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Author(s): Weaver, Colin Andrew
Rising, Michael Evan
Kulesza, Joel A.
Perfetti, Christopher Michael
Vaquer, Pablo Andres

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Analytic Sensitivity Coefficients for General Multigroup Infinite Medium k-Eigenvalue Problems

Colin A. Weaver [1,*], Michael E. Rising[1], Joel A. Kulesza[1], Christopher M. Perfetti[2], Pablo A. Vaquer[1]

[1]Los Alamos National Laboratory, Los Alamos, NM; [2]University of New Mexico, Albuquerque, NM

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ABSTRACT

The general multigroup infinite medium k-eigenvalue neutron transport equation is used to derive analytic expressions for the infinite medium k-eigenvalue, the scalar neutron flux and adjoint, and the sensitivity of k_∞ to perturbations in the multigroup nuclear data of a single species isotropic elastic scattering material. In the appendix, we present the multigroup nuclear data for U-235 and U-238 along with the corresponding k-eigenvalue, flux, adjoint, and sensitivity profiles, which include the sensitivity of k_∞ to the total, fission, capture, and scattering macroscopic cross sections as well as to the group-to-group scattering cross section matrix, group neutron production, and the unconstrained and constrained fission neutron energy distribution.

Keywords: analytic, sensitivity coefficient, mulitgroup, infinite medium, k-eigenvalue

1. INTRODUCTION

Analytic benchmarks are used in the nuclear engineering community to verify the numerical results of neutron transport simulations. The neutron transport equation is intractable to analytic solutions except under certain stringent conditions. The art of benchmarking is to find a balance between simplifying the mathematics of the underlying equations representing a nuclear system and remaining true to some description of the real-world, i.e., we do not want to simplify our problem so much that it does not correspond to any physical system. This paper addresses a gap in our verification test sets, namely, we are limited in our methods for verifying that nuclear data sensitivity calculations are correct. The most popular approach is to make multiple direct perturbations of the nuclear data, calculate the resulting k-eigenvalues, and extract sensitivity coefficients from the perturbed data set. This method is an art of its own and has its own challenges, e.g., large perturbations can activate non-linear effects, there is statistical uncertainty associated with the results, and calculating the perturbed data set is computationally expensive. The work presented in this paper offers a new verification method. We continue the theory established in a well-known analytical benchmark test set for criticality code verification [1] and expand it to include analytic nuclear data sensitivity coefficients.

2. THEORY

Without derivation, we begin by writing down the general multigroup infinite medium k-eigenvalue problem for a single species isotropic elastic scattering material.

$$\overline{\overline{\Sigma_T}}\,\overline{\phi} = \overline{\overline{\Sigma_S}}\,\overline{\phi} + \frac{1}{k_\infty}\overline{\chi}\,\overline{\nu\Sigma_F}\,\overline{\phi} \tag{1}$$

*caweaver@lanl.gov

In this work, we consider G energy groups with G being the fastest energy group and one being the slowest. The notation we have employed in Equation (1) emphasizes that this is a matrix-vector-scalar equation with the following terms defined:

- total neutron macroscopic cross section

$$\overline{\overline{\Sigma_T}} = \begin{pmatrix} \Sigma_{GT} & 0 & 0 & 0 \\ 0 & \Sigma_{(G-1)T} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \Sigma_{1T} \end{pmatrix} = G \times G \text{ matrix} \tag{2}$$

- neutron scattering macroscopic cross section, $\Sigma_{g'gS}$, from energy group g to energy group g'

$$\overline{\overline{\Sigma_S}} = \begin{pmatrix} \Sigma_{GGS} & 0 & 0 & 0 \\ \Sigma_{(G-1)GS} & \Sigma_{(G-1)(G-1)S} & 0 & 0 \\ \vdots & \vdots & \ddots & 0 \\ \Sigma_{1GS} & \Sigma_{1(G-1)S} & \cdots & \Sigma_{11S} \end{pmatrix} = G \times G \text{ matrix} \tag{3}$$

  Notice that, without loss of generality, we have assumed neutrons do not up-scatter, i.e., they do not gain energy from scattering, hence, the scattering matrix is lower triangular. We require that summing over all out-going energies, i.e., summing the columns of the scattering matrix, results in a vector of neutron scattering macroscopic cross sections, $\Sigma_{gS} = \sum_{g'=1}^{G} \Sigma_{g'gS}$.
- fission neutron energy distribution

$$\overline{\chi} = \begin{pmatrix} \chi_G \\ \chi_{(G-1)} \\ \vdots \\ \chi_1 \end{pmatrix} = G \times 1 \text{ vector} \tag{4}$$

