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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

This work presents a general set of equations that can be used to rapidly generate new benchmarks to verify nuclear data sensitivity calculations. 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 flux, and the sensitivity of k_∞ to perturbations in the multigroup nuclear data of a single species, isotropic and elastic scattering, material. The multigroup nuclear data for U-235 and U-238 is presented along with their corresponding k-eigenvalues, forward flux, adjoint flux, 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-wise fission 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., one does not want to simplify the problem so much that it does not correspond to any physical system. This paper addresses the limitation of current verification test sets to rapidly verify that nuclear data sensitivity calculations are correct. A 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 has its own challenges to overcome, 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 analytic verification method. The theory established in a well-known analytical benchmark test set for criticality code verification [1] is expanded to include analytic nuclear data sensitivity coefficients.

2. THEORY

One can begin by writing down the general multigroup infinite medium k-eigenvalue problem for a single species, isotropic and elastic scattering, material as

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

*caweaver@lanl.gov

where the derivation leading to this point is available in [1].

In this work, G energy groups are considered with G being the fastest energy group and one being the slowest. The notation employed in Equation (1) emphasizes that this is a matrix-vector-scalar equation with the variables of the equation defined in the list below.

- The total neutron macroscopic cross section, which is a $G \times G$ matrix, is

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

- The neutron scattering macroscopic cross section, $\Sigma_{g'gS}$, from energy group g to energy group g', which is a $G \times G$ matrix, is

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

  Without loss of generality, it is assumed that neutrons do not up-scatter, i.e., they do not gain energy from scattering, hence, the scattering matrix is lower triangular. It is required that summing over all outgoing energies, i.e., summing the columns of the scattering matrix, results in a vector of energy integrated neutron scattering macroscopic cross sections, $\Sigma_{gS} = \sum_{g'=1}^{G} \Sigma_{g'gS}$.
- The fission neutron energy distribution, which is a $G \times 1$ vector, is

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

- The average number of neutrons emitted from each fission event is $\bar{\nu}$, and the neutron fission macroscopic cross section is Σ_F. When multiplied together they form a $1 \times G$ vector,

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

- The scalar neutron flux, which is a $G \times 1$ vector, is

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

- The infinite medium k-eigenvalue, which is a scalar, is k_∞.

It is required in the present work that there are no $(\mathrm{n}, x\mathrm{n}')$ reactions, $x > 1$, included in Σ_S and the scattering cross section includes only isotropic, elastic scattering and no higher order moments. Hence, the neutron capture cross section, i.e., zero neutrons emitted, is written as $\Sigma_C = \Sigma_T - \Sigma_S - \Sigma_F$. Thus, for each energy group g, the total neutron macroscopic cross section is the sum over its constituents,

$$\Sigma_{gT} = \Sigma_{gC} + \Sigma_{gF} + \sum_{g'=1}^{G} \Sigma_{g'gS}. \tag{7}$$

2.1. Derivation of the Infinite Medium k-Eigenvalue

Given these definitions, one can derive an analytic expression for k_∞. Start by grouping the total and scattering macroscopic cross section matrices on the left-hand side of Equation (1),

$$\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right) \overline{\phi} = \frac{1}{k_\infty} \overline{\chi}\, \overline{\nu\Sigma_F}\, \overline{\phi}. \tag{8}$$

Apply the inverse of the resulting matrix to both sides of the equation to isolate the scalar neutron flux, notice that this is tantamount to solving the neutron transport equation itself,

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

Left multiply by $\overline{\nu\Sigma_F}$ to obtain

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

Realize that $\overline{\nu\Sigma_F}\, \overline{\phi}$ is a scalar and can be cancelled out on both sides of the equation. This leaves an analytic expression for k_∞ that is independent of the scalar neutron flux,

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

which requires only one matrix inversion to calculate. Recall that $\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)$ is non-singular when every entry on the diagonal of this lower-triangular matrix is non-zero. Hence, if the nuclear data is non-zero in every energy group, then it will always be possible to calculate the inverse and compute k_∞.

Equation (11) shows that the k-eigenvalue of the infinite medium system under scrutiny is 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 (11) 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, the transport operator is explicitly inverted instead, and the scalar neutron flux has been cancelled out of the equation.

