Title: **A New Mathematical Adjoint for the Modified SAAF- S_N Equations**

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A New Mathematical Adjoint for the Modified SAAF- S_N Equations

Sebastian Schunert, Yaqi Wang, Richard Martineau

Abstract

We present a new adjoint FEM weak form, which can be directly used for evaluating the mathematical adjoint, suitable for perturbation calculations, of the self-adjoint angular flux S_N equations (SAAF- S_N) without construction and transposition of the underlying coefficient matrix. Stabilization schemes incorporated in the described SAAF- S_N method make the mathematical adjoint distinct from the physical adjoint, i.e. the solution of the continuous adjoint equation with SAAF- S_N .

This weak form is implemented into RattleSnake, the MOOSE (Multiphysics Object-Oriented Simulation Environment) based transport solver.

Numerical results verify the correctness of the implementation and show its utility both for fixed source and eigenvalue problems.

Keywords: Linear Transport Equation, Adjoint, SAAF- S_N equations

1 Introduction

We present a new approach to directly derive the mathematical adjoint of the self-adjoint angular flux S_N equations (SAAF- S_N) without construction and transposition of the underlying coefficient matrix associated with the SAAF- S_N equations. The new approach is directly embedded into the finite-element framework that finds its expression in the weak form of the SAAF- S_N equations. This makes it convenient for implementation into the multiphysics code framework Moose [1], in particular into the designated radiation transport solver Rattle S_N ake.

The solution of the adjoint transport equations is of great interest in the nuclear engineering community for a variety of applications. In the early days of nuclear computational science two applications stood out which are both outlined in [2]: first, the change of the multiplication factor due to a change in the cross sections data, and second the repeated computation of a detector response in case of a changing distributed source or boundary conditions. In both cases, using the adjoint solution avoids repeated solution of the forward problem saving valuable execution time. More recently, the push towards augmenting nuclear engineering calculations with a comprehensive sensitivity and uncertainty analysis on a regular basis has led to increased interest in the solution of the adjoint equation because it is the basis of the efficient Adjoint Sensitivity Analysis Procedure, [3]. For the named reasons, solution of the adjoint linear transport equation is an active field of research and is a mode available in most production level codes, for example TORT [4] and DENOVO [5].

The solution of the transport equation on a digital computer, adjoint or forward, requires the discretization of the applicable form of the transport equation. For the adjoint transport equation, the order in which to apply the discretization and adjoint can be switched:

- Physical adjoint: Obtain the continuous adjoint equations from the continuous

forward equations and then discretize the continuous adjoint equations.

- Mathematical adjoint: Discretize the forward equations and then obtain the adjoint equations by transposing the coefficient matrix of the fully discretized forward equation.

In general, the discretization and adjoint operations do not commute and thus physical and mathematical adjoint fluxes are different. The mathematical adjoint has the advantage over the physical adjoint that identities involving forward and adjoint solutions derived for the continuum equations still hold exactly even in the presence of discretization errors. The same is not true for the physical adjoint flux.

The SAAF equation considered in this work belongs to the group of second order linear transport equations which also comprises the even and odd-parity forms of the transport equations [6]. It is derived by formally solving the first order transport equation for the angular flux and substitution of the resulting expression into the streaming term of the original equation. As is also the case for the even/odd-parity transport equations, division by the total interaction cross section creates a singularity in void regions. The particular method used within this work modifies the SAAF- S_N equations to account for void regions[7] and will therefore be referred to as modified SAAF- S_N equations. Discretization of energy and angle for these equations will be performed using the multigroup formalism and the S_N method leading to the multigroup SAAF- S_N equations.

Although the SAAF- S_N within-group equations without scattering are self-adjoint, various reasons make the equations asymmetric, such as weakly imposed reflective boundary conditions, source-iteration-consistent scattering treatment, modifications for void regions and scattering and fission terms.

This paper presents a new approach to derive the mathematical adjoint equations of the stabilized, multigroup SAAF- S_N forward equations that is based on direct manipulation of their transport weak form. The implemented mathematical adjoint

will be instrumental for incorporating sensitivity and uncertainty analysis tools into the MOOSE/RattleSnake framework.

The work is organized as follows: in Sec. 2 the multigroup forward and adjoint transport equations are introduced. In Sec 3, the SAAF- S_N equations and their weak form are introduced followed by the main development of the new methodology. In Sec. 4, the consistency of the mathematical and physical eigenvalue and eigenfunctions are examined. Numerical results demonstrating correctness and utility of the new mathematical adjoint of the SAAF- S_N equations are presented in Sec. 5. Finally, conclusions are drawn in Sec. 6.

