# ADJOINT-BASED SENSITIVITY FOR RADIATION TRANSPORT USING AN EDDINGTON TENSOR FORMULATION

A Thesis

by

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ABSTRACT

Adjoint methods can provide a first-order approximation of the response a physical system experiences due to a perturbation in the system's parameters. However, when applying the method to time dependent transport, memory costs can quickly become a concern, and a fully angular dependent flux must be stored at each timestep. In this thesis, a lower-order Variable Eddington Tensor formulation of the transport equation is considered to remove the angular dependence of the stored solution and reduce memory costs. Indeed, given the Eddington tensor, the Eddington tensor approach yields the same flux solution as the full transport solution.

In the case of perturbations, one may make some simplifying assumption regarding the Eddington tensor: for instance, keep it unperturbed or assuming a functional variation of the Eddington tensor over the input parameter space. An unperturbed Eddington assumption may introduce error in the sensitivity calculation. A simple linear interpolation scheme for the Eddington over the uncertain parameter range is devised for use in certain scenarios, at the cost of requiring a few additional angular solves to parameterize the Eddington tensor. An alternate formulation using an Eddington tensor derived from the adjoint transport is also presented. Comparison of the derived Eddington methods and transport methods is done using simple slab geometry test cases.

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NOMENCLATURE

| | |
|---|---|
| VET | Variable Eddington Tensor |
| aVET | Adjoint Variable Eddington Tensor |
| SN | Discrete Ordinate Method |
| $\langle \bullet, \bullet \rangle$ | Volumetric Inner Product $\int_V dV$ |
| $\langle\langle \bullet, \bullet \rangle\rangle$ | Volumetric-Angular Inner Product $\int_V \int_{4\pi} d\Omega dV$ |
| $[\bullet, \bullet]$ | Boundary Inner Product $\oint_{\partial V} dS$ |
| $[\![\bullet, \bullet]\!]$ | Boundary-Angular Inner Product $\oint_{\partial V} \int_{4\pi} d\Omega dS(\vec{\Omega} \cdot \vec{n})$ |
| $\psi$ | Forward Angular Flux |
| $\phi$ | Forward Scalar Flux |
| $\varphi$ | Forward-like Flux from aVET formulation |
| $\psi^\dagger$ | Adjoint Angular Flux |
| $\phi^\dagger$ | Adjoint Scalar Flux |
| $\varphi^\dagger$ | Adjoint-like Flux from VET formulation |
| $\mathbb{E}$ | Eddington Tensor |
| $\mathbb{E}^\dagger$ | Adjoint Eddington Tensor |

CONTRIBUTORS AND FUNDING SOURCES

## Contributors

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# 1. INTRODUCTION

## 1.1 Introduction

Computational simulations have become important tools for engineers and scientists across a wide array of disciplines. These simulations allow for researchers to examine significantly complex and long life systems in a way that is frequently more economical in both time and money than construction of the real world system, if even feasible. An important step in creating one of these methods is confirmation that the results can be trusted to reasonably approximate the real life scenario. This can be accomplished using three processes outlined by the National Research Council [1]

- Verification - How accurately does the computation solve the underlying equations of the model for the quantities of interest?
- Validation - How accurately does the model represent reality for the quantities of interest?
- Uncertainty Quantification (UQ) - How do the various sources of error and uncertainty feed into uncertainty in the model-based prediction of the quantity of interest?

Adjoint methods are of particular interest for UQ. In general, adjoint methods provide a mechanism for propagating uncertainty and error in the system variables to the uncertainty in the desired quantity of interest. Adjoint methods accomplish this in a particularly economical way, sometimes requiring only two differential system solves which can then be used for any combination of sources of error, as opposed to performing an independent solve for each individual error scenario. These adjoint methods have been applied across various complex and time dependent systems. An example of adjoint methods applied to hydrodynamic systems with shocks can be found in Wildey et al. [2]. A more relevant adjoint example to neutron transport occurs in Stripling et al. in the form of reactor burn-up equations [3].

Application of the adjoint method to time-dependent transport can pose a major technical limitation. In general, the adjoint method applied to radiation transport requires storing six-dimensional data (the forward angular flux) at each time step. When dealing with high resolution in these six dimensions and many time steps, this can potentially require an unreasonable amount of memory for data storage, rendering the method functionally unusable.

Typically, a checkpointing method can be employed to alleviate some of the memory limitations of a time dependent adjoint system [4] [5]. In this scheme, the forward solution, i.e., the angular flux in the case of transport, is stored at checkpoint timesteps when performing a forward solve from $t = 0$ to $T$. The adjoint method then initializes at the final time step, which sweeps in the reverse time direction. At any point the forward solution is needed in the reverse sweep for a quantity of interest calculation the forward solution is reconstructed by performing a forward solve starting with the nearest checkpoint. Ultimately, this becomes a balancing act of memory usage for storing checkpoints and additional computation time for recomputing the forward solution from checkpoints. An efficient checkpointing scheme which chooses the checkpoints in a binomial fashion is presented by Griewank and Walther [5]. However this method still requires the storing of the primary time-dependent variable, the angular flux, at the checkpoint times. For large phase-space solutions, this can severely limit the number of checkpoints that can be stored in memory, resulting in a increase in compute time for calculating the uncertainty propagation.

Moreover, many quantities of interest in transport can be computed from the scalar flux and do not require the angular flux. Having to store and recompute the angular flux only for it to be integrated over angle and converted to a scalar flux for use can be a computational burden. A potential solution to the memory requirement for the time-dependent transport adjoint formulation is the use of a quasi-diffusion method to reduce the overall dimensionality of the transport problem, from 6D+time (space, direction, energy, time for transport) to 4D+time (space, energy, time for quasi-diffusion). The quasi-diffusion method examined in this work is termed as a "Variable Eddington Tensor" (VET) formulation and uses the unperturbed forward angular flux to compute the Eddington tensor needed in the quasi-diffusion approach. While not the focus of this thesis, in the VET formulation the primary time-dependent variable is the scalar flux. Therefore, with the proper adjoint formulation a checkpointing method could be applied to the VET formulation in which scalar flux are checkpointed as a method to further reduce memory requirements.

This thesis is organized as follows. In Chapter 2 the typical transport adjoint method is demonstrated and the inner products required for sensitivity calculations are derived. Then in Chapter 3 a quasi-diffusion formulation is taken of the transport equation. This quasi-diffusion approach then undergoes an adjoint treatment to derive sensitivity inner products that do not require storing any angular fluxes. An alternate quasi-diffusion method is proposed in Chapter 4, a quasi-diffusion formulation is taken of the adjoint transport equation and a similar approach is taken in an attempt to derive another set of inner products to use for sensitivity. The three methods and the relation between them are shown in Figure 1.1. In Chapter 5 the methods are tested against each other on simple system to verify expected behavior and examine their accuracy. Conclusions about the derived methods based on the test cases are presented in Chapter 6.

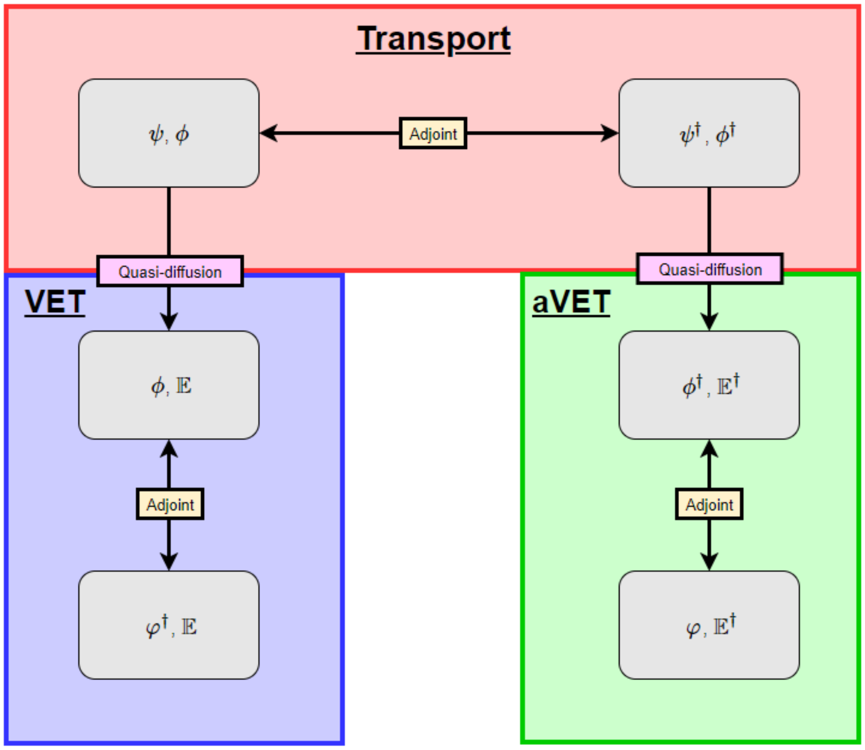


Figure 1.1: Diagram showing relations between various formulations in this thesis.

# 2. BACKGROUND (TRANSPORT)

This work will focus on a relatively simple transport equation form, the one-group steady-state transport equation. Examination of effectiveness of an adjoint formalism using the quasi-diffusion approximation instead of the full transport solution in this setting will provide insight to the advantages and shortcomings of the technique when applied to multigroup, time-dependent transport equation. A cursory formulation of the one-group time-dependent quasi-diffusion equation can be found in Appendix A, which shows some terms shared with the steady state formulation. In the following chapter, the forward steady-state one-group transport equation is presented, the corresponding adjoint equation is derived, then sensitivity inner products are derived using a first order approximation.

## 2.1 Steady-state One-group Neutron Transport Equation

The one-group steady-state transport equation with isotropic sources and isotropic scattering for a volume $V$ bounded by its surface $\partial V$ is given below.

$$\vec{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, \vec{\Omega}) + \sigma_t(\vec{r}) \psi(\vec{r}, \vec{\Omega}) = \frac{1}{4\pi} \sigma_s(\vec{r}) \phi(\vec{r}) + \frac{1}{4\pi} q(\vec{r}), \quad \forall \vec{r} \in V \tag{2.1}$$

$$\psi(\vec{r}, \vec{\Omega}) = \psi^{\text{inc}}(\vec{r}, \vec{\Omega}) \quad \vec{r} \in \partial V^- = \{\vec{r} \in \partial V, \text{ s.t. }, \vec{\Omega} \cdot \vec{n}(\vec{r}) < 0\} \tag{2.2}$$

The possibly uncertain parameters in this system are: the total and scattering cross sections $\sigma_t$ and $\sigma_s$, the volumetric source term $q$, and the incident angular flux on the system given by $\psi^{\text{inc}}$. The unknowns (dependent variables) are the angular flux $\psi(\vec{r}, \vec{\Omega})$ and the scalar flux $\phi(\vec{r})$ given by

$$\phi(\vec{r}) = \int_{4\pi} d\Omega \, \psi(\vec{r}, \vec{\Omega}) \, .$$

### 2.1.1 Quantity of Interest, Response Functions, and Inner Products

Frequently, the solution to the transport equation is not the sought after value, but rather some Quantity of Interest (*QoI*), a functional that depends on the transport solution. Given $\psi(\vec{r},\vec{\Omega})$, the solution of the one-group steady-state transport (Eq. (2.1)), and $R(\vec{r},\vec{\Omega})$, a "response function" specific to the desired ***QoI***, the quantity of interest is defined as

$$QoI := \int_V dV \int_{4\pi} d\vec{\Omega}\, R(\vec{r},\vec{\Omega})\psi(\vec{r},\vec{\Omega}) \tag{2.3}$$

The response function $R$ can take on physically defined forms, such as the cross section of a detector; or it may take a form of a mathematical construct, such as $R(\vec{r},\vec{\Omega}) = 1/v$ to return the total number of neutrons present in the system. Another example is to let $R(\vec{r},\vec{\Omega}) = \sigma\chi(\vec{r})$ to obtain the total reaction rate in a portion of the domain ($\chi(\vec{r}) = 1$ if $\vec{r} \in$ region of interest, and 0 otherwise). Note that the response function will frequently be expressed as $q^\dagger$, the adjoint source, as we have already noted that there is a relationship between the solution, the adjoint solution, and their respective source terms.

Two volumetric inner products are defined using $\langle\langle \bullet, \bullet \rangle\rangle$ and $\langle \bullet, \bullet \rangle$ notations. These two inner-products are for use with angular and scalar fluxes, respectively.

$$\langle\langle \psi, f \rangle\rangle = \int_V dV \int_{4\pi} d\Omega\, \psi(\vec{r},\vec{\Omega}) f(\vec{r},\vec{\Omega})\,, \tag{2.4a}$$

$$\langle \phi(\vec{r}), f \rangle = \int_V dV\, \phi(\vec{r}) g(\vec{r})\,. \tag{2.4b}$$

For later use, two additional inner products are also defined as surface integrals over the domain boundary $\partial V$. The second definition is used to distinguish between incoming and outgoing surface integrals.

$$[\![\psi, f]\!] = \int_{\partial V} dS \int_{4\pi} d\Omega \, \vec{\Omega} \cdot \vec{n}(\vec{r}) \, \psi(\vec{r}, \vec{\Omega}) f(\vec{r}, \vec{\Omega}) \,, \tag{2.5a}$$

$$[\![\psi, f]\!]_{\pm} = \int_{\partial V} dS \int_{\vec{\Omega}\cdot\vec{n} \gtrless 0} d\Omega \, \vec{\Omega} \cdot \vec{n}(\vec{r}) \, \psi(\vec{r}, \vec{\Omega}) f(\vec{r}, \vec{\Omega}) \,. \tag{2.5b}$$

Therefore, with this notation, the quantity of interest can be compactly expressed as shown below.

$$QoI := \left\langle\!\!\left\langle \psi(\vec{r}, \vec{\Omega}), q^\dagger(\vec{r}) \right\rangle\!\!\right\rangle = \left\langle \phi(\vec{r}), q^\dagger(\vec{r}) \right\rangle \tag{2.6}$$

### 2.1.2 Sensitivity Coefficients

A hurdle in utilizing the transport equation numerically to make real world predictions is that the system's parameters ($\sigma_t$, $\sigma_s$, $q$, and $\psi^{inc}$) may not be known exactly. This uncertainty in the system parameters is expected to translate to an uncertainty in the *QoI* value. Ideally, a reasonable error range would be determined for each system parameter and the system simulation would run over a finely discretized parameter space, using the resulting *QoI* values to generate an error range for the *QoI*. However, this straightforward method tends to be resource-intensive, requiring a complete forward solve of the transport equation for each input uncertainty scenario. Adjoint methods offer a way to drastically reduce the number of solves, while generally remaining fairly accurate for small perturbations around base or nominal values of the parameters.

## 2.2 Adjoint Sensitivity

Adjoint operators can provide a useful tool for sensitivity calculations. Using inner product notation consider the system of interest $\mathbf{A}\psi = q$. Call this this the forward system, with forward operator $\mathbf{A}$. Consider a test function $\psi^\dagger$, the adjoint operator $\mathbf{A}^\dagger$ is defined such that $\langle\!\langle \mathbf{A}\psi, \psi^\dagger \rangle\!\rangle = \langle\!\langle \psi, \mathbf{A}^\dagger\psi^\dagger \rangle\!\rangle$. For differential operators, derivation of $\mathbf{A}^\dagger$ generally relies on application of the divergence theorem (integration by parts), typically resulting in boundary terms ($BC$). Using the response function of the desired ***QoI***, the adjoint system can be constructed as $\mathbf{A}^{\dagger}\psi^{\dagger} = q^{\dagger}$, leading to an alternate expression of the ***QoI*** using the adjoint solution $\psi^{\dagger}$.

$$QoI = \left\langle\!\left\langle \psi, q^{\dagger} \right\rangle\!\right\rangle = \left\langle\!\left\langle \psi, \mathbf{A}^{\dagger}\psi^{\dagger} \right\rangle\!\right\rangle = \left\langle\!\left\langle \mathbf{A}\psi, \psi^{\dagger} \right\rangle\!\right\rangle + BC = \left\langle\!\left\langle q, \psi^{\dagger} \right\rangle\!\right\rangle + BC \tag{2.7}$$

Using the ***QoI*** definition, we formulate an approximation to the change in the quantity of interest ($\delta QoI$) using only perturbations in the initial system, i.e., using perturbation to the forward operator $\delta\mathbf{A}$ and forward source $\delta q$, but omitting changes in the forward solution itself [6]. Derivation of this approximation to the sensitivity coefficient begins with the perturbed system $\mathbf{A}_p\psi_p = q_p$ multiplied by the adjoint function $\psi^{\dagger}$ defined above. After expressing the perturbations in a $\delta$ form a first order approximation of $\delta\mathbf{A}\delta\psi = 0$ is used. An integration by parts is used to transpose $\mathbf{A}$ to $\mathbf{A}^{\dagger}$, resulting in boundary terms appearing.

$$\begin{aligned}
\left\langle\!\left\langle \mathbf{A}_p\psi_p, \psi^{\dagger} \right\rangle\!\right\rangle &= \left\langle\!\left\langle q_p, \psi^{\dagger} \right\rangle\!\right\rangle \\
\left\langle\!\left\langle (\mathbf{A} + \delta\mathbf{A})\left(\psi + \delta\psi\right), \psi^{\dagger} \right\rangle\!\right\rangle &= \left\langle\!\left\langle q + \delta q, \psi^{\dagger} \right\rangle\!\right\rangle \\
\left\langle\!\left\langle \mathbf{A}\psi + \delta\mathbf{A}\psi + \mathbf{A}\delta\psi, \psi^{\dagger} \right\rangle\!\right\rangle &\approx \left\langle\!\left\langle q + \delta q, \psi^{\dagger} \right\rangle\!\right\rangle \\
\left\langle\!\left\langle \mathbf{A}\psi + \mathbf{A}\delta\psi, \psi^{\dagger} \right\rangle\!\right\rangle &= \left\langle\!\left\langle q + \delta q - \delta\mathbf{A}\psi, \psi^{\dagger} \right\rangle\!\right\rangle \\
\left\langle\!\left\langle \psi + \delta\psi, \mathbf{A}^{\dagger}\psi^{\dagger} \right\rangle\!\right\rangle &= \left\langle\!\left\langle q + \delta q - \delta\mathbf{A}\psi, \psi^{\dagger} \right\rangle\!\right\rangle + BC \\
\left\langle\!\left\langle \psi_p, q^{\dagger} \right\rangle\!\right\rangle &= \left\langle\!\left\langle q + \delta q - \delta\mathbf{A}\psi, \psi^{\dagger} \right\rangle\!\right\rangle + BC
\end{aligned} \tag{2.8}$$

The left side of the final step of the above derivation is the perturbed *QoI*. Subtracting Eq. (2.7) from this yields the desired expression for the $\delta QoI$.

$$\delta QoI \approx \left\langle\left\langle \delta q - \delta \mathbf{A}\psi, \psi^{\dagger} \right\rangle\right\rangle + \delta BC \tag{2.9}$$

The advantage of the above expression for $\delta QoI$ is that two solves, one for the forward and another for the adjoint, can be used to approximate the sensitivity for a variety of operator and source perturbations, $\delta\mathbf{A}$ and $\delta q$.

