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Adjoint-Based Eigenvalue Sensitivity to Geometry Perturbations, and a Warning

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INTRODUCTION

Recently [1], the sensitivity of the λ eigenvalue ($\lambda = 1/k_{eff}$) to the location of a material interface was derived from the standard adjoint-based sensitivity formula. The equation applies only to uniform expansions or contractions of a surface, not to surface translations or rotations. However, for a flat surface (a plane), a translation in the direction of the normal (or in the opposite direction) is equivalent to an expansion or contraction, so the equation could apply to the translation of a body in the direction of its bounding surfaces, if they are flat. A related perturbation expression for the change in λ (not the derivative) was recently found to be ill-suited to describe the translation of a sphere [2]. In this paper, the sensitivity equation is used to estimate the effect of a uniform expansion of a solid fissile cylinder and of the location of the bottom half of a cylindrical critical assembly.

ADJOINT-BASED SENSITIVITY ANALYSIS FOR SURFACES

The sensitivity of the λ eigenvalue to a parameter u_n is related to the derivative, which can be shown to be [3]

$$\frac{d\lambda}{du_n} = \frac{\left\langle \psi_0^*, \left(\frac{dL}{du_n} - \lambda_0 \frac{dF}{du_n} \right) \psi_0 \right\rangle}{\left\langle \psi_0^*, F_0 \psi_0 \right\rangle}, \tag{1}$$

where subscript 0 indicates the initial, unperturbed configuration; ψ_0 and ψ_0^* are the forward and adjoint angular fluxes, respectively; and L and F are the transport and fission operators, respectively.

Let u_n represent a surface I_n (an internal interface or an external surface). The derivative of the λ eigenvalue with respect to the location of I_n is [1, 2]

$$\frac{d\lambda}{dI_n} = \frac{1}{m_f} \int_{I_n} dS \sum_{g=1}^{G} \left\{ W_g(r_n) - \sum_{g'=1}^{G} \left[W_{s,g' \to g}(r_n) + \lambda_0 W_{f,g' \to g}(r_n) \right] \right\}. \tag{2}$$

In Eq. (2), r_n represents the perturbed points on I_n; g is the energy-group index and $g' \to g$ represents an energy-group transfer; subscripts s and f refer to scattering and fission; m_f is the usual adjoint-weighted fission neutron production rate; and the W terms are forward-adjoint flux products integrated over angle convolved with cross-section differences across interface I_n [1, 2]. The derivation [1] of Eq. (2) involves a Dirac delta function that converts the forward-adjoint product volume integral in the numerator of Eq. (1) to a surface integral on the unperturbed surface.

In the derivation [1] of Eq. (2), it was assumed that each point on I_n that is perturbed is perturbed the same amount in the same direction (relative to its local surface normal). Thus, Eq. (2) applies only to uniform expansions or contractions of a surface. For a spherical or cylindrical surface, the derivative is the rate of change of λ as the radius increases. For flat surfaces, however, the derivative is the rate of change of λ as the surface is translated in the direction of its normal or in the opposite direction, whichever is positive in the coordinate system.

Thus, Eq. (2) can be used for certain translations of certain bodies as well as uniform expansions or contractions of any body.

APPLICATION TO A SOLID URANIUM CYLINDER

First, we apply Eq. (2) to the bounding surfaces of a solid uranium right circular cylinder. This problem is similar to the application to the bounding surface of a solid uranium sphere in [1], for which Eq. (2) was very accurate. The material is highly enriched uranium (HEU; 94.73 wgt% ^{235}U, 5.27 wgt% ^{238}U) with a mass density of 18.74 g/cm^3. The radius and height of the cylinder are 7 and 10 cm, respectively, and its mass is 28.85 kg.

The derivatives computed using Eq. (2) were compared with central-difference derivatives estimated by perturbing the dimensions by ±0.1 cm. Calculations were done using the PARTISN multigroup discrete ordinates code [4] with S_{16} quadrature, P_3 scattering, and the MENDF6 30-group library uncorrected for self-shielding. The unperturbed k_{eff} was 0.81938286.

The derivative of λ with respect to the location of the cylindrical surface was –0.09344135 from Eq. (2) and –0.09325011 from the central difference, a 0.2% difference. The derivative of λ with respect to the location of the top surface was –0.04298977 from Eq. (2) and –0.04370721 from the central difference, a 1.6% difference. Note that $dk_{eff}/du_n = (-k_{eff}^2)\, d\lambda/du_n$, so raising the top surface or increasing the radius has the effect of

decreasing λ and raising k_{eff}, as expected because these changes increase the mass of the fuel. The derivative of λ with respect to the location of the bottom surface was equal to the derivative for the top surface but opposite in sign, reflecting the fact that raising the bottom surface decreases the mass.

The larger difference for the flat surface is [1] due to the fact that W_g , which should be computed using angular fluxes, is estimated using flux moments, the number of which is limited (in PARTISN) to the number used in the expansion of the scattering source, and this is not necessarily enough to accurately reconstruct W_g. A Monte Carlo formulation would not suffer this deficiency.

