# ADJOINT-BASED SENSITIVITY ANALYSIS FOR FLUX-LIMITED DIFFUSION

A Thesis

by

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# ABSTRACT

Uncertainty quantification and sensitivity analysis (UQSA) is becoming an essential component for engineering and physics modeling. The growth of UQSA can be attributed to improved statistical methodologies and computational capabilities. Recent advancements in computer engineering are focused on increasing the CPU count, allowing for more operations to be performed per second. Increased computational speed often comes at the cost of a decrease in memory; this has a direct impact on the way large scale codes are developed. This work is focused on the adjoint-based sensitivity analysis, a notoriously memory intensive method. The adjoint approach to sensitivity analysis provides an efficient means for computing sensitivities when many parameters are perturbed. In the adjoint approach, a set of forward and adjoint equations are solved once, and the sensitivity of a quantity of interest with respect to any parameter can be found by computing known derivatives and evaluating inner products. This is computationally more efficient than the standard computation of sensitivities, which requires solving the forward system twice per perturbed parameter. The adjoint based sensitivity analysis is performed on systems described by flux-limited diffusion. The nonlinearity introduced by including a flux-limited diffusion coefficient complicates the expressions for the sensitivities. Where appropriate, approximations are suggested that simplify the differentiation; examples demonstrate that this does not introduce significant error. The adjoint method requires storing the full forward and adjoint solutions, in addition to any time-dependent parameters. For high-dimensional transient problems, this often requires more memory than available on standard computers, thus it is necessary to read and write to files. To avoid this time-consuming process, a method is proposed that treats the adjoint solution as

if it is in a “quasi-steady state". This allows the forward and adjoint equations to be solved in tandem, and eliminates the need to store excessive amounts of data. The proposed methods are applied to a one-dimensional radiative diffusion problem and a two-dimensional cylindrical multiphysics model. The data reduction storage method produces accurate sensitivities for systems in which the steady-state assumption for the adjoint system is valid; however it does not produce acceptable approximations for highly transient problems or quantities of interest that vary rapidly with time.

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# NOMENCLATURE

UQ : Uncertainty quantification

SA : Sensitivity analysis

QOI : Quantity of interest

Abs. : Absorption

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# 1. INTRODUCTION

Uncertainty quantification and sensitivity analysis (UQSA) has grown significantly in recent years, in part due to improved computing capabilities that have greatly increased the speed and accuracy to which UQSA calculations can be performed. The current trend in computer engineering is focused on increasing the CPU count such that more operations can be performed per second; the cost of the increased computation speed is a reduction in available memory [7]. Low memory has a significant impact on how large-scale codes are developed; this work is focused on the adjoint-based for sensitivity analysis, a notoriously memory intensive method. An adjoint equation, derived from the equations that govern the physical system, is solved and its solution is used to calculate sensitivities by evaluating inner products. As will be shown, this technique is necessary for systems with many unknown parameters, but it has a high memory demand for multidimensional, transient problems. In this work, sensitivity analyses are performed on systems that can be described by flux-limited diffusion. The nonlinearity of the flux-limited diffusion equation introduces complications when computing sensitivities; where appropriate, simplifications are proposed that retain the accuracy of the resulting quantities of interest. Finally, a method which reduces the memory required to perform adjoint and sensitivity calculations is proposed and examined for time-dependent systems.

# 2. THEORY

There are two common approaches to performing a sensitivity analysis. The simplest method by which the sensitivity of a quantity of interest can be examined requires solving the problem twice: compute the quantity of interest using one value for the parameter under consideration, then solve the problem a second time using a slightly different value of that parameter. The change in the resulting quantities of interest can be divided by the change in the parameter value to quantify the sensitivity. This is a direct and intuitive method, and requires little effort, as the only change required in the code is that of the parameter value. However, in many physical systems there are a large number of parameters for which we would like to compute sensitivities. The direct approach requires the code to be executed twice per perturbed variable; for systems with hundreds of parameters, this quickly becomes an unfeasible task. An approach better suited for systems with a large number of parameters is the adjoint-based method, which uses the solution of the adjoint equation to efficiently compute sensitivities of a quantity of interest with respect to any arbitrary parameter.

The first application of adjoint functions in perturbation theory was performed on problems in neutron transport by Wigner in 1945 [3]. He showed that the effects of perturbing material properties in a nuclear reactor could be studied efficiently using the adjoint neutron flux; the solution to the adjoint neutron transport equation. Wigner also identified the adjoint flux as the neutron "importance"; this will be illustrated later in this section. Wigner's initial work laid the foundation for performing systematic and deterministic uncertainty quantification and sensitivity analysis in the field of radiation transport; the ideas have since been applied to fields beyond

nuclear science.

This section will begin by introducing the diffusion approximation and the various forms of the radiation diffusion equation that will be used to describe the systems under consideration. Then the adjoint operator will be introduced, followed by the procedure for deriving adjoint equations, and how they can be utilized in sensitivity analyses.

## 2.1 The Diffusion Approximation

The movement of particles, such as neutrons or photons, is described by a transport equation. In its most complex form, the transport equation is a differential equation with as many as seven independent variables: three spatial coordinates, two directional angles, time, and energy [1]. The radiation transport equation has been extensively studied and can be solved for reasonably complex systems. However, for large scale, highly non-homogeneous systems, such as a nuclear reactor, the transport equation is far too complicated to solve with high fidelity. Therefore, many approximate forms of the transport equation have been derived that yield results in agreement with transport theory, but are easily solved for large systems. One of the most popular simplifications of the transport equation is the diffusion approximation. The time-dependent diffusion equation is given by Eq. (2.1):

$$\frac{1}{v(E)}\frac{\partial\phi(\vec{r},E,t)}{\partial t} - \nabla\cdot D(\vec{r},E,t)\nabla\phi(\vec{r},E,t) + \sigma_a(\vec{r},E,t)\phi(\vec{r},E,t) = Q(\vec{r},E,t). \tag{2.1}$$

The particle flux, $\phi$, is defined as the particle track length per unit volume, per unit time; it is the product of the particle speed and the particle density. The diffusion coefficient is denoted $D$; it is a variable introduced when making the diffusion approximation and is typically taken to be the inverse of the three times the transport

cross section. The term $\sigma_a$ is the absorption cross section, and $Q$ is the source. Each of these variables can, and typically do, depend on space, particle energy, and time. Often only a few of these dependencies is considered in order to simplify the set of equations to be solved. In the following sections a few particular forms of the diffusion equation are presented, and discretization for programming applications are discussed. Last, a particular choice of the diffusion coefficient, the flux-limited form, is presented and its benefits highlighted.

### *2.1.1 1-D Diffusion*

The one dimensional form of the diffusion equation in Cartesian coordinates is given by:

$$-\frac{d}{dx}\left(D(x)\frac{d}{dx}\phi(x)\right)+\sigma(x)\phi(x)=Q(x). \tag{2.2}$$

The energy dependence will be omitted in what follows, but spatial and temporal dependencies of all variables is considered. Equation (2.2) can readily be solved numerically by expressing it in matrix form and using an iterative technique, such as the Gauss-Seidel method or successive over relaxation [2].

To solve this problem numerically, the $x$ axis is discretized so that the $x$ position is given by

$$x_i = i\Delta x, \tag{2.3}$$

where $i$ is an integer and $\Delta x$ is the step size between successive cells. Integer values of $i$ are located at cell centers, and half integer values are at the boundaries. Material properties can vary between cells, but are assumed constant within the cell. The differential equation (2.2) can be converted to a finite difference equation using the

following approximations for the derivative:

$$\left(\frac{df}{dx}\right)_{i+1/2} \approx \frac{f(x_{i+1}) - f(x_i)}{\Delta x}, \tag{2.4}$$

Using equation (2.4) to evaluate the derivatives of the diffusion coefficient and flux, and denoting $f(x_i)$ as $f_i$, the one dimensional finite difference diffusion equation becomes:

$$\frac{-1}{\Delta x}\left[D_{i+1/2}\left(\frac{\phi_{i+1} - \phi_i}{\Delta x}\right) - D_{i-1/2}\left(\frac{\phi_i - \phi_{i-1}}{\Delta x}\right)\right] + \sigma_a(x_i)\phi(x_i) = Q(x_i), \tag{2.5}$$

where the diffusion coefficient at the interface is the harmonic mean of the values in each cell:

$$D_{i+1/2} = \frac{2D_{i+1}D_i}{Di + 1 + D_i}. \tag{2.6}$$

The finite difference form of the boundary conditions for the flux is derived in a similar way:

$$\begin{aligned} a\phi_0 - b\frac{\phi_1 - \phi_0}{\Delta x} &= 0, \\ a\phi_{N-1} + b\frac{\phi_N - \phi_{N-1}}{\Delta x} &= 0, \end{aligned} \tag{2.7}$$

which can be re-arranged to match the form of Eq. (2.5):

$$\begin{aligned} \left(a + \frac{b}{\Delta x}\right)\phi_0 - \frac{b}{\Delta x}\phi_1 &= 0, \\ \left(a - \frac{b}{\Delta x}\right)\phi_{N-1} + \frac{b}{\Delta x}\phi_N &= 0. \end{aligned} \tag{2.8}$$

Equations (2.5) and (2.8) can be combined into a single matrix equation of the form $A\phi$=$Q$ that is readily solved.

