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Verification of k-Eigenvalue Sensitivity Coefficient Calculations Using Adjoint-Weighted Perturbation Theory in MCNP

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Abstract

The adjoint-weighted perturbation capability in MCNP6 is employed to calculate sensitivity coefficients of k-eigenvalue to cross sections. The results from MCNP6 are compared against analytic solutions, discrete ordinates calculations, and with results generated by TSUNAMI-3D.

Overview

- **Calculating Sensitivity Coefficients**

- **Verification**
  - Analytic, infinite-medium solutions
  - Discrete ordinates calculations
  - TSUNAMI-3D comparisons

Sensitivity Coefficients

Review of Sensitivity Coefficients

- **Sensitivity to cross section σ_x a system response R is**

$$S_{R,\sigma_x} = \frac{\sigma_x}{R}\frac{\partial R}{\partial \sigma_x}$$

- **Here, R is the k-eigenvalue,**

$$S_{k,\sigma_x} = \frac{\sigma_x}{k}\frac{\partial k}{\partial \sigma_x} \approx \frac{\sigma_x}{k}\frac{\Delta k}{\Delta \sigma_x}$$

- **Approximation holds for small perturbation**

Review of Adjoint-Based Perturbations

- **Adjoint-based perturbation theory provides the following:**

$$k\Delta\rho = -\frac{\left\langle \psi^{\dagger}, P\psi \right\rangle}{\left\langle \psi^{\dagger}, F\psi \right\rangle}$$

- **where**

$$P = \Delta\Sigma_t - \Delta S - k^{-1}\Delta F$$

- **This can be estimated with continuous-energy Monte Carlo. (See Kiedrowski, Brown, Wilson, PHYSOR 2010)**

- **Approximation: <u>no scattering law perturbation</u>!**

Computing Sensitivity Coefficients

- Express change in cross section as

$$\Delta\sigma_x = f\sigma_x$$

- Apply the relationship

$$\Delta k = k\frac{k\Delta\rho}{1-k\Delta\rho}$$

- Compute sensitivity coefficients by

$$S_{k,\sigma_x} \approx \frac{1}{f}\frac{k\Delta\rho}{1-k\Delta\rho}$$

- Quantity $k\Delta\rho$ scales linearly with *f*; can make arbitrarily small until sensitivity becomes sufficiently precise.

Analytic Verification Problem

Reference Problem

- **Infinite-medium, multigroup problem:**
  - Closed-form solutions simple to obtain

- **Two-group cross sections:**

g	Σ_t	Σ_c	Σ_f	ν	χ	Σ_{sg1}	Σ_{sg2}
1	2	1/2	1/2	3/4	1	1/2	1/2
2	3	1	1	9/2	0	0	1

Analytic Solutions

- **Solution for *k*:**

$$k = \frac{\nu\Sigma_{f1}}{\Sigma_{R1}} + \frac{\nu\Sigma_{f2}}{\Sigma_{R2}}\frac{\Sigma_{s12}}{\Sigma_{R1}} = 1$$

- **Forward and adjoint solutions:**

$$\psi_1 = 1 \qquad \psi_2 = \frac{\Sigma_{s12}}{\Sigma_{R2}}$$

$$\psi_1^{\dagger} = \frac{\Sigma_{R2}}{\nu\Sigma_{f2}} \qquad \psi_2^{\dagger} = 1$$

