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Adjoint-Based Eigenvalue Sensitivity to Geometry Perturbations

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INTRODUCTION

Recently [1], the sensitivity of the k_{eff} eigenvalue to the location of a material interface was derived from the standard adjoint-based sensitivity formula. The equation derived in [1] applies only to uniform expansions or contractions of a surface, not to surface translations or rotations. However, the equation is related to an earlier first-order estimate for the change in the λ eigenvalue ($\lambda = 1/k_{eff}$) resulting from a more general change in the location of an interface [2]. It was suggested in [1] that the first-order $\Delta\lambda$ equation of [2] might be used to calculate the k_{eff} sensitivity to surface translations or rotations. In this paper, this idea is applied to estimate the sensitivity of k_{eff} to the translation of a sphere.

ADJOINT-BASED SENSITIVITY ANALYSIS FOR INTERNAL INTERFACES

The k_{eff} sensitivity to an interface location requires forward-adjoint inner products evaluated on the unperturbed interface multiplied groupwise by cross-section differences across the interface. First, define the macroscopic cross section difference for reaction x and energy group g across interface I_n as

$$\Delta\Sigma^g_{x,n} \equiv \Sigma^g_{x,n} - \Sigma^g_{x,n+1}, \tag{1}$$

where the region on the negative side of I_n has cross section $\Sigma^g_{x,n}$ and the region on the positive side has cross section $\Sigma^g_{x,n+1}$. The positive side of I_n is in the direction of the outward normal at any point. Define the following forward-adjoint inner products on the points r_n on surface I_n:

$$W_g(r_n) \equiv \Delta\Sigma^g_{t,n} \int_{4\pi} d\hat{\mathbf{\Omega}}\, \psi^{*g}_0(r_n, -\hat{\mathbf{\Omega}})\psi^g_0(r_n, \hat{\mathbf{\Omega}}), \tag{2}$$

$$W_{s,g'\to g}(r_n) \equiv \sum_{m=1}^{M} (2l_m+1)\Delta\Sigma^{g'\to g}_{sl_m,n}\varphi^{*g}_{0,m,IP}(r_n)\varphi^{g'}_{0,m}(r_n), \tag{3}$$

and

$$W_{f,g'\to g}(r_n) \equiv \Delta[\chi^{g'\to g}\nu\Sigma^{g'}_f]_n \varphi^{*g}_{0,0,IP}(r_n)\varphi^{g'}_{0,0}(r_n). \tag{4}$$

In Eqs. (2), (3), and (4), subscript 0 indicates the initial, unperturbed configuration; $\psi^g_0(r,\hat{\mathbf{\Omega}})$ and $\psi^{*g}_0(r,\hat{\mathbf{\Omega}})$ are the forward and adjoint angular fluxes, respectively; $\varphi^g_{0,m}(r)$ and $\varphi^{*g}_{0,m,IP}(r)$ are the usual forward flux moments and the inner product adjoint flux moments [1], respectively; and the other notation is standard. Define the combination of group-dependent Ws as

$$W(r_n) \equiv \sum_{g=1}^{G}\Big\{ W_g(r_n) - \sum_{g'=1}^{G}\Big[W_{s,g'\to g}(r_n) + \lambda_0 W_{f,g'\to g}(r_n)\Big]\Big\}, \tag{5}$$

and define the adjoint-weighted fission neutron production rate as

$$m_f \equiv \int dV \sum_{g=1}^{G}\sum_{g'=1}^{G} \chi^{g'\to g}_0(r)\nu\Sigma^{g'}_{f,0}(r)\varphi^{*g}_{0,0,IP}(r)\varphi^{g'}_{0,0}(r). \tag{6}$$

Using these equations, the "first-order eigenvalue change due to the interior boundary (interface) perturbation" [2] is

$$\Delta\lambda = \frac{1}{m_f}\int_{I_n} dS\; X_I(r_n) W(r_n), \tag{7}$$

where $X_I(r_n)$ is "an arbitrary first-order change in the interface points" in the direction of (or opposite) the surface normal at each point.