### *2.1.2 1-D Extension to Cylindrical and Spherical Geometries*

In one dimensional systems there is a convenient way to express the finite difference equations for the forward and adjoint flux such that the general formulation is geometry-independent. To switch between Cartesian, cylindrical, and spherical coordinate systems, it is only necessary to modify two coefficients. To derive this formulation, we explicitly impose continuity of the current, $J$, at the cell interface. Consider the interface at $\mathrm{x}_{i-1/2}$:

$$J_{i-1/2,left} = \frac{-2D_{i-1}}{\Delta x}(\phi_{i-1/2} - \phi_{i-1}), \tag{2.9}$$

$$J_{i-1/2,right} = \frac{-2D_{i}}{\Delta x}(\phi_{i} - \phi_{i-1/2}). \tag{2.10}$$

These equations must be equal; simple manipulations give us the expression:

$$J_{i-1/2} = \frac{-D_{i-1/2}}{\Delta x}(\phi_{i} - \phi_{i-1}), \tag{2.11}$$

where $D_{i-1/2}$ is again the harmonic mean of $D_i$ and $D_{i-1}$. The neutron balance equation for the cell can be written as:

$$A_{i+1/2}J_{i+1/2} - A_{i-1/2}J_{i-1/2} + \sigma_{a,i}\phi_i V_i = Q_i V_i, \tag{2.12}$$

where the coefficients are geometry specific:

$$\begin{aligned} Cartesian : A_{i-1/2} = 1, V_i = \Delta x \\ Cylindrical : A_{i-1/2} = 2\pi r_{i-1/2}, V_i = \pi((r_{i+1/2})^2 - (r_{i-1/2})^2) \\ Spherical : A_{i-1/2} = 4\pi r_{i-1/2}^2, V_i = (4/3)\pi((r_{i+1/2})^3 - (r_{i-1/2})^3). \end{aligned} \tag{2.13}$$

In terms of the flux, the diffusion equation is:

$$-A_{i+1/2}\frac{D_{i+1/2}}{\Delta x}(\phi_{i+1} - \phi_i) + A_{i-1/2}\frac{D_{i-1/2}}{\Delta x}(\phi_i - \phi_{i-1}) + \sigma_{a,i}\phi_i V_i = Q_i V_i. \tag{2.14}$$

### *2.1.3 2-D Diffusion*

The extension from one to two spatial dimensions is straightforward. We are particularly interested in two dimensional Cartesian *(x,y)* and cylindrical *(ρ,z)* geometries. The forward diffusion equations for these geometries are as follows:

$$-\frac{\partial}{\partial x}\left(D(x,y)\frac{\partial}{\partial x}\phi(x,y)\right) + \sigma(x,y)_a\phi(x,y) = Q(x,y), \tag{2.15}$$

$$\begin{aligned} -\frac{\partial D(\rho,z)}{\partial \rho}\frac{\partial \phi(\rho,z)}{\partial \rho} - \frac{D(\rho,z)}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial \phi}{\partial \rho}\right) - \frac{\partial D(\rho,z)}{\partial z}\frac{\partial \phi(\rho,z)}{\partial z} \\ -D(\rho,z)\frac{\partial^2 \phi(\rho,z)}{\partial z^2} + \sigma_a(\rho,z)\phi(\rho,z) = Q(\rho,z). \end{aligned} \tag{2.16}$$

These equations and the corresponding boundary conditions can be discretized using the same method of differentiation implemented in the one dimensional case.

### *2.1.4 Flux-Limited Diffusion*

Flux-limited diffusion coefficients are designed to correct for non-physical results related to the speed of propagation of information. Many forms of diffusion coefficients

have been proposed; the Larsen coefficient is used in this work, it is given by the expression [7]:

$$D = \left( (3\kappa\rho)^n + \left( \frac{1}{E_R} \left| \frac{\partial E_R}{\partial x} \right| \right)^n \right)^{-1/n}. \tag{2.17}$$

Typically $n$ is chosen to be 2, but can be adjusted such that the diffusion solution agrees more closely with transport. For optically thick problems the gradient of the flux is small compared to the transport cross section, $\sigma_{tr}$, and the diffusion equation reduces to its traditional form. For optically thin problems, the gradient of the flux dominates the expression and the speed is limited to the value defined by the current:

$$J = -D\nabla\phi. \tag{2.18}$$

Inclusion of the flux-limited diffusion coefficient makes the diffusion equation nonlinear. In practice, nonlinear equations are solved iteratively; an initial guess for the flux is provided, the diffusion coefficient is computed, and an improved approximation to the flux is determined by solving the diffusion equation with the current guess for the coefficient. The process is repeated until the flux and the diffusion coefficient converge, meaning that the change in the vector values for $D$ and $\phi$ do not change an appreciable amount between successive iterations.

## 2.2 The Adjoint Approach to Sensitivity Analysis

The adjoint approach to performing sensitivity analyses is a powerful, analytic method for identifying parameters that have the greatest influence on a particular quantity of interest. The method requires deriving and solving the adjoint equation, and using the solution to compute integrals that produce sensitivity coefficients. The adjoint flux carries a particular physical significance for particle transport. While the forward flux describes where particles are located, the adjoint flux describes the

particle's importance in contributing to a particular quantity of interest. This will be further addressed later in the section. With this physical interpretation, the adjoint flux can be used to determine where the contributions to a quantity of interest are highest, providing insight into the system behavior. This section will begin by defining the adjoint operator and deriving the adjoint diffusion equations, followed by a physical interpretation of the adjoint particle flux. The utility of the adjoint solution in computing sensitivities will be examined, and disadvantages to this approach will be discussed. Finally, a few of the sensitivities computed in this work will be derived to explicitly illustrate the method.

### *2.2.1 Adjoint Operators*

For two well behaved functions, $f(\vec{r})$ and $g(\vec{r})$, a formally self-adjoint operator $L$, is defined by the equality of the inner products:

$$(Lf, g) = (f, Lg), \tag{2.19}$$

where the inner product for two functions is given by:

$$(f, g) = \int f(\vec{r})g(\vec{r})d\vec{r}, \tag{2.20}$$

with the integral taken over the domain of the problem. Note that this domain could include spatial dimensions, time, energy, and angular variables, etc. If the functions $f(\vec{r})$ and $g(\vec{r})$ also satisfy the same boundary conditions, the operator $L$ is simply said to be self-adjoint. If an operator $L$ is not self-adjoint, it is possible to define $L^{\dagger}$, the operator adjoint to $L$, by the following relationship:

$$(Lf, g) = (f, L^{\dagger}g). \tag{2.21}$$

$L^\dagger$ operates on *g($\vec{r}$)*, the adjoint function, which satisfies boundary conditions that may be the same or different than those satisfied by the function *f($\vec{r}$)*, on which $L$ operates.

### *2.2.2 Steady State Adjoint Diffusion Equation*

As a simple, illustrative example, consider the one energy group diffusion equation:

$$-\nabla \cdot D(\vec{r})\nabla\phi(\vec{r}) + \sigma_a(\vec{r})\phi(\vec{r}) = Q(\vec{r}). \tag{2.22}$$

This can be written in a compact operator form:

$$L\phi = Q, \tag{2.23}$$

where the differential operator $L$ is given by:

$$L = -\nabla \cdot D(\vec{r})\nabla + \sigma_a(\vec{r}). \tag{2.24}$$

The corresponding adjoint problem can be written in a similar form:

$$L^\dagger\phi^\dagger = Q^\dagger. \tag{2.25}$$

From the definition of the adjoint operator, $L^\dagger$ must satisfy the equation:

$$(\phi^\dagger, L\phi) = (\phi, L^\dagger\phi^\dagger), \tag{2.26}$$

therefore the task is to find the correct form of $L^\dagger$ such that:

$$\int [-\phi^\dagger(\vec{r})\nabla \cdot D(\vec{r})\nabla\phi(\vec{r}) + \phi^\dagger(\vec{r})\sigma_a(\vec{r})\phi(\vec{r})]d\vec{r} = \int \phi(\vec{r})L^\dagger\phi^\dagger(\vec{r})d\vec{r}. \tag{2.27}$$

The term involving the absorption cross section is already of the correct form, as switching the order of $\phi$ and $\phi^\dagger$ does not change the value of the term. The diffusion term can be rewritten using integration by parts to move the derivative operators off of $\phi$ and onto $\phi^\dagger$. By this method, we have (suppressing function arguments):

$$-\int \phi^\dagger \nabla \cdot D\nabla\phi d\vec{r} = -\int \nabla \cdot (\phi^\dagger D\nabla\phi)d\vec{r} + \int (\nabla\phi^\dagger)\cdot D(\nabla\phi)d\vec{r}. \tag{2.28}$$