- ν = number of neutrons emitted from each fission event
  Σ_F = neutron fission macroscopic cross section

$$\overline{\nu\Sigma_F} = \begin{pmatrix} \nu\Sigma_{GF} & \nu\Sigma_{(G-1)F} & \cdots & \nu\Sigma_{1F} \end{pmatrix} = 1 \times G \text{ vector} \tag{5}$$

- scalar neutron flux

$$\overline{\phi} = \begin{pmatrix} \phi_G \\ \phi_{(G-1)} \\ \vdots \\ \phi_1 \end{pmatrix} = G \times 1 \text{ vector} \tag{6}$$

- infinite medium k-eigenvalue

$$k_\infty = \text{scalar} \tag{7}$$

We require that there are no (n, xn') reactions, $x > 1$, included in Σ_S, and the scattering cross section includes only isotropic elastic scattering and no higher order moments. Hence, we write $\Sigma_C = \Sigma_T - \Sigma_S - \Sigma_F$, where Σ_C is the neutron capture cross section, i.e., zero neutrons emitted. Thus, for each energy group g the total neutron macroscopic cross section is the sum over its constituents.

$$\Sigma_{gT} = \Sigma_{gC} + \Sigma_{gF} + \sum_{g'=1}^{G} \Sigma_{g'gS} \tag{8}$$

2.1. Derivation of the Infinite Medium k-Eigenvalue

With these definitions in place, we can now turn to deriving an analytic expression for k_∞. We start by grouping the total and scattering macroscopic cross section matrices on the left hand side of Equation (1).

$$\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right) \overline{\phi} = \frac{1}{k_\infty} \overline{\chi} \, \overline{\nu\Sigma_F} \, \overline{\phi} \tag{9}$$

We then apply the inverse of the resulting matrix to both sides of the equation in order to isolate the scalar neutron flux. Notice that this is tantamount to solving the neutron transport equation itself.

$$\overline{\phi} = \frac{1}{k_\infty} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1} \overline{\chi} \, \overline{\nu\Sigma_F} \, \overline{\phi} \tag{10}$$

Next, we introduce a mathematical trick in order to eliminate the scalar neutron flux from this equation. Left multiply the equation by $\overline{\nu\Sigma_F}$.

$$\overline{\nu\Sigma_F} \, \overline{\phi} = \frac{1}{k_\infty} \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1} \overline{\chi} \, \overline{\nu\Sigma_F} \, \overline{\phi} \tag{11}$$

Realize that $\overline{\nu\Sigma_F} \, \overline{\phi}$ is a scalar and can be cancelled out on both sides of the equation. This leaves us with an analytic expression for k_∞, which requires only one matrix inversion to calculate. Recall that by assumption $\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)$ is a lower triangular matrix, which is non-singular when every entry on the diagonal is non-zero. Hence, if the assumptions are satisfied, we should always be able to calculate the inverse and compute k_∞. In other words, in-group scattering must be non-zero for any of the equations derived in this paper to certainly be computationally tractable.

$$k_\infty = \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1} \overline{\chi} \tag{12}$$

Equation (12) is a powerful statement that says the k-eigenvalue of the infinite medium system under scrutiny can be expressed solely as a function of the multigroup nuclear data set. This result immediately indicates that the sensitivity of k_∞ to perturbations in any of the nuclear data on the right hand side of Equation (12) can also be analytically determined without appealing to advanced adjoint based sensitivity methods [2]. In fact, the only reason the adjoint flux is necessary in these methods is to invert the transport operator, $\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)$, and calculate the indirect effect that perturbing system parameters has on the flux itself. Here, we are explicitly inverting the transport operator instead, and the scalar neutron flux has been cancelled out of the equation.

2.2. Calculating the Scalar Neutron Flux and Adjoint

Before turning our attention to deriving these analytic sensitivity coefficients, we will briefly discuss how we can calculate the scalar neutron flux and the adjoint. With k_∞ known by Equation (12), we can gather all of the terms in Equation (1) on the left hand side.

$$\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} - \frac{1}{k_\infty} \overline{\chi} \, \overline{\nu\Sigma_F} \right) \overline{\phi} = \overline{\overline{L}} \, \overline{\phi} = \overline{0} \tag{13}$$

Next, we notice that the kernel of the linear map $\overline{\overline{L}}$, which is also known as the null space of $\overline{\overline{L}}$, is the flux vector we are interested in calculating.

$$\ker\left(\overline{\overline{L}} \right) = \left\{ \overline{\phi} \in \mathbb{R}^G \mid \overline{\overline{L}} \, \overline{\phi} = \overline{0} \right\} = \overline{\overline{L}}^{-1} \, \overline{0} \tag{14}$$

There are two notes on the practicality of performing this calculation. First, realize that you have to take the outer product of $\overline{\chi}$ and $\overline{\nu\Sigma_F}$ to generate a $G \times G$ matrix that can be combined with the other matrices. Second, it is actually quite easy to compute the kernel of $\overline{\overline{L}}$ using a scientific numerical code library such as Python's "SciPy" package, e.g., `flux = scipy.linalg.null_space(L)`, where we recognize that the sign ambiguity of the resulting vector may need to be removed if we use this method.