### 2.2.1 Adjoint Formulation for Transport

In a fairly straightforward application of the adjoint method previously shown,

$$\begin{aligned}
\left\langle\left\langle \frac{q}{4\pi}, \psi^{\dagger} \right\rangle\right\rangle &= \left\langle\left\langle \vec{\Omega}\cdot\vec{\nabla}\psi + \sigma_t\psi - \frac{\sigma_s}{4\pi}\phi, \psi^{\dagger} \right\rangle\right\rangle \\
&= \left\langle\left\langle \vec{\Omega}\cdot\vec{\nabla}\psi, \psi^{\dagger} \right\rangle\right\rangle + \left\langle\left\langle \sigma_t\psi, \psi^{\dagger} \right\rangle\right\rangle - \left\langle\left\langle \frac{\sigma_s}{4\pi}\phi, \psi^{\dagger} \right\rangle\right\rangle \\
&= -\left\langle\left\langle \psi, \vec{\Omega}\cdot\vec{\nabla}\psi^{\dagger} \right\rangle\right\rangle + \left\langle\left\langle \psi, \sigma_t\psi^{\dagger} \right\rangle\right\rangle - \left\langle\left\langle \psi, \frac{\sigma_s}{4\pi}\phi^{\dagger} \right\rangle\right\rangle + [[\psi^{\dagger}, \psi]] \\
&= \left\langle\left\langle \psi, -\vec{\Omega}\cdot\vec{\nabla}\psi^{\dagger} + \sigma_t\psi^{\dagger} - \frac{\sigma_s}{4\pi}\phi^{\dagger} \right\rangle\right\rangle + [[\psi^{\dagger}, \psi]] \\
&= \left\langle\left\langle \psi, q^{\dagger} \right\rangle\right\rangle + [[\psi^{\dagger}, \psi]]
\end{aligned} \tag{2.10}$$

the adjoint equation which corresponds to the transport formulation with adjoint source (response function) $q^{\dagger}$ is

$$-\vec{\Omega}\cdot\vec{\nabla}\psi^{\dagger} + \sigma_t\psi^{\dagger} = \frac{\sigma_s}{4\pi}\phi^{\dagger} + q^{\dagger} \tag{2.11a}$$

$$\psi^{\dagger}(\vec{r}) = \psi^{\dagger,\text{out}}(\vec{r}) = 0 \quad \vec{r} \in \partial V^{+} = \{\vec{r} \in \partial V, \quad \vec{\Omega}\cdot\vec{n} > 0\} \tag{2.11b}$$

where the definition of the adjoint scalar flux $\phi^{\dagger}$ is analogous to that of the forward scalar flux. It is worth noting that the adjoint equation is in the form of the standard transport equation, only with the direction of travel reversed ($\vec{\Omega} \to -\vec{\Omega}$). This often allows for forward transport solvers to be easily adapted to solving the adjoint transport system. Once the adjoint solution is obtained, the corresponding *QoI* can be calculated with a simple inner product with the forward source term, as follows from equations Eq. (2.7) and Eq. (2.10).

$$QoI := \langle\langle \psi, q^\dagger \rangle\rangle = \left\langle\left\langle \psi^\dagger, \frac{q}{4\pi} \right\rangle\right\rangle - [[\psi^\dagger, \psi]] \tag{2.12}$$

The surface interval in (2.12) can be split into incoming and outgoing flux integrals,

$$[[\psi^\dagger, \psi]]_- = [[\psi^\dagger, \psi^{\text{inc}}]]_- + [[\psi^{\dagger,\text{out}}, \psi]]_+$$

which are handled by the forward and adjoint boundary conditions respectively. Setting $\psi^{\dagger,\text{out}} = 0$ removes the outgoing flux integral:

$$\begin{aligned} QoI &= \left\langle\left\langle \psi^\dagger, \frac{q}{4\pi} \right\rangle\right\rangle - [[\psi^\dagger, \psi^{\text{inc}}]]_- \\ &= \left\langle \phi^\dagger, \frac{q}{4\pi} \right\rangle - [[\psi^\dagger, \psi^{\text{inc}}]]_- \ . \end{aligned} \tag{2.13}$$

### 2.2.2 Transport Adjoint Sensitivity

Now consider perturbations to our system. Specifically perturbations of $\delta\sigma_t$, $\delta\sigma_s$, and $\delta q$ to the total cross section, scattering cross section and angular source term respectively. In addition, the incident angular flux is also perturbed by $\delta\psi^{inc}$. These perturbations result in a perturbed solution to the SN-transport equation $\psi_p$.

$$\vec{\Omega} \cdot \vec{\nabla}\psi_p + \sigma_{t,p}\psi_p = \frac{\sigma_{s,p}}{4\pi}\phi_p + \frac{q_p}{4\pi}, \quad \forall \vec{r} \in V \tag{2.14}$$

$$\psi_p(\vec{r}) = \psi_p^{\text{inc}}(\vec{r}), \quad \forall \vec{r} \in \partial V^- \tag{2.15}$$

Any quantity with a subscript $p$ is to be understood as the perturbed value, that is, as the sum of the unperturbed value and the perturbation amount: $a_p = a + \delta a$.

This perturbation may result in a change to the *QoI*, now given by $QoI_p = \left\langle \psi_p, q^\dagger \right\rangle$. Note that we assumed that the response function (adjoint source) was not affected by the perturbation. Using the *unperturbed* adjoint equation given in Eq. (2.11a), the perturbed *QoI* can be expressed as:

$$\begin{aligned} QoI_p &= \left\langle\left\langle \psi_p, q^\dagger \right\rangle\right\rangle \\ &= \left\langle\left\langle \psi_p, -\vec{\Omega}\cdot\vec{\nabla}\psi^\dagger + \sigma_t\psi^\dagger - \frac{\sigma_s}{4\pi}\phi^\dagger \right\rangle\right\rangle \end{aligned} \tag{2.16}$$

Next, we perform an integration by parts and obtain:

$$QoI_p = \left\langle\left\langle \vec{\Omega}\cdot\vec{\nabla}\psi_p + \sigma_t\psi_p - \frac{\sigma_s}{4\pi}\phi_p, \psi^\dagger \right\rangle\right\rangle - \left[\left[\psi_p, \psi^\dagger\right]\right] \tag{2.17}$$

Note that the cross sections are unperturbed in Eq. (2.17). Using a $\delta$ notation for the perturbed system variables ($\sigma_{s,p} = \sigma_s + \delta\sigma_s$ for example), we can introduce the perturbed quantities:

$$\begin{aligned} QoI_p &= \left\langle\left\langle \vec{\Omega}\cdot\vec{\nabla}\psi_p + (\sigma_{t,p} - \delta\sigma_t)\psi_p - \frac{\sigma_{s,p} - \delta\sigma_s}{4\pi}\phi_p, \psi^\dagger \right\rangle\right\rangle - \left[\left[\psi_p, \psi^\dagger\right]\right] \\ &= \left\langle\left\langle \frac{q_p}{4\pi} - \delta\sigma_t\psi_p + \frac{\delta\sigma_s}{4\pi}\phi_p, \psi^\dagger \right\rangle\right\rangle - \left[\left[\psi_p, \psi^\dagger\right]\right] \end{aligned} \tag{2.18}$$

Next, note that the cross section terms have double perturbations terms $\delta\sigma_t\delta\psi$ and $\delta\sigma_s\delta\psi$ once it is observed that $\psi_p = \psi + \delta\psi$. In a first-order approximation, these doubly perturbed terms are ignored, yielding:

$$QoI_p \approx \left\langle\left\langle \frac{q + \delta q}{4\pi} - \delta\sigma_t\psi + \frac{\delta\sigma_s}{4\pi}\phi, \psi^\dagger \right\rangle\right\rangle - \left[\left[\psi_p, \psi^\dagger\right]\right] \ . \tag{2.19}$$

Subtraction of the unperturbed *QoI* expression in Eq. (2.12) supplies a final equation for computing the change in *QoI* using only the system perturbations and the unperturbed forward solution $\psi$ and the adjoint unperturbed solution $\psi^\dagger$, removing the need to solve the perturbed forward equation. Furthermore the boundary terms can be split into incoming and outgoing contributions. Using a zero outgoing boundary condition for the adjoint flux (thus $\left[\delta\psi, \psi^{\dagger,\text{out}}\right]_+ = 0$), one obtains the final form of the perturbation in the *QoI*.

$$\begin{aligned}
\delta QoI &= \left\langle\!\!\left\langle \frac{\delta q}{4\pi} - \delta\sigma_t\psi + \frac{\delta\sigma_s}{4\pi}\phi, \psi^\dagger \right\rangle\!\!\right\rangle - \left[\!\left[\delta\psi, \psi^\dagger\right]\!\right] \\
&= \left\langle\!\!\left\langle \frac{\delta q}{4\pi} - \delta\sigma_t\psi + \frac{\delta\sigma_s}{4\pi}\phi, \psi^\dagger \right\rangle\!\!\right\rangle - \left[\!\left[\delta\psi^{\text{inc}}, \psi^\dagger\right]\!\right]_- \\
&= \left\langle \frac{\delta q}{4\pi} + \frac{\delta\sigma_s}{4\pi}\phi, \phi^\dagger \right\rangle - \langle\!\langle \delta\sigma_t\psi, \psi^\dagger \rangle\!\rangle - \left[\!\left[\delta\psi^{\text{inc}}, \psi^\dagger\right]\!\right]_- \ .
\end{aligned} \tag{2.20}$$

Note that in the final formula, only the forward and adjoint scalar fluxes are required to evaluate the first-order sensitivity due to perturbations in either the isotropic external source or the isotropic scattering source term. However, the forward angular fluxes are needed to evaluate sensitivities due to perturbations in the total cross section. Additionally, the adjoint incident flux is also needed to assess sensitivity due to the boundary source, but these inner products concern only the domain boundary and the memory storage requirements for these are small compared to volumetric inner products.

# 3. VARIABLE EDDINGTON TENSOR FORMULATIONS FOR ADJOINT-BASED UNCERTAINTY QUANTIFICATION

## 3.1 Motivation for Sensitivity Analysis based on Variable Eddington Tensor Formulations

While the adjoint transport sensitivity formulation given by Eq. (2.20) provides a first-order accurate method to determine the sensitivity to multiple perturbation scenarios using only one forward transport solve and one adjoint transport solve, it can quickly run into limitations for time-dependent systems, where the forward and adjoint systems in space, energy, and angle must be stored at various time moments for subsequent retrieval to compute the sensitivities $\delta QoI$. For a 3-d geometry, this translates to storing the angular flux data across 6-dimensions (space/energy/angle). For time independent systems, Stripling [3] showed that a converged scattering source can be stored to reconstruct the forward steady-state transport solution on the fly. For time-dependent problems, one possibility to circumvent the storage issues is to employ a Variable Eddington Tensor (VET) approach (which only requires storing a space/energy, hence 4-d, solution at various moments in time), provided that input parameter perturbations do not affect the values of the Eddington tensor. In this work, we investigate this question in the simpler setting of a steady-state system.

### 3.1.1 Forward VET Formulation

A VET formulation will reduce the memory requirements when using the adjoint method for sensitivity evaluations. To present the VET formulation, the zero-th and first angular moments of steady-state transport equation are computed by application of the $\int d\Omega$ and $\int d\Omega\,\vec{\Omega}$ operators to Eq. (5.2a), respectively. Using the notation

$$\phi(\vec{r}) = \int d\Omega\,\psi(\vec{r},\vec{\Omega}), \quad \vec{J}(\vec{r}) = \int d\Omega\,\vec{\Omega}\psi(\vec{r},\vec{\Omega})\,, \tag{3.1}$$

the zero-th and first angular moment transport equations are :

$$\vec{\nabla}\cdot\vec{J} + (\sigma_t - \sigma_s)\phi = q\,, \tag{3.2a}$$

and

$$\vec{\nabla}\cdot\left(\int d\Omega\vec{\Omega}\vec{\Omega}\psi\right) + \sigma_t\vec{J} = 0\,. \tag{3.2b}$$

The Eddington Tensor $\mathbb{E}$ is then introduced to relate the second angular moment term in equation (3.2b) to the scalar flux. The caveat to the Eddington Tensor is that it requires the angular flux solution be known.

$$\mathbb{E}(\vec{r}) = \frac{\int d\Omega\vec{\Omega}\vec{\Omega}\psi(\vec{r},\vec{\Omega})}{\phi(\vec{r})}\,. \tag{3.3}$$

Note that the Eddington tensor is spatially dependent. The inclusion of the Eddington tensor allows Eq. (3.2b) to be expressed as

$$\vec{J} = -\frac{1}{\sigma_t}\vec{\nabla}\cdot\mathbb{E}\phi\,. \tag{3.4}$$

If $\psi(\vec{r},\vec{\Omega})$ is a linear function in angle, then $\mathbb{E}(\vec{r}) = \frac{1}{3}\mathbb{I}$ and one recovers Fick's law for the neutron diffusion current, $\vec{J} = -\frac{1}{3\sigma_t}\vec{\nabla}\phi$ (note the change from $\vec{\nabla}\cdot$ to $\vec{\nabla}$). Using Eq. (3.4) for the definition of $\vec{J}$ allows us to convert Eq. (3.2a) to the form shown in (3.5), which only has the scalar flux as an unknown. The substitution $\sigma_a = \sigma_t - \sigma_s$ was also used.

$$-\vec{\nabla}\cdot\left(\frac{1}{\sigma_t}\vec{\nabla}\cdot\mathbb{E}\phi\right) + \sigma_a\phi = q\,. \tag{3.5}$$

The known incident angular flux can be used to generate a suitable boundary conditions using a "Boundary Eddington Factor" $B(\vec{r})$ [7]. To derive the VET boundary condition for, begin by multiplying the transport boundary condition, Eq. (2.2), by $2|\vec{\Omega} \cdot \vec{n}|$. We obtain, for $\vec{r} \in \partial V$,

$$2J^{\text{inc}}(\vec{r}) \equiv 2 \int_{\vec{\Omega}\cdot\vec{n}<0} d\Omega \, |\vec{\Omega} \cdot \vec{n}| \psi^{\text{inc}}(\vec{r}, \vec{\Omega}) = 2 \int_{\vec{\Omega}\cdot\vec{n}<0} d\Omega \, |\vec{\Omega} \cdot \vec{n}| \psi(\vec{r}, \vec{\Omega}) \,. \tag{3.6}$$

$J^{\text{inc}}$ is the partial incoming current. Manipulating the second half-range integral yields:

$$2J^{\text{inc}}(\vec{r}) = \int_{4\pi} d\Omega \, \left( |\vec{\Omega} \cdot \vec{n}| - \vec{\Omega} \cdot \vec{n} \right) \psi(\vec{r}, \vec{\Omega}) = B(\vec{r})\phi(\vec{r}) - \vec{n}(\vec{r}) \cdot \vec{J}(\vec{r}) \tag{3.7}$$

with $\vec{J}$ the net current. The boundary Eddington factor is defined as

$$B(\vec{r}) = \frac{\int_{4\pi} d\Omega \, |\vec{\Omega} \cdot \vec{n}| \psi}{\phi}, \quad \vec{r} \in \partial V \,. \tag{3.8}$$

$\vec{J}$ can substituted using (3.4) to get the final form of the VET forward boundary condition:

$$2J^{\text{inc}} = B\phi + \vec{n} \cdot \frac{1}{\sigma_t} \vec{\nabla} \cdot \mathbb{E}\phi \,. \tag{3.9}$$

Note that the Robin boundary conditions for diffusion is recovered when $\mathbb{E} = \frac{1}{3}\mathbb{I}$ and $B = \frac{1}{2}$:

$$2J^{\text{inc}} = \frac{\phi}{2} + \vec{n} \cdot \frac{1}{3\sigma_t} \vec{\nabla}\phi \,.$$

### 3.1.2 Adjoint VET Formulation

Since the VET formulation generates a new forward equation to describe the system, a new adjoint corresponding to Eq. (3.5) must also be formulated. The typical adjoint process is followed in which the forward equation is multiplied by a test function and all operators are transferred to the test function using integration by parts. The following notation is used: $(\vec{\nabla}\vec{\nabla}u)_{ij} = \partial_{x_i}\partial_{x_j}u$ and a tensor dot product $\mathbb{A} : \mathbb{B} = \sum_i \sum_j A_{ij}B_{ij}$. Next, we compute $\left\langle q, \varphi^\dagger \right\rangle$ and use the forward VET balance equation, Eq. (3.5):

$$\begin{aligned}
\left\langle q, \varphi^\dagger \right\rangle &= -\left\langle \vec{\nabla} \cdot \left( \frac{1}{\sigma_t} \vec{\nabla} \cdot \mathbb{E}\phi \right), \varphi^\dagger \right\rangle + \left\langle \sigma_a \phi, \varphi^\dagger \right\rangle \\
&= \left\langle \frac{1}{\sigma_t} \vec{\nabla} \cdot \mathbb{E}\phi, \vec{\nabla}\varphi^\dagger \right\rangle + \left\langle \phi, \sigma_a \varphi^\dagger \right\rangle - \left[ \vec{n} \cdot \frac{1}{\sigma_t} \vec{\nabla} \cdot \mathbb{E}\phi, \varphi^\dagger \right] \\
&= -\left\langle \phi, \mathbb{E} : \left( \vec{\nabla} \left( \frac{1}{\sigma_t} \vec{\nabla} \varphi^\dagger \right) \right) \right\rangle + \left\langle \phi, \sigma_a \varphi^\dagger \right\rangle \\
&\qquad - \left[ \vec{n} \cdot \frac{1}{\sigma_t} \vec{\nabla} \cdot \mathbb{E}\phi, \varphi^\dagger \right] + \left[ \phi, \vec{n} \cdot \mathbb{E} \cdot \frac{1}{\sigma_t} \vec{\nabla} \varphi^\dagger \right] ,
\end{aligned} \tag{3.10}$$

where the new boundary inner product for use with VET is defined as

$$[\phi(\vec{r}), g(\vec{r})] = \int_{\partial V} dS\, \phi(\vec{r}) g(\vec{r}) \, . \tag{3.11}$$