We can apply integration by parts a second time to each of these terms. This gives us the following expressions:

$$\begin{aligned} -\int \nabla \cdot (\phi^\dagger D\nabla\phi)d\vec{r} = -\int \nabla\cdot\nabla(\phi^\dagger D\phi)d\vec{r} + \int \nabla\cdot((\nabla\phi^\dagger)D\phi)d\vec{r} \\ + \int \nabla\cdot(\phi^\dagger(\nabla D)\phi)d\vec{r}, \end{aligned} \tag{2.29}$$

and

$$\begin{aligned} \int (\nabla\phi^\dagger)\cdot D(\nabla\phi)d\vec{r} = \int \nabla\cdot((\nabla\phi^\dagger)D\phi)d\vec{r} - \int (\nabla^2\phi^\dagger)D\phi d\vec{r} \\ - \int (\nabla\phi^\dagger)\cdot(\nabla D)\phi d\vec{r}. \end{aligned} \tag{2.30}$$

Putting these expressions into Eq. (2.28) and combining terms gives:

$$\begin{aligned} \int \phi L^\dagger \phi^\dagger d\vec{r} = -\int \phi D\nabla^2\phi^\dagger d\vec{r} - \int \phi(\nabla D)(\nabla\phi^\dagger)d\vec{r} + \int \phi\sigma_a\phi^\dagger d\vec{r} \\ - \int \nabla\cdot(\phi^\dagger D\nabla\phi)d\vec{r} + \int \nabla\cdot(\phi D\nabla\phi^\dagger d\vec{r}. \end{aligned} \tag{2.31}$$

The first three terms on the right hand side of Eq. (2.31) form the adjoint operator:

$$L^\dagger = -\nabla\cdot D\nabla + \sigma_a, \tag{2.32}$$

implying that $L{=}L^{\dagger}$. We would like for the one-group diffusion operator to be self-adjoint, so we require that the last two terms vanish [1]. These terms can be rewritten using the divergence theorem:

$$-\int \nabla\cdot(\phi^{\dagger}D\nabla\phi)d\vec{r}+\int \nabla\cdot(\phi D\nabla\phi^{\dagger})d\vec{r}=-\oint(\phi^{\dagger}D\nabla\phi)\cdot d\vec{S}+\oint(\phi D\nabla\phi^{\dagger})\cdot d\vec{S}. \tag{2.33}$$

Requiring that these two terms vanish allows us to determine the necessary boundary conditions that must be satisfied by the adjoint flux. On the boundary, we must have:

$$\phi^{\dagger}D\nabla\phi=\phi D\nabla\phi^{\dagger}. \tag{2.34}$$

For adjoint calculations, the boundary conditions of the diffusion equation are typically of the form:

$$a\phi+b\nabla\phi=0. \tag{2.35}$$

It can be shown that the adjoint flux satisfies identical boundary conditions

$$a\phi^{\dagger}+b\nabla\phi^{\dagger}=0, \tag{2.36}$$

by direct substitution of (2.35) and (2.36) into (2.34).

In the case of nonhomogeneous boundary conditions for the forward equation, the adjoint boundary conditions are not as simple to derive. Consider again equation (2.33). If, for example, the problem of interest had fixed flux boundary conditions, we could determine the value of the second integral on the right hand side given the adjoint solution. However, there is no known information on the derivative of the forward flux at the boundary. In order for the adjoint flux to be independent of the

forward flux, which is typically (but not always) desired, we can require the adjoint flux vanish at the boundary, thus eliminating the unknown term. The second term on the right hand side is still nonzero, and will affect the derivation of the sensitivity expressions.

### *2.2.3 Time-Dependent Adjoint Diffusion Equation*

The time dependent, one group neutron diffusion equation is:

$$\frac{1}{v}\frac{\partial\phi(\vec{r},t)}{\partial t} - \nabla\cdot D(\vec{r},t)\nabla\phi(\vec{r},t) + \sigma_a(\vec{r},t)\phi(\vec{r},t) = Q(\vec{r},t), \tag{2.37}$$

where $v$ is the particle velocity, and the expressions for the coefficients and the flux can now be functions of time. Including time-dependence requires on a simple modification to the finite difference form of the diffusion equation. The time derivative term can be expressed as:

$$\frac{1}{v}\frac{\partial\phi}{\partial t} \simeq \frac{\phi_{n+1}-\phi_n}{v\Lambda t}, \tag{2.38}$$

where *n*, *n+1* are discrete time coordinates. The diffusion equation is solved using the implicit Euler method. The remaining terms in Eq. 64 are evaluated at time step n+1; the equation can be written in the form:

$$\left(\frac{1}{v\Delta t} - \nabla\cdot D\nabla + \sigma_a\nabla\right)\phi_{n+1} = Q + \frac{\phi_n}{v\Delta t}. \tag{2.39}$$

This can be interpreted as adding the term *1/(v$\Delta$t)* to the absorption cross section and the term $\phi_n$/ *(v$\Delta$t)* to the source. This new "effective source" term is a function of the flux at the previous time step, thus this information must be stored in the source array before the solution at the next time step can be found. When an initial value of the flux is given at all spatial locations, the solution of the diffusion equation

is solved forward in time by first converging the non-linear diffusion coefficient, using this expression to find the scalar flux at a particular time step, and then using this to calculate the source at the next time step. This iterative process is repeated to move the solution forward to the desired final time.

Unlike the steady state one group neutron diffusion operator, the time-dependent operator is not self-adjoint. The time-dependent adjoint operator can be determined using the same methodology used to derive the steady state operator. Equation (2.27) is modified to include the time derivative of the forward flux:

$$\int \left[ \phi^\dagger \frac{1}{v} \frac{\partial \phi}{\partial t} - \phi^\dagger \nabla \cdot D \nabla \phi + \phi^\dagger \sigma_a \phi \right] d\vec{r} = \int \phi L^\dagger \phi^\dagger d\vec{r}. \tag{2.40}$$

The operators can be split into the time-dependent and steady state components:

$$\begin{aligned} \frac{1}{v} \frac{\partial \phi}{\partial t} + L_{ss}\phi &= Q, \\ L_t^\dagger \phi^\dagger + L_{ss}^\dagger \phi^\dagger &= Q^\dagger. \end{aligned} \tag{2.41}$$

Next, multiply the first equation in (2.41) by $\phi^\dagger$ and the second equation by $\phi$, and integrate over all space. It has been shown that:

$$\int \phi^\dagger L_{ss} \phi d\vec{r} = \phi L_{ss}^\dagger \phi^\dagger d\vec{r}, \tag{2.42}$$

and that

$$\int \phi^\dagger Q d\vec{r} = \phi Q^\dagger d\vec{r}. \tag{2.43}$$

We are left with

$$\int \phi L_t^\dagger \phi^\dagger d\vec{r} = -\int \phi^\dagger \frac{1}{v} \frac{\partial \phi}{\partial t} d\vec{r}. \tag{2.44}$$

The right hand side of Eq. (2.44) can be rewritten as:

$$-\int \phi^\dagger \frac{1}{v}\frac{\partial \phi}{\partial t} d\vec{r} = -\int \frac{1}{v}\frac{\partial \phi \phi^\dagger}{\partial t} d\vec{r} + \int \phi \frac{1}{v}\frac{\partial \phi^\dagger}{\partial t} d\vec{r}. \tag{2.45}$$

The first term on the right hand side of this equation vanishes due to orthogonality properties of the forward and adjoint flux, leaving [1]:

$$\int \phi^\dagger \frac{1}{v}\frac{\partial \phi}{\partial t} d\vec{r} = -\int \phi \frac{1}{v}\frac{\partial \phi^\dagger}{\partial t} d\vec{r}. \tag{2.46}$$

Using this result, the adjoint equation for one group neutron diffusion is:

$$-\frac{1}{v}\frac{\partial \phi^\dagger(\vec{r},t)}{\partial t} - \nabla \cdot D(\vec{r},t)\nabla\phi^\dagger(\vec{r},t) + \sigma_a(\vec{r},t)\phi^\dagger(\vec{r},t) = Q^\dagger(\vec{r},t). \tag{2.47}$$

The difference between the forward and adjoint operators is the change in sign of the time derivative term; the adjoint equation runs physics backwards in time to determine the importance of each event in contributing to a quantity of interest. Care must be taken when solving the forward and adjoint equations; the discretization method must be chosen such that the adjoint equation remains formally adjoint to the forward equation after discretization. The consequence of the sign change in the time derivative of the adjoint flux is that the adjoint equation is solved backward in time. Many Runge-Kuttta discretizations have been demonstrated to possess symmetries that preserve the adjoint properties and can be used to integrate forward and backward in time without requiring modifications to the algorithm. For example, the same numerical solver can be used to solve the forward problem with appropriate *initial* condition and the adjoint problem with the appropriate *final* condition. The implicit, explicit, and modified Euler, as well as the 4th order Runge-Kutta method, are discretization schemes that exhibit this symmetry [8]. In this work, the implicit

Euler method is used to solve the forward and adjoint problem.

Further complications in performing the sensitivity analysis arise on time-dependent problems due to the time evolution of parameters other than the flux. For example, the flux-limited diffusion coefficient is dependent on the forward flux, which is time dependent. The value of the diffusion coefficient at each space and time step must then be stored for later use in the adjoint equation. Since the physics runs backwards in time for the adjoint problem, the values of the diffusion coefficient must be used starting from the final time step back to the initial time. This is true for other time dependent parameters as well, such as cross sections, sources, etc.