Next, we turn to calculating the adjoint flux vector. Again, without derivation, we will write down the general multigroup infinite medium *adjoint* k-eigenvalue problem.

$$\overline{\overline{\Sigma_T}}\ \overline{\phi}^{\dagger} = \overline{\overline{\Sigma_S}}^{T}\ \overline{\phi}^{\dagger} + \frac{1}{k_\infty}\overline{\nu\Sigma_F}^{T}\ \overline{\chi}^{T}\ \overline{\phi}^{\dagger} \tag{15}$$

Here, we have used superscript-T to denote the matrix-vector transpose operation. We can also solve this equation to find an analytic expression for k_∞.

$$k_\infty = \overline{\chi}^{T}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}^{T}\right)^{-1} \overline{\nu\Sigma_F}^{T} \tag{16}$$

Notice that this expression has to give you the same result for k_∞ as Equation (12). Use this fact to check that the implementation of these equations is correct. Finally, we can use Equation (15) to define the linear map, $\overline{\overline{L}}^{\dagger}$, that is needed to calculate the adjoint flux vector.

$$\ker\left(\overline{\overline{L}}^{\dagger}\right) = \left\{\overline{\phi}^{\dagger} \in \mathbb{R}^G \mid \overline{\overline{L}}^{\dagger}\ \overline{\phi}^{\dagger} = \overline{0}\right\} = \left(\overline{\overline{L}}^{\dagger}\right)^{-1}\ \overline{0} \tag{17}$$

where

$$\overline{\overline{L}}^{\dagger} = \overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}^{T} - \frac{1}{k_\infty}\overline{\nu\Sigma_F}^{T}\ \overline{\chi}^{T} \tag{18}$$

2.3. Derivation of the Analytic Sensitivity Coefficients

We now turn our attention to deriving the analytic sensitivity coefficients of k_∞ with respect to any one of the multigroup nuclear data. The sensitivity coefficients that we are interested in describe the fractional change in k_∞ due to a fractional change in a system parameter, α. Here, we have used α to represent any one of the multigroup nuclear data.

$$S_{k_\infty,\alpha} = \frac{\alpha}{k_\infty}\frac{\partial k_\infty}{\partial \alpha} \tag{19}$$

This is done, in practice, by directly taking the first partial derivative of Equation (12) with respect to α.

$$\frac{\partial k_\infty}{\partial \alpha} = \frac{\partial}{\partial \alpha}\left\{\overline{\nu\Sigma_F}\right\}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} + \overline{\nu\Sigma_F}\ \frac{\partial}{\partial \alpha}\left\{\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\right\}\overline{\chi} + \overline{\nu\Sigma_F}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial \overline{\chi}}{\partial \alpha} \tag{20}$$

Note that all we have done is applied the triple product rule from differential calculus to Equation (12).

2.3.1. Neutron Emission Sensitivities

Conceptually, the ν and χ sensitivity coefficients are the easiest to understand. In both cases, Equation (20) reduces substantially. Consider the sensitivity coefficients for ν and χ in group g.

$$S_{k_\infty,\nu_g} = \frac{\nu_g}{k_\infty}\frac{\partial}{\partial \nu_g}\left\{\overline{\nu\Sigma_F}\right\}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} = \frac{1}{k_\infty}\left[\overline{\nu\Sigma_F}\right]_g\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} \tag{21}$$

$$S_{k_\infty,\chi_g} = \frac{\chi_g}{k_\infty}\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\chi}}{\partial\chi_g} = \frac{1}{k_\infty}\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}[\overline{\chi}]_g \tag{22}$$

Here, we have used $[\cdot]_g$ to denote vectors where all of the entries have been zeroed out except for the data in the gth energy group. Hence, we can interpret these sensitivity coefficients as the ratio of two k-eigenvalues, where the k-eigenvalue in the numerator corresponds to the system in which we have zeroed out all of the entries in the ν or χ vectors except for energy group g. In other words, this tells us how much the ν or χ data in group g impacts the overall k-eigenvalue. This means that both sensitivity profiles should sum to one over all of the energy groups, i.e., $\sum_{g=1}^{G} S_{k_\infty,\nu_g} = 1$ and $\sum_{g=1}^{G} S_{k_\infty,\chi_g} = 1$. However, we recall that the χ fission neutron energy distribution is a discrete probability distribution with the natural constraint that it also sums to one over all of the energy groups, i.e., $\sum_{g=1}^{G} \chi_g = 1$. Thus, the "correct" χ sensitivity profile will reflect this constraint. We accomplish this by applying the following formula [3].

$$\widetilde{S}_{k_\infty,\chi_g} = S_{k_\infty,\chi_g} - \chi_g\sum_{g'=1}^{G} S_{k_\infty,\chi_{g'}} = S_{k_\infty,\chi_g} - \chi_g \tag{23}$$

This constrained sensitivity profile now has the property that it sums to zero over all of the energy groups, i.e., $\sum_{g=1}^{G} \widetilde{S}_{k_\infty,\chi_g} = 0$. Use these sums to check that the implementation of these equations is correct.

