VARIATIONAL SENSITIVITY ANALYSIS -- THEORY AND APPLICATION

by

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ABSTRACT

The theory underlying the variational sensitivity formalism is reviewed. Some general characteristics of uncertainties in fast reactor parameters as a function of nuclear data uncertainties are discussed. Numerical studies based on the variational sensitivity theory and the statistical theory are reviewed.

I. INTRODUCTION

It is often necessary to evaluate the effects of changes or uncertainties in design parameters, processing methods or nuclear data upon integral reactor physics parameters. Such effects can generally be determined by performing detailed calculations for each configuration, but such an approach may not be desirable from an economic viewpoint and may be impractical if the changes of interest are small or local in character and/or of a statistical nature. These considerations have led to the development of methods which permit the use of fluxes and adjoints calculated for a reference system in performing sensitivity studies for a variety of alterations.

The most direct procedure for performing sensitivity studies corresponds to the well-known first-order perturbation theory. In this method the expression defining the integral parameter of interest is evaluated directly using the exact mathematical operators along with the neutron flux and adjoint from the reference system. A generalized perturbation theory introduced by Usachev (1) and extended by Gandini (2) introduces corrections to account for the change in the neutron flux and adjoint as a result of the system change. Using a variational formalism (3), Stacey (4) developed methods to give estimates of reactivity worths and reaction rate ratios which gave second-order errors with respect to the flux change. Using Stacey's results, Hwang (5) has developed a means for treating statistical uncertainties in nuclear data. In this paper the work of Stacey and Hwang will be reviewed. Numerical examples based on earlier studies relating to data and methods uncertainties are presented.

II. VARIATIONAL PERTURBATION THEORY

The variational perturbation theory developed by Stacey may be used to estimate general bilinear ratios and linear flux ratios. Examples of the former include reactivity worth, prompt-neutron lifetime, delayed-neutron fraction, and reactivity worth ratios, while the latter includes breeding ratio

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and reaction rate ratios. We shall consider only the estimation of reactivity worth as it is not difficult to generalize to general bilinear or linear ratios.

Consider a critical reactor described by the equation

$$A\phi = \lambda B\phi. \quad (1)$$

In Eq. (1) the operator A represents neutron transport, scattering, and absorption, and B represents fission. ϕ is the neutron flux and $\lambda = 1/k$ where k is the effective multiplication constant. The adjoint, ϕ^* , for the system is described by

$$A^*\phi^* = \lambda B^*\phi^*, \quad (2)$$

where

$$\langle \phi^*, A\phi \rangle = \langle A^*\phi^*, \phi \rangle$$

defines the operators A^* and B^* , $\langle \cdot, \cdot \rangle$ represents an inner product notation, and it is assumed that the bilinear concomitant vanishes. If a reactivity perturbation is introduced into the system, the operators A and B change by ΔA and ΔB ,

$$A' = A + \Delta A, \quad B' = B + \Delta B, \quad (3)$$

and the perturbed system may be described by

$$A'\phi' = \lambda' B'\phi'. \quad (4)$$

Using Eqs. (2) and (4), an exact expression for the reactivity worth of the perturbation, $\rho = -\Delta\lambda$, is found,

$$\Delta\lambda = -\frac{k' - k}{kk'} = \frac{\langle \phi^*, (\Delta A - \lambda \Delta B)\phi' \rangle}{\langle \phi^*, B'\phi' \rangle}. \quad (5)$$

If ϕ' is assumed to be given by the unperturbed flux ϕ , the first-order perturbation theory expression results,

$$(\Delta\lambda)_0 = \frac{\langle \phi^*, (\Delta A - \lambda \Delta B)\phi \rangle}{\langle \phi^*, B\phi \rangle}. \quad (6)$$

It is well known that this estimate of $\Delta\lambda$ has errors which are first-order with respect to $\Delta\phi \equiv \phi' - \phi$. An estimate which is second order with respect to $\Delta\phi$ is given by the functional

$$(\Delta\lambda)_V = \frac{\langle \psi^*, (\Delta A - \lambda \Delta B)\psi \rangle}{\langle \psi^*, B\psi \rangle} \left[1 - \langle \psi^*, (A - \lambda B)\Gamma \rangle - \langle \Gamma^*, (A' - \lambda' B')\psi \rangle \right]. \quad (7)$$