2.2. Derivation of the Analytic Sensitivity Coefficients

The sensitivity coefficients of interest describe the fractional change in k_∞ due to a fractional change in a system parameter, α, which is used to represent any one of the multigroup nuclear data,

$$S_{k_\infty,\alpha} = \frac{\alpha}{k_\infty} \frac{\partial k_\infty}{\partial \alpha}. \tag{12}$$

This is determined by directly taking the first partial derivative of Equation (11) with respect to α,

$$\frac{\partial k_\infty}{\partial \alpha} = \frac{\partial \overline{\nu\Sigma_F}}{\partial \alpha} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1} \overline{\chi} + \overline{\nu\Sigma_F} \frac{\partial}{\partial \alpha} \left\{ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1} \right\} \overline{\chi} + \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1} \frac{\partial \overline{\chi}}{\partial \alpha}. \tag{13}$$

Notice that this expression was found by applying the triple product rule from differential calculus to Equation (11).

2.2.1. Neutron Emission Sensitivities

Conceptually, the $\bar{\nu}$ and χ sensitivity coefficients are the easiest to understand. In both cases, Equation (13) reduces substantially. The sensitivity coefficients for $\bar{\nu}$ and χ in group g are

$$S_{k_\infty,\bar{\nu}_g} = \frac{\bar{\nu}_g}{k_\infty}\frac{\partial\overline{\nu\Sigma_F}}{\partial\bar{\nu}_g}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} = \frac{1}{k_\infty}\left[\overline{\nu\Sigma_F}\right]_g\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} \tag{14}$$

and

$$S_{k_\infty,\chi_g} = \frac{\chi_g}{k_\infty}\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\frac{\partial\overline{\chi}}{\partial\chi_g} = \frac{1}{k_\infty}\overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\left[\overline{\chi}\right]_g. \tag{15}$$

Here, $[\cdot]_g$ represents the Kronecker delta function for energy group g and is used to denote vectors where all of the entries have been zeroed out except for the data in the gth energy group. Hence, these sensitivity coefficients can be interpreted as the ratio of two k-eigenvalues, where the k-eigenvalue in the numerator corresponds to the system in which all of the entries in the $\bar{\nu}$ or χ vectors have been zeroed out except for energy group g. In other words, this says how much the $\bar{\nu}$ 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., $\sum_{g=1}^{G} S_{k_\infty,\bar{\nu}_g} = 1$ and $\sum_{g=1}^{G} S_{k_\infty,\chi_g} = 1$. However, 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. This is accomplished by applying the following formula [3],

$$\widetilde{S}_{k_\infty,\chi_g} = S_{k_\infty,\chi_g} - \chi_g\sum_{g'=1}^{G} S_{k_\infty,\chi_{g'}} = S_{k_\infty,\chi_g} - \chi_g. \tag{16}$$

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

2.2.2. Cross Section Sensitivities

Now, the analytic sensitivity coefficients for the multigroup nuclear cross section data are derived. Only the first two terms on the right-hand side of Equation (13) are relevant because $\overline{\chi}$ is not a macroscopic cross section,

$$\frac{\partial k_\infty}{\partial\alpha} = \frac{\partial\overline{\nu\Sigma_F}}{\partial\alpha}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} + \overline{\nu\Sigma_F}\frac{\partial}{\partial\alpha}\left\{\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\right\}\overline{\chi}. \tag{17}$$

Differentiate the inverse matrix with respect to α,

$$\frac{\partial k_\infty}{\partial\alpha} = \frac{\partial\overline{\nu\Sigma_F}}{\partial\alpha}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} - \overline{\nu\Sigma_F}\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\left(\frac{\partial\overline{\overline{\Sigma_T}}}{\partial\alpha} - \frac{\partial\overline{\overline{\Sigma_S}}}{\partial\alpha}\right)\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi}. \tag{18}$$

Apply the distributive property to the difference of matrices to recover three terms that correspond to the contributon components of the overall sensitivity, which are often discussed in advanced adjoint-based sensitivity methods [2],

$$\frac{\partial k_\infty}{\partial \alpha} = \frac{\partial \overline{\nu\Sigma_F}}{\partial \alpha} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi} - \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \frac{\partial \overline{\overline{\Sigma_T}}}{\partial \alpha} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi} + \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \frac{\partial \overline{\overline{\Sigma_S}}}{\partial \alpha} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi}. \quad (19)$$

