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

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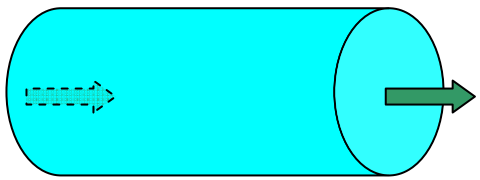
Introduction

- Recently (Favorite and Bledsoe, *Annals of Nuclear Energy*, April 2010), 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.

- These derivatives can be used in sensitivity/uncertainty analysis when dimensions are uncertain.

- The equation applies only to uniform expansions or contractions of a surface, not to surface translations or rotations.

- However, the expansion or contraction of a flat surface is equivalent to a translation parallel to its normal.



- Objectives:
  1. Discuss the adjoint-based sensitivity of λ to geometry perturbations.
  2. Provide examples of situations with uniform expansions or contractions of a surface.
  3. Discuss the importance of interactions among multiple perturbations (warning).

Sensitivity Theory (1 of 2)

- The derivative of the λ-eigenvalue with respect to parameter u_n is

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

L and F are the transport and fission operators, respectively.

- From Fig. 1, the cross section in the vicinity of an interface can be written

$$\Sigma(r) = \Sigma_n + H(r - r_n)(\Sigma_{n+1} - \Sigma_n).$$

- The derivative with respect to the interface location r_n is

$$\frac{d\Sigma(r_n)}{dr_n} = -\delta(r - r_n)(\Sigma_{n+1} - \Sigma_n).$$

- Define $\Delta\Sigma_n \equiv \Sigma_n - \Sigma_{n+1}$ and get

$$\frac{d\Sigma(r_n)}{dr_n} = \delta(r - r_n)\Delta\Sigma_n.$$

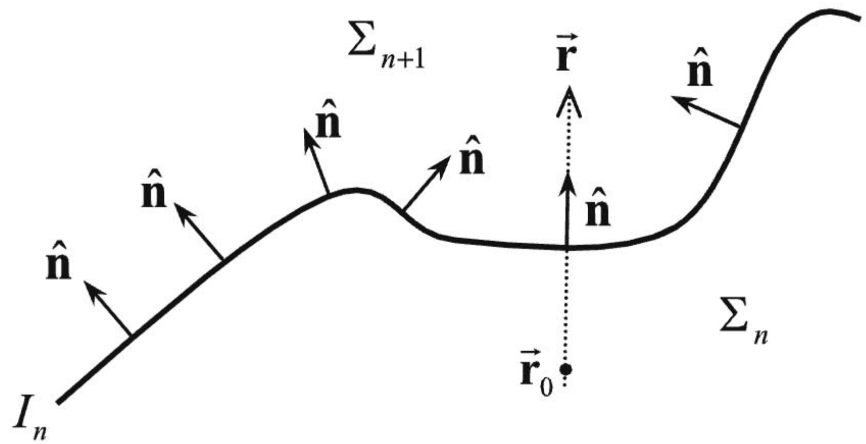


Fig. 1. Crossing an interface I_n in the outward normal direction.

Sensitivity Theory (2 of 2)

- Using $\frac{d\Sigma(r_n)}{dr_n} = \delta(r - r_n)\Delta\Sigma_n$ yields

$$\left\langle \psi_0^*, \frac{dL}{dr_n}\psi_0 \right\rangle = \sum_{g=1}^{G}\sum_{m=1}^{M}(2l_m + 1)\int_{I_n} dS\ \Delta\Sigma_{t,n}^{g}\varphi_{0,m,IP}^{*g}(r_n)\varphi_{0,m}^{g}(r_n)$$

$$-\sum_{g=1}^{G}\sum_{g'=1}^{G}\sum_{m=1}^{M}(2l_m + 1)\int_{I_n} dS\ \Delta\Sigma_{sl_m,n}^{g'\to g}\varphi_{0,m,IP}^{*g}(r_n)\varphi_{0,m}^{g'}(r_n)$$

and

$$\left\langle \psi_0^*, \frac{dF}{dr_n}\psi_0 \right\rangle = \sum_{g=1}^{G}\sum_{g'=1}^{G}\int_{I_n} dS\ \Delta[\chi^{g'\to g}\nu\Sigma_f^{g'}]_n\varphi_{0,0,IP}^{*g}(r_n)\varphi_{0,0}^{g'}(r_n).$$

- Forward moments are the usual ones: $\varphi_m^g(r) \equiv \int_{4\pi} d\hat{\mathbf{\Omega}}\ R_m(\hat{\mathbf{\Omega}})\psi^g(r,\hat{\mathbf{\Omega}})$.