It is not difficult to show that $(\Delta\lambda)_V$ is stationary about the functions

$\psi^* = \phi^*$ and $\psi = \phi$ of Eqs. (2) and (4) while the Euler equations for Γ^* and Γ are

$$(\Lambda - \lambda B)\Gamma_S = \frac{(\Delta A - \lambda \Delta B)\psi}{\langle \psi^*, (\Delta A - \lambda \Delta B)\psi \rangle} - \frac{B^* \psi}{\langle \psi^*, B^* \psi \rangle}, \quad (8)$$

$$(A^* - \lambda^* B^*)\Gamma_S^* = \frac{(\Delta A^* - \lambda \Delta B^*)\psi^*}{\langle \psi^*, (\Delta A - \lambda \Delta B)\psi \rangle} - \frac{B^* \psi^*}{\langle \psi^*, B^* \psi \rangle}. \quad (9)$$

The stationary value of $(\Delta\lambda)_V$ is given by Eq. (5) so that Eq. (7) provides an estimate of the reactivity worth of the perturbation which is accurate to second-order with respect to errors in ψ , ψ^* , Γ , and Γ^* . When the unperturbed flux and adjoint of Eqs. (1) and (2) are used as trial functions, then the variational estimate $(\Delta\lambda)_V$ is given by

$$(\Delta\lambda)_V = (\Delta\lambda)_0 \left\{ 1 - \left\langle \Gamma^*, \left[\Delta A - \Delta(\lambda B) \right] \phi \right\rangle \right\}, \quad (10)$$

with Γ^* defined by Eq. (9) with $\psi^* = \phi^*$ and $\psi = \phi$. It is convenient to approximate Γ^* so as to avoid the need to estimate λ^* , by the expression

$$(A^* - \lambda B^*)\Gamma^* = \frac{(\Delta A^* - \lambda \Delta B^*)\phi^*}{\langle \phi^*, (\Delta A - \lambda \Delta B)\phi \rangle} - \frac{B^* \phi^*}{\langle \phi^*, B\phi \rangle}, \quad (11)$$

which satisfies the biorthogonality property

$$\langle \Gamma^*, B\phi \rangle = 0. \quad (12)$$

Stacey (4) has shown that the factor multiplying $(\Delta\lambda)_0$ of Eq. (10) is a correction factor which accounts for the effect of the perturbation upon the flux.

Equation (10) thus provides an estimate of the reactivity worth of the perturbation which is more accurate than first-order perturbation theory but requires the solution of Eq. (11) in lieu of solving for the perturbed flux using Eq. (4). Although there may be situations where Eq. (11) is easier to solve than Eq. (4), the real incentive for use of the variational formalism appears when one considers estimates of reactivity perturbations in an altered system defined by the operators

$$\bar{A} = A + \delta A, \quad \bar{B} = B + \delta B.$$

The reactivity perturbation in the altered system is described by the operators

$$\bar{\Delta A} = \Delta A + \delta A, \quad \bar{\Delta B} = \Delta B + \delta B.$$

Stacey has shown that the reactivity worth of the perturbation in the altered system may be estimated as

$$(\bar{\Delta\lambda})_V = (\Delta\lambda)_0 \bar{h} \left(1 + \bar{f}_{adj} + \bar{f}_{flux} \right), \quad (13)$$

where $\bar{h}$ accounts for the effect of the alteration in system properties upon the first-order perturbation estimate

$$\bar{h} \approx \frac{1 - (\delta\lambda)_0 \frac{\langle \phi^*, \Delta B \phi \rangle + \langle \phi^*, dB \phi \rangle + \langle \phi^*, (dA - \lambda dB) \phi \rangle}{\langle \phi^*, (\Delta A - \lambda \Delta B) \phi \rangle} + \frac{\langle \phi^*, (dA - \lambda dB) \phi \rangle}{\langle \phi^*, (\Delta A - \lambda \Delta B) \phi \rangle}}{1 + \frac{\langle \phi^*, \delta B \phi \rangle + \langle \phi^*, dB \phi \rangle}{\langle \phi^*, (B + \Delta B) \phi \rangle}}, \quad (14)$$

with

$$(\delta\lambda)_0 = \frac{\langle \phi^*, (\delta A - \lambda \delta B) \phi \rangle}{\langle \phi^*, (B + \delta B) \phi \rangle}, \quad (15)$$