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 negative sensitivity coefficients can be achieved, i.e., positively perturbing the removal operator of the neutron transport equation will decrease the k-eigenvalue, and similarly for the other contributons, positively perturbing the fission and scattering source operators will increase the k-eigenvalue. Notice that the cross section sensitivities are also constrained quantities. Indeed, Equation (7) provides the constraint, which is the relationship between the total macroscopic cross section and its constituents. In this case, however, the constraint is implicitly accounted for when the collisional contributon is calculated for the constituent cross sections and when the fission and scattering source contributons are calculated for the total cross section. This process is demonstrated first for the capture cross section sensitivity,

$$\begin{aligned} S_{k_\infty, \Sigma_{gC}} &= -\frac{\Sigma_{gC}}{k_\infty} \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \frac{\partial \overline{\overline{\Sigma_T}}}{\partial \Sigma_{gC}} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi} \\ &= -\frac{1}{k_\infty} \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \left[\overline{\overline{\Sigma_C}}\right]_{g,g} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi}. \end{aligned} \quad (20)$$

Here, $[\cdot]_{g,g}$ denotes matrices where all of the entries have been zeroed out except for the data in the (g, g)th energy group, i.e., the capture cross section data in the gth energy group has been put 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. The fission cross section sensitivity is

$$\begin{aligned} S_{k_\infty, \Sigma_{gF}} &= \frac{\Sigma_{gF}}{k_\infty} \left[\frac{\partial \overline{\nu\Sigma_F}}{\partial \Sigma_{gF}} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi} - \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \frac{\partial \overline{\overline{\Sigma_T}}}{\partial \Sigma_{gF}} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi}\right] \\ &= \frac{1}{k_\infty} \left[\left[\overline{\nu\Sigma_F}\right]_g \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi} - \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \left[\overline{\overline{\Sigma_F}}\right]_{g,g} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi}\right], \end{aligned} \quad (21)$$

and the scattering cross section sensitivity is

$$\begin{aligned} S_{k_\infty, \Sigma_{g'gS}} &= \frac{\Sigma_{g'gS}}{k_\infty} \left[-\overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \frac{\partial \overline{\overline{\Sigma_T}}}{\partial \Sigma_{g'gS}} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi} \right. \\ &\qquad \left. + \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \frac{\partial \overline{\overline{\Sigma_S}}}{\partial \Sigma_{g'gS}} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi}\right] \\ &= \frac{1}{k_\infty} \left[-\overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \left[\Sigma_{g'gS}\right]_{g,g} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi} \right. \\ &\qquad \left. + \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \left[\overline{\overline{\Sigma_S}}\right]_{g',g} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1} \overline{\chi}\right]. \end{aligned} \quad (22)$$

The notation $\left[\ \Sigma_{g'gS}\ \right]_{g,g}$ means that the $\Sigma_{g'gS}$ group-to-group scattering cross section has been put 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 the scattering cross section matrix has been zeroed out except for the (g',g)th entry. This sensitivity matrix can be collapsed by summing over all of the outgoing neutron energies to find the sensitivity of k_∞ to the energy integrated neutron scattering macroscopic cross section Σ_{gS},

$$S_{k_\infty,\Sigma_{gS}} = \sum_{g'=1}^{G} S_{k_\infty,\Sigma_{g'gS}}. \tag{23}$$

Finally, the total cross section sensitivity is

$$\begin{aligned} S_{k_\infty,\Sigma_{gT}} = \frac{\Sigma_{gT}}{k_\infty}\Bigg[& \frac{\partial\overline{\nu\Sigma_F}}{\partial\Sigma_{gT}}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} \\ & -\overline{\nu\Sigma_F}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\ \frac{\partial\overline{\overline{\Sigma_T}}}{\partial\Sigma_{gT}}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\ \overline{\chi} \\ & +\overline{\nu\Sigma_F}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\ \frac{\partial\overline{\overline{\Sigma_S}}}{\partial\Sigma_{gT}}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\ \overline{\chi}\Bigg]. \end{aligned} \tag{24}$$

Recognize that $\Sigma_T\frac{\partial\Sigma_X}{\partial\Sigma_T} = \Sigma_X$, where Σ_X is a constituent of Σ_T, which reflects the fact that perturbing Σ_T perturbs each of its constituents by the same relative amount,

$$\begin{aligned} S_{k_\infty,\Sigma_{gT}} = \frac{1}{k_\infty}\Bigg[& \left[\ \overline{\nu\Sigma_F}\ \right]_g\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\overline{\chi} \\ & -\overline{\nu\Sigma_F}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\ \left[\ \overline{\overline{\Sigma_T}}\ \right]_{g,g}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\ \overline{\chi} \\ & +\overline{\nu\Sigma_F}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\ \sum_{g'=1}^{G}\left[\ \overline{\overline{\Sigma_S}}\ \right]_{g',g}\ \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}\right)^{-1}\ \overline{\chi}\Bigg]. \end{aligned} \tag{25}$$