A more detailed derivation of the boundary terms along with the double gradient term is given in appendix B. Note that we used the fact that the Eddington tensor is symmetric, $\mathbb{E}^T = \mathbb{E}$. This leads to the adjoint equation of the VET formulation, given in Eq. (3.12). Of particular note is that the double divergence term present in the forward equation contributes to a double gradient term in the adjoint equation below. The VET adjoint solution is represented by $\varphi^\dagger$ to avoid confusion with $\phi^\dagger$, which is the adjoint scalar flux from the transport method.

$$-\mathbb{E} : \left( \vec{\nabla} \left( \frac{1}{\sigma_t} \vec{\nabla} \varphi^\dagger \right) \right) + \sigma_a \varphi^\dagger = q^\dagger \tag{3.12}$$

By inspection of the boundary terms in Eq. (3.10) and for reasons that will become apparent during sensitivity calculations, the boundary condition chosen for the adjoint equation is given in Eq. (3.13).

$$2J^{\dagger,\text{out}} = B\varphi^\dagger + \vec{n}\cdot\mathbb{E}\cdot\frac{1}{\sigma_t}\vec{\nabla}\varphi^\dagger \quad \vec{r}\in\partial V \tag{3.13}$$

Note that the Robin boundary conditions are recovered for the adjoint diffusion problem, when $\mathbb{E} = \frac{1}{3}\mathbb{I}$ and $B = \frac{1}{2}$:

$$2J^{\dagger,\text{out}} = \frac{\varphi^\dagger}{2} + \vec{n}\cdot\frac{1}{3\sigma_t}\vec{\nabla}\varphi^\dagger\ .$$

In contrast to the adjoint transport formulation, the VET adjoint equation does not take the form of the forward VET equation, therefore the forward VET solver cannot necessarily be re-used to solve the adjoint equation. To obtain the *QoI* using this formulation, we substitute the adjoint equation definition into Eq. (3.10) and use the forward and adjoint boundary conditions.

$$\begin{aligned}\left\langle q,\varphi^\dagger\right\rangle &= \left\langle \phi,q^\dagger\right\rangle - \left[\vec{n}\cdot\frac{1}{\sigma_t}\vec{\nabla}\cdot\mathbb{E}\phi,\varphi^\dagger\right] + \left[\phi,\vec{n}\cdot\mathbb{E}\cdot\frac{1}{\sigma_t}\vec{\nabla}\varphi^\dagger\right] \\ &= QoI - \left[2J^{\text{inc}} - B\phi,\varphi^\dagger\right] + \left[\phi,2J^{\dagger,\text{out}} - B\varphi^\dagger\right]\ .\end{aligned} \tag{3.14}$$

The $B$ terms negate and yield a relatively compact form for the *QoI*

$$QoI = \left\langle q,\varphi^\dagger\right\rangle - \left[\phi,2J^{\dagger,\text{out}}\right] + \left[\varphi^\dagger,2J^{\text{inc}}\right] \tag{3.15}$$

In order to have a *QoI* that can be expressed entirely in terms of the adjoint solution, it is advantageous to set $J^{\dagger,\text{out}} = 0$ in the adjoint boundary condition, yielding the final expression

$$QoI = \left\langle q,\varphi^\dagger\right\rangle + \left[\varphi^\dagger,2J^{\text{inc}}\right]\ . \tag{3.16}$$

### 3.1.3 VET Adjoint Sensitivity

As was done for the transport formulation, we consider perturbations to the system parameters. However, in contrast to the transport case, the assumption is also made that the Eddington factor remains unperturbed under these system perturbations. This is an approximation because, in the general case, changing the system's parameters should change the angular flux solution, and hence the Eddington tensor may be altered as well. Because the Eddington tensor is an integrated quantity, we conjecture that it is less prone to perturbations. The effects of perturbations on $\mathbb{E}$ are considered later.

A total mean free path notation $\ell_t = \frac{1}{\sigma_t}$ is used for the total cross section to allow the $\delta$ notation to be used in a straightforward fashion. The relation between $\delta\ell_t$ and $\delta\sigma_t$ is shown.

$$\delta\ell_t = \ell_{t,p} - \ell_t = \frac{1}{\sigma_t + \delta\sigma_t} - \frac{1}{\sigma_t} = \frac{-\delta\sigma_t}{\sigma_t^2 + \sigma_t(\delta\sigma_t)} \approx \frac{-\delta\sigma_t}{\sigma_t^2}\left(1 - \frac{\delta\sigma_t}{\sigma_t}\right) \tag{3.17}$$

The perturbed VET forward problem is given below.

$$-\vec{\nabla} \cdot \left((\ell_t + \delta\ell_t)\vec{\nabla} \cdot \mathbb{E}\phi_p\right) + (\sigma_a + \delta\sigma_a)\phi_p = q + \delta q \quad \vec{r} \in V \tag{3.18a}$$

$$2J_p^{\text{inc}} = B\phi_p + \vec{n} \cdot (\ell_t + \delta\ell_t)\vec{\nabla} \cdot (\mathbb{E}\phi_p) \quad \vec{r} \in \partial V \tag{3.18b}$$

The usual adjoint process is performed, starting with the perturbed *QoI* definition using the response function (adjoint source) and the perturbed forward solution. Then, the left-hand side of the adjoint equation is inserted and the operators are carried over to the perturbed forward solution (integration by parts):

$$\begin{aligned}
QoI_p &= \left\langle \phi_p, q^\dagger \right\rangle \\
&= \left\langle \phi_p, -\mathbb{E} : \left( \vec{\nabla} \ell_t \vec{\nabla} \varphi^\dagger \right) + \sigma_a \varphi^\dagger \right\rangle \\
&= \left\langle -\vec{\nabla} \cdot \ell_t \vec{\nabla} \cdot (\mathbb{E}\phi_p) + \sigma_a \phi_p, \varphi^\dagger \right\rangle - \left[ \phi_p, \vec{n} \cdot \left( \mathbb{E} \cdot \ell_t \vec{\nabla} \varphi^\dagger \right) \right] \\
&\quad + \left[ \varphi^\dagger, \vec{n} \cdot \left( \ell_t \vec{\nabla} \mathbb{E} \phi_p \right) \right]
\end{aligned} \tag{3.19}$$

A first-order perturbation approximation of Eq. (3.18a) [1] is then used to substitute into the sensitivity Eq. (3.19), yielding a form independent of the perturbed forward solution in the volumetric inner products:

$$\begin{aligned}
QoI_p &= \left\langle q + \delta q + \vec{\nabla} \cdot \delta \ell_t \vec{\nabla} \cdot (\mathbb{E}\phi_p) - \delta\sigma_a \phi_p, \varphi^\dagger \right\rangle - \left[ \phi_p, \vec{n} \cdot \left( \mathbb{E} \cdot \ell_t \vec{\nabla} \varphi^\dagger \right) \right] \\
&\quad + \left[ \varphi^\dagger, \vec{n} \cdot \left( \ell_t \vec{\nabla} \cdot \mathbb{E} \phi_p \right) \right] \\
&\approx \left\langle q, \varphi^\dagger \right\rangle + \left\langle \delta q + \vec{\nabla} \cdot \delta \ell_t \vec{\nabla} \cdot (\mathbb{E}\phi) - \delta\sigma_a \phi, \varphi^\dagger \right\rangle \\
&\quad - \left[ \phi_p, \vec{n} \cdot \left( \mathbb{E} \cdot \ell_t \vec{\nabla} \varphi^\dagger \right) \right] + \left[ \varphi^\dagger, \vec{n} \cdot \left( \ell_t \vec{\nabla} \cdot \mathbb{E} \phi_p \right) \right]
\end{aligned} \tag{3.20}$$

The first surface term in Eq. (3.20) can be dealt with readily using the adjoint boundary condition ($\phi_p$ will be dealt with shortly). For the second surface term, we use a first-order approximation of the perturbed forward boundary condition

$$2J_p^{\text{inc}} = B\phi_p + \sigma_{t,p}^{-1} \vec{\nabla} \cdot \mathbb{E}\phi_p = B\phi_p + (\ell_t + \delta\ell_t) \vec{\nabla} \cdot \mathbb{E}\phi_p \approx B\phi_p + \ell_t \vec{\nabla} \cdot \mathbb{E}\phi_p + \delta\ell_t \vec{\nabla} \cdot \mathbb{E}\phi$$

[1] Eq. (3.18a) can be viewed as $A_p\phi_p = q + \delta q = A\phi_p + \delta A \phi + O(\delta^2)$, hence $A\phi_p \simeq q + \delta q - \delta A \phi$

Reporting back in the surface terms, we obtain:

$$
\begin{aligned}
&-\left[\phi_p, \vec{n}\cdot\left(\mathbb{E}\cdot\ell_t\vec{\nabla}\varphi^\dagger\right)\right] + \left[\varphi^\dagger, \vec{n}\cdot\left(\ell_t\vec{\nabla}\cdot\mathbb{E}\phi_p\right)\right] \\
&= -\left[\phi_p, 2J^{\dagger,\text{out}} - B\varphi^\dagger\right] + \left[\varphi^\dagger, 2J_p^{\text{inc}} - B\phi_p - \vec{n}\cdot\left(\delta\ell_t\vec{\nabla}\cdot\mathbb{E}\phi_p\right)\right] \\
&\approx -\left[\phi_p, 2J^{\dagger,\text{out}}\right] + \left[\varphi^\dagger, 2J_p^{\text{inc}} - \vec{n}\cdot\left(\delta\ell_t\vec{\nabla}\cdot\mathbb{E}\phi\right)\right]
\end{aligned}
\tag{3.21}
$$

Note that the first-otder approximation was used in the first step. However, the last step is a true equality and we have exact cancelation of $\left[\phi_p, B\varphi^\dagger\right] - \left[\varphi^\dagger, B\phi_p\right] = 0$. Finally, a first-order expression for the sensitivity in the ***QoI*** is as follows:

$$
\begin{aligned}
\delta QoI =& QoI_p - QoI \\
=& \left\langle\delta q, \varphi^\dagger\right\rangle - \left\langle\vec{\nabla}\cdot\delta\ell_t\vec{\nabla}\cdot(\mathbb{E}\phi) + \delta\sigma_a\phi, \varphi^\dagger\right\rangle - \left[\delta\phi, 2J^{\dagger,\text{out}}\right] + \left[\varphi^\dagger, 2\delta J^{\text{inc}}\right] \\
&- \left[\varphi^\dagger, \vec{n}\cdot\left(\delta\ell_t\vec{\nabla}\cdot\mathbb{E}\phi\right)\right] .
\end{aligned}
\tag{3.22}
$$

Again, it is advantageous to use $J^{\dagger,\text{out}} = 0$ in the adjoint boundary condition to remove a dependency on the perturbed forward VET solution. Integration by parts can be applied to condense the $\delta\ell_t$ terms. The result is the the final form for computing the ***QoI*** response using the adjoint VET flux $\varphi^\dagger$. The accuracy of this method is one of the primary foci of this work.

$$
\delta QoI = \left\langle\delta q - \delta\sigma_a\phi, \varphi^\dagger\right\rangle - \left\langle\delta\ell_t\vec{\nabla}\cdot(\mathbb{E}\phi), \vec{\nabla}\varphi^\dagger\right\rangle + \left[\varphi^\dagger, 2\delta J^{\text{inc}}\right] . \tag{3.23}
$$

### 3.1.4 Response Function Perturbation

We have ignored the possibility of a perturbation in the response function $q^\dagger$. Assuming the unperturbed scalar flux $\phi$ is known, which is true for VET and transport, this term is trivial to obtain using a first order approximation.

$$\begin{aligned} QoI_p &= \left\langle \phi_p, q_p^\dagger \right\rangle \\ &= \left\langle \phi + \delta\phi, q^\dagger + \delta q^\dagger \right\rangle \\ &\approx \left\langle \phi, q^\dagger \right\rangle + \left\langle \delta\phi, q^\dagger \right\rangle + \left\langle \phi, \delta q^\dagger \right\rangle \end{aligned} \tag{3.24}$$

The last inner-product $\left\langle \phi, \delta q^\dagger \right\rangle$ is simply added to any of the derived methods where $\phi$ is known, which is true for all but one method in this thesis. This method where the inner-product due to $\delta q^\dagger$ is no longer trivial is defined later, and the term is dealt with in more detail.

### 3.2 Refinements on the VET Approach for Sensitivity Estimation

In this section, attempts are made to reduce the error between the VET adjoint method and the transport adjoint method. In general, these come at the cost of extra solves, but still do not require storing angular fluxes. At the heart of it, the main source of difference between transport and VET is the assumption that the Eddington remained unperturbed in the VET method, so we begin with examining Eddington perturbation ($\delta\mathbb{E}$) terms.

#### 3.2.1 Error From Unperturbed Eddington Assumption

To observe the terms that were dropped in the unperturbed Eddington approximation, consider a reformulation of the perturbed forward equation, this time introducing $\delta\mathbb{E}$ and $\delta B$ terms.

$$-\vec{\nabla} \cdot \left( (\ell_t + \delta\ell_t) \vec{\nabla} \cdot (\mathbb{E} + \delta\mathbb{E}) \phi_p \right) + (\sigma_a + \delta\sigma_a)\phi_p = q + \delta q \ , \quad \vec{r} \in V \tag{3.25a}$$

$$2J_p^{\text{inc}} = (\ell_t + \delta\ell_t) \vec{\nabla} \cdot ((\mathbb{E} + \delta\mathbb{E})\phi_p) + (B + \delta B)\phi_p \ , \quad \vec{r} \in \partial V \tag{3.25b}$$

The above can be substituted into Eq. (3.19) to yield an expanded $QoI$ equation, including the Eddington perturbation terms.

$$\begin{aligned} QoI_p = &\left\langle q + \delta q + \vec{\nabla} \cdot \delta\ell_t \vec{\nabla} \cdot (\mathbb{E}_p \phi_p) + \vec{\nabla} \cdot \ell_{t,p} \vec{\nabla} \cdot (\delta\mathbb{E}\phi_p) - \delta\sigma_a \phi, \varphi^\dagger \right\rangle \\ &- \left[\phi_p, \mathbb{E} \cdot \ell_t \vec{\nabla} \varphi^\dagger\right] + \left[\varphi^\dagger, \ell_t \vec{\nabla} \cdot \mathbb{E}\phi_p\right] \end{aligned} \tag{3.26}$$

The boundary condition for the perturbed forward solution takes on a slightly more complex form, as the additional $\delta\mathbb{E}$ and $\delta B$ terms come into play, but the derivation of the sensitivity proceeds similarly to the case ignoring Eddington perturbations. Once again a first order approximation is taken, and the 2nd and 3rd order delta terms are ignored.

$$\begin{aligned} \delta QoI = &\left\langle \delta q + \vec{\nabla} \cdot \delta\ell_t \vec{\nabla} \cdot (\mathbb{E}\phi) + \vec{\nabla} \cdot \ell_t \vec{\nabla} \cdot (\delta\mathbb{E}\phi) - \delta\sigma_a \phi, \varphi^\dagger \right\rangle \\ &- \left[2\delta\phi, J^{\dagger,\text{out}}\right] + \left[2\varphi^\dagger, \delta J^{\text{inc}}\right] - \left[\varphi^\dagger, \delta\ell_t \vec{\nabla} \cdot \mathbb{E}\phi\right] \\ &- \left[\varphi^\dagger, \ell_t \vec{\nabla} \cdot \delta\mathbb{E}\phi\right] - \left[\varphi^\dagger, \delta B\phi\right] \end{aligned} \tag{3.27}$$

Comparing the above formulation with the unperturbed Eddington case shows that the terms lost by the unperturbed Eddington assumption are

$$\left\langle \vec{\nabla} \cdot \ell_t \vec{\nabla} \cdot (\delta\mathbb{E}\phi), \varphi^\dagger \right\rangle - \left[\varphi^\dagger, \ell_t \vec{\nabla} \cdot \delta\mathbb{E}\phi\right] - \left[\varphi^\dagger, \delta B\phi\right] , \tag{3.28}$$

more compactly expressed in the form

$$- \left\langle \ell_t \vec{\nabla} \cdot (\delta\mathbb{E}\phi), \vec{\nabla}\varphi^\dagger \right\rangle - \left[\varphi^\dagger, \delta B\phi\right] . \tag{3.29}$$

### 3.2.2 Blending $\phi^\dagger$ and $\varphi^\dagger$

As a brief recap, two adjoint methods of determining sensitivity have been considered. The first is a transport approach with sensitivity approximated by Eq. (2.20), which utilizes the forward transport solutions $\psi$ and $\phi$ in conjunction with the transport adjoint solutions $\psi^\dagger$ and $\phi^\dagger$. This equates to two angular transport solves as well as storing two angular flux solutions for use.

The second method is the VET formulation in which sensitivity is approximated by Eq. (3.23). This method utilizes the forward solution $\phi$ as well as the VET adjoint solution $\varphi^\dagger$, in total this requires a forward SN solve to determine $\phi$ and the unperturbed Eddington $\mathbb{E}$ followed by a scalar VET solve for $\varphi^\dagger$, but importantly no angular flux solution $\psi$ is stored.