### *2.2.4 Physical Interpretation of the Adjoint Flux*

To understand the physical significance of the adjoint flux, consider neutron transport in a steady state, subcritical system with a source. Suppose there is a neutron detector with a response proportional to the detector material cross section. If the source is taken to be a delta function, a point source, the adjoint flux is given by:

$$\phi^{\dagger} = (\phi, \sigma_d), \tag{2.48}$$

according to Eq. (2.26), where $\sigma_d$ is the detector material cross section. Thus, the adjoint flux is proportional to the detector response to a unit source. It is proportional to the "importance" of a particle in contributing to the response of the detector. This physical interpretation is consistent with the boundary conditions: there is zero outgoing adjoint flux at a free surface- any particle leaving the system is not important as it can no longer contribute to the detector response [1].

### *2.2.5 Sensitivity Analysis Using Adjoints*

Our motivation in deriving the adjoint equation for the scalar flux is its utility in efficiently determining the sensitivity of a given quantity of interest ($QOI$) to the parameters that characterize a system. We can do this as follows:
In nuclear systems, we are often interested in quantities of interest of the form

$$\int w(\vec{r})\phi(\vec{r})d\vec{r}, \tag{2.49}$$

where $w(\vec{r})$ is a weighting function. For example, if the $QOI$ is the fission rate the appropriate weighting function would be the fission cross section. From equations (2.37) and (2.47) that define the forward and adjoint equation, and (2.38)-(2.39) which relates the two when the boundary conditions are homogeneous, we have:

$$(\phi^{\dagger}, Q) = (\phi, Q^{\dagger}) \equiv QOI. \tag{2.50}$$

The right-hand side of Eq. (2.50) is the quantity of interest when the adjoint source is defined to be the appropriate weighting function. To see how this can be used to determine the sensitivity of the $QOI$ on a particular parameter, consider a small perturbation to equation (2.23):

$$(L + \delta L)(\phi + \delta\phi) = (Q + \delta Q). \tag{2.51}$$

Expanding Eq. (2.51) and keeping only the terms of first order in $\delta$ gives:

$$L\delta\phi + \delta L\phi = \delta Q, \tag{2.52}$$

where Eq. (2.23) was used to cancel $L\phi$ and $Q$. Using the definition of the adjoint we can write:

$$(L\delta\phi, \phi^\dagger) = (\delta\phi, L^\dagger\phi^\dagger) = (\delta Q, \phi^\dagger) - (\delta\phi, \phi^\dagger). \tag{2.53}$$

The perturbed quantity of interest is

$$QOI + \delta(QOI) = \int (w\phi)d\vec{r} + \int (w\delta\phi)d\vec{r} + \int (\delta w\phi)d\vec{r}. \tag{2.54}$$

Equation (2.49) can be used to cancel the first terms on each side of Eq. (2.54), while Eq. (2.53) lets us rewrite the remaining terms in (2.54) to find the result:

$$\delta(QOI) = (\phi, \delta w) + (\delta Q, \phi^\dagger) - (\delta L\phi, \phi^\dagger). \tag{2.55}$$

The perturbation can be taken to be a small change in a quantity $\theta$, then the response of the $QOI$ can be taken to be a partial derivative with respect to $\theta$:

$$\frac{\partial(QOI)}{\partial\theta} = (\phi, \frac{\partial w}{\partial\theta}) + (\frac{\partial Q}{\partial\theta}, \phi^\dagger) - (\frac{\partial L}{\partial\theta}\phi, \phi^\dagger). \tag{2.56}$$

### *2.2.6 Non-homogeneous Boundary Conditions*

The previously presented sensitivity analysis was dependent on homogeneous boundary conditions (vanishing, vacuum, or reflecting) for the forward and adjoint flux. In the case of non-homogeneous, non-vanishing boundary conditions, the derivation of the sensitivity coefficients does not hold. An additional term, which accounts for the boundary conditions, is required. In general, we have:

$$\left(\phi^\dagger, L\phi\right) - \left(\phi, L^\dagger\phi^\dagger\right) = \oint \left[\phi D\nabla\phi^\dagger - \phi^\dagger D\nabla\phi\right] \cdot d\vec{S} \tag{2.57}$$

The surface integral term must be carried along in the derivation of the sensitivity, $\partial(QOI)/\partial\theta$. Again, consider a small perturbation to equation (2.23):

$$(L + \delta L)(\phi + \delta\phi) = (Q + \delta Q). \tag{2.58}$$

Expanding equation (2.58) and keeping only the terms of first order in delta gives:

$$L\delta\phi + \delta L\phi = \delta Q, \tag{2.59}$$

where Eq. (2.23) was used to cancel L $\phi$ and Q. Using the definition of the adjoint we can write:

$$(\phi^\dagger, L\delta\phi) = (L^\dagger\phi^\dagger, \delta\phi) + \delta \oint \left[\phi D\nabla\phi^\dagger - \phi^\dagger D\nabla\phi\right] \cdot d\vec{S}. \tag{2.60}$$

Take the inner product of $\phi^\dagger$ with equation (2.59) and combine it with the previous equation to give:

$$(L^\dagger\phi^\dagger, \delta\phi) + \delta \oint \left[\phi D\nabla\phi^\dagger - \phi^\dagger D\nabla\phi\right] \cdot d\vec{S} = (\phi^\dagger, \delta Q) - (\phi^\dagger, \delta L\phi). \tag{2.61}$$

From the previous derivation, the perturbed quantity of interest is:

$$\delta(QOI) = (\phi, \delta w) + (\delta Q, \phi^\dagger) - (\delta L\phi, \phi^\dagger). \tag{2.62}$$

The perturbation can be taken to be a small change in a quantity $\theta$, then the response of the $QOI$ can be taken to be a partial derivative with respect to $\theta$. Equation (2.61) can then be used to eliminate the unknown derivatives in the inner products to give

the final result:

$$\frac{\partial(QOI)}{\partial\theta} = (\phi, \frac{\partial w}{\partial\theta}) + (\frac{\partial Q}{\partial\theta}, \phi^\dagger) - (\frac{\partial L}{\partial\theta}\phi, \phi^\dagger) - \frac{\partial}{\partial\theta}\oint \left[\phi D\nabla\phi^\dagger - \phi^\dagger D\nabla\phi\right] \cdot d\vec{S}. \quad (2.63)$$

The key benefit of the adjoint approach is that the unknown derivatives in $\partial(QOI)/\partial\theta$, such as $\partial\phi/\partial\theta$, can be replaced with a known derivative using the adjoint equation. Equation (2.63) does not retain this feature due to the surface integral. In order to solve the sensitivity problem with non-homogeneous boundary conditions, enough information must be provided on the forward boundary so that $\phi$ or $\nabla\phi$ is known, and the adjoint boundary conditions can be chosen such that the term containing unknown information about $\phi$ vanishes. However, the surface integral must be incorporated into the sensitivity calculations, which can be cumbersome. Thus, though it is possible to handle non-homogeneous boundary conditions, it is typically avoided. It should be noted that in transport theory the problem presents itself differently; the forward boundary condition is a specified value of the incoming angular flux. The surface integral above takes the form:

$$\begin{aligned} &\oint \psi\psi^\dagger\, \hat{\Omega}\cdot\hat{n}\, dS\, d\Omega \quad && (\hat{\Omega}\cdot\hat{n} < 0), \\ &\oint \psi\psi^\dagger\, \hat{\Omega}\cdot\hat{n}\, dS\, d\Omega \quad && (\hat{\Omega}\cdot\hat{n} > 0). \end{aligned} \quad (2.64)$$

The outgoing adjoint flux is taken to be zero since any particle leaving the system cannot contribute to the quantity of interest; thus the second integral vanishes. Applying this boundary condition is sufficient to solve for the adjoint flux, which can then be used in the first integral, along with the specified incoming forward flux, to compute the surface integral contribution to the sensitivities. However, taking the derivative of the surface integral is non-trivial; it will likely need to be evaluated

using numerical perturbations, thus limiting the advantages of the adjoint approach.

### *2.2.7 Data Storage Challenges*

The main disadvantage of the adjoint approach is that it requires having access to the complete forward solution and other time dependent parameters, in order to solve the adjoint equation running backwards in time. Furthermore, the forward and adjoint solutions along with parameter values must be accessible in order to perform the sensitivity calculations. Most problems of interest are 2- or 3-dimensional systems with time- and spatial- dependent parameters. As you improve your spatial and temporal resolution the memory required to store the information grows rapidly, and it is easy to exceed the memory available on even an appreciably sized computer. Thus, it is necessary to write the information to files and retrieve them as needed. This quickly increases the computational time required, as reading and writing to files is far more time-consuming than the simple floating point operations required to solve the systems of equations. One of the primary goals of this work is to determine if alternative methods of computing the sensitivity integrals can be devised such that it is not necessary to store large amounts of data or read and write to files. In the examples presented, a method which requires minimal data storage and computational time will be tested. This modified method will assume that the adjoint flux evolves much slower than the forward flux. Over a time period of interest, the adjoint flux will then be approximately constant, and the steady state adjoint equation can be solved in tandem with the forward equation. The forward equation for flux limited diffusion is given by Eq.(2.65):

$$\frac{1}{v}\frac{\partial\phi(\vec{r},t)}{\partial t} - \nabla\cdot D(\vec{r},t)\nabla\phi(\vec{r},t) + \sigma_a(\vec{r},t)\phi(\vec{r},t) = Q(\vec{r},t), \tag{2.65}$$

and the steady state adjoint equation is given by Eq. (2.66):

$$-\nabla \cdot D(\vec{r},t)\nabla\phi^{\dagger}(\vec{r},t) + \sigma_a(\vec{r},t)\phi^{\dagger}(\vec{r},t) = Q^{\dagger}(\vec{r},t). \tag{2.66}$$

The forward equation is solved for one time step; this provides a value for the source and the diffusion coefficient, which depend on the forward flux. This value of $Q$ and $D$ are passed to the adjoint equation, which is solved assuming it satisfies the steady state equation. This process is repeated for as many time steps as desired. Typically, the forward equation would be solved until the last time step, and the values for emph(Q) and $D$ would be called running backwards in time to solve the adjoint system. The assumption that time dependent parameters can be used in the adjoint equation as if they are evolving forward time can introduce significant errors in highly time dependent problems. This modified method will be used to compute sensitivities and the results will be compared to the correct answers to determine if this data reduction method is viable.