2.3.2. Cross Section Sensitivities

Next, we turn to deriving the analytic sensitivity coefficients for the multigroup nuclear cross section data. For this, we only need the first two terms on the right hand side of Equation (20).

$$\frac{\partial k_\infty}{\partial\alpha} = \frac{\partial}{\partial\alpha}\left\{\overline{\nu\Sigma_F}\right\}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} + \overline{\nu\Sigma_F}\frac{\partial}{\partial\alpha}\left\{\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\right\}\overline{\chi} \tag{24}$$

Now, we actually have to carry out differentiating the inverse matrix with respect to α.

$$\frac{\partial k_\infty}{\partial\alpha} = \frac{\partial}{\partial\alpha}\left\{\overline{\nu\Sigma_F}\right\}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} - \overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\left(\frac{\partial\overline{\overline{\Sigma_T}}}{\partial\alpha} - \frac{\partial\overline{\overline{\Sigma_S}}}{\partial\alpha}\right)\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} \tag{25}$$

If we apply the distributive property to the difference of matrices, then we recover three terms that correspond to the contributon components of the overall sensitivity, which are often discussed in advanced adjoint based sensitivity methods [2]. Thus, these equations can also be used to check that the components of a more advanced sensitivity method are working properly.

$$\begin{aligned}\frac{\partial k_\infty}{\partial\alpha} = \frac{\partial}{\partial\alpha}\left\{\overline{\nu\Sigma_F}\right\}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}& \\ - \overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\overline{\Sigma_T}}}{\partial\alpha}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}& \\ + \overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\overline{\Sigma_S}}}{\partial\alpha}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}&\end{aligned} \tag{26}$$

The first term on the right hand side corresponds to the *fission source contributon*, the second term corresponds to the *collisional contributon*, and the third term corresponds to the *scattering source contributon*. Notice that the collisional contributon is the only mechanism by which we can achieve negative sensitivity coefficients, i.e., positively perturbing the removal operator of the neutron transport equation will decrease the k-eigenvalue, similarly for the other contributons, positively perturbing the fission and scattering source operators will increase the k-eigenvalue. Before we write down the analytic sensitivity coefficients for each of the macroscopic cross sections, we note that these are also constrained sensitivities. Indeed, Equation (8) provides the constraint, which is the relationship between the total macroscopic cross section and its constituents. In this case, however, we explicitly account for the constraint when we calculate the collisional contributon for the constituent cross sections and when we calculate the fission and scattering source contributons for the total cross section. We will demonstrate this first for the capture cross section sensitivity.

$$\begin{aligned} S_{k_\infty,\Sigma_{gC}} &= -\frac{\Sigma_{gC}}{k_\infty}\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\overline{\Sigma_T}}}{\partial\Sigma_{gC}}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} \\ &= -\frac{1}{k_\infty}\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\left[\overline{\overline{\Sigma_C}}\right]_{g,g}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} \end{aligned} \tag{27}$$

Here, we have used $[\cdot]_{g,g}$ to denote matrices where all of the entries have been zeroed out except for the data in the (g,g)th energy group, i.e., we have taken the capture cross section data in the gth energy group and put it on the (g,g)th diagonal entry of the otherwise zero matrix. Notice that the capture cross section sensitivity does not require calculation of either the fission or scattering source contributon. This will not be true for the other sensitivity coefficients. We see this first for the fission cross section.

$$\begin{aligned} S_{k_\infty,\Sigma_{gF}} &= \frac{\Sigma_{gF}}{k_\infty}\left[\frac{\partial}{\partial\Sigma_{gF}}\left\{\overline{\nu\Sigma_F}\right\}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}-\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\overline{\Sigma_T}}}{\partial\Sigma_{gF}}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}\right] \\ &= \frac{1}{k_\infty}\left[\left[\overline{\nu\Sigma_F}\right]_g\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}-\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\left[\overline{\overline{\Sigma_F}}\right]_{g,g}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}\right] \end{aligned} \tag{28}$$

Next, we see this for the scattering cross section.

