a profile. σ_1^i, σ_2^i are the combined cross section for the first or second system, at enrichments ε_1 and ε_2 respectively. The above equation is not rigorously true, since ε is defined in terms of weight-percent and not volume-fraction, but is a reasonable approximation for our purposes. The nuclear cross sections σ_A^i, σ_B^i have experimental uncertainties associated with them, which we will denote δ_A^i and δ_B^i. Through use of the standard error propagation equation,

$$d\sigma^2 = (\partial\sigma/\partial\sigma_A)^2 \, d\sigma_A^2 + (\partial\sigma/\partial\sigma_B)^2 \, d\sigma_B^2 \qquad \text{(Eq.7)}$$

we derive the expressions for the total error in σ:

$$\delta_1^2 = \varepsilon_1^2 \delta_A^2 + (1-\varepsilon_1)^2 \delta_B^2 \qquad \text{(Eq.8)}$$
$$\delta_2^2 = \varepsilon_2^2 \delta_A^2 + (1-\varepsilon_2)^2 \delta_B^2,$$

where the indices for nuclear reactions and energy group have been dropped for simplicity.

To derive the sensitivity coefficients, the functional dependence of k_{eff} on the cross section must be determined. Let us suppose that the difference in k_{eff} depends only on the total cross section, that is, that everything about the two systems is identical except for the underlying nuclear cross sections and the enrichment. All the difference between the two systems is caused by this difference in the cross section data. Making a linear approximation, we write $k_{eff} = k_0 + \alpha\,(\sigma-\sigma_0) + O(\sigma^2)$. A non-linear approximation can be shown to produce a similar result due to weak dependence of correlation on the functional relationship. The sensitivity coefficients S_k are nothing more than the fraction change in k_{eff} produced by a corresponding change in the cross section of interest. $S_k = (\delta k/k)/(\delta\sigma/\sigma) = (\sigma/k)(\partial k/\partial\sigma)$. Substituting the above expressions for $k(\sigma)$:

$$S_{A1} = (\sigma_1/k)\,\alpha\varepsilon_1. \quad S_{B1} = (\sigma_1/k)\,\alpha(1-\varepsilon_1). \qquad \text{(Eq.9)}$$
$$S_{A2} = (\sigma_2/k)\,\alpha\varepsilon_2. \quad S_{B1} = (\sigma_2/k)\,\alpha(1-\varepsilon_2).$$

This gives us a 2x2 sensitivity matrix, in terms of the enrichments of the two systems. Although these appear to be linear equations in enrichment, note that the cross sections σ_1 and σ_2 are the total cross sections, themselves functions of enrichment. The advantage to the fact that the above equations are all linear in α (assumed constant) is that α can be removed from the matrix as a common factor, and cancels out when the ratio between the diagonal and off-diagonal elements is formed (Equation 11). Because the two cases are both benchmark critical experiments, we can further assume that $k_1 = k_2 = 1$, which also cancels.

The uncertainty matrix, C_{aa}, in the notation of the previous section and draft NUREG/CR-5593, is a diagonal 2x2 matrix with $C_{11} = \delta_A^2$, $C_{22} = \delta_B^2$. The off-diagonal elements are assumed zero, since the errors in the ^{235}U and ^{238}U cross sections are assumed to be uncorrelated. Forming the product $C_{kk} = S_k C_{aa} S_k^T$ for the propagated uncertainty matrix yields the following terms:

$$C_{11} = \sigma_1^2\varepsilon_1^2\delta_A^2 + \sigma_1^2(1-\varepsilon_1)^2\delta_B^2 \qquad \text{(Eq.10a)}$$
$$C_{12} = C_{21} = \sigma_1\sigma_2\varepsilon_1\varepsilon_2\delta_A^2 + \sigma_1\sigma_2(1-\varepsilon_1)(1-\varepsilon_2)\delta_B^2 \qquad \text{(Eq.10b)}$$
$$C_{22} = \sigma_2^2\varepsilon_2^2\delta_A^2 + \sigma_2^2(1-\varepsilon_2)^2\delta_B^2 \qquad \text{(Eq.10c)}$$