The former method holds a clear advantage when dealing with source perturbations, both volumetric $\delta q$ and boundary $\delta\psi^{\text{inc}}$. Neither of these perturbations required a first order approximation, therefore the adjoint method is exact. Additionally neither requires storing the angular flux; only the scalar flux. The transport derivation gives the exact $\delta QoI$ value. Given that source perturbations in general do cause perturbations in $\mathbb{E}$ and $B$, the two VET formulations below are not necessarily equal. In addition, there is a $4\pi$ factor separating the $\delta q$ term between the transport and VET formulation. From here it is clear to see that $\varphi^\dagger \neq \phi^\dagger$. For instance, the sensitivity due to external (volumetric and/or boundary) source perturbations are as follows for each method:

$$\delta QoI = \begin{cases} \left\langle \frac{\delta q}{4\pi}, \phi^\dagger \right\rangle - \left[\left[\delta\psi^{\text{inc}}, \psi^\dagger\right]\right]_- , & \text{Transport} \\ \left\langle \delta q, \varphi^\dagger \right\rangle + \left[\varphi^\dagger, 2\delta J^{\text{inc}}\right] , & \text{VET with } \delta\mathbb{E}, \delta B = 0 \\ \left\langle \delta q, \varphi^\dagger \right\rangle + \left[\varphi^\dagger, 2\delta J^{\text{inc}}\right] & \text{VET with no } \delta\mathbb{E}, \delta B \text{ assumption} \\ \quad - \left\langle \ell_t \vec{\nabla} \cdot (\delta\mathbb{E}\phi) , \vec{\nabla}\varphi^\dagger \right\rangle - \left[\varphi^\dagger, \delta B\phi\right] , & \end{cases} \tag{3.30}$$

From this, a "blended" method is proposed which uses the relevant transport inner products for source perturbation, and VET inner products for cross-section perturbation terms. Contrasted to the VET adjoint, this blended method requires an additional transport solve to determine $\phi^\dagger$. In a scenario where only sources are perturbed or only cross sections are perturbed, the blended method will match the results of the transport method or VET method. What is not clear is how the blended method fares when both sources an cross sections are perturbed.

$$\delta QoI = \left\langle \frac{\delta q}{4\pi}, \phi^\dagger \right\rangle - \left\langle \delta\sigma_a \phi, \varphi^\dagger \right\rangle - \left\langle \delta\ell_t \vec{\nabla} \cdot (\mathbb{E}\phi), \vec{\nabla}\varphi^\dagger \right\rangle - [\![\delta\psi^{\text{inc}}, \psi^\dagger]\!] \tag{3.31}$$

### 3.3 Estimating $\delta\mathbb{E}$

Both the transport and VET adjoint methods require a first-order perturbation assumption to be made, but the VET method also introduces the additional assumption that the Eddington remains unperturbed. As such, it seems reasonable that methods to approximate the Eddington perturbation $\delta\mathbb{E}$ may allow for reduced error in Eddington derived sensitivity, ideally approaching that of transport adjoint.

A linear approximation scheme is considered in this work. Let $\vec{p}$ be a point the parameter space, in this case $\{\sigma_s, \sigma_t, q, \psi^{\text{inc}}\}$ and $\delta p$ be the perturbation in that space.

$$\delta\mathbb{E} \approx \frac{\partial\mathbb{E}}{\partial\vec{p}} \cdot \delta\vec{p} \tag{3.32}$$

Since no algebraic analytical form is known for $\mathbb{E}(\vec{p})$, the derivative must be approximated using an additional value for $\mathbb{E}$ from an additional forward transport solve.

$$\frac{\partial\mathbb{E}}{\partial\vec{p}} \approx \frac{\mathbb{E}(\vec{p}_1) - \mathbb{E}(\vec{p}_0)}{\vec{p}_1 - \vec{p}_0} \tag{3.33}$$

The need for an additional transport solve to find $\mathbb{E}(\vec{p}_1)$ is the primary cost of performing this method, and a constraint in situations where this approximation is viable. An analogous process can be used to approximate $\delta B$. With approximations for $\delta\mathbb{E}$ and $\delta B$ in hand, Eq. (3.29) can be used to to refine the VET sensitivity calculation. For situations where many perturbation scenarios need to be considered, this approximation method could prove useful.

# 4. ALTERNATE VARIABLE EDDINGTON TENSOR FORMULATION USING ADJOINT TRANSPORT EDDINGTON

The process by which the VET adjoint equation was formulated involved first converting the angular dependent transport equation to the VET form, then taking the adjoint of the resulting VET quasi-diffusion equation. It is worth considering if performing the operations in a switched order would yield the same result, which is to say, first derive the adjoint angular flux and then apply the VET treatment. This method of transport adjoint derived VET will be termed aVET.

## 4.1 The aVET Formulation

The aVET formulation of the adjoint flux is analogous to the forward formulation shown above starting at Eq. (3.1), but starts with the adjoint transport formulation.

$$-\vec{\Omega}\cdot\vec{\nabla}\psi^{\dagger}+\sigma_t\psi^{\dagger}=\frac{\sigma_s}{4\pi}\phi^{\dagger}+q^{\dagger} \tag{4.1}$$

$$\psi^{\dagger,\text{out}}(\vec{r})=0 \quad \vec{r}\in\partial V^{+}=\{\vec{r}\in\partial V, \quad \vec{\Omega}\cdot\vec{n}>0\} \tag{4.2}$$

The zero-th and first angular moments of the adjoint expression are then taken and combined into a single system, as was done with the forward-derived VET method.

$$\vec{\nabla}\cdot\vec{J}^{\dagger}+(\sigma_t-\sigma_s)\phi^{\dagger}=4\pi q^{\dagger}\,, \tag{4.3a}$$

$$\vec{\nabla}\cdot\left(\int d\Omega\vec{\Omega}\vec{\Omega}\psi^{\dagger}\right)+\sigma_t\vec{J}^{\dagger}=0\,. \tag{4.3b}$$

Notable is that a factor of $4\pi$ exists in the zero-th order equation due to the integration of the scalar response. This carries through to the corresponding VET formulation.

$$-\vec{\nabla}\cdot\left(\frac{1}{\sigma_t}\vec{\nabla}\cdot\mathbb{E}^\dagger\phi^\dagger\right)+\sigma_a\phi^\dagger=4\pi q^\dagger\,. \tag{4.4a}$$

$$2J^{\dagger,\text{out}}(\vec{r})=B^\dagger(\vec{r})\phi^\dagger(\vec{r})+\vec{n}\cdot\frac{1}{\sigma_t}\vec{\nabla}\cdot\mathbb{E}^\dagger\phi^\dagger\,. \tag{4.4b}$$

In the above, an "Adjoint Eddington Tensor" and an "Adjoint Boundary Eddington Factor" terms are required, and defined as

$$\mathbb{E}^\dagger(\vec{r})=\frac{\int d\Omega\vec{\Omega}\vec{\Omega}\psi^\dagger(\vec{r},\vec{\Omega})}{\phi^\dagger(\vec{r})}\,,\quad \vec{r}\in V \tag{4.5}$$

$$B^\dagger(\vec{r})=\frac{\int_{4\pi}d\Omega\,|\vec{\Omega}\cdot\vec{n}|\psi^\dagger(\vec{r},\vec{\Omega})}{\phi^\dagger(\vec{r})}\,,\quad \vec{r}\in\partial V\,. \tag{4.6}$$

Since the above was directly derived from the transport adjoint equation, the *QoI* definition still holds.

$$QoI=\langle\langle\psi,q^\dagger\rangle\rangle=\left\langle\phi^\dagger,\frac{q}{4\pi}\right\rangle-[[\psi^\dagger,\psi]] \tag{4.7}$$

The above formulation also has a corresponding forward equation, with solution denoted by $\varphi$. Where as the forward-derived VET method retained the transport forward solution $\phi$ but generated an alternative adjoint $\varphi^\dagger$, the aVET method retains the transport adjoint solution $\phi$ and generates an alternate forward solution $\varphi$. The result is an alternate forward system that is analogous to the alternate adjoint system for $\varphi^\dagger$ from earlier.

$$-\mathbb{E}^\dagger:\vec{\nabla}\left(\frac{1}{\sigma_t}\vec{\nabla}\varphi\right)+\sigma_a\varphi=\frac{q}{4\pi} \tag{4.8a}$$

$$2J^{\text{inc}}=B^\dagger\varphi+\mathbb{E}^\dagger\cdot\frac{1}{\sigma_t}\vec{\nabla}\varphi\quad \vec{r}\in\partial V\,. \tag{4.8b}$$

A new expression for the *QoI* can be found by using Eq. (4.7) and Eq. (4.8a), this time expressed using the $\varphi$.

$$\begin{aligned} QoI = \left\langle \phi, q^\dagger \right\rangle &= \left\langle \phi^\dagger, \frac{q}{4\pi} \right\rangle - [[\psi^\dagger, \psi]] \\ &= \left\langle \phi^\dagger, -\mathbb{E}^\dagger : \vec{\nabla} \left( \frac{1}{\sigma_t} \vec{\nabla} \varphi \right) + \sigma_a \varphi \right\rangle - [[\psi^\dagger, \psi]] \\ &= \left\langle 4\pi q^\dagger, \varphi \right\rangle - [[\psi^\dagger, \psi]] - \left[ \mathbb{E}^\dagger \cdot \frac{1}{\sigma_t} \vec{\nabla} \varphi, \phi^\dagger \right] + \left[ \frac{1}{\sigma_t} \vec{\nabla} \cdot \mathbb{E}^\dagger \phi^\dagger, \varphi \right] \\ &= \left\langle 4\pi q^\dagger, \varphi \right\rangle - [[\psi^\dagger, \psi]] - \left[ \phi^\dagger, 2J^{\text{inc}} \right] + \left[ \varphi, 2J^{\dagger,\text{out}} \right] \end{aligned} \tag{4.9}$$

## 4.2 First-order Sensitivity Estimation Using the aVET Form

For sensitivity, a perturbed adjoint $\phi_p^\dagger$ is now considered. This is expanded to the first order using the $\delta$ notation, and the typical adjoint method is applied. A perturbation to the response is also introduced. For the previous methods, this could be dealt with trivially by the product $\delta QoI = \left\langle \phi, \delta q^\dagger \right\rangle$, however, since the value of $\phi$ isn't necessarily available in the aVET method, this type of perturbation requires additional attention. In addition $\delta q$ and $\delta \psi^{\text{inc}}$ perturbations may have occurred, but are not reflected in the perturbed adjoint equation below. As was done with the forward derived VET the assumption $\delta \mathbb{E}^\dagger$ is made.

$$-\vec{\nabla} \cdot \left( (\ell_t + \delta \ell_t) \vec{\nabla} \cdot \mathbb{E}^\dagger \phi_p^\dagger \right) + (\sigma_a + \delta \sigma_a) \phi_p^\dagger = 4\pi q^\dagger + 4\pi \delta q^\dagger \tag{4.10a}$$

$$2J^{\dagger,\text{out}} = B^\dagger \phi_p^\dagger + \vec{n} \cdot (\ell_t + \delta \ell_t) \vec{\nabla} \cdot \mathbb{E}^\dagger \phi_p^\dagger \quad \vec{r} \in \partial V \, . \tag{4.10b}$$

An inner-product with $\varphi$ is taken and the perturbation terms are collected on the RHS leaving the original operator on the LHS.

$$-\left\langle \vec{\nabla}\cdot\left(\ell_t\vec{\nabla}\cdot\mathbb{E}^{\dagger}\phi_p^{\dagger}\right),\varphi\right\rangle+\left\langle\sigma_a\phi_p^{\dagger},\varphi\right\rangle=\left\langle 4\pi q^{\dagger}+4\pi\delta q^{\dagger},\varphi\right\rangle+\left\langle\vec{\nabla}\cdot\left(\delta\ell_t\vec{\nabla}\cdot\mathbb{E}^{\dagger}\phi^{\dagger}\right),\varphi\right\rangle \\ -\left\langle\delta\sigma_a\phi^{\dagger},\varphi\right\rangle \tag{4.11}$$

The adjoint process is then applied to the RHS, resulting in boundary terms

$$\left\langle\phi_p^{\dagger},-\mathbb{E}^{\dagger}:\vec{\nabla}\left(\ell_t\vec{\nabla}\varphi\right)+\sigma_a\varphi\right\rangle=\left\langle 4\pi q^{\dagger}+4\pi\delta q^{\dagger},\varphi\right\rangle+\left\langle\vec{\nabla}\cdot\left(\delta\ell_t\vec{\nabla}\cdot\mathbb{E}^{\dagger}\phi^{\dagger}\right),\varphi\right\rangle \\ -\left\langle\delta\sigma_a\phi^{\dagger},\varphi\right\rangle-\left[\phi_p^{\dagger},\mathbb{E}\cdot\ell_t\vec{\nabla}\varphi\right]+\left[\varphi,\ell_t\vec{\nabla}\cdot\mathbb{E}\phi_p^{\dagger}\right] \tag{4.12}$$

Take a look at the boundary conditions. The assumption is made that $2J^{\dagger,\text{out}}$ remains unperturbed.

$$\begin{aligned}-\left[\phi_p^{\dagger},\mathbb{E}\cdot\ell_t\vec{\nabla}\varphi\right]+\left[\varphi,\ell_t\vec{\nabla}\cdot\mathbb{E}\phi_p^{\dagger}\right]&=-\left[\phi_p^{\dagger},2J^{\text{inc}}-B\varphi\right]\\&\quad+\left[\varphi,2J^{\dagger,\text{out}}-B\phi_p^{\dagger}-\delta\ell_t\vec{\nabla}\cdot\mathbb{E}\phi_p^{\dagger}\right]\\&\approx-\left[\phi_p^{\dagger},2J^{\text{inc}}\right]+\left[\varphi,2J^{\dagger,\text{out}}-\delta\ell_t\vec{\nabla}\cdot\mathbb{E}\phi^{\dagger}\right]\end{aligned} \tag{4.13}$$

Taking boundary conditions into account, Eq. (4.12) becomes

$$\begin{aligned}\left\langle\phi_p^{\dagger},\frac{q}{4\pi}\right\rangle&=\left\langle 4\pi q^{\dagger}+4\pi\delta q^{\dagger},\varphi\right\rangle+\left\langle\vec{\nabla}\cdot\left(\delta\ell_t\vec{\nabla}\cdot\mathbb{E}^{\dagger}\phi^{\dagger}\right),\varphi\right\rangle-\left\langle\delta\sigma_a\phi^{\dagger},\varphi\right\rangle\\&\quad-\left[\phi_p^{\dagger},2J^{\text{inc}}\right]+\left[\varphi,2J^{\dagger,\text{out}}-\delta\ell_t\vec{\nabla}\cdot\mathbb{E}\phi^{\dagger}\right]\quad.\end{aligned} \tag{4.14}$$

A important relation to keep in mind that the perturbed *QoI* can be expressed using the perturbed adjoint. A first order approximation must be made, namely $\left\langle\phi_p^{\dagger},\frac{\delta q}{4\pi}\right\rangle\approx\left\langle\phi^{\dagger},\frac{\delta q}{4\pi}\right\rangle$, however, for $\delta q$ and $\delta\psi^{\text{inc}}$ perturbations the adjoint system remains unperturbed so $\phi = \phi^\dagger$.

$$\begin{aligned} QoI_p = \left\langle \psi_p, \frac{q_p^\dagger}{4\pi} \right\rangle &= \left\langle \phi_p^\dagger, \frac{q_p}{4\pi} \right\rangle - \left[\!\left[ \psi_p^\dagger, \psi_p \right]\!\right] \\ &\approx \left\langle \phi_p^\dagger, \frac{q}{4\pi} \right\rangle + \left\langle \phi^\dagger, \frac{\delta q}{4\pi} \right\rangle - \left[\!\left[ \psi_p^\dagger, \psi_p \right]\!\right] \end{aligned} \tag{4.15}$$

The above relation can be combined with the unperturbed *QoI* form derived in Eq. (4.9) and the expression in Eq. (4.14) to give a sensitivity product.

$$\delta QoI = \left\langle \delta q^\dagger, \varphi \right\rangle - \left\langle \left( \delta\ell_t \vec{\nabla} \cdot \mathbb{E}^\dagger \phi^\dagger \right), \vec{\nabla}\varphi \right\rangle - \left\langle \delta\sigma_a \phi^\dagger, \varphi \right\rangle + \left\langle \delta q, \phi \right\rangle - \left[\!\left[ \psi_p^\dagger, \psi_p \right]\!\right] + \left[\!\left[ \psi^\dagger, \psi \right]\!\right] \tag{4.16}$$

The boundary terms can somewhat resolved using a first order approximation and the boundary adjoint boundary conditions.

$$\begin{aligned} - \left[\!\left[ \psi_p^\dagger, \psi_p \right]\!\right] + \left[\!\left[ \psi^\dagger, \psi \right]\!\right] &= - \left[\!\left[ \psi^\dagger + \delta\psi^\dagger, \psi + \delta\psi \right]\!\right] + \left[\!\left[ \psi^\dagger, \psi \right]\!\right] \\ &\approx - \left[\!\left[ \delta\psi^\dagger, \psi \right]\!\right] - \left[\!\left[ \psi^\dagger, \delta\psi \right]\!\right] \\ &= - \left[\!\left[ \delta\psi^\dagger, \psi^{\text{inc}} \right]\!\right]_- - \left[\!\left[ \psi^\dagger, \delta\psi^{\text{inc}} \right]\!\right]_- \end{aligned} \tag{4.17}$$

Laving the final $\delta$*QoI* form of

$$\begin{aligned} \delta QoI \approx{}& \left\langle \delta q^\dagger, \varphi \right\rangle - \left\langle \left( \delta\ell_t \vec{\nabla} \cdot \mathbb{E}^\dagger \phi^\dagger \right), \vec{\nabla}\varphi \right\rangle - \left\langle \delta\sigma_a \phi^\dagger, \varphi \right\rangle + \left\langle \delta q, \phi \right\rangle \\ & - \left[\!\left[ \delta\psi^\dagger, \psi^{\text{inc}} \right]\!\right]_- - \left[\!\left[ \psi^\dagger, \delta\psi^{\text{inc}} \right]\!\right]_- \quad . \end{aligned} \tag{4.18}$$

The problematic term in the above is $\left[\!\left[ \delta\psi^\dagger, \psi^{\text{inc}} \right]\!\right]_-$ since in general $\delta\psi^\dagger$ is not known. However two scenarios eliminate this term. The first is when $\delta\psi^\dagger = 0$, which can be guaranteed if only forward source perturbations are made to the system since these have no effect on the adjoint system, so the adjoint flux remains unperturbed. In this scenario the method is also exact since no first order approximations are needed and the adjoint

Eddingtion terms remain unperturbed. The second scenario where we need not worry about this inner-product term is when the unperturbed forward system has no incident flux, which constrains the use of this method.