$$\begin{aligned} S_{k_\infty,\Sigma_{g'gS}} &= \frac{\Sigma_{g'gS}}{k_\infty}\left[-\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\overline{\Sigma_T}}}{\partial\Sigma_{g'gS}}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}\right. \\ &\qquad\left.+\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\overline{\Sigma_S}}}{\partial\Sigma_{g'gS}}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}\right] \\ &= \frac{1}{k_\infty}\left[-\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\left[\Sigma_{g'gS}\right]_{g,g}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}\right. \\ &\qquad\left.+\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\left[\overline{\overline{\Sigma_S}}\right]_{g',g}\left(\overline{\overline{\Sigma_T}}-\overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}\right] \end{aligned} \tag{29}$$

The notation $\left[\Sigma_{g'gS}\right]_{g,g}$ means that we put the $\Sigma_{g'gS}$ group-to-group scattering cross section on the (g,g)th diagonal entry of the otherwise zero matrix. On the other hand, $\left[\overline{\overline{\Sigma_S}}\right]_{g',g}$ means that we have zeroed out the scattering cross section matrix except for the (g',g)th entry. Notice that we can collapse this sensitivity matrix by summing over all of the out-going energies to find the sensitivity of k_∞ to the multigroup macroscopic scattering cross section Σ_{gS}.

$$S_{k_\infty,\Sigma_{gS}} = \sum_{g'=1}^{G} S_{k_\infty,\Sigma_{g'gS}} \tag{30}$$

Finally, we write down the analytic expression for the sensitivity coefficient for the total cross section.

$$S_{k_\infty,\Sigma_{gT}} = \frac{\Sigma_{gT}}{k_\infty}\left[\frac{\partial}{\partial \Sigma_{gT}}\left\{\overline{\nu\Sigma_F}\right\}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} - \overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\overline{\Sigma_T}}}{\partial \Sigma_{gT}}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} + \overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\overline{\Sigma_S}}}{\partial \Sigma_{gT}}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}\right] \quad (31)$$

We need to recognize a stardard sensitivity trick before we can move forward. Namely, $\Sigma_T\frac{\partial\Sigma_X}{\partial\Sigma_T} = \Sigma_X$, where Σ_X is a constituent of Σ_T. This reflects the fact that perturbing Σ_T perturbs each of its constituents by the same amount.

$$S_{k_\infty,\Sigma_{gT}} = \frac{1}{k_\infty}\left[\left[\overline{\nu\Sigma_F}\right]_g\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} - \overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\left[\overline{\overline{\Sigma_T}}\right]_{g,g}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} + \overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\sum_{g'=1}^{G}\left[\overline{\overline{\Sigma_S}}\right]_{g',g}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}\right] \quad (32)$$

Notice that $\left[\overline{\overline{\Sigma_T}}\right]_{g,g}$ is a zero matrix except for the (g,g)th entry which is defined by Equation (8). This means that we can separate it into its constituent parts.

$$\left[\overline{\overline{\Sigma_T}}\right]_{g,g} = \left[\overline{\overline{\Sigma_C}}\right]_{g,g} + \left[\overline{\overline{\Sigma_F}}\right]_{g,g} + \sum_{g'=1}^{G}\left[\Sigma_{g'gS}\right]_{g,g} \quad (33)$$

Inserting this expression into the equation above and matching it to the other cross section sensitivities leads us to conclude that the total cross section sensitivity coefficient is a sum of the constituent cross section sensitivities.

$$S_{k_\infty,\Sigma_{gT}} = S_{k_\infty,\Sigma_{gC}} + S_{k_\infty,\Sigma_{gF}} + \sum_{g'=1}^{G} S_{k_\infty,\Sigma_{g'gS}} \quad (34)$$

However, we also know by examining Equation (12) that perturbing each of the cross sections by the same amount should cancel out and leave us with the original unperturbed value for k_∞. This means that we also expect the total cross section sensitivity to be zero for these infinite medium systems.

$$S_{k_\infty,\Sigma_{gT}} = 0 \quad (35)$$

These sensitivity properties should be used to check that the implementation of these equations was done correctly, i.e., check that Equation (32) and Equation (34) are both zero.

3. CONCLUSIONS

In this paper, we have derived analytic sensitivity coefficients for general multigroup infinite medium k-eigenvalue problems. The work presented here is entirely self-contained in that all of the assumptions and notation have been clearly stated and each step of the mathematical derivations have been explicitly recorded and commented upon. All that is left for the reader to do is to generate a set of multigroup nuclear data cross sections that is suitable to their needs and apply these equations judiciously. An example of this process is presented in Appendix A. The objective of this work is to give the nuclear engineering community a new method to verify that their sensitivity calculations agree with theory. This can be useful for verifying more advanced sensitivity and uncertainty analysis methods. In the future, we hope to extend these equations to account for multiple isotopic species and to investigate analytic sensitivity coefficients for multipole-multigroup nuclear data representations. We also hope to investigate the use of these equations in constructing an analytic upper sub-criticality limit benchmark.