Note that the diagonal terms C_{11} and C_{22} are the same expressions for the combined variance $\mathrm{Var}(\sigma_1)$ and $\mathrm{Var}(\sigma_2)$ as those we derived using the error propagation equation (Equation 7). The standard expression[6] for the correlation coefficient is $\rho_{12} = \mathrm{Cov}(\sigma_1,\sigma_2)/\sqrt{\mathrm{Var}(\sigma_1)}\sqrt{\mathrm{Var}(\sigma_2)} = C_{12}/\sqrt{C_{11}}\sqrt{C_{22}}$.

$$\rho = \frac{\left\{\sigma_1\sigma_2\varepsilon_1\varepsilon_2\delta_A^2 + \sigma_1\sigma_2(1-\varepsilon_1)(1-\varepsilon_2)\delta_B^2\right\}}{\sqrt{\left\{\sigma_1^2\varepsilon_1^2\delta_A^2 + \sigma_1^2(1-\varepsilon_1)^2\delta_B^2\right\}}\ \sqrt{\left\{\sigma_2^2\varepsilon_2^2\delta_A^2 + \sigma_2^2(1-\varepsilon_2)^2\delta_B^2\right\}}} \qquad \text{(Eq.11)}$$

This expression may be simplified by defining the vector $\mathbf{x_1} = (\sigma_1\varepsilon_1\delta_A,\ \sigma_1(1-\varepsilon_1)\delta_B)$ and $\mathbf{x_2} = (\sigma_2\varepsilon_2\delta_A,\ \sigma_2(1-\varepsilon_2)\delta_B)$, corresponding to the two configurations being compared.

It can be shown that the correlation parameter ρ is the dot product between these two vectors. That is,

$$\rho = (\mathbf{x}_1 \cdot \mathbf{x}_2)/|\mathbf{x}_1||\mathbf{x}_2|. \qquad \text{(Eq.12)}$$

Applications

We can make use of the above definition to demonstrate that this parameter ρ has all the properties that make it suitable for use as a correlation coefficient as defined in the standard S/U methodology. In order to be of use it must be self-consistent; that is, when $\varepsilon_1 = \varepsilon_2$, it should be true that $\rho = 1$. In addition, the parameter must be bounded between the values of 0 and 1 inclusive. That the first is the case can be shown by substituting $\varepsilon=\varepsilon_1=\varepsilon_2$ into Equation 11 or by virtue of Equation 12. That the second is the case can be seen readily by Equation 12.

Recall the underlying assumption, that the k_{eff} values of the two systems depend only on the magnitude of the cross section, or $k_{eff} = k(\sigma)$. This assumption implies that the two systems have identical moderation (H/X), average neutron energy (energy corresponding to average lethargy causing fission, of ECALCF), geometrical arrangement, materials, and all other parameters which influence k_{eff} except enrichment. In trending the behavior of the calculational bias as a function of enrichment, holding all other parameters of the system constant would be the ideal situation. The physical interpretation of the above "correlation parameter" is therefore that it represents the maximum degree of correlation –the degree of shared covariance– between two benchmark cases at different enrichments, that is, between two cases having identical physical and neutronic parameters and differing only in the enrichment. The actual correlation between any two systems would be less than ρ, in general, since the degree of shared covariance would be decreased due to factors other than the enrichment.

Figure 1 demonstrates the calculated correlation parameter $\rho(\varepsilon_1,\varepsilon_2)$ for two systems as a function of ε_2, with $\varepsilon_1 = 0.05$ (5wt% ^{235}U). Here we have assumed for simplicity $\sigma_A = \sigma_B = 1$ (arbitrary units). A more sophisticated treatment would utilize the actual group-wise cross section data and develop a profile $\rho(\varepsilon_1,\varepsilon_2;g_{ij})$ as a function of the neutron energy group i for nuclear reaction j, $i = 1,2,...,N$ and $j = c,s,f$ (capture, scattering, and fission.) Varying the relative values of σ_A, σ_B, shows that in general the correlation parameter is fairly insensitive to the ratio σ_A/σ_B.