If every surface point that is displaced is displaced the same (signed) distance, then $X_I(r_n) = r_n - r_0$ (a constant) on the surface to be perturbed and 0 elsewhere. Using this fact in Eq. (7) and identifying $\Delta\lambda = \lambda(r_n) - \lambda_0$, the derivative of λ with respect to the interface location is found to be

$$\frac{d\lambda}{dr_n} = \frac{1}{m_f}\int_{I_n} dS\; W(r_n), \tag{8}$$

where it is understood that the integral is only taken on the perturbed part of the surface. Equation (8) was derived previously [1] in a way that was independent of Ref. [2] and Eq. (7). It was pointed out [1] that this

equation applies only to uniform expansions or contractions of a surface, and it was suggested that Eq. (7) might be useful for other types of surface perturbations, such as translations or rotations.

APPLICATION TO THE TRANSLATION OF A SPHERE

Let the initial, unperturbed surface I_n be a one-dimensional sphere of radius R, as shown in Fig. 1; then $W(r_n)$ is a constant on I_n and it can be removed from under the integral in Eq. (7). Let Δr be the distance that the sphere, or some subset of its total surface, is translated. The displacement X_I of each point on the sphere can be written as a function of θ:

$$X_I(\theta) = \Delta r \cos\theta - R + \sqrt{R^2 - \Delta r^2 \sin^2\theta}. \tag{9}$$

The displacement X_I is signed, as indicated by arrows in Fig. 1; it is positive for $0 \le \theta < \theta_1$, 0 for $\theta = \theta_1 = \text{acos}(\tfrac{1}{2}\Delta r/R)$, and negative for $\theta_1 < \theta \le \pi$. Equation (7) becomes, in spherical coordinates,

$$\begin{aligned}\Delta\lambda &= \frac{W}{m_f}\int_0^{2\pi} d\omega \int_{\theta_a}^{\theta_b} d\theta\, R^2 \sin\theta\, X_I(\theta) \\ &= 2\pi R^2 \frac{W}{m_f}\int_{\theta_a}^{\theta_b} d\theta \sin\theta\, X_I(\theta),\end{aligned} \tag{10}$$

where θ_a and θ_b specify the portion of the range of θ over which the perturbation occurs. The integral has a closed-form analytic solution. The final equation for the change in λ due to the translation of that portion of a spherical surface between θ_a and θ_b a distance Δr in the $\theta = 0$ direction is

$$\begin{aligned}\Delta\lambda = 2\pi R^2 \frac{W}{m_f}\Bigg[& R\cos\theta - \frac{\Delta r}{2}\cos^2\theta \\ & + \frac{1}{4}\Bigg(\frac{2}{\Delta r}(\Delta r^2 - R^2)\ln\Big\{\sqrt{2}\,\Delta r\cos\theta \\ & + \sqrt{2R^2 - \Delta r^2 + \Delta r^2\cos(2\theta)}\Big\} \\ & - \cos\theta\sqrt{4R^2 - 2\Delta r^2 + 2\Delta r^2\cos(2\theta)}\Bigg)\Bigg]_{\theta_a}^{\theta_b}.\end{aligned} \tag{11}$$

The limit of Eq. (11) is 0 as Δr goes to 0. The difficult term is the logarithm divided by Δr. When the term in brackets is expanded as the difference between evaluations at θ_b and θ_a, the difference in logarithms becomes the logarithm of a ratio that equals one when Δr is 0, allowing the application of L'Hôpital's rule.

NUMERICAL RESULTS FOR PERTURBATIONS

We consider a two-region sphere. The inner region has a radius of 6.12745 cm and is pure ^{235}U at a density of 16.9 g/cm^3. The outer region has thickness 3.063725 cm and is water at a density of 1 g/cm^3. Scattering is isotropic. The k_{eff} calculated using PARTISN [3] with S_{64} quadrature and a 30-group library, slightly modified from MENDF6 to correct non-balancing absorption cross sections, was 0.99972692. The value calculated using MCNP [4] and the same 30-group library was 0.999682 ± 0.0000130. This comparison is important because W and m_f [Eqs. (5) and (6)] were calculated using PARTISN for the unperturbed one-dimensional sphere, but the exact perturbed values of k_{eff}, which require at least two-dimensional transport, were computed using MCNP (for this reason, the uncertainty is large when Δk_{eff} is small). MCNP was used instead of PARTISN in order to avoid orthogonal meshing of the curved surfaces.