The derivative of λ with respect to the size of the cylinder — that is, with respect to the uniform expansion of the entire boundary — is, in first-order perturbation theory, the derivative with respect to the cylindrical surface plus the derivative with respect to the top surface minus the derivative with respect to the bottom surface (since, for a uniform expansion, that surface moves in the negative axial direction). Thus the derivative of λ with respect to the uniform expansion of the cylinder is –0.1794209 from Eq. (2). The derivative using a central difference (perturbing all surfaces simultaneously) was –0.1806921, a 0.7% difference (with respect to the central difference).

APPLICATION TO ZEUS

Zeus [5] was a cylindrical stack of alternating HEU (93% enriched) and graphite plates (the outer radius of the stack was 26.67 cm) surrounded by rectangular copper blocks. "Configuration 1" had a critical mass of 125.6 kg HEU. It was assembled on a vertical assembly machine in which the moveable, bottom part of the assembly contained ~40% of the HEU mass. The two-dimensional geometry for configuration 1 as given in Appendix C of [5] was modified for use in this paper; in it, the rectangular copper reflector is converted to a cylindrical annulus. For this paper, the axial dimensions were rounded to 0.1 cm so that the bottom half of Zeus could be moved without changing the mesh spacing, and the bottom half was placed 0.1 cm below full assembly. Transport calculations were done using PARTISN with S_{16} quadrature, P_3 scattering, and the MENDF6 30-group cross section set uncorrected for self-shielding. The unperturbed k_{eff} was 0.96667242.

The derivative of λ with respect to the location of each axial (z) interface in the Zeus lower core was calculated using the adjoint-based equation [Eq. (2)] and a central difference with a perturbation of ±0.01 cm. Results are shown in Table I.

Table I shows that the adjoint-based derivatives [from Eq. (2)] match the central differences extremely well, except where the derivatives are very small, in which case the central differences are probably inaccurate. The separate sums of negative and positive quantities agree very well, but the overall sum has a 1.3% difference, because of the inaccuracy in subtracting similarly sized terms.

What is the derivative of λ with respect to the location of the entire Zeus lower core? The central-difference result, obtained by perturbing all surfaces simultaneously, was –0.0074363. The adjoint-based result is the sum of the independent derivatives for all surfaces, or –0.0098139 from Table I. The adjoint-based result is in error by 32%.

This problem demonstrates one of the well-known pitfalls of first-order perturbation and sensitivity theory. The first-order theory has no way to account for interacting effects of multiple perturbations. The true derivative of k_{eff} or λ with respect to the location of the Zeus lower core is not the simple sum of the derivatives with respect to the location of the individual surfaces.

SUMMARY AND CONCLUSIONS

The adjoint-based first-order sensitivity estimate of the λ eigenvalue with respect to the location of a surface [1] has been applied to the uniform expansion of a solid HEU cylinder. Each of the components of that expansion (the expansion of the cylindrical surface, the raising of the top, and the lowering of the bottom) were very accurately estimated by the adjoint-based equation (compared to central differences). The overall expansion of the cylinder is estimated in first-order theory as the simple sum of the individual components (with their correct sign), and the adjoint-based equation was quite accurate.

Table I. $d\lambda/dz_n$ for each material interface in the lower core of Zeus.

z (cm)	Central Diff.	Adjoint	Difference
57.6	–0.0067285	–0.0067374	0.132%
53.6[a]	–0.1251248	–0.1248847	–0.192%
53.3[b]	0.1242767	0.1240026	–0.221%
45.2[a]	–0.0964496	–0.0962740	–0.182%
44.9[b]	0.0953346	0.0951158	–0.229%
36.8[a]	–0.0639967	–0.0639009	–0.150%
36.5[b]	0.0629240	0.0627898	–0.213%
28.4[a]	–0.0366902	–0.0367146	0.066%
28.1[b]	0.0360359	0.0360658	0.083%
24.1	0.0006416	0.0006392	–0.362%
9.7	0.0000482	0.0000499	3.628%
5.9	0.0000000	0.0000000	0.
0	0.0000449	0.0000345	–23.135%
Sum	–0.0096840	–0.0098139	1.341%
Negatives	–0.338674	–0.338326	–0.103%
Positives	0.319306	0.318698	–0.190%

[a] Top of a fuel plate.
[b] Bottom of a fuel plate.

The adjoint-based theory was also applied to estimate the effect on λ of raising the lower core of the Zeus assembly (from a position 0.1 cm below full insertion). The effect of raising each surface independently was well estimated using the adjoint-based equation, but the effect of raising the entire lower core is not the simple sum of the effect of raising each surface. The adjoint-based equation cannot cope with interacting effects, and the equation yielded a poor estimate.

The adjoint-based equation for the sensitivity of λ to geometry perturbations can be a very powerful tool for the analysis of critical systems. For the uniform expansion or contraction of a body — for the size of a tank or slug, for example — the equation is quite robust. For the location of a body, there are competing additions and removals of reactivity [2], and the equation must be applied cautiously.

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