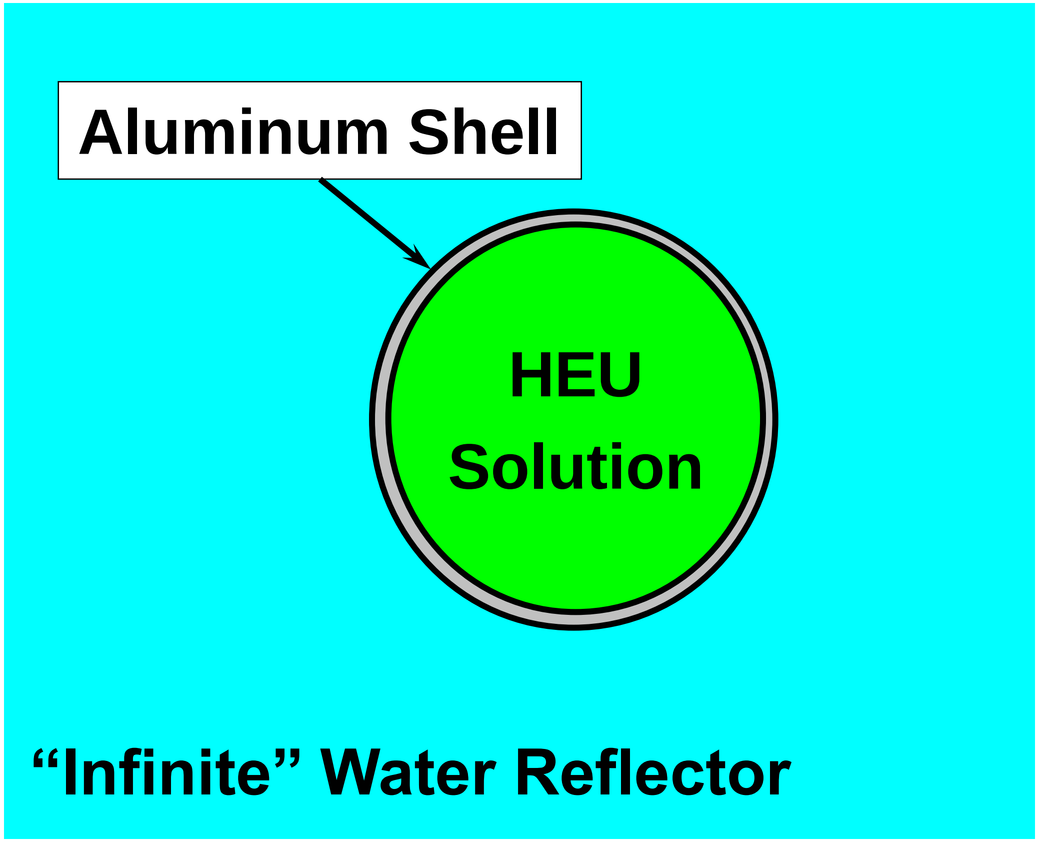
Sensitivity Coefficient Verification

	Exact	MCNP	C/R
σ_{c1}	-1/3	-0.333323 +/- 0.000135	0.99997
σ_{c2}	-3/8	-0.374922 +/- 0.000195	0.99979
σ_{f2}	3/8	+0.375192 +/- 0.000263	1.00051
σ_{s12}	5/12	+0.416644 +/- 0.000214	0.99995

Discrete Ordinates Verification

Benchmark Problem

- **Modeled HEU-SOL-THERM-012 from ICSBEP Handbook in both MCNP and Partisn**



Find sensitivity for water density variation.

Verification Result

- **Problem chosen because:**
  - Adjoint-based perturbation theory captures results compared to direct discrete ordinates calculation within 6 percent.
  - Differential operator perturbation technique is different from direct calculation with adjoint by about 66%.
  - Flux is nearly isotropic over large domain; approximation from no scattering law change should not have adverse impact

- **Result:**

Partisn	MCNP	C/R
0.0157639	0.0160498 +/- 0.0004630	1.01814

TSUNAMI-3D Comparison

TSUNAMI-3D Comparison

- **MCNP (ENDF-VI) compared against result generated by TSUNAMI-3D using 238-energy groups with KENO.**

- **Test problem: Bare, homogeneous sphere containing hydrogen, carbon, fluorine, and LEU (see B.T. Rearden, NS&E 2004).**
  - Anisotropic scattering is important!

Results

	TSUNAMI-3D	MCNP	C/R
Total	$+3.314 \times 10^{-1}$	$+3.173 \times 10^{-1}$	0.957
Capture	-5.081×10^{-1}	-5.019×10^{-1}	0.988
Fission	$+3.964 \times 10^{-1}$	$+3.978 \times 10^{-1}$	1.004
Elastic	$+4.115 \times 10^{-1}$	$+4.219 \times 10^{-1}$	1.025
Inelastic	$+2.950 \times 10^{-2}$	$+2.198 \times 10^{-2}$	0.745

Discussion

- **Fission and capture agree within 2%, inelastic scatter is different by more than 25%.**

- **Differences in scattering (both elastic and inelastic) are worse on a per-isotope sensitivity basis**

- **Evidence points to MCNP approximation of not perturbing energy/angle transfer laws**
  - Note: differential operator also struggles with scattering