# 5. RESULTS

## 5.1 Transport Solution Method

A discrete ordinates (SN) method can be used to solve the one-group steady-state transport equation (Eq. (2.1)). In the SN method, a discrete angular quadrature is used to represent the angular variable and carry out the angular integration. Using an angular quadrature with $D$ directions $\vec{\Omega}_d$, the transport equation is solved along each direction:

$$\vec{\Omega}_d \cdot \vec{\nabla}\psi_d + \sigma_t\psi_d = \frac{\sigma_s}{4\pi}\phi + \frac{q}{4\pi} \quad \vec{r} \in V,\ \forall d \in [1, D] \tag{5.1}$$

The scalar flux can be computed from the angular flux as follows

$$\phi(\vec{r}) \approx \sum_{d=1}^{D} w_d\psi_d(\vec{r})\,,$$

where $\psi_d(\vec{r}) = \psi(\vec{r}, \vec{\Omega}_d)$ and $w_d$ is the angular quadrature weight. This leads to a coupled system of $D$ equations of the form shown in Eq. (5.2a), where the system is coupled through the scattering source term. This system of equations, where both the angular flux and scalar flux are unknowns, is solved iteratively using source iteration as follows:

$$\vec{\Omega}_d \cdot \vec{\nabla}\psi_d^{(\ell+1)} + \sigma_t\psi_d^{(\ell+1)} = \frac{\sigma_s}{4\pi}\phi^{(\ell)} + \frac{q}{4\pi}\,, \tag{5.2a}$$

$$\phi^{(\ell+1)}(\vec{r}) = \sum_{d=1}^{D} w_d\psi_d^{(\ell+1)}(\vec{r})\,. \tag{5.2b}$$

Iteration terminates once $\left|\phi^{(\ell+1)} - \phi^{(\ell)}\right| \leq \text{Tol}$, which was set to $10^{-8}$ for this work.

The test cases in this writing use a slab geometry however, so with that in mind the above can be slightly simplified. Namely, the angular flux no longer needs to be function of the full $\vec{\Omega}$ angular range, but can be represented using a cosine factor $\mu \in [-1, 1]$. The main mathematical result of this is a factor of $2\pi$ resulting from the relation

$$\psi(\vec{r}, \vec{\Omega}) = \frac{1}{2\pi}\psi(\vec{r}, \mu) \,. \tag{5.3}$$

The SN method then discretizes this $\mu$ range into ordinates, and the system takes the form

$$\vec{\Omega}_d \cdot \vec{\nabla}\psi_d^{(\ell+1)} + \sigma_t\psi_d^{(\ell+1)} = \frac{\sigma_s}{2}\phi^{(\ell)} + \frac{q}{2} \,, \tag{5.4a}$$

$$\phi(\vec{r})^{(\ell+1)} = \sum_{d=1}^{D} w_d\psi_d^{(\ell+1)}(\vec{r}) \,. \tag{5.4b}$$

Within the VET formulations, this transform of $4\pi \rightarrow 2$ holds, as the source terms $q$ and $q^{\dagger}$ propagate this $2\pi$ factor through the VET formulation.

With the angular dependence handeled by the SN method for transport, each of the $D$ spatially dependent SN equations in Eq. (5.2a) is then solved using a discontinuous finite element method with up-winding [8]. For this work and $S_8$ angular quadrature used is used and the spatial domain is discretized into 2,000 uniformly-spaced elements.

## 5.2 VET Solution Method

Solution of the quasi-diffusion VET formulations are performed using a Discontinuous Galerkin (DG) method with an interior-penalty approach; see Arnold [9], for instance. Compared to a standard diffusion approach, slight modifications to the interior penalty terms are required to support quasi-diffusion. For standard diffusion the current terms used at the mesh interface would take the form $\frac{1}{3\sigma_t}\vec{\nabla}\phi$ but for the Eddington approach the current terms take the form $\frac{1}{\sigma_t}\vec{\nabla} \cdot (\mathbb{E}\phi)$. Linear basis functions are used as the finite element basis. As was the case for SN transport, the spatial domain is discretized into 2,000 uniform elements for the results shown in the following sections.

## 5.3 Results

We have presented 5 separate methods for unperturbed *QoI* calculation have been discussed:

1. forward and adjoint inner products for both SN and VET formulations (yielding a total of 4 different approaches), and,

2. the alternate aVET method in Eq. (4.9).

as well as 7 separate methods for $\delta QoI$ calculation:

1. forward and adjoint inner products for both SN and VET formulations (4 approaches),

2. the "blended" method presented in Eq. (3.31),

3. the method of approximating $\delta\mathbb{E}$ shown in Eq. (3.33), and,

4. the aVET inner product in Eq. (4.18).

The inner-products associated with the above $\delta QoI$ methods are given in Table 5.1.

| Method | $\delta QoI$ Inner Product |
|---|---|
| Transport | $\left\langle \phi_p, q^\dagger \right\rangle - \left\langle \phi, q^\dagger \right\rangle = \left\langle \delta\phi, q^\dagger \right\rangle$ |
| Transport Adjoint | $\left\langle \frac{\delta q}{4\pi}, \phi^\dagger \right\rangle - \left\langle\!\left\langle \delta\sigma_t \psi, \psi^\dagger \right\rangle\!\right\rangle + \left\langle \frac{\delta\sigma_s}{4\pi}\phi, \phi^\dagger \right\rangle - \left[\!\left[ \delta\psi^{\text{inc}}, \psi^\dagger \right]\!\right]_-$ |
| VET Forward | $\left\langle \phi_p^\star, q^\dagger \right\rangle - \left\langle \phi, q^\dagger \right\rangle = \left\langle \delta\phi, q^\dagger \right\rangle$ |
| VET Adjoint | $\left\langle \delta q, \varphi^\dagger \right\rangle - \left\langle \delta\sigma_a \phi, \varphi^\dagger \right\rangle - \left\langle \delta\ell_t \vec{\nabla} \cdot (\mathbb{E}\phi), \vec{\nabla}\varphi^\dagger \right\rangle + \left[ \varphi^\dagger, 2\delta J^{\text{inc}} \right]$ |
| VET Blended | $\left\langle \frac{\delta q}{4\pi}, \phi^\dagger \right\rangle - \left\langle \delta\sigma_a \phi, \varphi^\dagger \right\rangle - \left\langle \delta\ell_t \vec{\nabla} \cdot (\mathbb{E}\phi), \vec{\nabla}\varphi^\dagger \right\rangle - \left[\!\left[ \delta\psi^{\text{inc}}, \psi^\dagger \right]\!\right]_-$ |
| VET $\delta\mathbb{E}$ | VET Adj $- \left\langle \ell_t \vec{\nabla} \cdot (\delta\mathbb{E}\phi), \vec{\nabla}\varphi^\dagger \right\rangle - \left[ \varphi^\dagger, \phi\delta B \right]$ |
| aVET | $\left\langle \delta q^\dagger, \varphi \right\rangle - \left\langle \left( \delta\ell_t \vec{\nabla} \cdot \mathbb{E}^\dagger \phi^\dagger \right), \vec{\nabla}\varphi \right\rangle - \left\langle \delta\sigma_a \phi^\dagger, \varphi \right\rangle + \left\langle \delta q, \phi \right\rangle - \left[\!\left[ \delta\psi^\dagger, \psi^{\text{inc}} \right]\!\right]_- - \left[\!\left[ \psi^\dagger, \delta\psi^{\text{inc}} \right]\!\right]_-$ |

Table 5.1: Summary of Methods. For response perturbation $\delta q^\dagger$, the straightforward $\left\langle \phi, \delta q^\dagger \right\rangle$ had been omitted from all methods except aVET. For forward VET method, the perturbed scalar flux $\phi_p^\star$ is computed using the unperturbed Eddington.

When dealing with sensitivity calculations, techniques based on the forward solutions are expected to give the most exact answer simply because it involves an additional forward solve of the perturbed system for each perturbation case. The adjoint methods for sensitivity are relying on a first-order approximation (we dropped the double $\delta$ terms), however they only require a single forward solve and a single adjoint for use with all perturbation cases.

The seven methods were implemented in a MATLAB finite element method (FEM) solver. One-dimensional test cases were run, varying which parameter experienced a perturbation and the magnitude of that perturbation. The results of the five different sensitivity methods were analyzed to identify cases where the efficient VET adjoint showed promise as a time and memory efficient method for computing sensitivity. As a representation of this, the % *QoI* response is plotted against the % change in a given parameter $p$, which are defined as

$$\textit{QoI}\ \%\ \text{response} = \frac{\delta QoI}{QoI}\ , \tag{5.5a}$$

$$p\ \%\ \text{change} = \frac{\delta p}{p}\ . \tag{5.5b}$$

Any references to an "exact" solution for a method means that it agrees with the $\delta QoI$ value found by subtracting two forward (unperturbed and perturbed) SN transport answers.

### 5.3.1 Homogeneous System, Homogeneous Perturbation

To start, a test case consisting of a relatively simple system is chosen. The system is a homogeneous material with a volumetric source throughout and no incident flux. The response function is the center of the region sufficiently far from the boundaries. Towards the center of this region the infinite medium solution is approached, and $\phi \approx \phi^{\infty} = \frac{q}{\sigma_a}$. Note that this system should not show any significant response to perturbations in the scattering cross section. The following values are chosen for the entire region $x \in [0, 10]$: $q = 2$, $\sigma_a = 1$, and $\sigma_s = 1$. For the response function $q^{\dagger} = 1$ for $x \in [4, 6]$ and $0$ elsewhere. Therefore the predicted *QoI* for this, using the infinite medium approximation is

$$QoI \approx \langle q^{\dagger}, \phi \rangle = \int_4^6 dx\, \frac{q}{\sigma_a} = 4 \tag{5.6}$$

The unperturbed scalar fluxes are shown in Figure 5.1. These plots show both the true scalar flux $\phi$ obtained using the SN and VET methods (which should be equal), as well as the "forward-like" flux $\varphi$ obtained as the adjoint of the aVET method. Similarly, the scalar adjoint flux $\phi^{\dagger}$ obtained using SN and aVET are shown on the same plot as the "adjoint-like" $\varphi^{\dagger}$ from the VET formulation. Looking at the graphs it becomes clear that $\phi^{\dagger} \neq \varphi^{\dagger}$ and $\phi \neq \varphi$, providing a succinct confirmation that the solution of the adjoint of the VET formulation is not the same as the solution to the VET formulation of the transport adjoint. At a glance it may appear that the difference between the scalar flux solutions $\phi$, $\phi^{\dagger}$ and the flux-like $\varphi$, $\varphi^\dagger$ is a simple factor of 2 due to source normalization, but that is not the case and plots which take the factor of 2 into account are presented in Appendix C.

For perturbations, the entire system is perturbed uniformly, resulting in another homogeneous system, so therefore the perturbed ***QoI*** can be easily predicted as $QoI_p \approx (6-4)\phi_p^\infty = 2\frac{q_p}{\sigma_{a,p}}$. Given the simple form of the expected flux in the center, the derivatives can be taken to get an expected sensitivity.

$$\frac{\partial \phi}{\partial q} = \frac{1}{\sigma_a} \tag{5.7a}$$

$$\frac{\partial \phi}{\partial \sigma_a} = -\frac{q}{\sigma_a^2} \tag{5.7b}$$

$$\frac{\partial \phi}{\partial \sigma_s} = 0 \tag{5.7c}$$

The seven methods of $QoI$ perturbation calculation were applied to this system for perturbations in $q$, $\sigma_s$, and $\sigma_t$. Perturbation in the system parameters were taken in the range of $\pm 10\%$. The % response results over this range are plotted in Figure 5.2. $\delta QoI$ values for selected perturbations are given in Table 5.2.

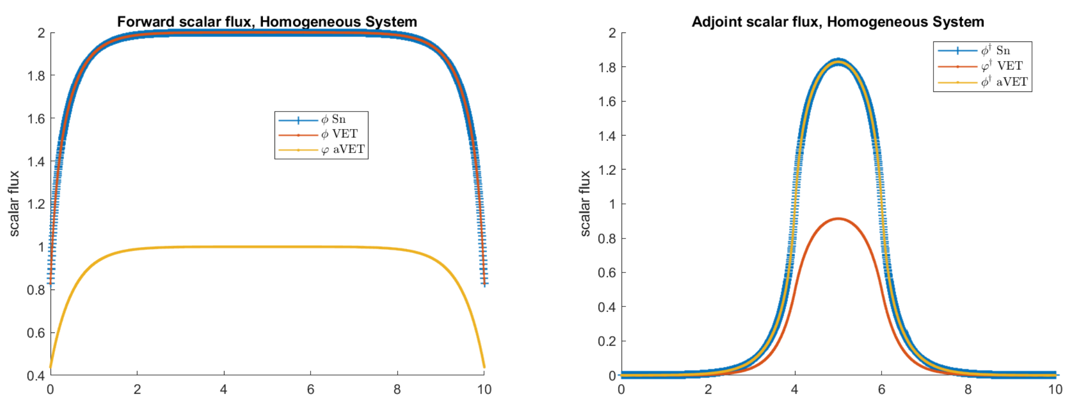


Figure 5.1: Plots of unperturbed scalar fluxes for the homogeneous system. This include "forward" fluxes $\phi$ and $\varphi$ show on the left, and "adjoint" fluxes $\phi^\dagger$ and $\varphi^\dagger$ on the right.

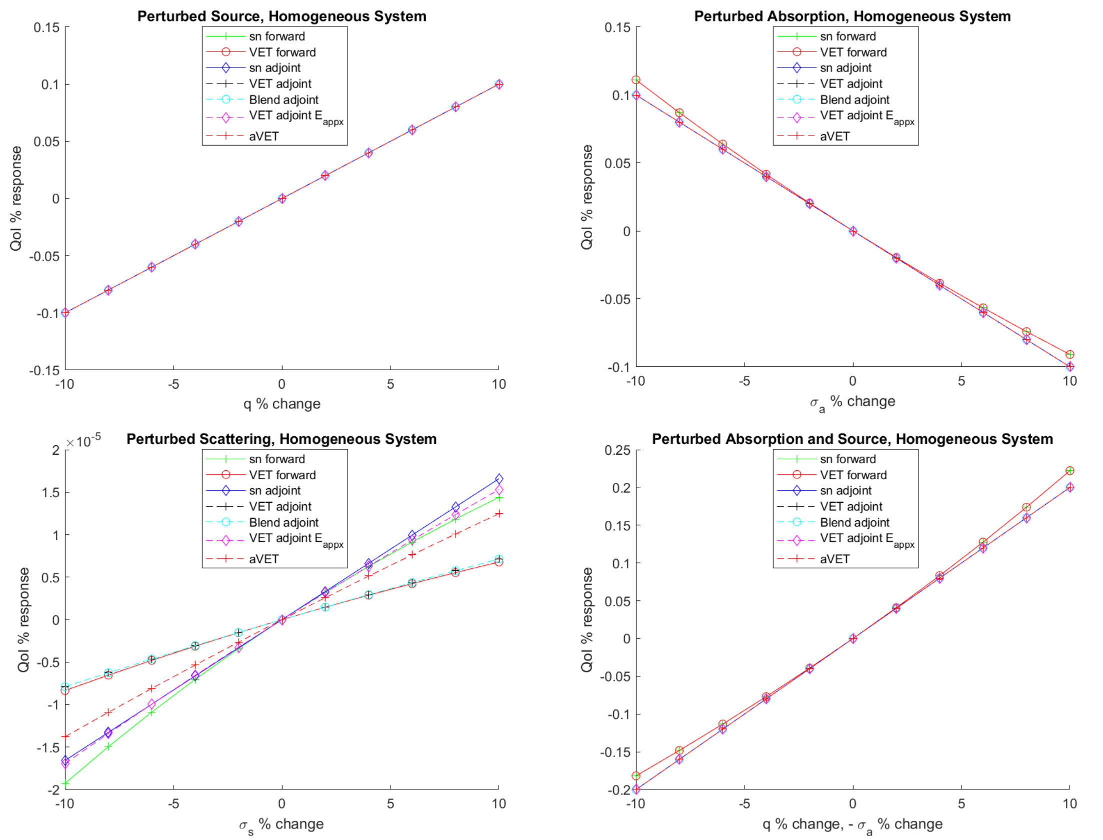


Figure 5.2: *QoI* response to various perturbation scenarios for the homogeneous system under various homogeneous perturbations. For the unperturbed system $q = 2$, $\sigma_a = 1$, and $\sigma_s = 1$.

The unperturbed *QoI* value was the same for all methods, agreeing with the prediction. In both the unperturbed and perturbed state, the Eddington is essentially at the infinite medium limit, so the unperturbed Eddington approximation should be a safe assumption in this scenario. The results of the $q$ and $\sigma_a$ perturbations seem to support this. For the source perturbations, no first-order approximation is needed, so all methods appear to give the same result, which is exact. The $\sigma_a$ perturbations begin to show the effects of the first-order approximation, where both the transport and VET adjoint methods depart from the exact forward found $\delta QoI$. As expected, the system does not show strong sensitivity to $\sigma_s$

perturbations.

| Method | $QoI$ | $+10\%q$ | $-10\%\sigma_a$ | $+10\%\sigma_s$ | $+10\%q, -10\%\sigma_a$ |
|---|---|---|---|---|---|
| SN Fwd | 3.99976 | 0.39998 | 0.44419 | 5.7577e-05 | 0.88858 |
| VET Fwd | 3.99976 | 0.39998 | 0.44428 | 2.7131e-05 | 0.88868 |
| SN Adj | 3.99976 | 0.39998 | 0.39983 | 6.6307e-05 | 0.79980 |
| VET Adj | 3.99976 | 0.39998 | 0.39988 | 2.8534e-05 | 0.79986 |
| Blended | - | 0.39998 | 0.39988 | 2.8534e-05 | 0.79986 |
| VET $\delta\mathbb{E}$ | - | 0.39998 | 0.39983 | 6.124e-05 | 0.79980 |
| aVET | 3.99976 | 0.39998 | 0.39980 | 4.986e-05 | 0.79978 |

Table 5.2: Table of selected $\delta QoI$ values for the homogeneous system under homogeneous perturbations. The unperturbed $QoI$ for various methods is given in the first column.

### 5.3.2 Homogeneous System, Inhomogeneous Perturbation

For the next test case, the same initial homogeneous system is used for the unperturbed state. However, we attempt to introduce Eddington perturbations by perturbing the system to an inhomogeneous state, there by introducing a boundary layer into the system. This is done by only perturbing the $q$, $\sigma_a$, $\sigma_s$ terms on the region $x \in [0, 6]$, so that the region of interest is within the perturbed region, but on one of its boundaries. In this perturbed state, the infinite medium limit can no longer be applied. By introducing a $\delta\mathbb{E}$, we hope to begin differentiating the transport and VET adjoint methods, as the $\delta\mathbb{E} = 0$ was the major assumption that had to be made in VET. Response plots are shown in Figure 5.3 and selected $\delta QoI$ values in Table 5.3. Refer to Figure 5.1 for the unperturbed fluxes.