### *2.2.8 Sensitivities for the Included Examples*

The expression for the sensitivity of a quantity of interest with respect to a parameter $\theta$ using the adjoint approach is given by Eq. (2.67) :

$$\frac{\partial(QOI)}{\partial\theta} = \left(\phi, \frac{\partial w}{\partial\theta}\right) + \left(\frac{\partial Q}{\partial\theta}, \phi^{\dagger}\right) - \left(\frac{\partial L}{\partial\theta}\phi, \phi^{\dagger}\right). \tag{2.67}$$

In this study the primary quantity of interest is the total absorption, *Abs.*:

$$Abs. = \int \sigma_a \phi \; d^3r \, dt,$$

thus the appropriate adjoint source is the absorption cross section. As as example, consider the sensitivity of the absorption rate with respect to changes in the absorption cross section. Eq. (2.67) becomes:

$$\frac{\partial(Abs.)}{\partial\sigma_a} = \left(\phi, \frac{\partial\sigma_a}{\partial\sigma_a}\right) + \left(\frac{\partial Q}{\partial\sigma_a}, \phi^\dagger\right) - \left(\frac{\partial L}{\partial\sigma_a}\phi, \phi^\dagger\right). \tag{2.68}$$

The first term on the right hand side is just the integral of the flux over the spatial and temporal domain, the second term vanishes, but the third term is not as trivial to compute. Recall that the flux-limited diffusion coefficient depends nonlinearly on the absorption cross section and the scalar flux. The derivative that must be evaluated is:

$$\frac{\partial}{\partial\sigma_a}\left(-\frac{\partial}{\partial x}\left(\left\{(3\sigma_a)^n + \left(\frac{1}{\phi}\left|\frac{\partial\phi}{\partial x}\right|\right)^n\right\}^{-1/n}\frac{\partial\phi}{\partial x}\right) + \sigma_a\phi\right). \tag{2.69}$$

The flux-limited form of the diffusion coefficient severely complicates the spatial derivative. To avoid performing this derivative analytically, a second-order centered finite difference approximation is employed. The proposed derivative expression was compared to a finite difference sensitivity estimation to ensure the error introduced in the approximation was negligible. For the finite difference sensitivity, the forward problem is solved for two slightly different values of $\sigma_a$ and the sensitivity is computed by taking the ratio of the change in the absorption rate to the change in the cross section. The expression for the numerical derivative that gave a sensitivity that agreed well with the finite difference method is given by:

$$\frac{\partial}{\partial\sigma_a}\left(\frac{\partial}{\partial x}D\frac{\partial\phi}{\partial x}\right)_i \approx \frac{1}{\Delta x}\left(\left(\frac{\partial D}{\partial\sigma_a}\frac{\partial\phi}{\partial x}\right)_{i+1/2} - \left(\frac{\partial D}{\partial\sigma_a}\frac{\partial\phi}{\partial x}\right)_{i-1/2}\right), \tag{2.70}$$

where $\Delta x$ is the discretization step size and $i \pm 1/2$ subscripts denote where on the discretized domain the functions should be evaluated. The derivatives of the diffusion coefficient with respect to the absorption cross section are calculated analytically.

It is also interesting to examine the sensitivity of the absorption rate to the model parameter, $n$. Unlike the absorption cross section, the parameter $n$ is non-physical; it is chosen arbitrarily such that the diffusion solution agrees with transport theory. Typically, a value of $n = 2$ is chosen. However, for some systems, fractional values of $n$ yield behavior that closely agrees with transport simulations. The sensitivity of the absorption rate with respect to small changes in $n$ can be determined using the analytical expression:

$$\frac{\partial(Abs.)}{\partial n} \approx \frac{1}{\Delta x}\left(\left(\frac{\partial D}{\partial n}\frac{\partial \phi}{\partial x}\right)_{i+1/2} - \left(\frac{\partial D}{\partial n}\frac{\partial \phi}{\partial x}\right)_{i-1/2}\right), \tag{2.71}$$

where $\partial D/\partial n$ is expressed analytically. It should be noted that typical choices of $n$ are integer values; small perturbations to $n$ are not considered in practice. However, the sensitivities will still provide insight into how big of an effect changing $n$ might have on the resulting quantities of interest.

# 3. RESULTS

Sensitivity analyses are performed for multiple systems described by flux-limited diffusion. In the following sections, the particular forms of the forward and adjoint diffusion equations are presented and the expressions for the sensitivity coefficients are derived. To evaluate the potential for reducing the amount of data that must be stored to perform the sensitivity analysis, the results from a modified approach are compared to the true sensitivity coefficients. In the modified method, which the adjoint system is taken to be "quasi-steady state" and is solved in tandem with the forward equation. The method eliminates the need to store time-dependent parameters that would traditionally be used backward in time to solve the adjoint equation. Additionally, contributions to the integrals used to compute sensitivity coefficients can be computed at the end of each time step, allowing the forward and adjoint solutions to be discarded after each time step.

## 3.1 1-D Flux-Limited Diffusion

A sensitivity analysis was performed for a system in which the flux-limited diffusion coefficient plays a crucial role. It has been shown that the choice of a fractional value of the exponent, $n$, provided a diffusion solution for a radiative shock profile through a cooling layer that agreed with transport theory [5]. In this study, an analogous problem for neutron transport is studied using the typical choice of $n=2$ and the value $n=1/3$ that was shown to yield a more accurate solution for this problem. The source for the forward diffusion equation is as follows:

$$Q(\tau) = \begin{cases} 0.85 & \tau < 2 \\ 1 & \tau \in [2, 2.5] \\ 0.78 & \tau > 2.5 \end{cases},$$

.

The spatial variable is expressed in terms of mean free paths: $\tau{=}\sigma_a x$, and the flux goes to zero at the boundaries. The absorption cross section is unity throughout the domain of the system. The quantity of interest is the absorption reaction rate, thus the adjoint source is the absorption cross section. All parameters are constant in time; the initial condition for the forward flux is set to zero, and the final condition in the adjoint problem is taken to be zero, indicating that the final time step is the point at which the source is turned off and the absorption rate goes to zero. Figure 3.1 illustrates the forward and adjoint flux solutions for both values of $n$ taken at $t = 2.5s$. The distinctive peak in the forward flux for $n = 1/3$ in the middle region is what is expected from transport theory, that the diffusion coefficient with $n = 2$ does not accurately depict. In the adjoint solution, the effect of the flux limiter is to increase the gradient of the adjoint flux at the domain boundaries.

The sensitivity of the time-integrated absorption reaction rate with respect to small changes in the absorption cross section, source, and choice of $n$ is computed using the adjoint and finite difference methods. Figures 3.2 and 3.3 illustrates the convergence of the sensitivities as the discretization size $dx$ is decreased, with the ratio $dx/dt$ held constant for each choice of $n$.

The Wynn-epsilon acceleration method is used to compute the values to which the sensitivities are converging in the limit that the step size is taken to zero. For $n = 1/3$, the sensitivity of the absorption rate with respect to changes in the source is 20.7,

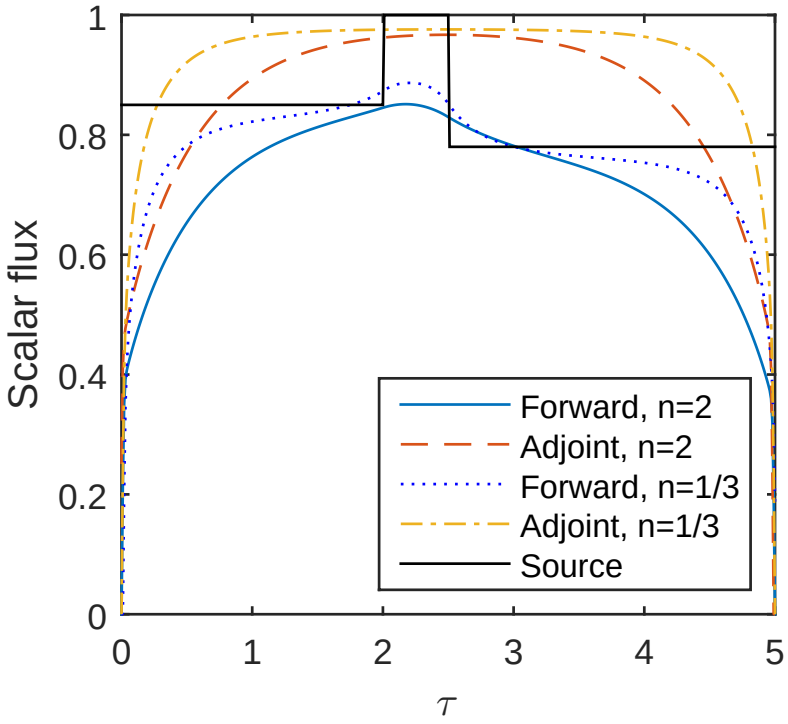


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Figure 3.1: Forward and adjoint flux solutions for n=2, n=1/3.