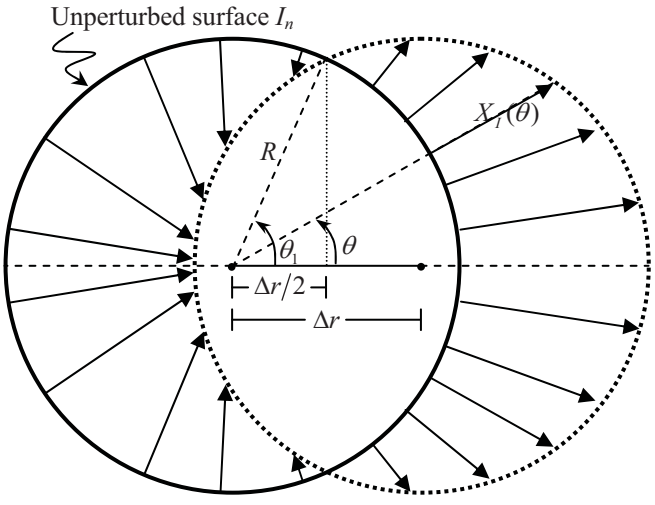

Fig. 1. The translation of a sphere a distance Δr. $\theta_1 = \text{acos}(\tfrac{1}{2}\Delta r/R)$.

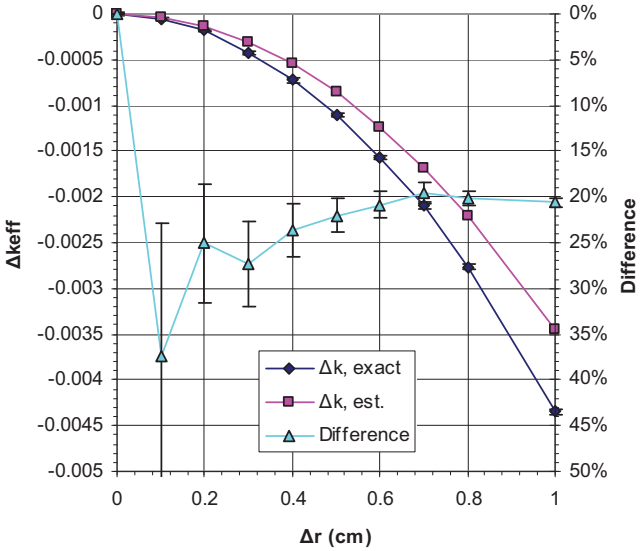

Fig. 2. The change in k_{eff} as a function of the translation of the ^{235}U sphere. 1σ error bars are shown in all figures.

First, consider the effect on k_{eff} when the entire ^{235}U sphere is translated. Results are shown in Fig. 2. The estimate of Eq. (7) gives the right shape but is too small (in magnitude) by ~ 20% over the range of perturbations.

The perturbation formula of Eq. (11) [derived from Eq. (7)] can be used to treat the translation of the entire sphere as two separate perturbations, one a "bulge" for $(\theta_a, \theta_b) = (0, \theta_1)$, and the other a "collapse" for $(\theta_a, \theta_b) = (\theta_1, \pi)$. The bulge is the portion of the dotted sphere corresponding to the outward arrows in Fig. 1, and the collapse is the portion of the dotted sphere corresponding to the inward arrows. In first-order perturbation theory, the estimated effect of the translation of the entire sphere, $(\theta_a, \theta_b) = (0, \pi)$, is the sum of these two components.

Results for the bulge are shown in Fig. 3 and results for the collapse are shown in Fig. 4. The perturbation theory is much more accurate for each of the pieces than it is for the whole, being in error by only ~ 2% for small perturbations and ~ 10% for large perturbations.

In a similar problem in which there was a gap between the fuel and the reflector and translation of the fuel did not perturb the reflector, the agreement of the perturbation results for the bulge and the collapse was as good as those of Figs. 3 and 4, but the agreement of the perturbation result for the translation of the entire fuel sphere was much worse, having the wrong sign.