Corrections for the change in the flux due to the introduction of the reactivity perturbation and due to the alteration in the system are accounted for by the term

$$\begin{aligned} \bar{F}_{\text{flux}} \approx & - \langle \Gamma^*, (\delta A - \lambda \delta B) \phi \rangle - \langle \Gamma^*, (dA - \lambda dB) \phi \rangle \\ & - \langle \Gamma^*, (\Delta A - \lambda \Delta B) \phi \rangle + \left[(\delta\lambda)_0 + (\overline{\Delta\lambda})_0 \right] \\ & \cdot \left[\langle \Gamma^*, \delta B \phi \rangle + \langle \Gamma^*, \Delta B \phi \rangle + \langle \Gamma^*, dB \phi \rangle \right], \end{aligned} \quad (16)$$

where

$$(\overline{\Delta\lambda})_0 = \frac{\langle \phi^*, [\overline{\Delta A} - (\lambda + (\delta\lambda)_0) \overline{\Delta B}] \phi \rangle}{\langle \phi^*, (B + \overline{\Delta B}) \phi \rangle}. \quad (17)$$

Correction for the change in the adjoint due to the alteration in the system is accounted for by the term

$$\bar{F}_{\text{adj}} \approx - \langle \phi^*, (\Delta A - \lambda \Delta B) \Gamma \rangle + (\delta\lambda)_0 \langle \phi^*, \delta B \Gamma \rangle. \quad (18)$$

The generalized adjoint Γ^* is calculated from Eq. (11) and Γ is calculated from

$$(A - \lambda B) \Gamma = \frac{(\Delta A - \lambda \Delta B) \phi}{\langle \phi^*, (\Delta A - \lambda \Delta B) \phi \rangle} - \frac{B \phi}{\langle \phi^*, B \phi \rangle}, \quad (19)$$

$$\langle \phi^*, B \Gamma \rangle = 0. \quad (20)$$

Hence one set of trial functions ϕ , ϕ^* , Γ^* , and Γ may be calculated for the original system from Eqs. (1), (2), (11), and (19) and then used to evaluate the reactivity worth of a perturbation with only second-order errors for

many different alterations of the original system as well as the worth in the reference system. The computational advantage of such a scheme relative to computation of the unperturbed adjoint and perturbed flux for each system alteration is obvious.

The variational sensitivity theory developed by Stacey (4) is applicable to any representation of the operators A and B. An experimental code using a one-dimensional diffusion theory representation, VARI-1D (6), has been developed to test the method and is currently available through the Argonne Code Center. This code solves Eqs. (11) and (19) by a successive approximation method which may be shown to be equivalent to a standard power iteration without acceleration. A potential problem in the solution of these equations is that of fundamental mode contamination since Eqs. (12) and (20) should be satisfied. Numerical experience to date indicates no problem. Preliminary specifications for a two-dimensional diffusion theory capability have recently been completed. The two-dimensional capability will be oriented to reactor design applications. Initial studies have shown that the numerical methods of the VARI-1D code appear to be applicable to the two-dimensional problem.

III. STATISTICAL UNCERTAINTIES IN SENSITIVITY STUDIES

The variational sensitivity formalism developed by Stacey (4) provides a convenient way of relating any fractional change in reactivity coefficients or reaction rate ratios to an arbitrary change in cross sections. Such a relation is essential if one is to consider how uncertainties in nuclear data and their correlations affect design parameters. Hwang (5) has studied the characteristics of uncertainties in integral reactor parameters as a function of the corresponding uncertainties in nuclear data.

One can relate the fractional change in reactivity coefficient of type i (e.g. central worth) to changes in cross section as

$$\left(\frac{\rho - \rho_0}{\rho_0} \right)_i = \sum_{j=1}^N a_j^{(i)} \left[\frac{\sigma_j - \bar{\sigma}_j}{\bar{\sigma}_j} \right] + \left\{ \sum_{j=1}^N b_j^{(i)} \left[\frac{\sigma_j - \bar{\sigma}_j}{\bar{\sigma}_k} \right] \right\} \sum_{k=1}^N c_k^{(i)} \left[\frac{\sigma_k - \bar{\sigma}_k}{\bar{\sigma}_k} \right] + \dots, \quad (21)$$

where the coefficients $a_j^{(i)}$, $b_j^{(i)}$, and $c_k^{(i)}$ are functions of the reference cross-section data $\bar{\sigma}$ and may be obtained directly from the variational sensitivity theory code VARI-1D (6). The index N may be taken as the number of energy intervals over which cross-section changes are considered and the number of altered reaction cross-section types.