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APPENDIX A. URANIUM EXAMPLES

All of the analytic expressions derived in Section 2 are general and exact given the assumptions that we specified are satisfied. It is beneficial to understand the mathematical structure of these simple k-eigenvalue sensitivity coefficients, because it fosters the engineering intuition that is required to analyze more realistic systems. However, we realize that presenting examples will reinforce our understanding of the mathematics. To that end, we will look at the multigroup nuclear data and corresponding flux, adjoint, and sensitivity profiles for U-235 and U-238.

The multigroup nuclear data presented in Figure 2 was generated using the multigroup tally options in MCNP6®[4]. We set up two infinite medium k-eigenvalue problems consisting purely of U-235 and U-238. Energy dependent cell flux tallies were specified (`F4:n CELL`) as well as the following special treatments:

(`FT4 MGC 1`) calculates the multigroup cross sections; (`FT4 SPM 0`) calculates the angle integrated scattering probability matrix; and (`FT4 FNS 0`) calculates the prompt fission neutron energy distribution.

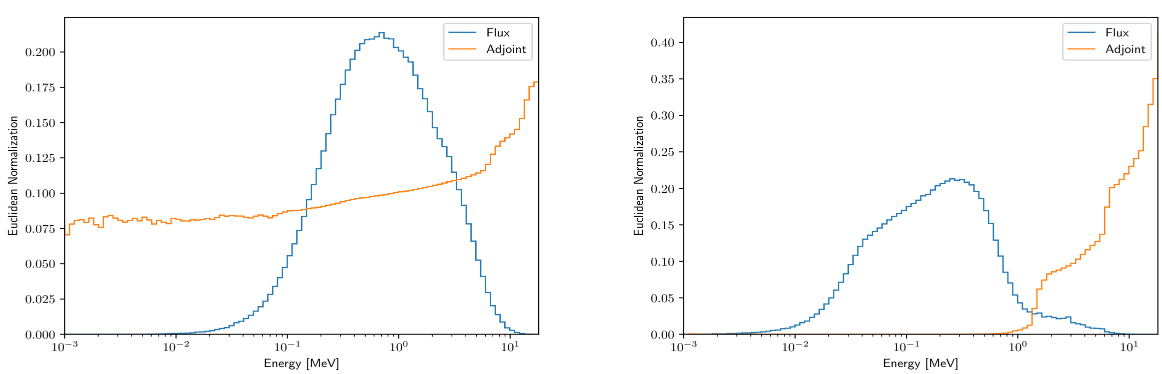
We compare the continuous energy k-eigenvalues calculated with MCNP6®to the multigroup k-eigenvalues calculated with Equation (12) in Table I. Notice that the additional physics not accounted for in our assumptions makes a relatively small but important impact on the k-eigenvalue. This is an interesting result that highlights the importance of including all relevant physics in our neutron transport simulations, because, in both cases, the k-eigenvalue is underestimated.

Table I. Continuous vs. Multigroup k-Eigenvalues

Isotope	Continuous	Multigroup
U-235	2.280142 ± 0.000042	2.268976
U-238	0.310186 ± 0.000060	0.303270