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 (7). This means that it can be separated into its constituent parts,

$$\left[\ \overline{\overline{\Sigma_T}}\ \right]_{g,g} = \left[\ \overline{\overline{\Sigma_C}}\ \right]_{g,g} + \left[\ \overline{\overline{\Sigma_F}}\ \right]_{g,g} + \sum_{g'=1}^{G}\left[\ \Sigma_{g'gS}\ \right]_{g,g}. \tag{26}$$

Insert this expression into the equation above it, match it to the other cross section sensitivities, and realize that the total cross section sensitivity coefficient is the sum of the constituent cross section sensitivities,

$$S_{k_\infty,\Sigma_{gT}} = S_{k_\infty,\Sigma_{gC}} + S_{k_\infty,\Sigma_{gF}} + \sum_{g'=1}^{G} S_{k_\infty,\Sigma_{g'gS}}. \tag{27}$$

However, examine Equation (11) and realize that perturbing each of the cross sections by the same amount cancels out and leaves the original unperturbed value for k_∞ as the result. This means that the total cross section sensitivity is expected to be zero for these infinite medium systems,

$$S_{k_\infty,\Sigma_{gT}} = 0. \tag{28}$$

2.3. Calculating the Scalar Neutron Flux and Adjoint Flux

Expressions for calculating the scalar neutron flux and adjoint flux are presented and used to show that the equations derived in this paper are equivalent to those from first-order perturbation theory. Keep in mind that k_∞ is known by Equation (11) and gather all of the terms in Equation (1) on the left-hand side,

$$\left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} - \frac{1}{k_\infty} \overline{\chi}\; \overline{\nu\Sigma_F} \right) \overline{\phi} = \overline{\overline{L}}\, \overline{\phi} = \overline{0}. \tag{29}$$

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 scalar neutron flux,

$$\ker\left(\overline{\overline{L}} \right) = \left\{ \overline{\phi} \in \mathbb{R}^G \mid \overline{\overline{L}}\, \overline{\phi} = \overline{0} \right\} = \overline{\overline{L}}^{-1}\, \overline{0}. \tag{30}$$

There are two notes on the practicality of performing this calculation. First, realize that one has 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 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 the sign ambiguity of the resulting vector may need to be removed if this method is used.

The adjoint flux vector can be calculated in a similar manner. The general multigroup infinite medium *adjoint* k-eigenvalue problem is

$$\overline{\overline{\Sigma_T}}\, \overline{\phi}^\dagger = \overline{\overline{\Sigma_S}}^\intercal\, \overline{\phi}^\dagger + \frac{1}{k_\infty} \overline{\nu\Sigma_F}^\intercal\, \overline{\chi}^\intercal\, \overline{\phi}^\dagger, \tag{31}$$

where $(\cdot)^\intercal$ is used to denote the matrix-vector transpose operation. This equation can also be used to find an analytic expression for k_∞,

$$k_\infty = \overline{\chi}^\intercal \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}^\intercal \right)^{-1} \overline{\nu\Sigma_F}^\intercal, \tag{32}$$

which gives the same result for k_∞ as Equation (11). Finally, use Equation (31) to define the linear map, $\overline{\overline{L}}^\dagger$, that is needed to calculate the adjoint flux vector,

$$\ker\left(\overline{\overline{L}}^\dagger \right) = \left\{ \overline{\phi}^\dagger \in \mathbb{R}^G \mid \overline{\overline{L}}^\dagger\, \overline{\phi}^\dagger = \overline{0} \right\} = \left(\overline{\overline{L}}^\dagger \right)^{-1} \overline{0}, \tag{33}$$

where

$$\overline{\overline{L}}^\dagger = \overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}^\intercal - \frac{1}{k_\infty} \overline{\nu\Sigma_F}^\intercal\, \overline{\chi}^\intercal. \tag{34}$$

This method for calculating the scalar neutron flux and adjoint flux highlights the fact that they both live in the null space of their respective k-eigenvalue transport matrices. However, there is a simpler approach to calculating the scalar neutron flux. Realize that k_∞ and $\overline{\nu\Sigma_F}\, \overline{\phi}$ in Equation (9) are constants, which means that the scalar neutron flux can be written as

$$\overline{\phi} \propto \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1} \overline{\chi}. \tag{35}$$