Figure 2 graphs $\rho(0.5, \varepsilon_2)$ for $\sigma_A/\sigma_B = 100$ (again, arbitrary units), to simulate the effect of having a highly thermal as opposed to intermediate or fast system. The 50wt% ^{235}U condition is chosen just to illustrate that the correlation curve is correctly normalized and well-behaved over the entire range. A comparison of Figures 1 and 2 shows that there is surprisingly little difference between the range for fast and thermal systems. Draft NUREG/CR-5593 derives the correlation coefficients C_{kk} for systems with 2, 3, 5, and 11wt% ^{235}U enrichments, over a wide variety of neutron energies, and shows that the 11wt% data available was only weakly coupled to the 5wt% data ($\Delta\varepsilon$~6%). If we adopt the criteria that two benchmarks can be considered correlated if $C_{kk} > 0.8$, the two figures show a maximum range of correlation of $\Delta\varepsilon$~40%. These results show that the dominant source of differences between the benchmark data can be attributed to factors other than the enrichment, and that it is *in principle* possible to correlate cases with enrichments over a relatively wide range. The practical matter, however, is that other considerations may well restrict the area of applicability significantly.

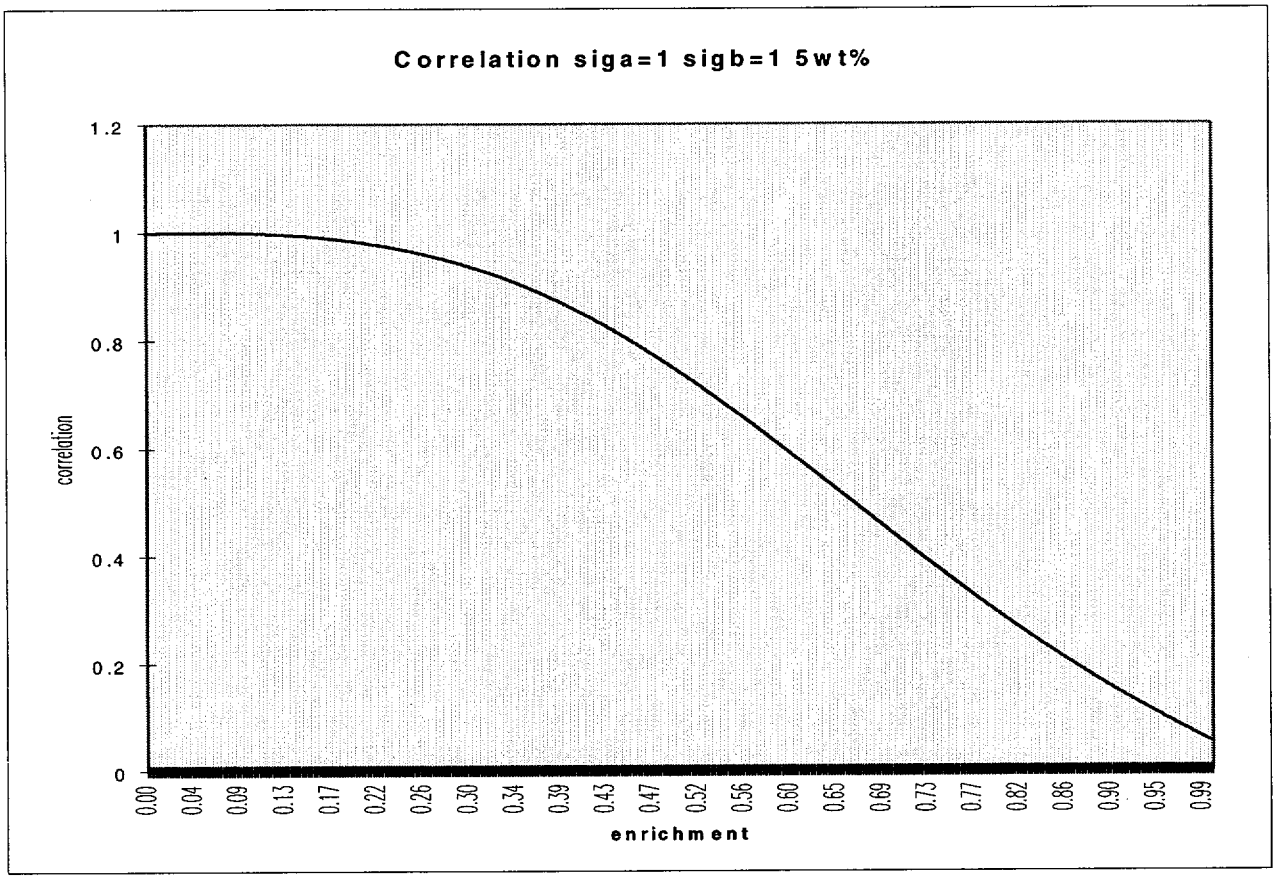

Figure 1

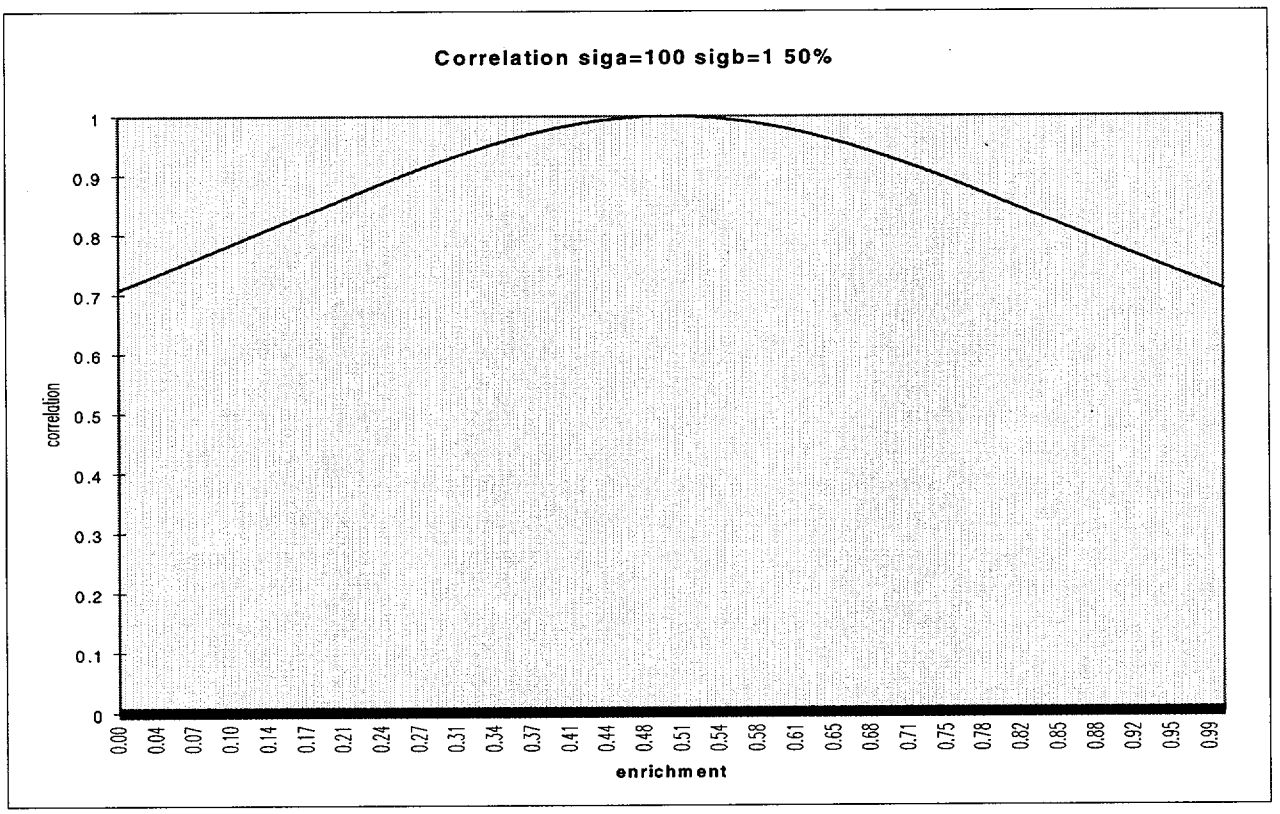

Figure 2

Possible Generalization

As stated initially, the enrichment was chosen as the trending parameter partly because the effect on the combined cross section of changing the enrichment is easily predicted and expressed in equation form. There is nothing unique about enrichment, however, and it is in