- Adjoint moments are “inner product moments”: $\varphi_{m,IP}^{*g}(r) \equiv \int_{4\pi} d\hat{\mathbf{\Omega}}\ R_m(\hat{\mathbf{\Omega}})\psi^{*g}(r,-\hat{\mathbf{\Omega}})$.

- The sensitivity of λ to an interface location involves forward-adjoint inner products on the unperturbed interface convolved with cross-section differences across the interface.

Relationship to Previous Work

- Our equation for $d\lambda/dr_n$ can be written

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

(with suitable definitions of the Ws).

- Rahnema (1984) gives the "first-order eigenvalue change due to the interior boundary (interface) perturbation" as

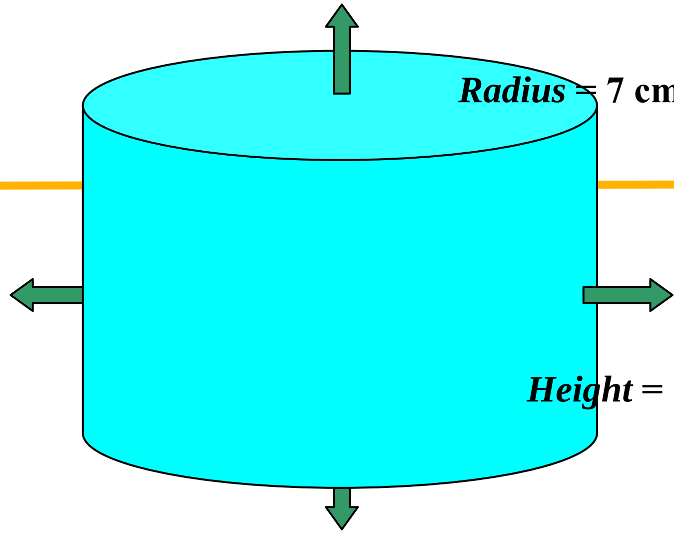
$$\Delta\lambda = \frac{1}{m_f}\int_{I_n} dS\ X_I(r_n)\sum_{g=1}^{G}\left\{W_g(r_n) - \sum_{g'=1}^{G}\left[W_{s,g'\to g}(r_n) + \lambda_0 W_{f,g'\to g}(r_n)\right]\right\},$$

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 each point on the perturbed interface is obtained by displacing each point on the unperturbed interface *the same* distance X_I in the direction of the surface normal at the point (X_I can be negative), then X_I is not a function of space, and our equation and Rahnema's are related by