Similarly, Equation (31) can be rearranged to show that

$$\overline{\phi}^\dagger \propto \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}}^\intercal \right)^{-1} \overline{\nu\Sigma_F}^\intercal, \tag{36}$$

and transposing this expression results in

$$\overline{\phi}^{\dagger\intercal} \propto \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1}. \tag{37}$$

These expressions for the scalar neutron flux and adjoint flux can be substituted into Equation (24) to recover the typical adjoint-weighted result found from first-order perturbation theory [2],

$$S_{k_\infty,\Sigma_{gT}} = \Sigma_{gT} \frac{\overline{\phi}^{\dagger\intercal} \left(\frac{1}{k_\infty} \overline{\chi} \frac{\partial \overline{\nu\Sigma_F}}{\partial \Sigma_{gT}} - \frac{\partial \overline{\overline{\Sigma_T}}}{\partial \Sigma_{gT}} + \frac{\partial \overline{\overline{\Sigma_S}}}{\partial \Sigma_{gT}} \right) \overline{\phi}}{\frac{1}{k_\infty} \overline{\phi}^{\dagger\intercal} \overline{\chi} \, \overline{\nu\Sigma_F} \, \overline{\phi}}, \tag{38}$$

where it has been recognized that

$$k_\infty^2 = \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1} \overline{\chi} \, \overline{\nu\Sigma_F} \left(\overline{\overline{\Sigma_T}} - \overline{\overline{\Sigma_S}} \right)^{-1} \overline{\chi} \propto \overline{\phi}^{\dagger\intercal} \overline{\chi} \, \overline{\nu\Sigma_F} \, \overline{\phi}. \tag{39}$$

Thus, it has been shown that the general set of equations derived in this paper are equivalent to their adjoint-based counterparts and can be used to verify not only the final sensitivity results of a non-analytic solution but the contributon components of that solution as well.

3. URANIUM EXAMPLES

All of the analytic expressions derived in Section 2 are general and exact given that the assumptions of the paper are met. 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, examples are presented to reinforce the reader's understanding of the mathematics. To that end, consider the multigroup nuclear data and corresponding k-eigenvalues, forward flux, adjoint flux, and sensitivity profiles for two infinite medium systems consisting of U-235 and U-238.

The multigroup nuclear data presented in Figure 2 was generated using the multigroup tally options in MCNP6.3 [4, 5]. Two infinite medium k-eigenvalue problems consisting purely of U-235 and U-238 were set up and energy dependent track-length flux tallies were specified (`F4:n CELL`). The following special treatments were specified to generate the multigroup nuclear data: (`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.

The continuous energy k-eigenvalues calculated with MCNP6.3 are compared to the multigroup k-eigenvalues calculated with Equation (11) in Table I. Notice that the physics not accounted for in Equation (1) makes a relatively small but important impact on the k-eigenvalue. This result highlights the importance of including all relevant physics in neutron transport simulations, because, in both cases, the k-eigenvalue is underestimated.

Table I. Continuous energy k-eigenvalues produced by MCNP6.3 [4] and analytic multigroup k-eigenvalues for two infinite medium systems consisting of U-235 and U-238

Isotope	Continuous MCNP	Analytic Multigroup	Multigroup / Continuous
U-235	2.28014 ± 0.00004	2.26898	0.99511
U-238	0.31019 ± 0.00006	0.30327	0.97769

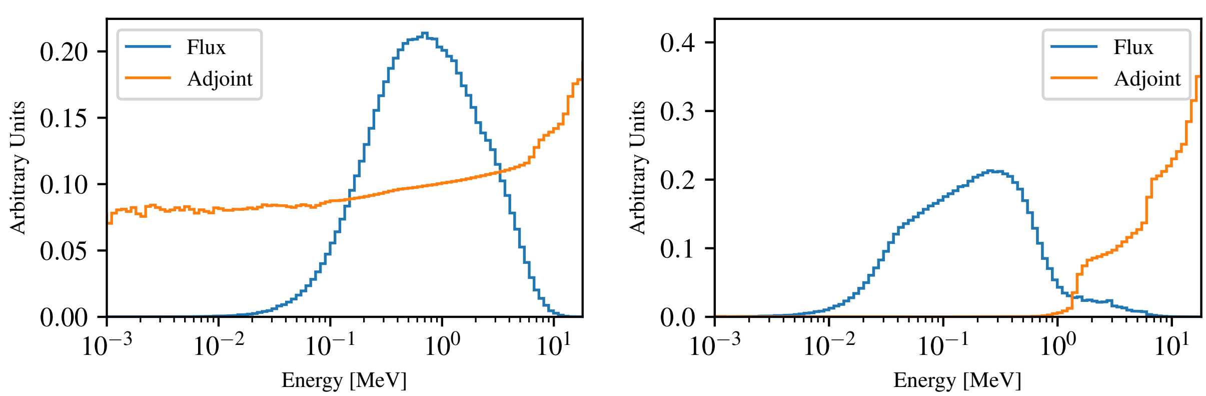
The energy integrated macroscopic cross section sensitivities calculated with the KSEN card in MCNP6.3 are compared to the analytic results calculated with the expressions developed in Section 2.2.2 in Table II.