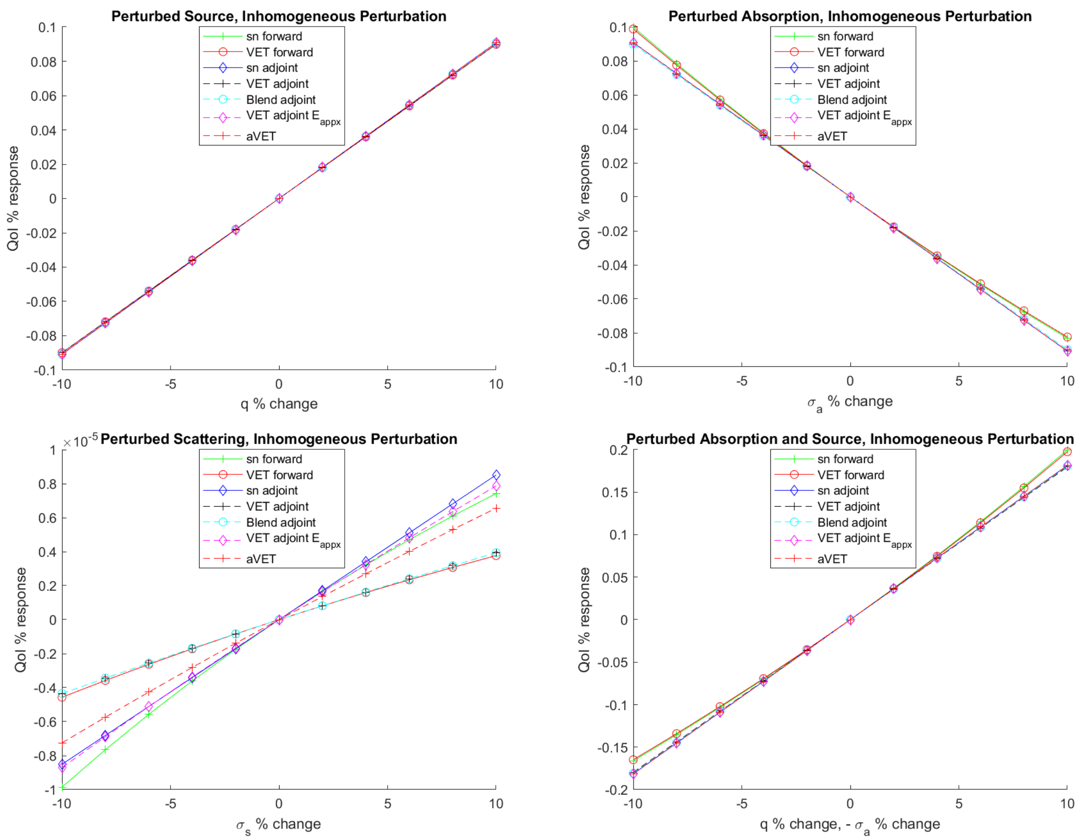


Figure 5.3: *QoI* response to various perturbation scenarios for the homogeneous system under various inhomogeneous perturbations. For the unperturbed system $q = 2$, $\sigma_a = 1$, and $\sigma_s = 1$.

As expected, the introduction of the boundary layer in the perturbed state begins to show differentiation in the selected methods. For source perturbations the transport and VET adjoint methods match their respective forward found values. The blended method matches the SN values for source perturbations and the VET values for cross-section perturbations as designed. The behavior of the blended method with both source and cross-section perturbations shows that it does provide an improvement over the VET method, however the found value still lies closer to the VET value than the transport adjoint value. The $\delta\mathbb{E}$ method shows more promise in this trial, as the addition of the $\delta\mathbb{E}$ terms begins to reconcile the VET adjoint method with the more exact transport adjoint. The aVET method shows its exact nature for the source perturbation, as well as providing a $\delta QoI$ value similar to the $\delta\mathbb{E}$ approximation method for $\sigma_a$ perturbations, despite the latter leveraging an additional transport solve.

| Method | $QoI$ | $+10\%q$ | $-10\%\sigma_a$ | $+10\%\sigma_s$ | $+10\%q, -10\%\sigma_a$ |
|---|---:|---|---|---|---:|
| SN Fwd | 3.99976 | 0.36309 | 0.39952 | 2.9680e-05 | 0.79915 |
| VET Fwd | 3.99976 | 0.35947 | 0.39517 | 1.5072e-05 | 0.79040 |
| SN Adj | 3.99976 | 0.36309 | 0.36301 | 3.4051e-05 | 0.72610 |
| VET Adj | 3.99976 | 0.35947 | 0.35941 | 1.5733e-05 | 0.71888 |
| Blended | - | 0.36309 | 0.35941 | 1.5733e-05 | 0.72250 |
| VET $\delta\mathbb{E}$ | - | 0.36295 | 0.36298 | 3.1479e-05 | 0.72603 |
| aVET | 3.99976 | 0.36309 | 0.36299 | 2.6234e-05 | 0.72609 |

Table 5.3: Table of selected $\delta QoI$ values for the homogeneous system under inhomogeneous perturbations. The unperturbed $QoI$ for various methods is given in the first column.

### 5.3.3 Shielded Incident Isotropic Flux

Next is a simple shielding case to test how the methods deals with a surface source as opposed to the volumetric source of the previous test cases. An isotropic flux is incident on the left boundary $x = 0$ of the system with no incident flux on the right boundary and no volumetric source is present. The incident flux passes though a shield from $x = [1, 2]$ with $\sigma_a = 0.5$ and $\sigma_s = 0.5$. The response is taken on the right side of the shield using a response $q^\dagger = 1$ for $x \in [3, 4]$ and 0 else. Response plots shown in Figure 5.5 and $\delta QoI$ values in Table 5.4. Also, this test case introduces streaming regions into the problem. For the VET formulations, there is a factor of $\ell_t = \frac{1}{\sigma_t}$ that is undefined for streaming where $\sigma_t = 0$. To avoid this, a value of $\sigma_t = 10^{-8}$ is used to signify a streaming region. Cross-section perturbations occur in the shielding material, while incident flux perturbations occur only for the flux incident at $x = 0$. Since there is an incident flux present, the aVET method cannot be applied in full for cross-section perturbations. As such the aVET method is excluded from cross-section sensitivity graphs in Figure 5.5 and the values given in Table 5.4 exclude the boundary term dependent on $\delta\psi^\dagger$ boundary term in Eq 4.18.

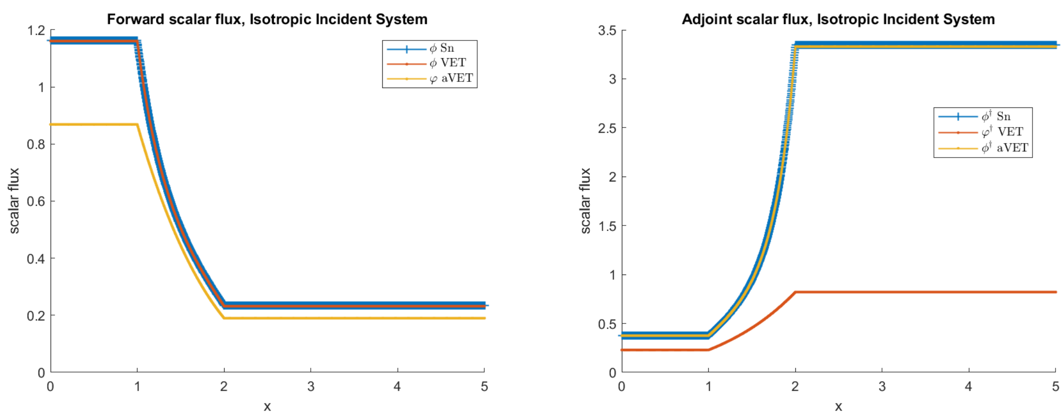


Figure 5.4: Plots of unperturbed scalar fluxes for the isotropic incident shielding system. Forward fluxes $\phi$ and $\varphi$ show on the left, and adjoint fluxes $\phi^\dagger$ and $\varphi^\dagger$ on the right.

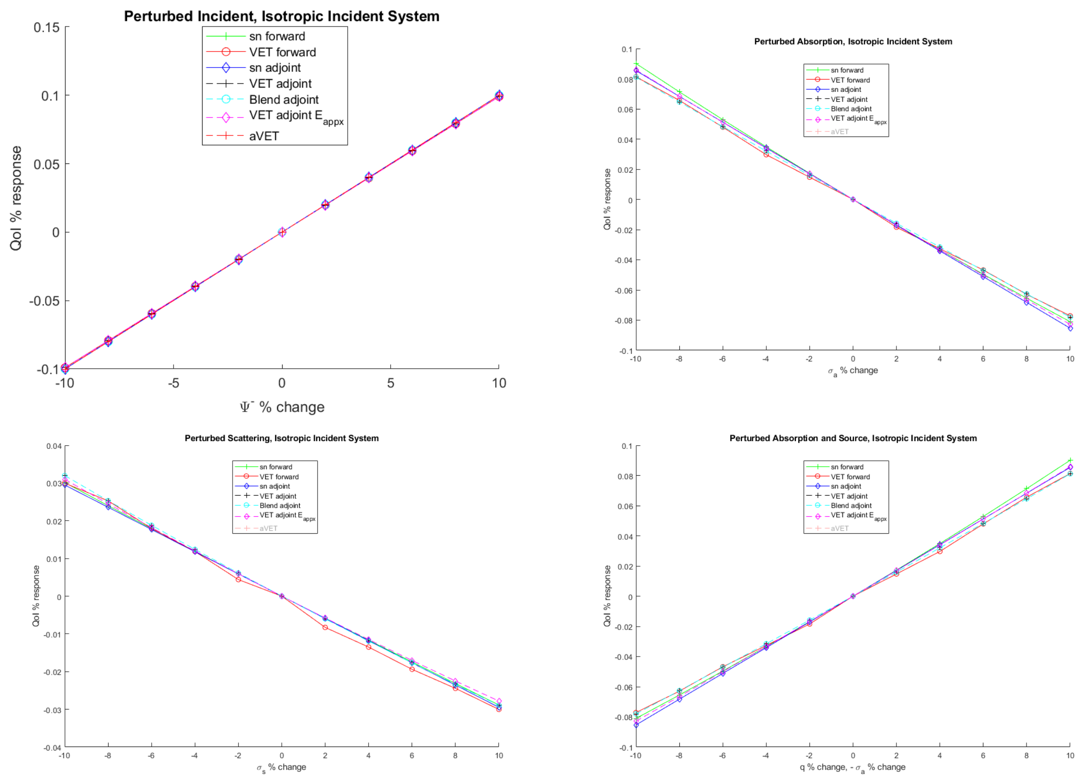


Figure 5.5: *QoI* response to various perturbation scenarios for the isotropic incident shielding system.

Response to perturbation in the incident flux behaves as expected, with transport adjoint, blended, and aVET all retrieving the exact $\delta QoI$. Response to $\sigma_s$ perturbations are a bit more pronounced here, but still fairly weak. In a higher dimensional system, scattering could be particularly important for shielding problems, as neutrons could scatter around the shield in some way. However, in the tested slab geometry this is not possible. The aVET method is predicted to have issues with this scenario and cross-section perturbations due to the $\delta\psi^\dagger$ boundary term and Table 5.4 seems to support this, as without this term the predicted sensitivity is almost twice that of those found with other methods, including VET.

| Method | $QoI$ | $+10\%\psi^-$ | $-10\%\sigma_a$ | $+10\%\sigma_s$ | $+10\%\psi^-, -10\%\sigma_a$ |
|---|---|---|---|---|---|
| SN Fwd | 0.234008 | 0.023401 | 0.021079 | -0.0067476 | 0.046588 |
| VET Fwd | 0.234008 | 0.023181 | 0.019670 | -0.0066481 | 0.044818 |
| SN Adj | 0.231931 | 0.023401 | 0.019975 | -0.0068956 | 0.043376 |
| VET Adj | 0.231698 | 0.023181 | 0.018981 | -0.0067751 | 0.042162 |
| Blended | - | 0.023401 | 0.018981 | -0.0067751 | 0.042381 |
| VET $\delta\mathbb{E}$ | - | 0.023170 | 0.020079 | -0.0065100 | 0.043249 |
| aVET | 0.234008 | 0.023401 | 0.035869$^\star$ | -0.012563$^\star$ | 0.059270$^\star$ |

Table 5.4: Table of selected $\delta QoI$ values for the isotropic incident shielding system under perturbations. The unperturbed $QoI$ for various methods is given in the first column. $^\star$excluding $\delta\psi^\dagger$ term for aVET methods.

### 5.3.4 Shielded Incident Beam

The next system is almost identical to the previous isotropic incident flux system, except that the incident flux is no longer isotropic, but a mono-directional grazing beam. The beam chosen is $mu = 0.1834$, which corresponds to $N = 5$ in the SN solver used for the transport solve. The aVET method is still not valid for cross-section perturbations in this scenario as an incident flux is still present.

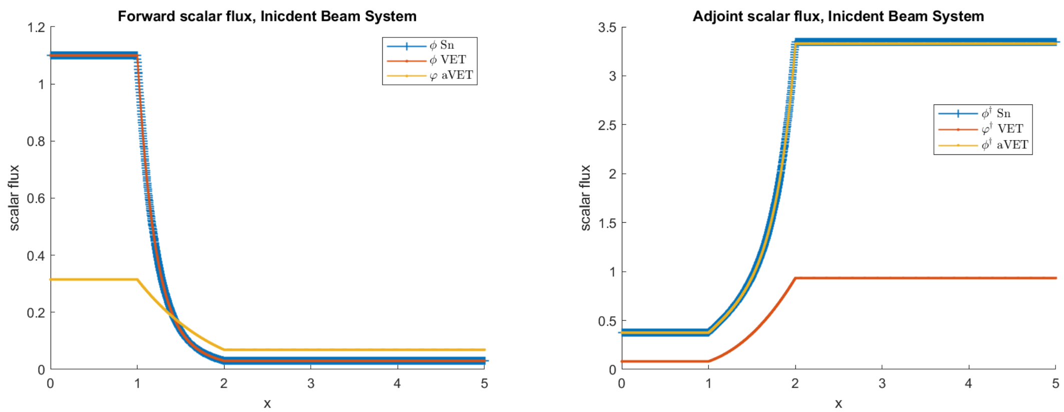


Figure 5.6: Plots of unperturbed scalar fluxes for the beam shielding system. Forward fluxes $\phi$ and $\varphi$ show on the left, and adjoint fluxes $\phi^\dagger$ and $\varphi^\dagger$ on the right.

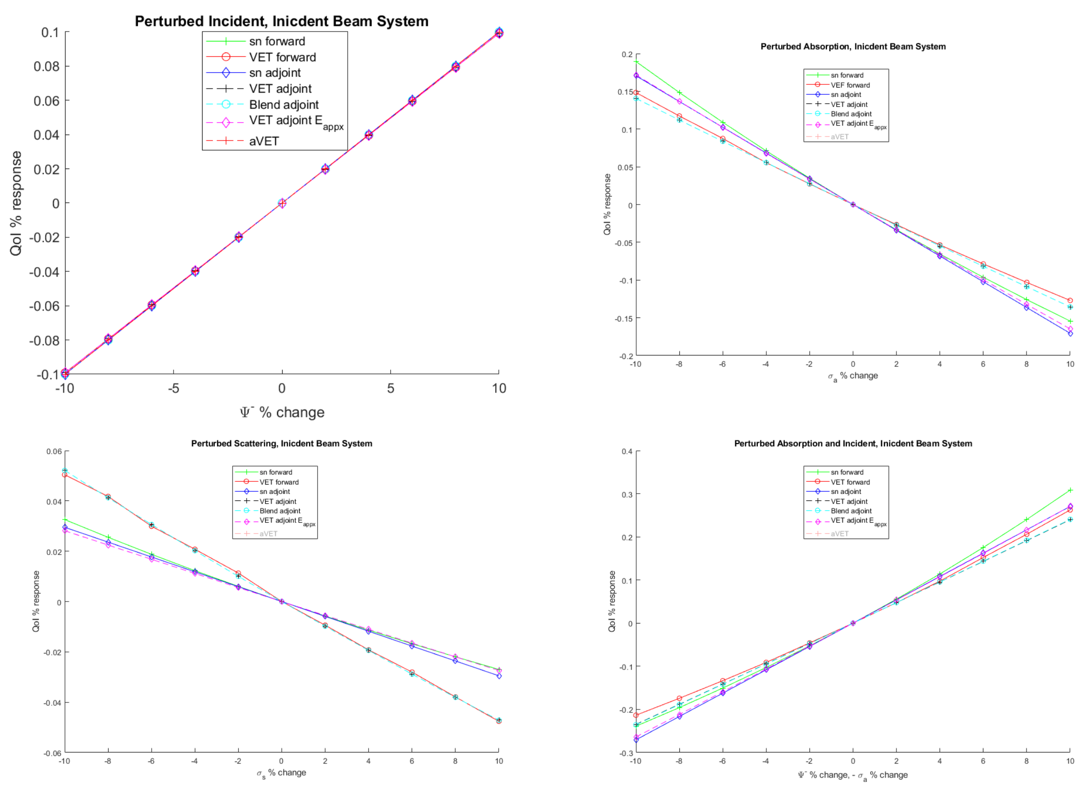


Figure 5.7: *QoI* response to various perturbation scenarios for the beam shielding system.

Compared to the isotropic case, the VET methods appear to behave somewhat worse for the incident beam case, particularly for scattering cross-section perturbations. However the $\delta\mathbb{E}$ approximation method seems to correct most of the error between the VET and transport adjoint, which begins to indicate that this method could be powerful, particularly in cases of scatting perturbations which up to this point have caused the greatest deviation between VET and transport.

| Method | $QoI$ | $+10\%\psi^-$ | $-10\%\sigma_a$ | $+10\%\sigma_s$ | $+10\%\psi^-, -10\%\sigma_a$ |
|---|---|---|---|---|---|
| SN Fwd | 0.234008 | 0.0030185 | 0.0057195 | -0.00081464 | 0.00931 |
| VET Fwd | 0.234008 | 0.0029948 | 0.0044783 | -0.0014368 | 0.007921 |
| SN Adj | 0.231931 | 0.0030185 | 0.0051489 | -0.00089097 | 0.0081674 |
| VET Adj | 0.231698 | 0.0029942 | 0.0042423 | -0.0014234 | 0.0072365 |
| Blended | - | 0.0030185 | 0.0042423 | -0.0014234 | 0.0072608 |
| VET $\delta\mathbb{E}$ | - | 0.0029942 | 0.0051834 | -0.00082693 | 0.0081776 |
| aVET | 0.234008 | 0.0030185 | 0.013009$^\star$ | -0.0045566$^\star$ | 0.016028$^\star$ |

Table 5.5: Table of selected $\delta QoI$ values for the beam shielding system under perturbations. The unperturbed $QoI$ for various methods is given in the first column. $^\star$excluding $\delta\psi^\dagger$ term for aVET methods.