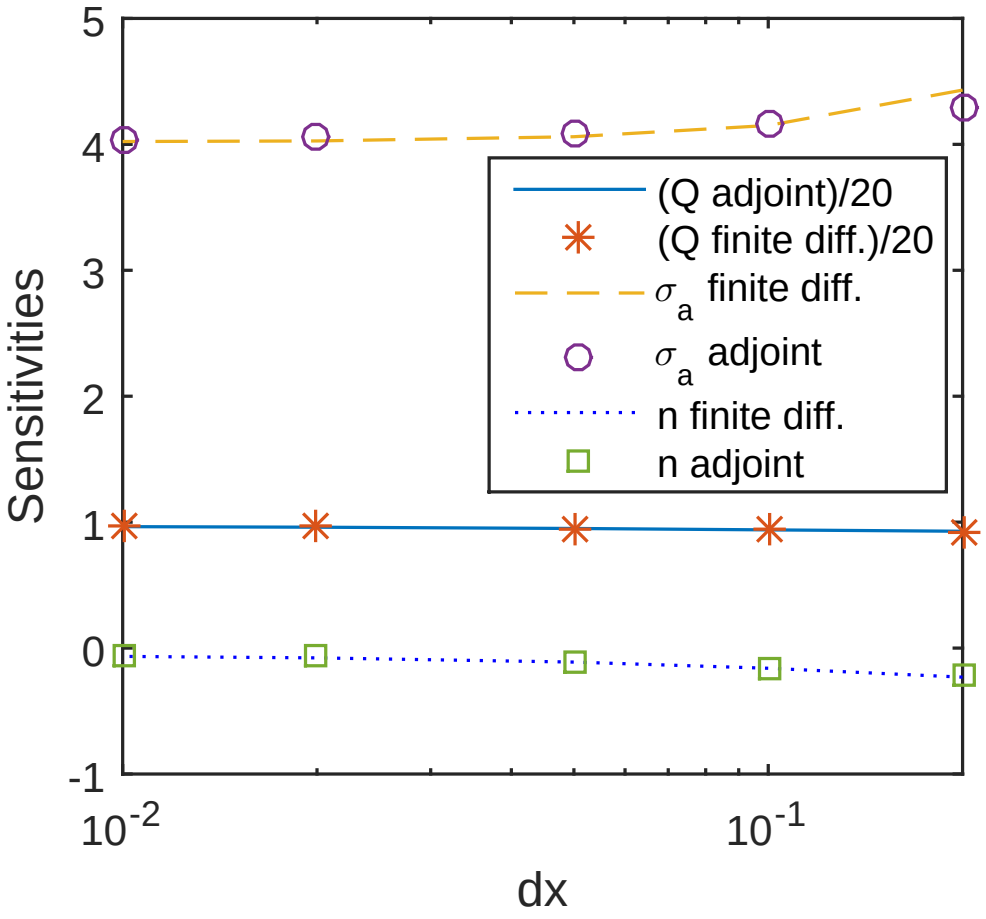


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Figure 3.2: Sensitivity convergence for n=2.

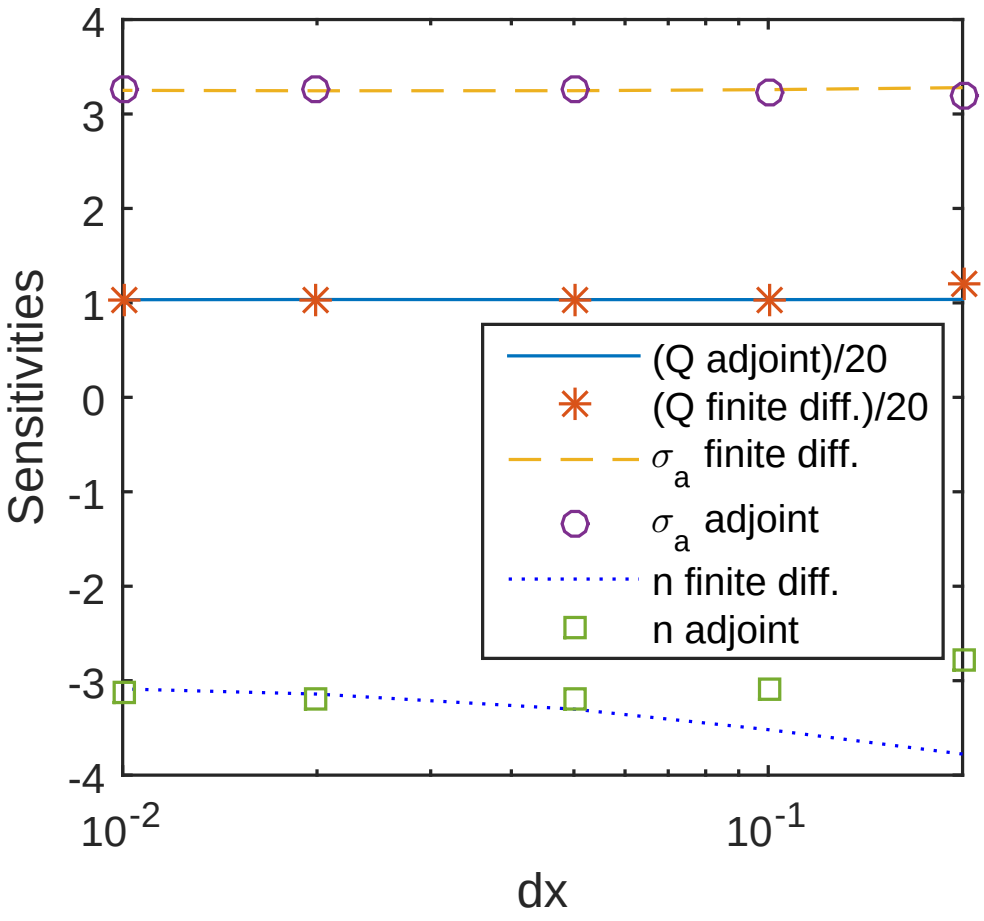


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Figure 3.3: Sensitivity convergence for n=1/3.

with respect to changes in the absorption cross section is 3.3, and with respect to changes in $n$ is -2.9. For $n = 2$, the sensitivity of the absorption rate with respect to changes in the source is 20.7, with respect to changes in the absorption cross section is 4.1, and with respect to changes in $n$ is -0.05. The sensitivity of the absorption rate with respect to changes in the source is independent of $n$ as expected. The sensitivity to changes in the cross section are comparable for the two values of $n$, but changes in $n$ have a substantially greater influence for fractional values of $n$ than for the commonly chosen value of $n = 2$. The Wynn-epsilon acceleration method predicts that the finite difference and adjoint sensitivities converge to the same value with less than 6% difference, demonstrating the accuracy of the adjoint method even when numerical differentiation schemes were employed to reduce complexity in expressions, such as in Eq. (2.71).

## 3.2 2-D Cylindrical "Crooked Pipe"

The "crooked pipe" or "top hat" problem introduced by Lawerence Livermore National Laboratory is a popular test for radiation transport and diffusion codes [4]. The system is a cylindrical duct composed of optically thin and thick materials. In the traditional problem, a high temperature source is located at the left inlet, producing incoming flux on the boundary. The geometry is illustrated in Figure 3.4. In order to avoid the complications discussed for nonhomogeneous boundaries, a modified problem is considered here. In lieu of an incoming flux, the boundaries are left open and a source of fixed temperature is placed at the left inlet. As radiation diffuses through the medium, the material heats up and radiates itself, producing a source related to the material temperature. This system is described by a set of coupled differential equations:

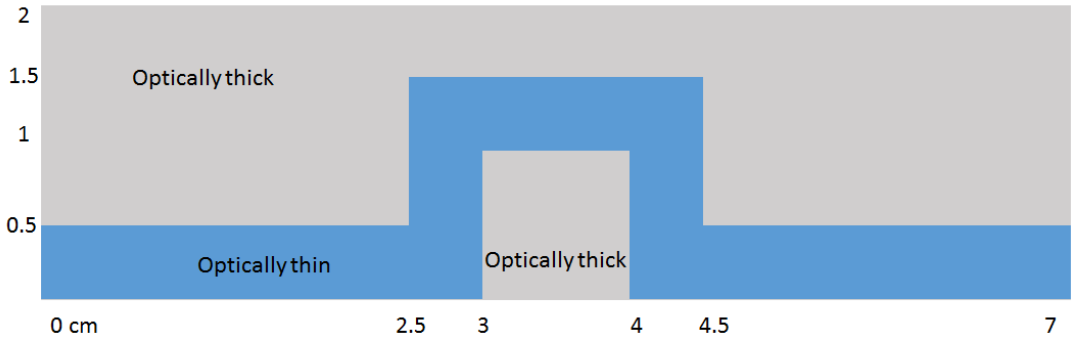


Figure 3.4: Geometry for crooked pipe radiative diffusion example.