What hurts the perturbation result for the entire sphere translation (Fig. 2)? Clearly, first-order perturbation theory is sufficient for the separate components but not for the entire sphere. The first-order estimate is the sum of the components, but the exact perturbed result is not the sum because the perturbations interact, an effect that the first-order theory misses.

NUMERICAL RESULTS FOR SENSITIVITIES

For sensitivity analysis, the derivative of k_{eff} with respect to a surface translation by bulging or collapsing may be estimated as recently suggested [1]. For example, fitting a quadratic polynomial through the first four points of Figs. 3 and 4 results in perturbation estimates of the derivative at $\Delta r = 0$ of +/–0.01584 for bulging/collapsing, respectively. Fitting the exact points results in derivatives of 0.01547 and –0.01599, respectively, so the perturbation estimates of the sensitivity are in error by ~ 2%. For the translation of the entire sphere, the derivative of k_{eff} with respect to Δr at $\Delta r = 0$ clearly must be 0 due to symmetry, and the estimate shows that behavior (Fig. 2).

SUMMARY AND CONCLUSIONS

The translation of a body has a positive component (the bulging in the direction of the translation, in "front" of the body) and a negative component (the collapsing "behind"). In two related spherical test problems, interface perturbation theory worked very well for each component separately, but it did not work well for the total translation. The theory has been shown to be very accurate for uniform spherical and cylindrical contractions and expansions [1]. More work needs to be done to understand the accuracy limits of the theory.

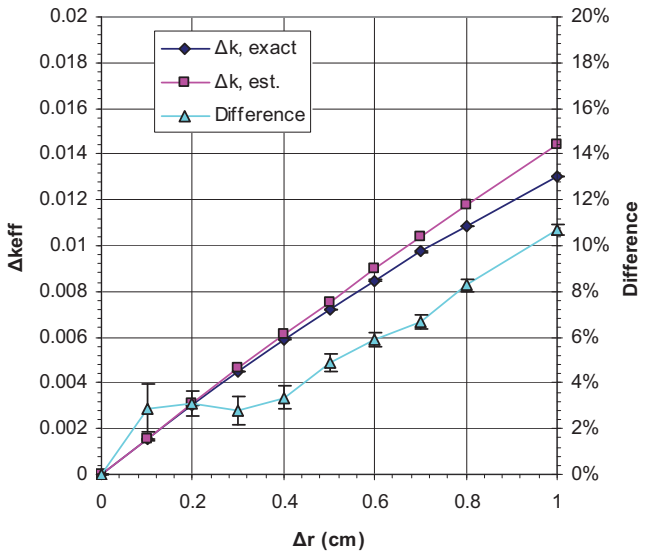

Fig. 3. The change in k_{eff} as a function of the "bulging" displacement of the right side of the ^{235}U sphere.

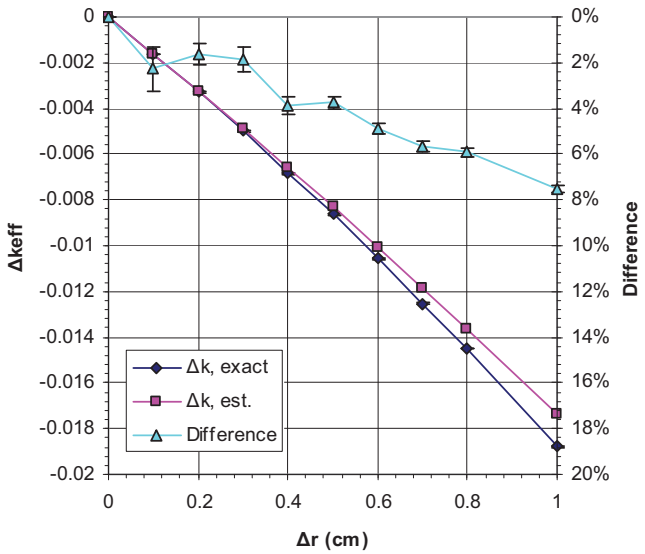

Fig. 4. The change in k_{eff} as a function of the "collapsing" displacement of the left side of the ^{235}U sphere.

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