### 5.3.5 Reed Problem

A more varied and complex problem (Reed's problem, [10]) is used next. The domain is split into 5 regions of unequal length with properties given below. As for perturbations, the focus of this series of tests will be placed on perturbations to the scattering cross section in regions 4 and 5.

$$\text{Region 1: } x \in [0, 2), \quad \sigma_a = 50,\ \sigma_s = 0,\ q = 50$$

$$\text{Region 2: } x \in [2, 3), \quad \sigma_a = 5,\ \sigma_s = 0,\ q = 0$$

$$\text{Region 3: } x \in [3, 5), \quad \sigma_a = 10^{-8}\,\sigma_s = 0,\ q = 0$$

$$\text{Region 4: } x \in [5, 6), \quad \sigma_a = 0.1,\ \sigma_s = 0.9,\ q = 1$$

$$\text{Region 5: } x \in [6, 8], \quad \sigma_a = 0.1,\ \sigma_s = 0.9,\ q = 0$$

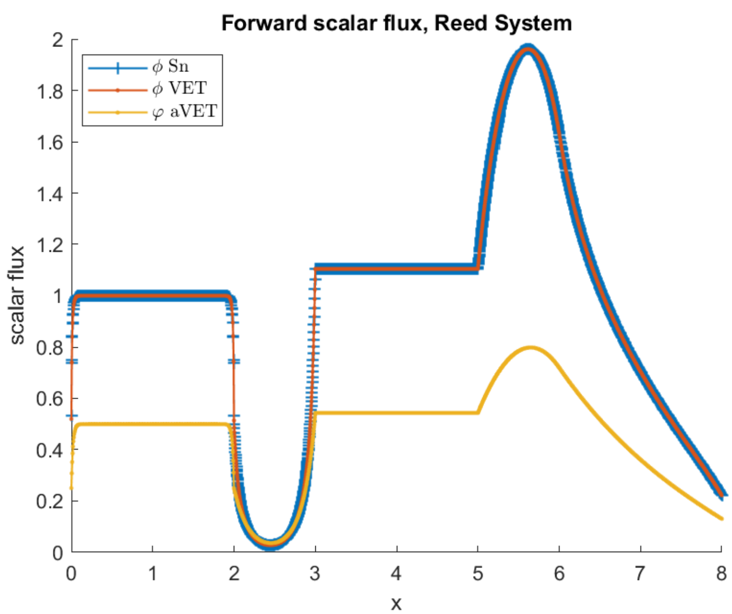


Figure 5.8: Plot of unperturbed forward scalar flux for the Reed's problem.

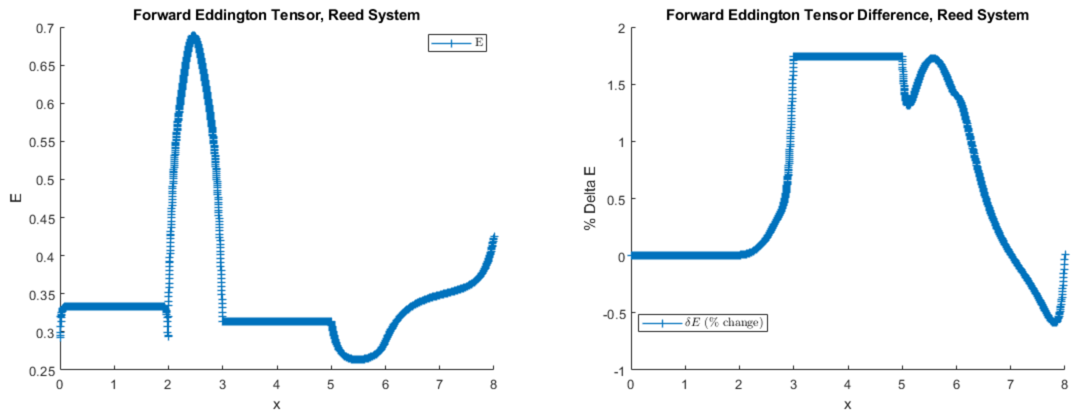


Figure 5.9: Plots of unperturbed Eddington Tensor for Reed's problem as well as the Eddington perturbation $\delta\mathbb{E}$ for a $+10\%$ scattering perturbation in regions 4 and 5.

Five separate response functions are considered, corresponding to the average flux in each of the 5 regions. The corresponding five adjoint fluxes and the computed sensitivities are given in Figures 5.10 through 5.14.

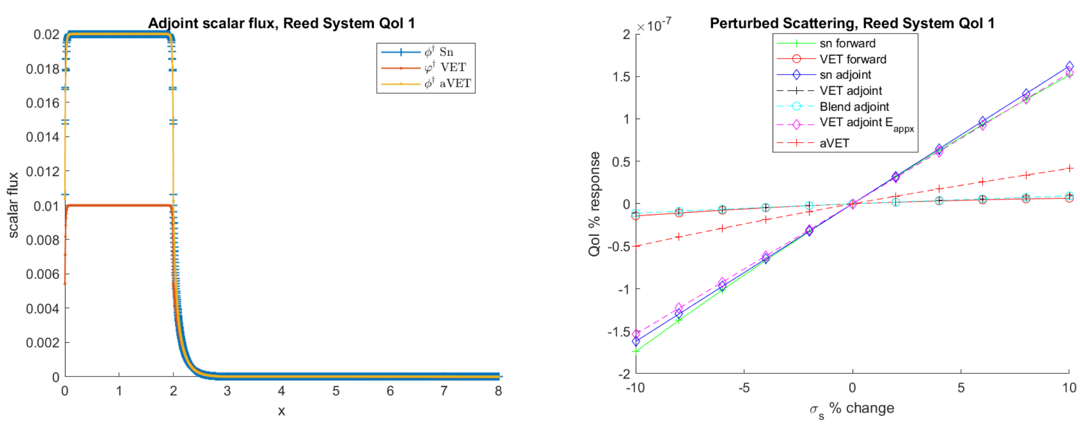


Figure 5.10: Scattering response and adjoint flux for Reed problem with *QoI* in region 1.

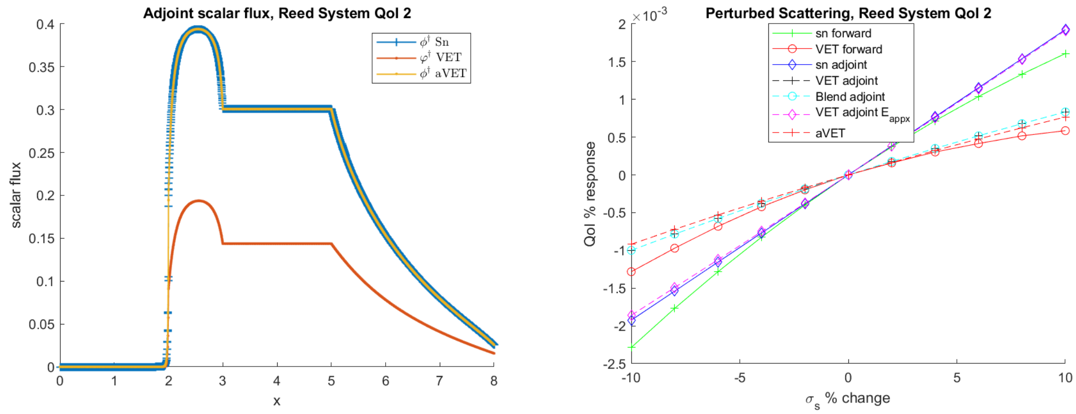


Figure 5.11: Scattering response and adjoint flux for Reed problem with *QoI* in region 2.

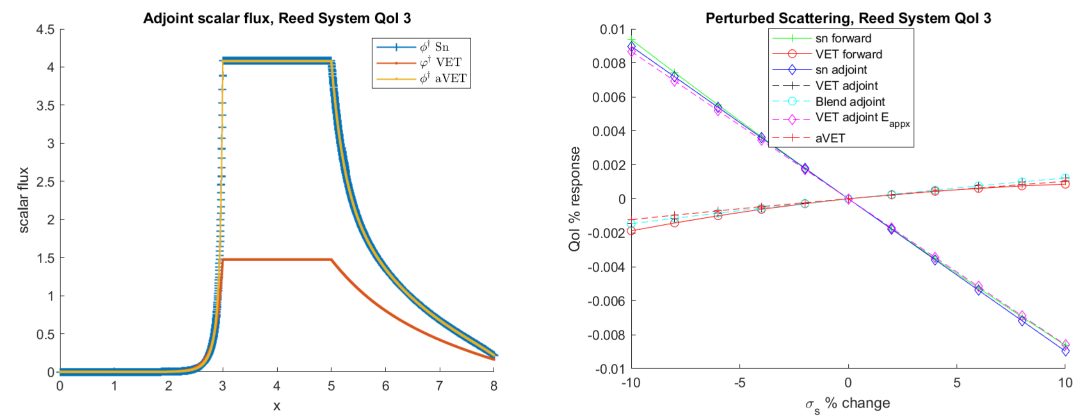


Figure 5.12: Scattering response and adjoint flux for Reed problem with *QoI* in region 3.

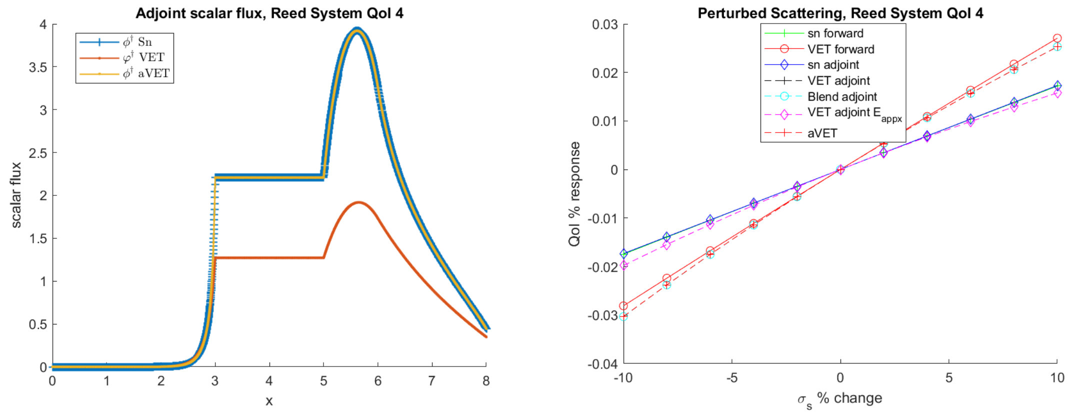


Figure 5.13: Scattering response and adjoint flux for Reed problem with *QoI* in region 4.

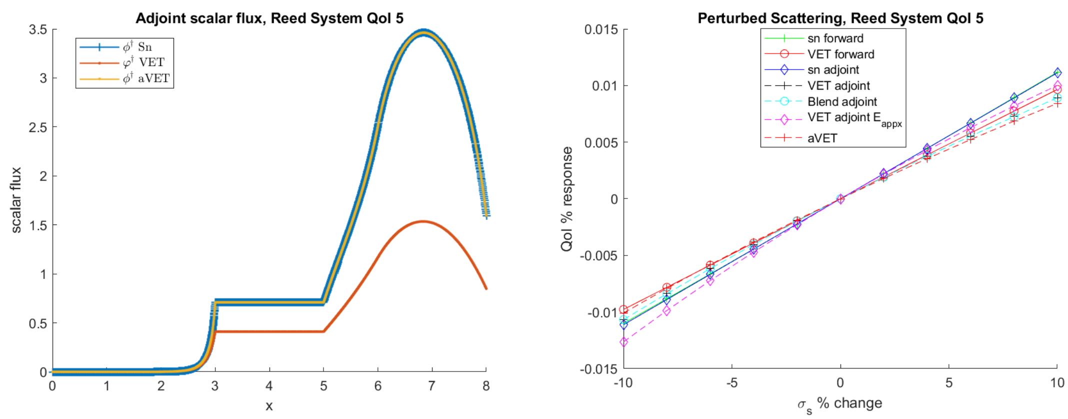


Figure 5.14: Scattering response and adjoint flux for Reed problem with *QoI* in region 5.

With the *QoI* in regions 1 and 2 the overall response to the scattering perturbation is small, on the order of $10^{-7}$ and $10^{-3}$ respectively. In these regions the VET methods (excluding $\delta\mathbb{E}$ approximation) appear to underestimate the small response to the perturbation; this appears to be reconciled well using the $\delta\mathbb{E}$ though. With the *QoI* in regions 4 and 5, where the scattering perturbations take place, the response to the scattering is of slightly higher magnitude, and the VET methods appear to overestimate the response. Once again the $\delta\mathbb{E}$ approximation method resolves much of the difference between VET and transport adjoint. The most problematic region appears to be when the *QoI* is in the void of region 3. In this scenario the transport methods show a response similar in magnitude to the response of *QoI* in regions 4 and 5, but the VET method shows a response of relatively small magnitude in the opposite direction. The $\delta\mathbb{E}$ approximation however, goes a long way to improving the VET method so that it agrees fairly well with transport adjoint. Looking at the $\delta\mathbb{E}$ inner-product term $\left\langle \ell_t \vec{\nabla} \cdot (\delta\mathbb{E}\phi), \vec{\nabla}\varphi^\dagger \right\rangle$ of Eq. (3.27) can give insight to why $\delta\mathbb{E}$ plays such a large role in these scenarios. The total mean free path term $\ell_t$ is very large in voids ($10^8$ in this case) and results in the term blowing up even for quite small perturbations in $\delta\mathbb{E}$ as shown in Figure 5.9.

| Term | *QoI* 1 | *QoI* 2 | *QoI* 3 | *QoI* 4 | *QoI* 5 |
|---|---:|---:|---:|---:|---:|
| Unperturbed *QoI* | 0.994951 | 0.158209 | 1.10511 | 1.75802 | 0.766009 |
| $+\left\langle \delta q, \varphi^\dagger \right\rangle$ | 0 | 0 | 0 | 0 | 0 |
| $-\left\langle \delta\sigma_a \phi, \varphi^\dagger \right\rangle$ | 0 | 0 | 0 | 0 | 0 |
| $-\left\langle \delta\ell_t \vec{\nabla} \cdot (\mathbb{E}\phi), \vec{\nabla}\varphi^\dagger \right\rangle$ | 9.26678e-09 | 0.000132024 | 0.00135357 | 0.0444895 | 0.00682825 |
| $+\left[\varphi^\dagger, 2\delta J^{\text{inc}}\right]$ | 0 | 0 | 0 | 0 | 0 |
| $-\left\langle \ell_t \vec{\nabla} \cdot (\delta\mathbb{E}\phi), \vec{\nabla}\varphi^\dagger \right\rangle$ | 1.44e-07 | 0.000169373 | -0.0108674 | -0.0167694 | 0.000788856 |
| $-\left[\varphi^\dagger, \phi\delta B\right]$ | 7.97272e-11 | 1.13587e-06 | 1.16455e-05 | 2.51421e-05 | 6.12292e-05 |

Table 5.6: Term by Term comparison of VET method and $\delta\mathbb{E}$ approximation method for the Reed QoI's under a $+10\%$ scattering perturbation in regions 4 and 5.

### 5.3.6 Detector in void

We will now focus in the *QoI* in a void, using Reed's problem presented in the previous section. The *QoI* used in the previous example was the average flux within the void.

However, in a non-simulation experiment the void flux may be detected by detector of some non-zero cross-section placed within the void region. This presence of a non-zero cross section may help dampen the effect of the $\delta\mathbb{E}$ term by reducing the $\ell_t$ value and reshaping the adjoint flux. To test this more realistic scenario, the previous Reed's system has the void region broken into two void regions of almost half the original length, and a small absorption region inserted in the middle to represent a detector. The width of this detector is one mean free path.

Region 1: $x \in [0, 2)$, $\quad \sigma_a = 50$, $\sigma_s = 0$, $q = 50$

Region 2: $x \in [2, 3)$, $\quad \sigma_a = 5$, $\sigma_s = 0$, $q = 0$

Region 3: $x \in [3, 3.95)$, $\quad \sigma_a = 10^{-8}\, \sigma_s = 0$, $q = 0$

Region 4: $x \in [3.95, 4.05)$, $\quad \sigma_a = 10\, \sigma_s = 0$, $q = 0$

Region 5: $x \in [4.05, 5)$, $\quad \sigma_a = 10^{-8}\, \sigma_s = 0$, $q = 0$

Region 6: $x \in [5, 6)$, $\quad \sigma_a = 0.1$, $\sigma_s = 0.9$, $q = 1$

Region 7: $x \in [6, 8]$, $\quad \sigma_a = 0.1$, $\sigma_s = 0.9$, $q = 0$

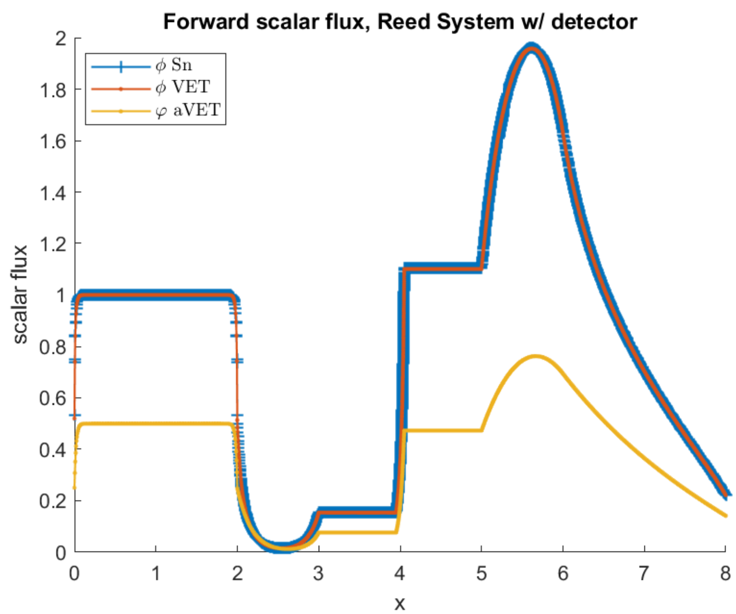


Figure 5.15: Plot of unperturbed forward scalar flux for the Reed's problem with detector in void.