principle possible to extend the technique to explore the development of the correlation between benchmark cases as a function of other parameters. Typically, the neutron energy (ECALCF) and moderation level (H/X) will have a stronger influence on the bias than the enrichment alone. This may be done by generalizing the above equations. Let k_{eff} be a function of N nuclear variables, thus: $k_{eff} = k(\xi_1, \xi_2,...,\xi_N)$. Linearizing, we approximate k_{eff} for the i^{th} benchmark by $k_i(\xi_1, \xi_2,...,\xi_N) = k_{0i} + \alpha_1\xi_{i1} + \alpha_2\xi_{i2} + ... + \alpha_N\xi_{iN}$. The S_{ij} ($i = i^{th}$ benchmark case, $j = j^{th}$ nuclear of physical parameter) can be defined as $S_{ij} = (\xi_{ij}/k_i)(\partial k_i/\partial\xi_{ij}) = \alpha_j\xi_{ij}/k_i$. If these are all critical experiments, we can make the further approximation that $k_1=k_2=...=k_N=1$ and then $S_{ij} = \alpha_j\xi_{ij}$. The $C_{\alpha\alpha}$ matrix is a diagonal matrix consisting of the variances $\delta\xi_j^2$. We can then derive the propagated uncertainty matrix in similar fashion by defining $C_{kk} = SC_{\alpha\alpha}S^T$. Then $\rho(\xi_{11},\xi_{12},...,\xi_{1N}; \xi_{21},\xi_{22},...,\xi_{2N})$ can be defined as $C_{12}/\sqrt{C_{11}}\sqrt{C_{22}}$.

In terms of the sensitivity vectors, we can show that $\mathbf{x}_1 = (\alpha_1\xi_{11}\delta\xi_1, \alpha_2\xi_{12}\delta\xi_2,...,\alpha_N\xi_{1N}\delta\xi_N)$ and $\mathbf{x}_2 = (\alpha_1\xi_{21}\delta\xi_1, \alpha_2\xi_{22}\delta\xi_2,...,\alpha_N\xi_{2N}\delta\xi_N)$. Alternately, we can express these in terms of the sensitivity coefficients as $\mathbf{x}_1 = (S_{11}\delta\xi_1, S_{12}\delta\xi_2,...,S_{1N}\delta\xi_N)$ and $\mathbf{x}_2 = (S_{21}\delta\xi_1, S_{22}\delta\xi_2,...,S_{2N}\delta\xi_N)$. We can see from Equation 9 that these relations are also true for the specific solution when k_{eff} is expressed in terms of the enrichment ε. Then one can show by matrix multiplication that Equation 12 still holds; that is, that $\mathrm{Var}(k_i)=|\mathbf{x}_i|^2$ and that the correlation parameter $\rho = (\mathbf{x}_1 \cdot \mathbf{x}_2)/|\mathbf{x}_1||\mathbf{x}_2|$. This is somewhat more difficult to solve than that for enrichment, because multiple parameters may be involved and it is thus necessary to determine the α_i. But assuming that the behavior of k_{eff} can be parameterized in terms of the underlying parameters, this technique can yield a semi-quantitative measure of the correlation between benchmarks which differ according to these parameters.

Conclusion

This paper demonstrates that it is possible to derive a first-order correlation parameter expressing the shared covariance between two benchmark cases, identical except for ^{235}U enrichment, in the form of an analytical equation which is simply the dot product between two *sensitivity vectors*. Although this method currently provides a bounding estimate of the degree of correlation between two systems which differ only in enrichment, it also demonstrates that it is possible to estimate this correlation quantitatively without the derivation of the forward and adjoint flux data required by the full S/U methodology. Further work is needed to extend this method to second-order terms in k_{eff} and a full linear treatment in multiple parameters.

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