Equation (21) can be generalized to the treatment of statistical uncertainties in terms of mean-square deviations. Without loss of generality one can write

$$E \left[\left(\frac{\rho - \rho_0}{\rho_0} \right)_i^2 \right] = \underline{a}^{(i)T} K \underline{a}^{(i)} + H, \quad (22)$$

where K is the covariance matrix,

$$K_{jk} = E \left[\left(\frac{\sigma_j - \bar{\sigma}_j}{\bar{\sigma}_j} \right) \left(\frac{\sigma_k - \bar{\sigma}_k}{\bar{\sigma}_k} \right) \right]. \quad (23)$$

H accounts for high-order terms in Eq. (21) and E represents the mean-square deviation. As long as the covariance matrix K is non-negative definite, the quadratic form in Eq. (22) is always true independent of the distribution function assumed whereas H requires an assumption about the distribution function. Hwang (5) has shown that if one assumes the usual multivariate normal distribution function, then Eq. (22) is completely specified once the covariance matrix is given.

Given K, the question of practical interest is whether the mean-square deviation of the reactivity ratio exceeds some tolerance set by the reactor designer. Is

$$E \left[\left(\frac{\rho - \rho_0}{\rho_0} \right)_i^2 \right] \leq \epsilon_i ?$$

In practical terms this question might take the form, "Accounting for all data uncertainties and their correlations, are the data good enough to give 10% accuracy on a central worth calculation?"

In order to study this problem qualitatively, Hwang (5) introduced a region of tolerance for the reactor parameter of type i defined by the equation

$$\underline{X}_A^{T(i)} \underline{X} = 1, \quad (24)$$

where

$$A_{jk}^{(i)} = a_j^{(i)} r_{jk} a_k^{(i)} / \epsilon_i^2,$$

$$r_{jk} = K_{jk} / \sqrt{K_{jj} K_{kk}},$$

$$|r_{jk}| \leq 1, \quad j \neq k,$$

$$r_{jk} = 1, \quad j = k,$$

$$x_j = \left\{ E \left[\frac{(\sigma_j - \bar{\sigma}_j)^2}{\bar{\sigma}_j^2} \right] \right\}^{1/2}_{\text{max tol.}} \quad (25)$$

Equation (24) represents a "hyper-ellipsoid" surface in the N-dimensional space of X and the size of the region depends on the matrix A . If I is the total number of reactor parameters of interest, the region of tolerance can be pictured as the common region bound by all I surfaces defined by the quadratic form of Eq. (24).

Hwang proceeded to study the region of tolerance for a number of special cases and he found that the region of tolerance can be extremely sensitive to the choice of the correlation matrix especially when it approaches the positive semi-definite limit. As detailed information on the nature of the correlation matrix, such as those proposed for the error file in ENDF/B, become available, quantitative studies on the role of statistical uncertainties will be pursued. Such data must, however, satisfy the non-negative definiteness requirements in order for it to be physically meaningful and valuable in any actual study.

IV. VARIATIONAL SENSITIVITY STUDIES

The variational sensitivity code VARI-1D (6) has been used extensively in determining the sensitivity of integral neutronics properties of LMFBR critical assemblies to changes in data and methods. Some limited results from these studies will be reviewed to indicate the scope of applications for which sensitivity theory is appropriate.