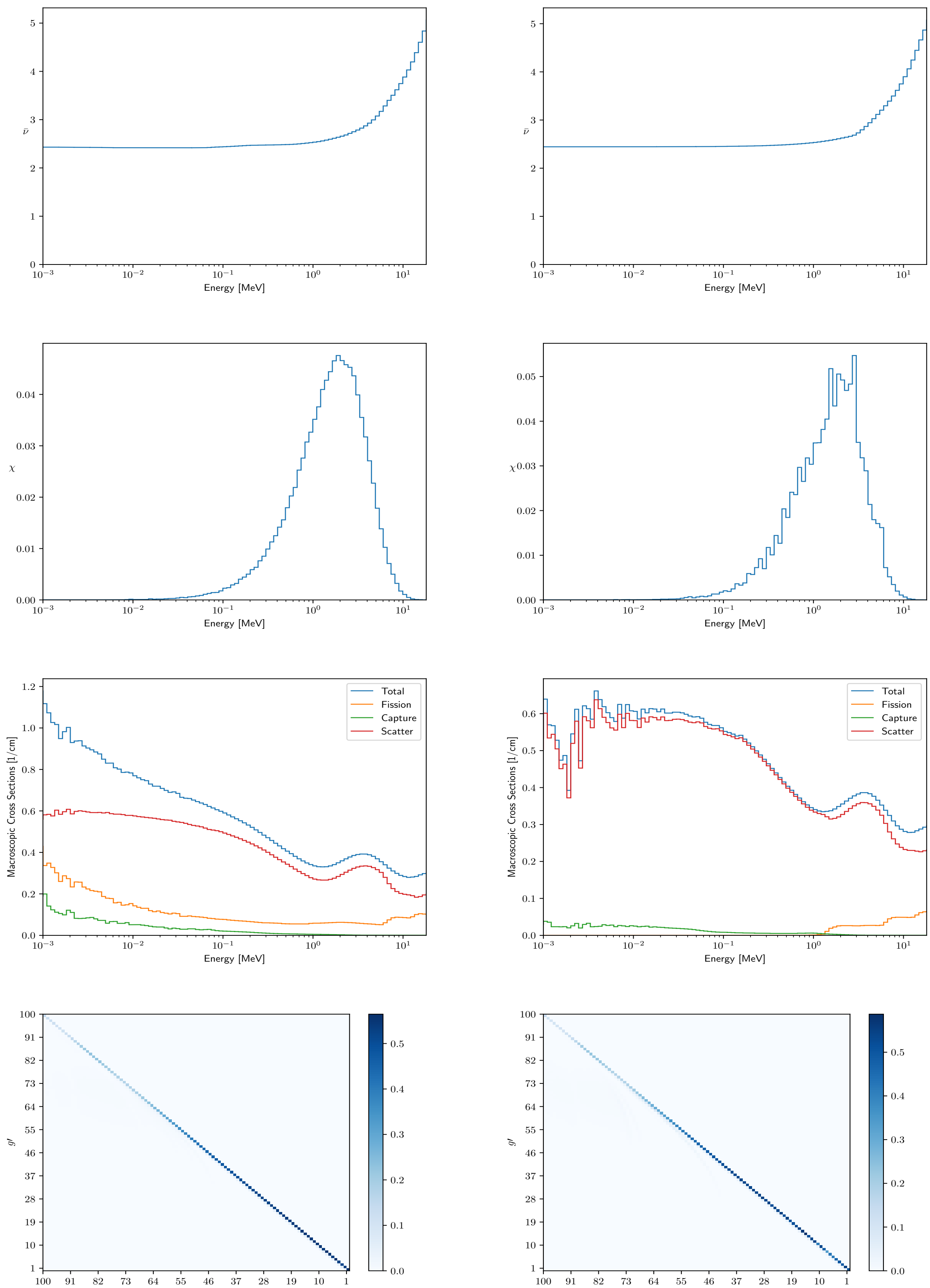
Figure 1 compares the scalar neutron flux and adjoint for both systems. We find that these are non-self adjoint systems, with U-238 only having a non-zero adjoint beyond the fission energy threshold. Figure 3 compares the sensitivity profiles for each uranium isotope. We see common behavior between the two sets of profiles, e.g., the constituent cross section sensitivities both sum to zero, which is what we expected from theory. However, the scattering cross section sensitivity matrices deserve some special attention. The results agree with intuition, i.e., k_∞ is not sensitive to in-group scattering. This means that the integrated scattering sensitivity profile is solely a function of out-group scattering. We also find that the infinite medium k-eigenvalue is particularly sensitive to certain scattering pathways. This could be a result of neutrons avoiding fission resonances or neutrons heading towards capture resonances. Hence, accurate knowledge of the nuclear data cross section resonances is important to the sensitivity and uncertainty analysis of nuclear systems. Thus, investigation of the analytic multipole-multigroup sensitivity coefficients is warranted to further understand the dominant sensitivity mechanisms of our k-eigenvalue problems.