$$\begin{aligned} \frac{1}{v}\frac{\partial \phi}{\partial t} - \nabla \cdot D\nabla\phi + \sigma_a \phi &= Q, \\ \rho C_v \frac{\partial T}{\partial t} &= \sigma_a \left(\phi - acT^4\right). \end{aligned} \tag{3.1}$$

To derive the adjoint equations for the coupled system, we use the Lagrangian approach to forming the sensitivity expression. The differential equations will be combined to form the operator F:

$$F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} = \begin{pmatrix} \dot{\phi}/v - f(\phi) \\ \dot{T} - g(T) \end{pmatrix} = 0, \tag{3.2}$$

with

$$\begin{aligned} f(\phi) &= \nabla \cdot D\nabla\phi - \sigma_a\phi + Q, \\ g(T) &= \frac{\sigma_a}{\rho C_v}(\phi - acT^4). \end{aligned} \tag{3.3}$$

To find the adjoint system for the coupled set of equations, the work of Stripling [8]

is followed. The derivation begins by forming a Lagrangian:

$$\mathcal{L} = \int \left[ QOI - \langle \lambda, F \rangle \right] dt, \tag{3.4}$$

where the angular brackets denote integrals over all space. Take the derivative of $\mathcal{L}$ with respect to an arbitrary parameter, $\theta$:

$$\frac{\partial \mathcal{L}}{\partial \theta} = \int \left[ QOI_\theta + QOI_x x_\theta - \frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle \dot{x}_\theta - \frac{\partial}{\partial x} \langle \lambda, F \rangle x_\theta - \frac{\partial}{\partial \theta} \langle \lambda, F \rangle \right] dt. \tag{3.5}$$

Using integration by parts, the integral can be rewritten as:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \theta} = & \left[ -\frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle x_p \right]_{t_0}^{t_f} + \int \left[ \langle QOI_\theta \rangle - \frac{\partial}{\partial \theta} \langle \lambda, F \rangle \right] dt, \\ & + \int \left[ \langle QOI_x \rangle + \frac{d}{dt} \left( \frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle \right) - \frac{\partial}{\partial x} \langle \lambda, F \rangle \right] x_\theta dt, \end{aligned} \tag{3.6}$$

where x=$(\phi \ \mathrm{T})^T$ and subscripts denote partial derivatives. The only term that cannot be computed directly is $x_p$. The adjoint equations are the conditions that are imposed on $\lambda$=$(\phi^\dagger \ \mathrm{T}^\dagger \ )^T$ such that the integrand of the final term is eliminated. The initial and final conditions can be used to eliminate the first term.

The adjoint equations are:

$$\langle QOI_x \rangle + \frac{d}{dt} \left( \frac{\partial}{\partial \dot{x}} \langle \lambda, F \rangle \right) - \frac{\partial}{\partial x} \langle \lambda, F \rangle = 0. \tag{3.7}$$

This is split into the components for $\phi$ and T, and the expressions for F and the QOI

(absorption) are plugged in, resulting in the following coupled adjoint equations:

$$\begin{aligned} -\frac{1}{v}\frac{\partial \phi^\dagger}{\partial t} - \nabla\cdot(D\nabla\phi^\dagger) + \sigma_a\phi^\dagger &= \sigma_a + \frac{\sigma_a}{\rho C_v}T^\dagger, \\ -\frac{\partial T^\dagger}{\partial t} &= -\frac{4\sigma_a T^3}{\rho C_v}T^\dagger + \frac{\partial}{\partial T}\left(\sigma_a\phi\right) - \frac{\partial}{\partial T}\left(\sigma_a\phi\phi^\dagger\right). \end{aligned} \tag{3.8}$$

The coupled forward and adjoint equations are solved for the cylindrical crooked pipe problem and multiple quantities of interest are examined. The parameters for this problem are summarized in Table 3.1. Figures 3.5 and 3.6 illustrate the forward and adjoint flux at a particular time step.

Sensitivities are computed for various quantities of interest related to absorption in the system. The QOIs are the energy absorption over different time periods, and within various volumes. The correct adjoint approach, in which the forward problem is solved, the data is stored, and the adjoint problem is solved backward, is compared to the traditional perturbation theory result; the method in which the problem is solved twice, with two slightly different values of the parameter under scrutiny. The results for each are given in Tables 3.2-3.7. In the table, the "forward" method refers to the direct method in which the code is ran twice per parameter; the "adjoint"

Table 3.1: Parameter values for cylindrical crooked pipe example.

| | |
|---|---|
| dr=dz | 0.05 (cm) |
| dt | 0.01 (ns) |
| $\rho$ (thin) | 0.01 (g/cc) |
| $\rho$ (thick) | 10 (g/cc) |
| $C_v$ (thin) | 0.05 (E16 erg/g/keV) |
| $C_v$ (thick) | 0.05 (E16 erg/g/keV) |
| $\sigma_a$ | 20 ($cm^{-1}$) |
| $T_{initial}$ | 0.005 (keV) |
| Q | 0.1 ($GJ/cm^3/s$) |

method refers to the adjoint sensitivity calculations. The "forward absorption" is computed by integrating $(\phi, \sigma_a)$ over the region and time period of interest, while the "adjoint absorption" is computed by integrating $(\phi^\dagger, Q)$ over the region and time period of interest. Regions 1 and 2 are indicated in Figures 3.7 and 3.8.

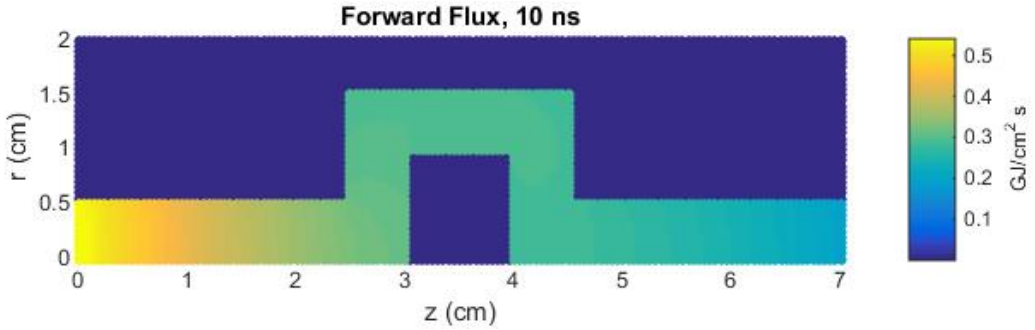


Figure 3.5: Forward flux.

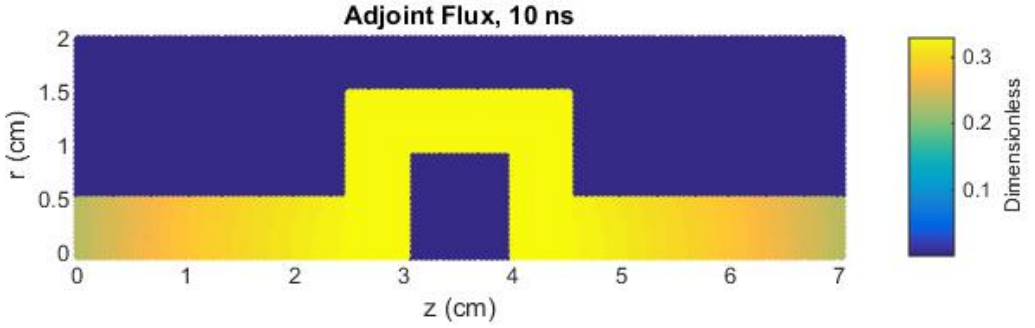


Figure 3.6: Adjoint flux.

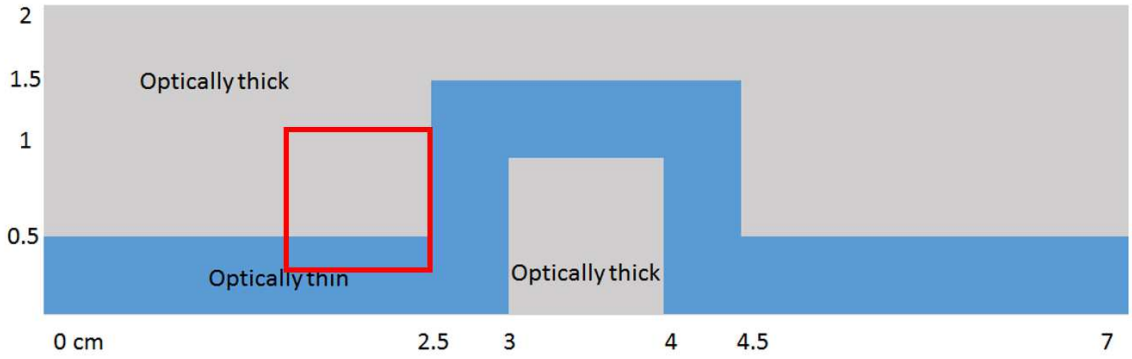


Figure 3.7: Region 1.