$$\Delta\lambda = \frac{d\lambda}{dr_n} X_I.$$

Uniform Expansion of a Cylinder



- Bare HEU cylinder, 28.85 kg

- Unperturbed $k_{eff} = 0.81938286$
  + PARTISN, S_{16}, P_3, 30 groups

- Assuming linearity,

$d\lambda/dr_{size} = d\lambda/dr_{cyl} + d\lambda/dr_{top} - d\lambda/dr_{bot}$

- Results

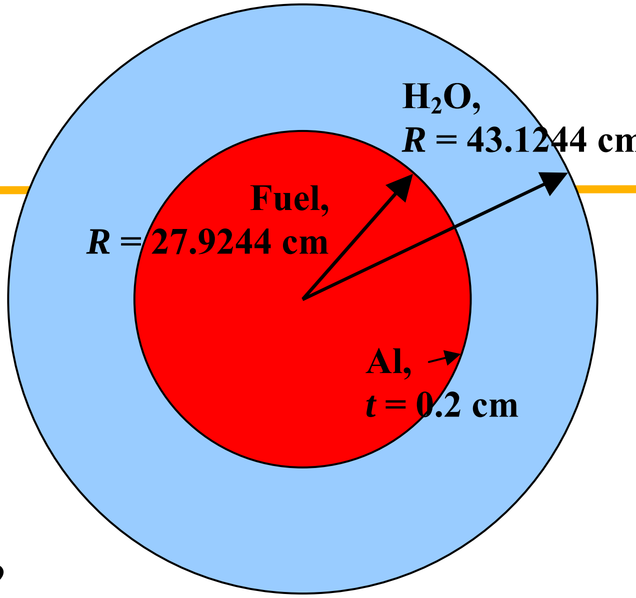
Surface	$d\lambda/r_n$, adjoint	$d\lambda/r_n$, central diff.	Difference
Cylinder	–0.09344135	–0.09325011	0.2%
Top	–0.04298977	–0.04370721	1.6%
Bottom	0.04298977	0.04370721	1.6%
"Size" (uniform expansion)	–0.1794209	–0.1806921	0.7%
Simple sum	–0.1794209	–0.1806645	0.7%

Recall $\lambda = 1/k_{eff}$, so

$$\frac{dk_{eff}}{du_n} = (-k_{eff}^2)\frac{d\lambda}{du_n}$$

- Agreement for the flat surfaces is poor because W_g, which is defined 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.

Size of a tank/Location of a spherical shell



- ICSBEP, HEU-SOL-THERM-012.
- HEU-oxyfluoride solution contained in a thin aluminum tank; infinite water reflector.
- What is the sensitivity of k_{eff} to the fuel radius? – or, equivalently, to the location (inner radius) of the aluminum tank?

	Shell location (inner radius)
r_0, Δr (cm)	27.9244, ±0.1
$k_{eff}(r_-)$ $k_{eff,0}$ $k_{eff}(r_+)$ dk_{eff}/dr_n (fit) C^2 of the fit	1.0343074 1.0354058 1.0364955 1.094050×10^{-2} 0.999995
Sensitivity (direct pert.)	0.29506
$d\lambda/dr_n$ dk_{eff}/dr_n	-1.020717×10^{-2} 1.094275×10^{-2}
Sensitivity (sens. theory)	0.29512
Difference	0.0206%

- The sensitivity is the sum of two terms, a sensitivity each for the inner and outer aluminum radius:
  - $r_{out} = r_{in} + t$ (fixed)
  - $d\lambda/dr_{shell} = d\lambda/dr_{in} + d\lambda/dr_{out}$