Figure 1. Scalar Neutron Flux and Adjoint



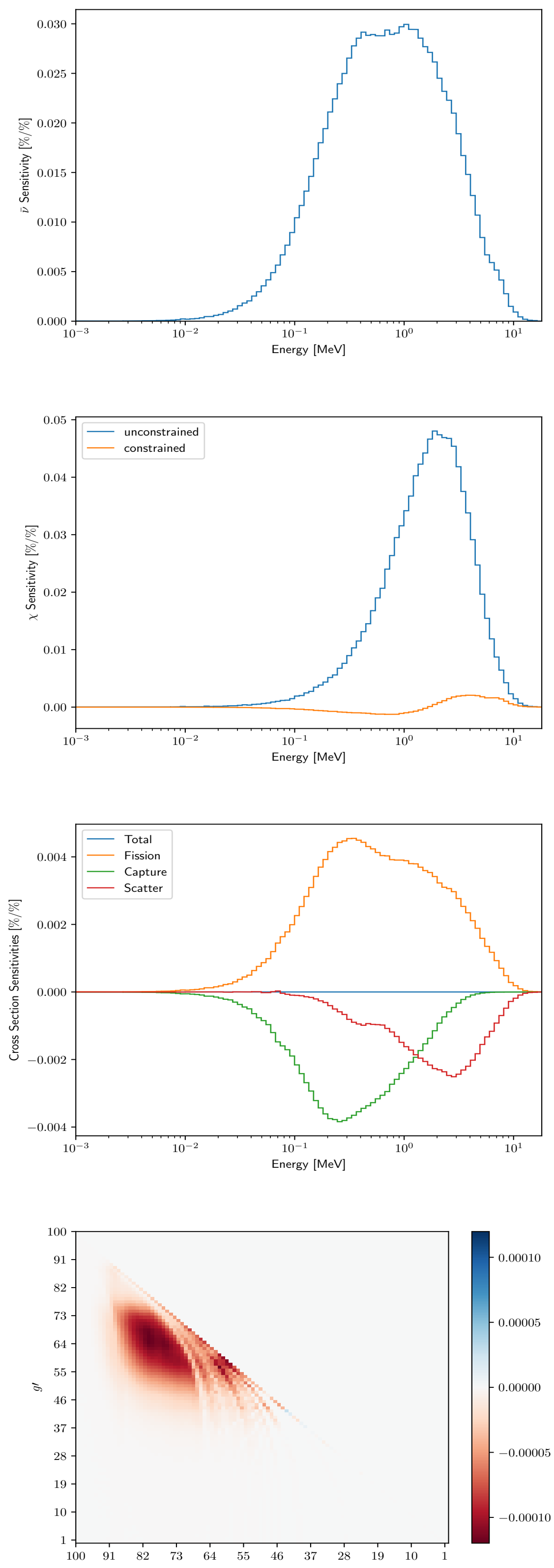
(a) U-235 **(b) U-238**

Figure 2. Nuclear Data
(Top to Bottom: Neutron Emission, Cross Sections, Scattering Matrix)

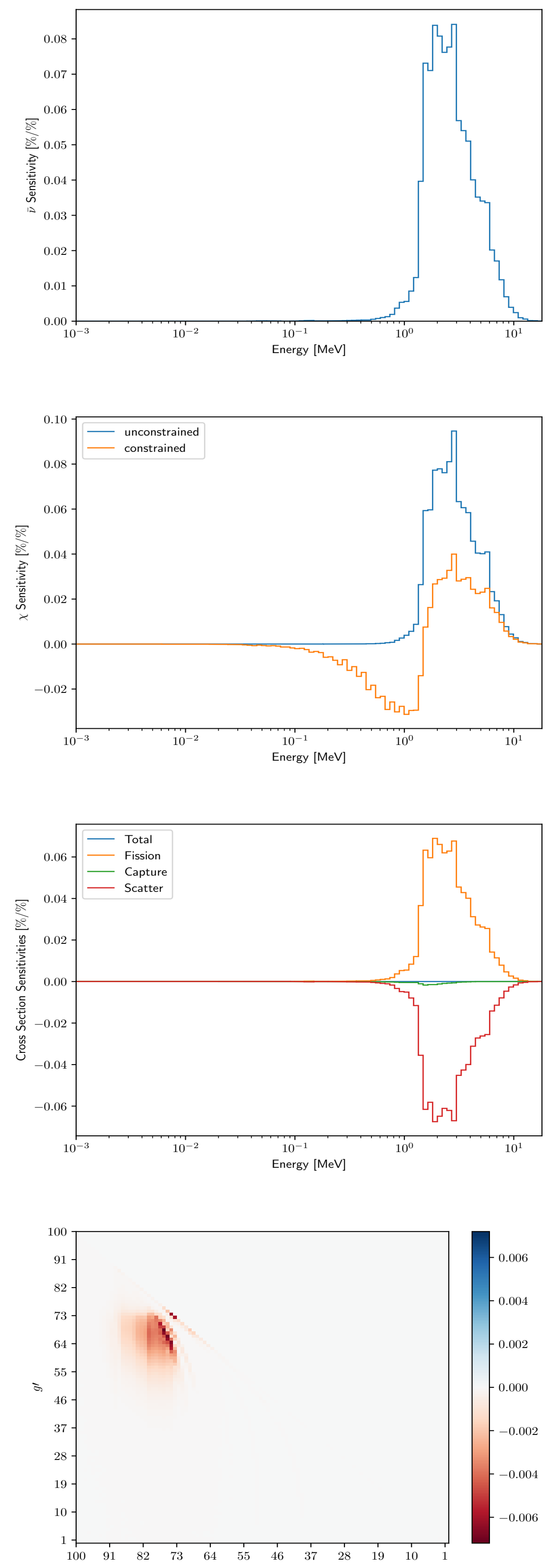


(a) U-235 **(b) U-238**

Figure 3. Sensitivity Profiles
(Top to Bottom: Neutron Emission, Cross Sections, Scattering Matrix)



(a) U-235



(b) U-238