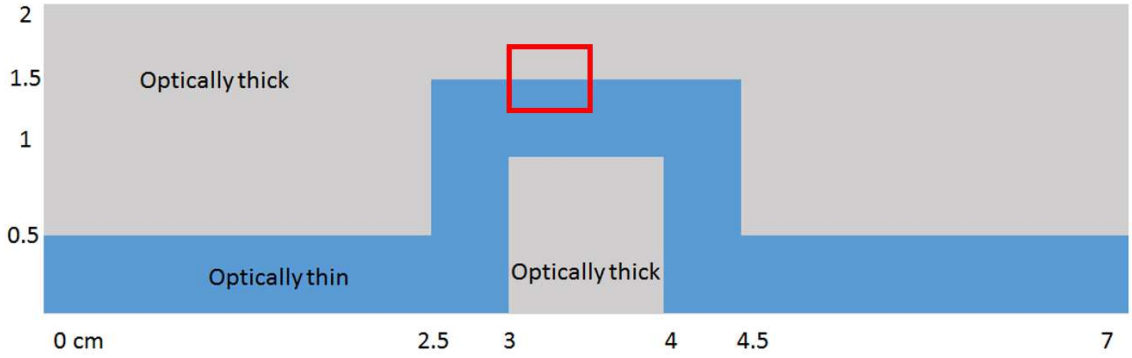


Figure 3.8: Region 2.

Table 3.2: Forward and adjoint sensitivities of total energy absorption in the system, integrated over the first 10 ns.

| | | Percent Difference |
|---|---|---|
| Forward Absorption | 0.59596 | |
| Adjoint Absorption | 0.59985 | 0.653 |
| Forward dQOI/d$\sigma_a$ | 0.232 | |
| Adjoint dQOI/d$\sigma_a$ | 0.242 | 4.525 |
| Forward dQOI/dQ | 0.5944 | |
| Adjoint dQOI/dQ | 0.5998 | 0.917 |

Table 3.3: Forward and adjoint sensitivities of total energy absorption in the system, integrated over the first 100 ns.

| | | Percent Difference |
|---|---|---|
| Forward Absorption | 6.0214 | |
| Adjoint Absorption | 6.0426 | 0.352 |
| Forward dQOI/d$\sigma_a$ | 2.2202 | |
| Adjoint dQOI/d$\sigma_a$ | 2.2983 | 3.518 |
| Forward dQOI/dQ | 6.0161 | |
| Adjoint dQOI/dQ | 6.0425 | 0.439 |

Table 3.4: Forward and adjoint sensitivities of total energy absorption in region 1, integrated over the first 10 ns.

| | | Percent Difference |
|---|---|---|
| Forward Absorption | 0.00487 | |
| Adjoint Absorption | 0.00490 | 0.768 |
| Forward dQOI/d$\sigma_a$ | -0.0106 | |
| Adjoint dQOI/d$\sigma_a$ | -0.0101 | 5.085 |
| Forward dQOI/dQ | 0.00501 | |
| Adjoint dQOI/dQ | 0.004934 | 1.517 |

Table 3.5: Forward and adjoint sensitivities of total energy absorption in region 1, integrated over the first 100 ns.

| | | Percent Difference |
|---|---|---|
| Forward Absorption | 0.0493 | |
| Adjoint Absorption | 0.0497 | 0.876 |
| Forward dQOI/d$\sigma_a$ | -0.107 | |
| Adjoint dQOI/d$\sigma_a$ | -0.102 | 4.533 |
| Forward dQOI/dQ | 0.04835 | |
| Adjoint dQOI/dQ | 0.0497 | 2.796 |

The direct and adjoint methods agree to around 5% or less for the sensitivities computed for this example. The approximation to the derivative of the QOI with respect to the cross section discussed previously did not introduce appreciable error. The same problem is solved using the data storage reduction method. The adjoint equation is solved in tandem with the forward equation. The results are summarized in Tables 3.8-3.9.

Table 3.6: Forward and adjoint sensitivities of total energy absorption in region 2, integrated over the first 10 ns.

| | | Percent Difference |
|---|---|---|
| Forward Absorption | 0.00172 | |
| Adjoint Absorption | 0.00173 | 0.581 |
| Forward dQOI/d$\sigma_a$ | -0.00235 | |
| Adjoint dQOI/d$\sigma_a$ | -0.00240 | 2.128 |
| Forward dQOI/dQ | 0.0156 | |
| Adjoint dQOI/dQ | 0.0153 | 1.929 |

Table 3.7: Forward and adjoint sensitivities of total energy absorption in region 2, integrated over the first 100 ns.

| | | Percent Difference |
|---|---|---|
| Forward Absorption | 0.0176 | |
| Adjoint Absorption | 0.0177 | 0.568 |
| Forward dQOI/d$\sigma_a$ | -0.0237 | |
| Adjoint dQOI/d$\sigma_a$ | -0.0224 | 5.405 |
| Forward dQOI/dQ | 0.01799 | |
| Adjoint dQOI/dQ | 0.01775 | 1.3175 |

Table 3.8: Comparison of sensitivities computed using the modified data storage reduction method (Mod.) to the forward sensitivities. Integration time is 10 ns.

| Region | dQOI/d$\sigma_a$ | Mod. dQOI/d$\sigma_a$ | % Error |
|---|---|---|---|
| All space | 0.2424 | 0.8558 | 43.98 |
| Region 1 | -0.01006 | 0.22 | 2289 |
| Region 2 | -0.0024 | -0.00237 | 1.292 |
| Region | dQOI/dQ | Mod. dQOI/dQ | % Error |
| All space | 0.5944 | 0.6001 | 0.959 |
| Region 1 | 0.00501 | 0.6001 | 11878 |
| Region 2 | 0.0153 | 0.00176 | 88.51 |

Table 3.9: Comparison of sensitivities computed using the modified data storage reduction method (Mod.) to the forward sensitivities. Integration time is 100 ns.

| Region | dQOI/d$\sigma_a$ | Mod. dQOI/d$\sigma_a$ | % Error |
|---|---|---|---|
| All space | 2.2981 | 2.217 | 3.529 |
| Region 1 | -0.1022 | 2.217 | 2270 |
| Region 2 | -0.0219 | -0.0236 | 7.429 |
| Region | dQOI/dQ | Mod. dQOI/dQ | % Error |
| All space | 6.016 | 6.043 | 0.444 |
| Region 1 | 0.0483 | 6.0428 | 12399 |
| Region 2 | 0.01798 | 0.01776 | 1.2563 |

When integrating over the entire volume, the data storage reduction method yields sensitivities that are of the correct order of magnitude. This is also true for region 2, which is far from the source. At this location, it is reasonable to expect that the forward and adjoint flux are not changing rapidly over the time period of integration, therefore the "quasi-steady state" approximation is reasonable. However, for region 1 near the source, the system is changing notably at early times and the adjoint flux cannot be assumed to be in a steady state, thus the high error for the sensitivities in this region. The data storage reduction method is a promising technique for systems in which the steady state criteria for the adjoint flux are met. For highly transient problems or quantities of interest that are sensitive to time, the method does not estimate sensitivities to an acceptable level of error.

# 4. CONCLUSIONS

Sensitivity analyses were performed for physical systems described by flux-limited diffusion. The adjoint-based sensitivity analysis is preferred for these systems as it the method is computationally efficient when many parameters are to be varied. However, the nonlinearity of the flux-limited diffusion equation results in complicated expressions for the sensitivity integrals. The cumbersome analytical expressions are estimated using simple numerical approximations; the sensitivities calculated with the proposed approximations agree well with the true values. The adjoint method is a simple and efficient way to compute sensitivities, but becomes computationally expensive for high-dimensional and high fidelity models. To evaluate the sensitivity integrals, it is necessary to have access to the full forward and adjoint solutions, as well as any time- and spatially-dependent variables. For transient problems, the memory demand required to store such information is too large for most computers. Furthermore, writing the information to files and reading it as needed to compute the sensitivities becomes unreasonably time consuming. A method by which the amount of data that needs to be stored in order to compute sensitivities with high accuracy is desired. In this work, such a method was explored for transient radiative diffusion problems. The adjoint equation was treated as being in a "quasi-steady state"; it was assumed that the adjoint solution changed slowly with respect to time relative to the forward solution. In this approximation, the adjoint solution could be computed in tandem with the forward solution; this is compared to the correct way in which the adjoint solution is solved backwards in time using the full forward solution. For problems that exhibited strong time dependence, such as the "crooked pipe" problem, this approximation did not produce sensitivities with acceptable accuracy. However

the method does hold promise for systems in which the slow time evolution of the adjoint solution holds.

## 4.1 Future Work

Alternative data storage reduction techniques should be explored in the future. Possibilities include selective saving of the forward and adjoint solutions, where solutions from a reduced number of time steps are stored and interpolation is used to reconstruct the missing data. This method would be particularly well suited for problems with slow or monotonic changes where interpolation techniques can accurately estimate the solution at the missing time steps.

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