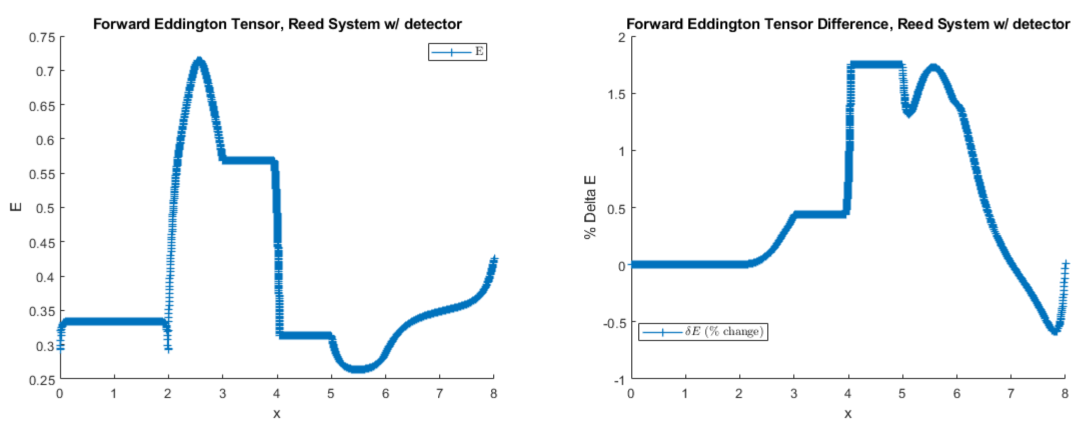


Figure 5.16: Plots of unperturbed Eddington Tensor for Reed's problem with detector as well as the Eddington perturbation $\delta\mathbb{E}$ for a $+10\%$ scattering perturbation in regions 4 and 5.

The response considered is then the average flux in the detector region. Once again the focus is placed on scattering perturbations.

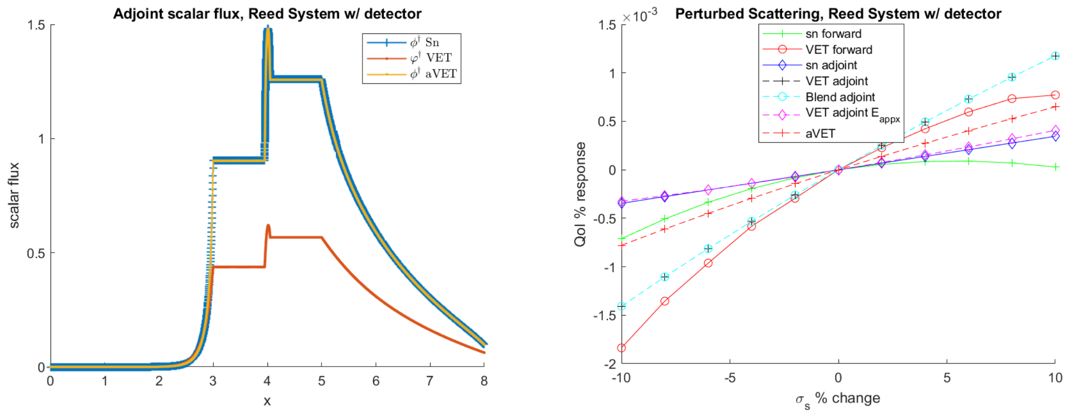


Figure 5.17: Scattering response and adjoint flux for Reed problem with detector in void region.

While the behavior of the VET method are not ideal in this test case, they are improved over the void average flux *QoI* of the previous section, in the sense that the VET response is on the same order of magnitude and direction as the transport adjoint method. The $\delta\mathbb{E}$ approximation method once again proves to be a powerful tool for reconciling VET and transport adjoint methods. The aVET method appears to fair a bit better in this case when compared to VET.

# 6. CONCLUSIONS AND OUTLOOK

For the systems tested, the VET method shows some promise for use in sensitivity calculations, however it appears that void regions could pose a problem for VET in certain scenarios. The blended method demonstrated an approach to increase the accuracy, particularly for source perturbations, at the cost of an additional SN solve to obtain $\phi^\dagger$. The $\delta\mathbb{E}$ approximation approach was even more accurate in most cases, but requires at least 1 extra SN solve for each perturbed system property, making it viable in scenarios where many perturbation scenarios must be tested.

Scattering perturbations showed possibly the most interesting behavior. The deviation of the VET and SN methods is stronger (relative to the SN sensitivity) in most of the test case when $\sigma_s$ is perturbed. Unfortunately, the testing of heavy scatting systems in one spacial dimension can be a bit limited. In a two or three dimensions, the ability for particles to scatter around objects exists in general, while this is not available in slab geometry. Expanding the discussed concepts to higher spatial dimensions would be a worthwhile next step, particularly in observing the effects of scattering on the VET method.

For the test cases with only a volumetric source, the aVET method utilizing $\varphi$ showed some advantages by way of its exact nature for source perturbations and while having similar accuracy to VET for cross section perturbations. This method however, cannot be used with in incident flux scenarios as formulated, so it's use case is limited.

Overall the $\delta\mathbb{E}$ approximation method appeared to fare the best of all VET methods, and frequently was close to the sensitivity found by transport adjoint. However, it is also the most costly of the VET methods, as additional transport solves are required to populate sample $\mathbb{E}$ values in the perturbation space. In scenarios where there are only a few perturbed variables, but many different perturbation values must be tested, the $\mathbb{E}$ seems like the best overall choice. However, as the number of independently perturbed parameters increases, the population of the perturbation space with sample $\mathbb{E}$ values becomes more intensive, and at a certain point the memory issues we seek to avoid using VET begin to show again.

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# APPENDIX A

## TIME DEPENDENT VET

While out of scope for this writing, a major goal of this method is the application towards time-dependent systems. As such, it is worth taking a brief look at how the VET formulation would look in a time dependent system. As with the steady state, the starting point is the one-group transport equation, now with the time derivative factor.

$$\frac{1}{v}\frac{\partial}{\partial t}\psi(\vec{r},\vec{\Omega},t) + \vec{\Omega}\cdot\vec{\nabla}\psi(\vec{r},\vec{\Omega},t) + \sigma_t\psi(\vec{r},\vec{\Omega},t) = \frac{1}{4\pi}\sigma_s\phi(\vec{r},t) + q(\vec{r},\vec{\Omega},t) \tag{A.1}$$

$$\psi(\vec{r},\vec{\Omega},t) = \psi^{\text{inc}}(\vec{r},\vec{\Omega},t) \quad \vec{r}\in\partial V^- = \{\vec{r}\in\partial V,\ \text{s.t. },\vec{\Omega}\cdot\vec{n}(\vec{r}) < 0\} \tag{A.2}$$

$$\psi(\vec{r},\vec{\Omega},0) = \psi_0(\vec{r},\vec{\Omega}) \tag{A.3}$$

The zero-th and first angular moments are taken of the time dependent system. The Eddington Tensor is used in the 1st order equation.

$$\frac{1}{v}\frac{\partial}{\partial t}\phi + \vec{\nabla}\cdot\vec{J} + (\sigma_a)\phi = q\,, \tag{A.4a}$$

$$\frac{1}{v}\frac{\partial}{\partial t}\vec{J} + \vec{\nabla}\cdot(\mathbb{E}\phi) + \sigma_t\vec{J} = 0\,. \tag{A.4b}$$

The moments are then combined in the same fashion used in the steady-state case

$$\frac{1}{v}\frac{\partial}{\partial t}\phi - \vec{\nabla}\cdot\left(\frac{1}{v\sigma_t}\frac{\partial}{\partial t}\vec{J}\right) - \vec{\nabla}\cdot\left(\frac{1}{\sigma_t}\vec{\nabla}\cdot(\mathbb{E}\phi)\right) + (\sigma_a)\phi = q. \tag{A.5}$$

Note that the same double divergence term shows up the the time dependent equation as it does in the steady state formulation. So it is conceivable that insight gained from the steady state treatment will carry over to the time-dependent problem.

## APPENDIX B

## DETAILED VET BOUNDARY TERM DERIVATION

Represent the value $\ell_t\vec{\nabla}\cdot\mathbb{E}\phi$ by some vector $\vec{v}$.

$$
\begin{aligned}
-\left\langle \vec{\nabla}\cdot\left(\ell_t\vec{\nabla}\cdot\mathbb{E}\phi\right),\varphi^\dagger\right\rangle &= -\int_V dV\,\varphi^\dagger\left(\vec{\nabla}\cdot\left(\ell_t\vec{\nabla}\cdot\mathbb{E}\phi\right)\right)\\
&= -\int_V dV\,\varphi^\dagger\left(\vec{\nabla}\cdot\vec{v}\right)
\end{aligned} \tag{B.1}
$$

Then use a product rule $\vec{\nabla}\cdot(\vec{v}\varphi^\dagger) = \varphi^\dagger(\vec{\nabla}\cdot\vec{v}) + \vec{v}\cdot(\vec{\nabla}\varphi^\dagger)$. Use the divergence theorem on the $\vec{\nabla}\cdot(\vec{v}\varphi^\dagger)$ term to convert to a surface integral

$$
\begin{aligned}
-\int_V dV\,\varphi^\dagger\left(\vec{\nabla}\cdot\vec{v}\right) &= -\int_V dV\,\vec{\nabla}\cdot(\vec{v}\varphi^\dagger) + \int_V dV\,\vec{v}\cdot(\vec{\nabla}\varphi^\dagger)\\
&= -\oint_{\partial V} dS\,(\vec{v}\varphi^\dagger)\cdot\vec{n} + \int_V dV\,\vec{v}\cdot(\vec{\nabla}\varphi^\dagger)\\
&= -\oint_{\partial V} dS\,\left(\left(\ell_t\vec{\nabla}\cdot\mathbb{E}\phi\right)\varphi^\dagger\right)\cdot\vec{n} + \int_V dV\,\left(\ell_t\vec{\nabla}\cdot\mathbb{E}\phi\right)\cdot(\vec{\nabla}\varphi^\dagger)\\
&= -\left[\left(\ell_t\vec{\nabla}\cdot\mathbb{E}\phi\right)\cdot\vec{n},\varphi^\dagger\right] + \int_V dV\,\left(\ell_t\vec{\nabla}\cdot\mathbb{E}\phi\right)\cdot(\vec{\nabla}\varphi^\dagger)
\end{aligned} \tag{B.2}
$$

Turn focus to the remaining volume integral. Define the vector $\vec{u} = \ell_t \vec{\nabla}\varphi^\dagger$. Breakout $\mathbb{E}$ into component vectors $\vec{E}$

$$\begin{aligned}
\int_V dV \, \left(\ell_t \vec{\nabla} \cdot \mathbb{E}\phi\right) \cdot (\vec{\nabla}\varphi^\dagger) &= \int_V dV \, \left(\vec{\nabla} \cdot \mathbb{E}\phi\right) \cdot \vec{u} \\
&= \int_V dV \sum_{n=x,y,z} \left(\vec{\nabla} \cdot \vec{E}_n \phi\right) u_n \\
&= \sum_{n=x,y,z} \int_V dV \, \left(\vec{\nabla} \cdot \vec{E}_n \phi\right) u_n \\
&= \sum_{n=x,y,z} \left[\int_V dV \, \vec{\nabla} \cdot \left(\vec{E}_n \phi u_n\right) - \int_V dV (\vec{E}_n \phi) \cdot \vec{\nabla} u_n\right] \\
&= \sum_{n=x,y,z} \left[\oint_{\partial V} dS \, \vec{E}_n \phi u_n \cdot \vec{n} - \int_V dV (\vec{E}_n \phi) \cdot \vec{\nabla} u_n\right] \\
&= \oint_{\partial V} dS \, \phi \left(\vec{E} \cdot \vec{u}\right) \cdot \vec{n} - \int_V dV \phi \left(\mathbb{E} : \vec{\nabla}\vec{u}\right) \\
&= \oint_{\partial V} dS \, \phi \left(\vec{E} \cdot \ell_t \vec{\nabla}\varphi^\dagger\right) \cdot \vec{n} - \int_V dV \phi \left(\mathbb{E} : \vec{\nabla}\ell_t \vec{\nabla}\varphi^\dagger\right) \\
&= \left[\phi, \vec{E} \cdot \ell_t \vec{\nabla}\varphi^\dagger \cdot \vec{n}\right] - \left\langle \phi, \mathbb{E} : \vec{\nabla}\ell_t \vec{\nabla}\varphi^\dagger \right\rangle
\end{aligned} \tag{B.3}$$

Putting everything together

$$\begin{aligned}
-\left\langle \vec{\nabla} \cdot \left(\ell_t \vec{\nabla} \cdot \mathbb{E}\phi\right), \varphi^\dagger \right\rangle = &-\left\langle \phi, \mathbb{E} : \vec{\nabla}\ell_t \vec{\nabla}\varphi^\dagger \right\rangle + \left[\phi, \vec{E} \cdot \ell_t \vec{\nabla}\varphi^\dagger \cdot \vec{n}\right] \\
&- \left[\left(\ell_t \vec{\nabla} \cdot \mathbb{E}\phi\right) \cdot \vec{n}, \varphi^\dagger\right]
\end{aligned} \tag{B.4}$$

## APPENDIX C

## ADDITIONAL FLUX GRAPHS SHOWING $2\varphi$ AND $2\varphi^\dagger$

Additional graphs showing $\varphi$ and $\varphi^\dagger$ scaled by a factor of 2, showing the difference between $\phi$ and $\varphi$ values is more than just the apparent factor of two

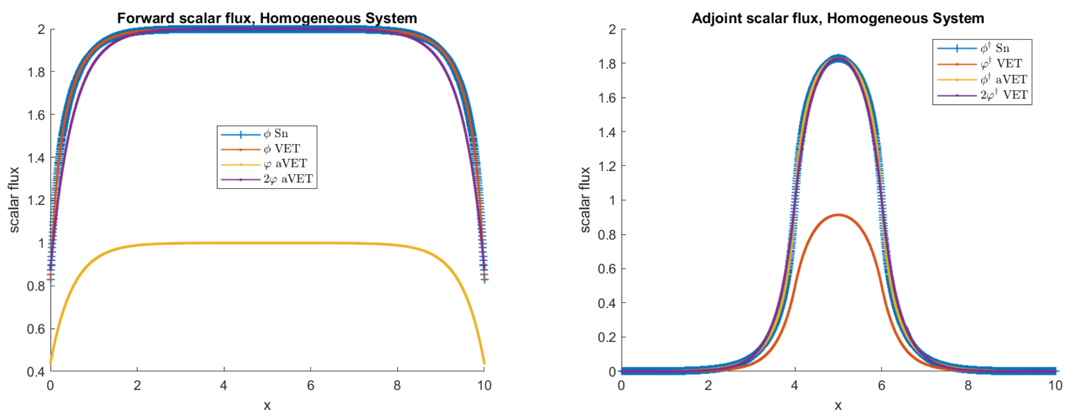


Figure C.1: Plots of unperturbed scalar fluxes for the homogeneous system, including $2\varphi$ and $2\varphi^\dagger$

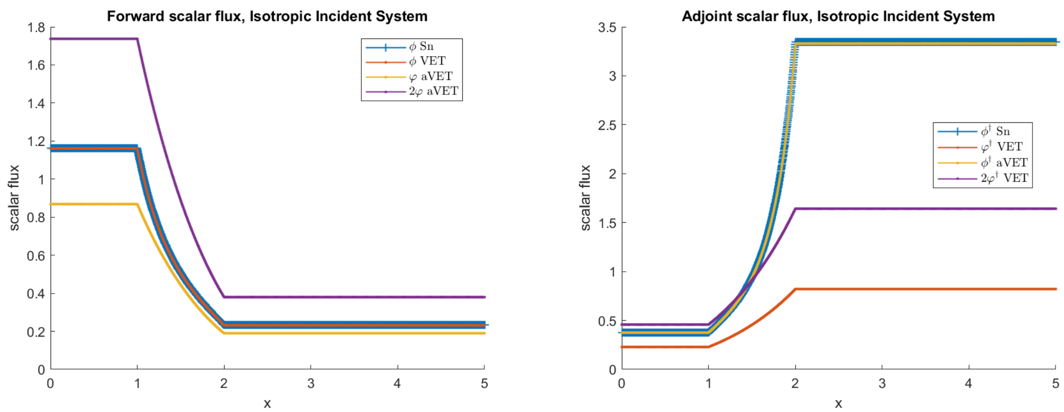


Figure C.2: Plots of unperturbed scalar fluxes for the shielding system, including $2\varphi$ and $2\varphi^\dagger$

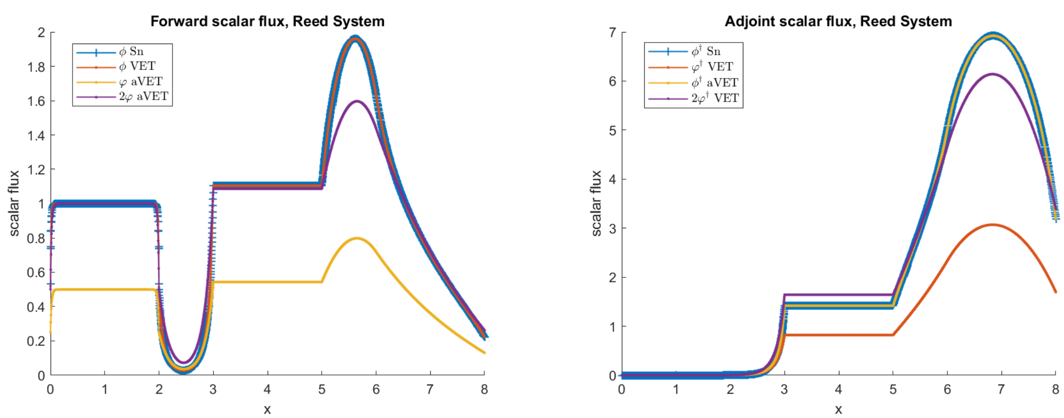


Figure C.3: Plots of unperturbed scalar fluxes for the Reed system, including $2\varphi$ and $2\varphi^\dagger$