Zeus Critical Assembly Machine

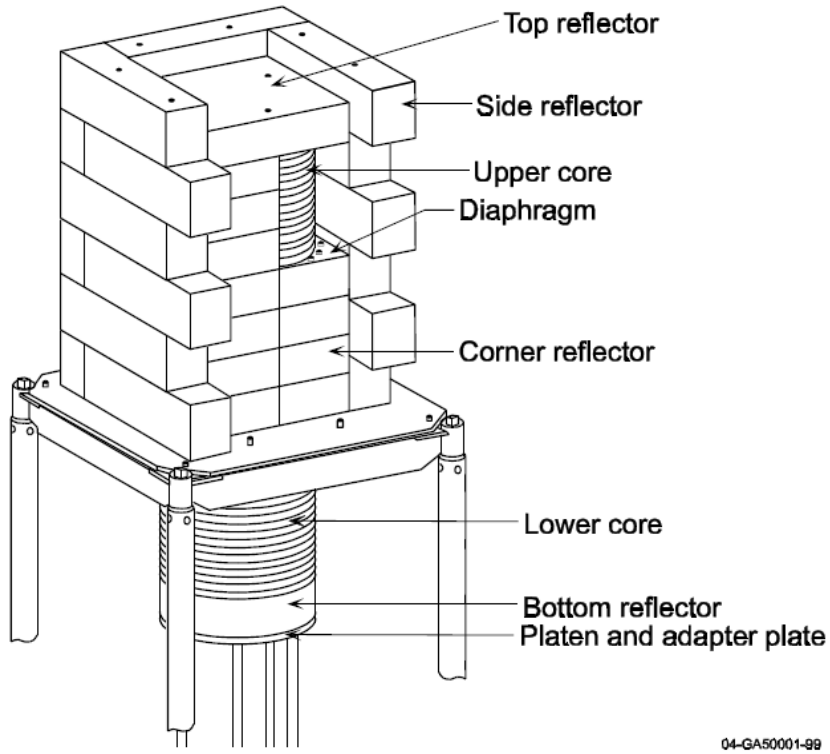


Figure 6. Schematic Cutaway of Zeus before Assembly.

- ICSBEP, HEU-MET-INTER-006.
- A two-dimensional PARTISN input file is given.
- Dimensions were rounded so that the lower core could be moved without changing the meshing.
- The lower core contains 4 fuel plates, 5 graphite plates, and a copper reflector.
- PARTISN with S_{16} quadrature, P_3 scattering, MENDF6 30-group cross sections (not corrected).
  - $k_{eff} = 0.96667$

Zeus Lower Core Results

- When the lower core is 0.1 cm below full assembly, $d\lambda / dz_n$ for each material interface in the lower core is:

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	0.000%
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.

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

- The exact (central-difference) derivative for the entire lower core is –0.0074363. The perturbation-theory estimate is … …a 32% difference.

- There are higher-order effects (interactions) that are not accounted for in the first-order theory.

Results for Zeus Radial Dimensions

- What is the total (group-summed) sensitivity of k_{eff} to the radius of the HEU plates alone, to the radius of the graphite plates alone, and to the radius of the stack of HEU and graphite plates together?

	HEU outer radius	Graphite outer radius	HEU + graphite outer radius
r_0, Δr (cm)	26.67, ±0.1	26.67, ±0.1	26.67, ±0.1
$k_{eff}(r_-)$	0.96613545	0.96548091	0.96422458
$k_{eff,0}$	0.96739805	0.96739805	0.96739805
$k_{eff}(r_+)$	0.96864860	0.96927697	0.97053377
dk_{eff}/dr_n (fit)	1.256575×10^{-2}	1.898030×10^{-2}	3.154595×10^{-2}
C^2 of the fit	0.999992	0.999966	0.999988
Sensitivity (direct pert.)	0.34642	0.52326	0.86968
$d\lambda/dr_n$	-1.345168×10^{-2}	-2.024678×10^{-2}	-3.369845×10^{-2}
dk_{eff}/dr_n	1.258888×10^{-2}	1.894813×10^{-2}	3.153700×10^{-2}
Sensitivity (sens. theory)	0.34706	0.52238	0.86944
Difference	0.1839%	0.1696%	0.0284%

- k_{eff} in the cylindrical Zeus is more sensitive to the radius of the graphite plates than to the radius of the HEU plates.

- Sensitivities here are additive.

Summary and Conclusions

- The derivative of λ with respect to an interface location involves forward-adjoint inner products on the unperturbed interface convolved with cross-section differences across the interface.

- A "simple" expression gives $d\lambda/dr_n$ for uniform expansions or contractions of a surface.

- These derivatives can be used in sensitivity/uncertainty analysis for dimensions.

- Adjoint-based perturbation theory results:
  - + Predicted $d\lambda/dr$ extremely well for the individual surfaces of a solid cylinder, and predicted $d\lambda/dr_{size}$ extremely well.
  - + Predicted $d\lambda/dr_{shell}$ extremely well for the location of a spherical shell in a spherical system (two surfaces).
  - + Predicted $d\lambda/dz_n$ extremely well for the individual surfaces in the Zeus lower core, but failed to predict $d\lambda/dz_n$ for moving the entire lower core.
  - + Predicted $d\lambda/dr$ extremely well for different groupings of radial surfaces in Zeus.
  - + (Last year) predicted components of a sphere translation extremely well, but failed to predict $\Delta\lambda$ for the full translation.

- Use caution, especially when components of a sum alternate in sign.