Hummel and Stacey (7) performed extensive data uncertainty studies for the plutonium-fueled ZPR-6 Assembly 7. Uncertainties of $\pm 20\%$ in central sodium-void worth, $\pm 5\%$ in breeding ratio, and $\pm 2\%$ in k_{eff} were found to result from current data uncertainties. Hwang (5) expanded on this work accounting for correlations among the data by assuming six different covariance matrices. In this study only intercorrelations of cross sections of the same type were considered and the number of energy regions was limited to three, thus limiting the size of the matrix A of Eq. (24). The linear coefficients were obtained from the VARI-1D code. For k_{eff} and breeding ratio the coefficients were all of the same sign so that no cancellation of error is expected and the region of tolerance is relatively insensitive to the intercorrelation of cross sections in various energy regions. For the central sodium worth, the coefficients were such as to expect significant cancellation of error. Hwang also found that the coefficients for ^{235}Pu fission and ^{238}U capture were of opposite sign so that error cancellation might be expected if the intracorrelations among these cross sections exist. The six correlation matrices assumed by Hwang had the form shown in Table I. Case 3 representing complete correlation corresponds to the study by Hummel and Stacey (7). Hwang assumed a standard deviation of $\pm 10\%$ for ^{239}Pu capture and fission and $\pm 5\%$, $\pm 10\%$, and $\pm 15\%$ for ^{238}U capture in the three energy regions. Table II gives Hwang's results for ZPR-6 Assembly 7. Table III gives similar results for the ZPPR-4 assembly which closely resembles the Demonstration Plant design. The results clearly show that the mean-square deviation is extremely sensitive to the correlations among the data uncertainties.

Studies were also performed to test the sensitivity of integral neutronics parameters to various multigroup preparation methods (8). The effects of in-sequence unresolved overlap corrections, fine-group pseudo-composition-independent libraries, resolved resonance attenuation methods, and space-dependent cross-section collapse were a few of the methods sensitivity studies performed. In that study it was shown that a difference in k_{eff} of 0.16% could be attributed to the choice of fine-group mesh structure in use of the MC² (19) code to generate multigroup cross sections. In view of the large differences found among various processing codes (10) in the calculation of k_{eff} for ZPR-6 Assembly 7, it is obvious that an intercomparison of these codes using sensitivity methods is desirable.

Another study using the VARI-1D code concluded that the effects of the $(n, \gamma n')$ reaction were sufficiently large to warrant inclusion of this reaction in the ²³⁸U inelastic matrix (11). Studies of the central-worth discrepancy in three critical assemblies concluded that errors in nuclear data and cross-section preparation methods could account for a significant portion of the discrepancy (12).

The studies noted above demonstrate the efficacy of the variational sensitivity theory in providing an economical means of studying the effects of changes in data, methods, and models on parameters of interest in the Fast Breeder Reactor design.

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TABLE I
Assumed Correlation Matrix

Case	r_{12}	r_{13}	r_{23}
1	0.	0.	0.
2	0.5	0.5	0.5
3	0.99	0.99	0.99
4	-0.2	-0.2	-0.2
5	-0.72617	0.18019	-0.37240
6	-0.49	-0.49	-0.49

TABLE II

Standard Deviations ($\pm\%$) for ZPR-6, Assembly 7, Corresponding
to the Estimated Uncertainties in Cross Sections

Case	k_{eff}			Central Na-Worth			BR		
	U-Capt.	^{239}Pu		U-Capt.	^{239}Pu		U-Capt.	^{239}Pu	
		Fiss.	Capt.		Fiss.	Capt.		Fiss.	Capt.
1	1.47	3.98	0.41	16.0	21.5	7.24	4.19	5.37	1.02
2	1.95	5.12	0.55	16.7	16.2	7.28	5.51	6.51	1.38
3	2.34	6.04	0.67	17.4	8.18	7.32	6.56	7.46	1.66
4	1.22	3.42	0.33	15.8	23.3	7.23	3.52	4.84	0.83
5	0.93	2.53	0.27	14.9	19.8	6.98	2.76	3.97	0.61
6	0.70	2.37	0.16	15.3	25.6	7.20	2.15	3.94	0.44

TABLE III

Standard Deviations ($\pm\%$) for ZPPR-4 (Demo Mockup) Corresponding
to the Estimated Uncertainties in Cross Sections

Case	k_{eff}			Central Na-Worth			BR		
	U-Capt.	Pu		U-Capt.	Pu		U-Capt.	Pu	
		Fiss.	Capt.		Fiss.	Capt.		Fiss.	Capt.
1	0.99	3.20	0.24	8.09	8.00	2.82	4.64	5.01	0.92
2	1.26	3.82	0.32	9.12	7.35	3.09	5.94	6.03	1.22
3	1.48	4.35	0.39	10.00	6.65	3.33	6.99	6.89	1.46
4	0.86	2.91	0.19	7.65	8.25	2.70	3.99	4.53	0.77
5	0.67	2.31	0.13	6.99	7.46	2.52	2.77	3.47	0.52
6	0.63	2.44	0.09	6.95	8.60	2.52	2.82	3.74	0.47