Forward/Adjoint P1 in a Similar Problem*

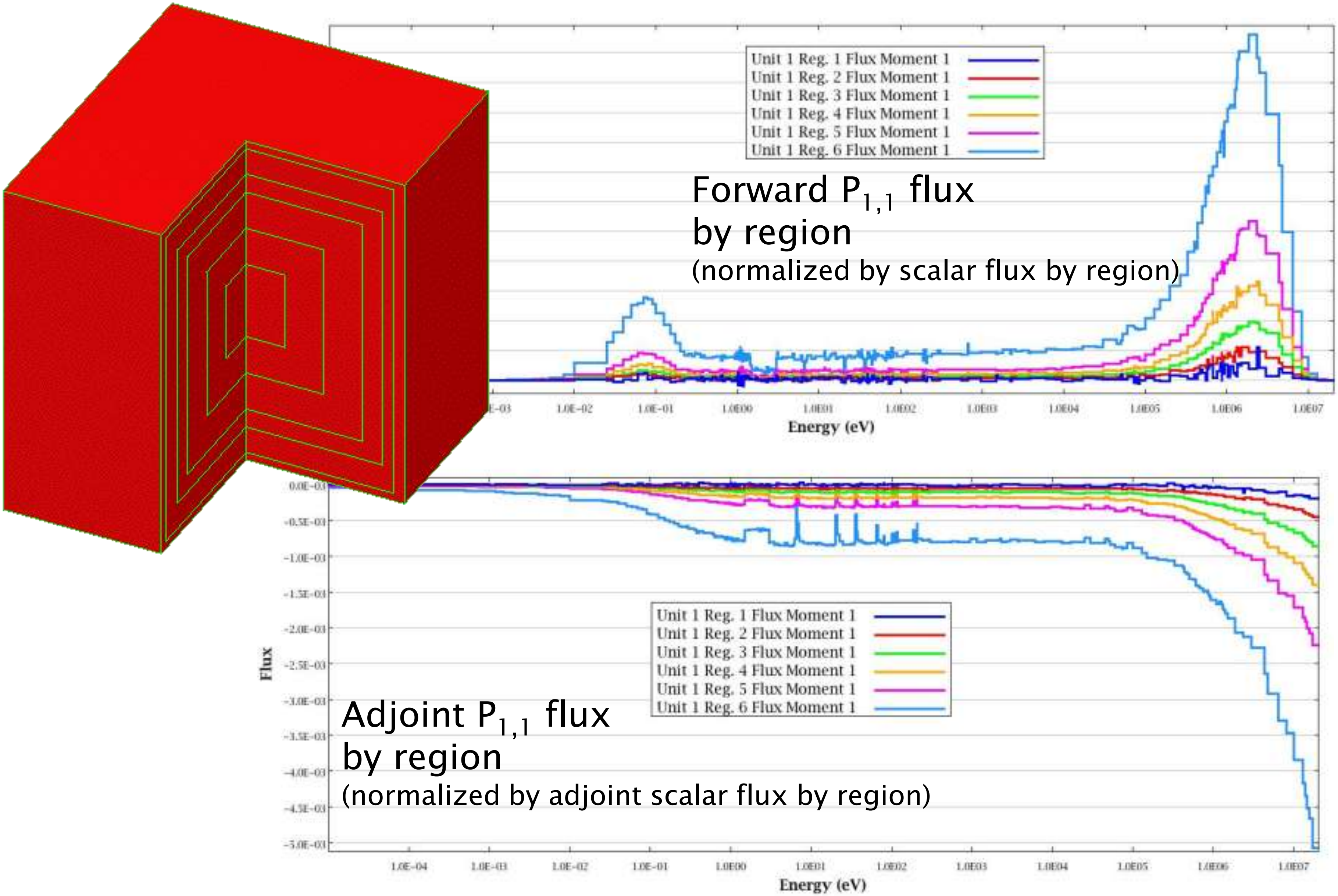


***Figure courtesy of B.T. Rearden of ORNL**

Summary

Conclusions

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- **MCNP adjoint-perturbation capability shows good agreement when scattering law perturbation is not significant (i.e., fission cross section perturbations)**

- **Future work is needed on perturbing continuous-energy scattering laws**

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Questions?