The results agree within statistics, which is evidenced by the ratios of the two values being near unity and the z-scores being less than one in all but one case. This is a simple example of how the analytic expressions developed in this paper can be used to generate benchmark test sets. A full test set would include verification of the k-eigenvalue, scalar neutron flux, adjoint flux, and the energy dependent sensitivity profiles.

Table II. MCNP6.3 [4] KSEN results and analytic energy integrated cross section sensitivities for two infinite medium systems consisting of U-235 and U-238 (N/A = not applicable)

Isotope	Cross Section	KSEN	Analytic	Analytic / KSEN	Z-Score
U-235	Total	−0.00015 ± 0.00144	0.00000	N/A	0.10078
	Fission	0.16022 ± 0.00038	0.16067	1.00284	1.18638
	Capture	−0.10363 ± 0.00007	−0.10358	0.99950	0.72832
	Scatter	−0.05673 ± 0.00123	−0.05710	1.00638	−0.29495
U-238	Total	−0.00045 ± 0.00103	0.00000	N/A	0.43625
	Fission	0.81334 ± 0.00012	0.81339	1.00006	0.42523
	Capture	−0.01471 ± 0.00004	−0.01472	1.00013	−0.04882
	Scatter	−0.79908 ± 0.00099	−0.79867	0.99950	0.40612

Figure 1 compares the scalar neutron flux and adjoint flux for both systems. These are non-self adjoint systems with U-238 only having a non-negligible adjoint flux beyond the classic fission energy threshold. Figure 3 compares the sensitivity profiles for each uranium isotope. There is common behavior between the two sets of profiles, e.g., the constituent cross section sensitivities both sum to zero, which is what was 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 energy integrated scattering sensitivity profile is solely a function of out-group scattering. Notice 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, it is important to have accurate knowledge of the nuclear data cross section resonances when performing the sensitivity analysis of a nuclear system. This means that the analytic multipole-multigroup sensitivity coefficients should be investigated to further understand the dominant sensitivity mechanisms of the k-eigenvalue problems at hand.



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

Figure 1. Analytic scalar neutron flux and adjoint flux for two infinite medium systems consisting of U-235 and U-238

4. CONCLUSIONS

In this paper, the analytic sensitivity coefficients for general multigroup infinite medium k-eigenvalue problems were derived. 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 meticulously recorded. The reader can apply these equations to a set of multigroup nuclear data cross sections that satisfy the assumptions given in this paper and use the results to verify that their numerical sensitivity calculations are correct. The objective of this work is to give the nuclear engineering community a new method to rapidly verify that sensitivity calculations agree with theory. In the future, these equations can be extended to account for multiple isotopic species, more reactions, and higher order sensitivity coefficients.

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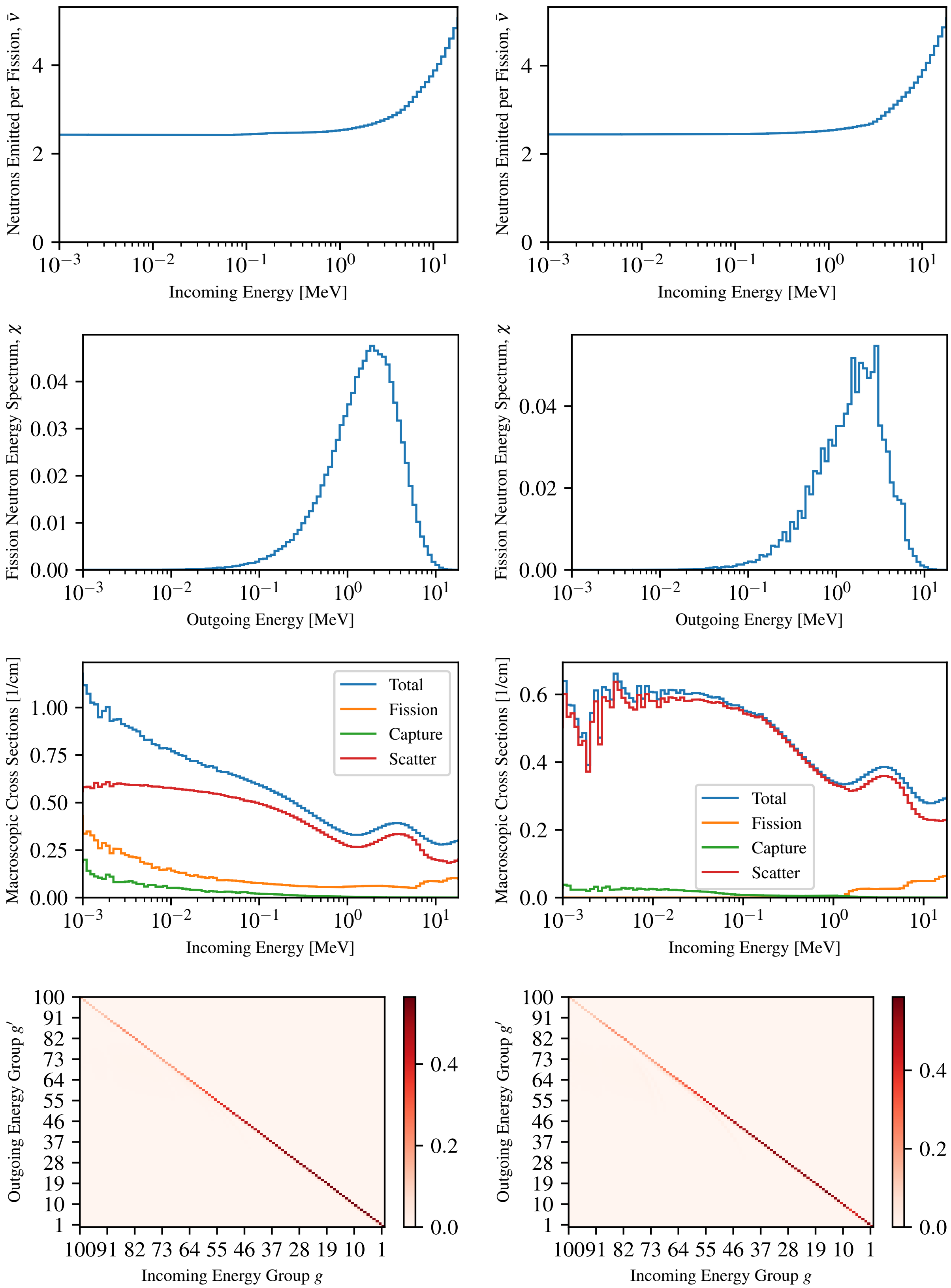
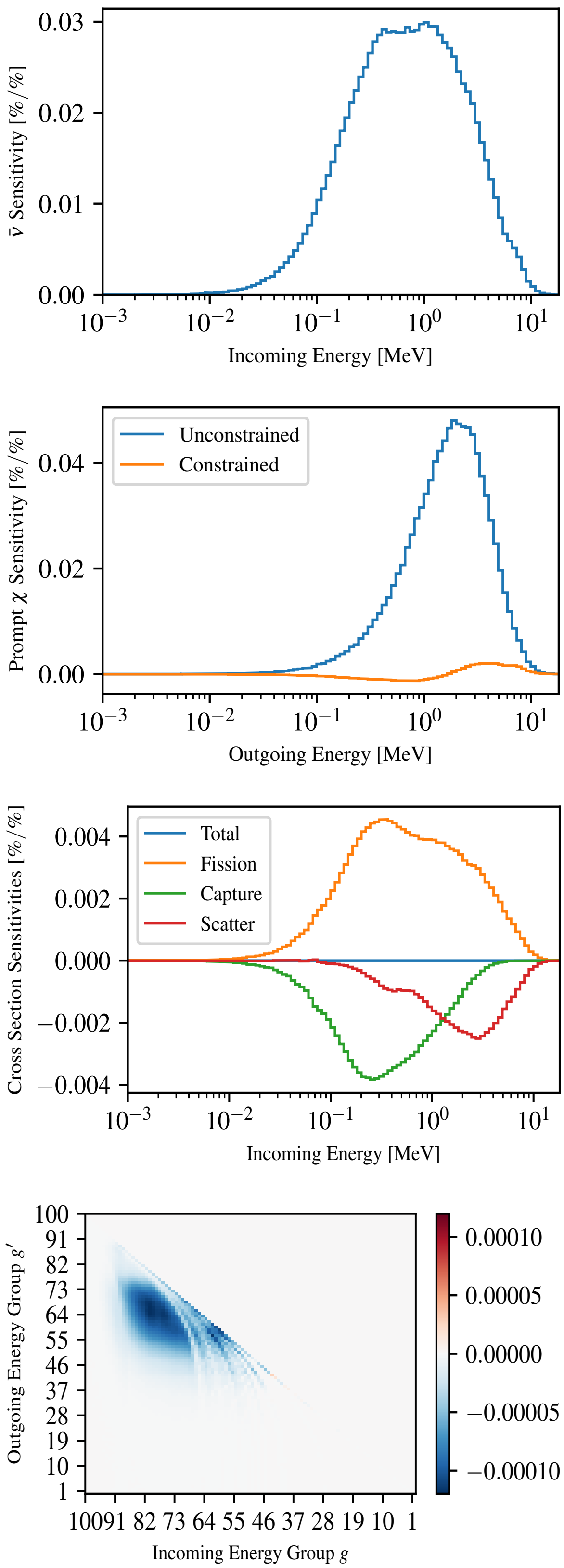
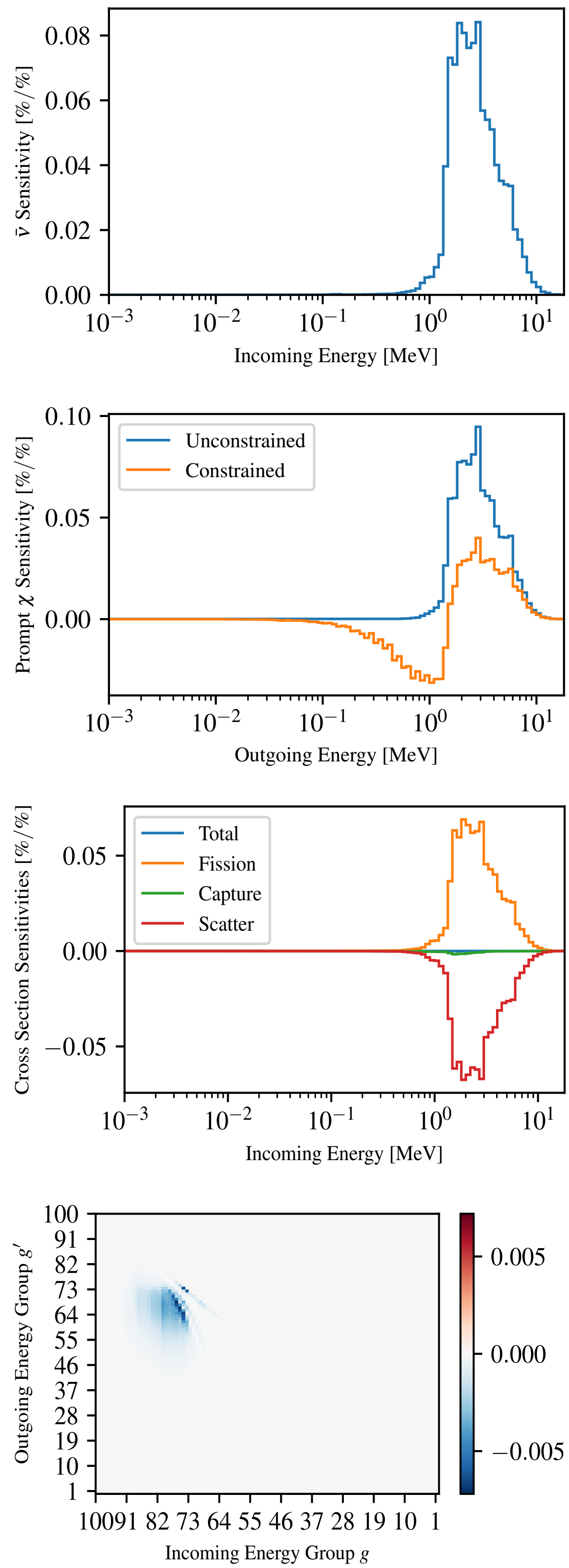


(a) U-235 **(b) U-238**

Figure 2. Multigroup nuclear data produced by MCNP6.3 [4] for two infinite medium systems consisting of U-235 and U-238



(a) U-235



(b) U-238

Figure 3. Analytic multigroup nuclear data sensitivity coefficients for two infinite medium systems consisting of U-235 and U-238