2 Steady State Multigroup Transport Equation - Forward and Adjoint

Within this work, the discussion shall be confined to the steady-state linear transport equation (LTE) because the presented framework for the derivation of a mathematical adjoint has not been extended to transient problems, yet. This is not a fundamental limitation of the presented approach and extension to transient problems may very likely constitute future work. The vast majority of particle transport problems is solved in steady-state because of the large demand of computational resources required for transient calculations. In addition, the steady-state adjoint can be used to generate consistent point-kinetics parameters for solving transient forward problems within the point-kinetic approximation.

First, in subsection 2.1, the first-order forward, multigroup LTE is introduced and common discretization methods are discussed and then, in subsection 2.4, multiple forms of the first-order adjoint LTE are derived from the forward LTE varying the order of discretization and adjoint operations.

2.1 The Forward Transport Equation

The inhomogeneous, steady-state, first-order, multigroup neutron transport equation with externally imposed body source is given by[6]:

$$\begin{aligned} \hat{\Omega} \cdot \nabla \psi_g + \sigma_{t,g} \psi_g(\vec{r}, \hat{\Omega}) &= \sum_{g'=1}^G \sum_{l=0}^L \frac{2l+1}{4\pi} \sum_{m=-l}^l \sigma_{s,l}^{g' \rightarrow g}(\vec{r}) \phi_{g',l,m}(\vec{r}) Y_{l,m}(\hat{\Omega}) \\ &+ \frac{\chi_g(\vec{r})}{4\pi} \sum_{g'=1}^G \nu \sigma_{f,g'} \phi_{g'}(\vec{r}) + \frac{Q_g(\vec{r}, \hat{\Omega})}{4\pi}, \end{aligned} \quad (1)$$

where:

- g : group index.
- $\psi_g(\vec{r}, \hat{\Omega})$: the multigroup angular flux.
- $\phi_{g,l,m}(\vec{r},) = \int_{4\pi} d\hat{\Omega} Y_{l,m}(\hat{\Omega}) \psi_g(\vec{r}, \hat{\Omega})$: the angular flux moment of order l, m .
- $Y_{l,m}(\hat{\Omega})$: spherical harmonics function of order l, m .
- $\vec{r}$: spatial coordinate.
- $\hat{\Omega}$: particle's direction of motion.
- $\sigma_{t,g}(\vec{r})$: total cross section in group g .
- $\sigma_{s,l}^{g' \rightarrow g}(\vec{r},)$: l -th Legendre moment of the scattering cross section from group g' to group g .
- χ_g : fission spectrum in group g .
- $\nu \sigma_{f,g}(\vec{r})$: fission production cross section in group g .
- $Q_g(\vec{r}, \hat{\Omega})$: external distributed source in group g .

Note, Eq. (1) only supports a solution if the configuration is subcritical because supercritical configurations featuring an external source cannot be in steady state. Frequently, the reactor physics community is interested in the solution of the k-eigenvalue problem emulating the question of how to scale the fission source with the eigenvalue k_{eff} in order to render a steady solution[6]:

$$\begin{aligned} \hat{\Omega} \cdot \nabla \psi_g + \sigma_{t,g} \psi_g(\vec{r}, \hat{\Omega}) &= \sum_{g'=1}^G \sum_{l=0}^L \frac{2l+1}{4\pi} \sum_{m=-l}^l \sigma_{s,l}^{g' \rightarrow g}(\vec{r}) \phi_{g',l,m}(\vec{r}) Y_{l,m}(\hat{\Omega}) \\ &+ \frac{\chi_g(\vec{r})}{4\pi k_{\text{eff}}} \sum_{g'=1}^G \nu \sigma_{f,g'} \phi_{g'}(\vec{r}). \end{aligned} \quad (2)$$

The formalism for the derivation of the mathematical adjoint works in conjunction with both types of LTE, Eq. (1) and (2). For a solution of the LTE boundary conditions must be given on the inflow boundaries:

$$\psi_g(\vec{r}, \hat{\Omega}) = \psi_{\text{BC},g}(\vec{r}, \hat{\Omega}) \text{ for } \vec{r} \in \partial\mathcal{D}^-. \quad (3)$$

Discretization of the forward equations typically proceeds by the discretization of $\hat{\Omega}$. Within this work, only the S_N method described e.g. in [6] shall be considered to this end. The S_N method solves the multigroup equations only along discrete directions $\hat{\Omega}_n$ for $n = 1, \dots, N$ and approximates integrals over the angular direction by a quadrature rule:

$$\int_{4\pi} d\hat{\Omega} \cdot \rightarrow \sum_{n=1}^N w_n \cdot. \quad (4)$$

Applying the S_N discretization to the multigroup equations Eq. (1) gives:

$$\begin{aligned}
\hat{\Omega}_n \cdot \nabla \psi_{g,n} + \sigma_{t,g} \psi_{g,n}(\vec{r}) &= \sum_{g'=1}^G \sum_{l=0}^L \frac{2l+1}{4\pi} \sum_{m=-l}^l \sigma_{s,l}^{g' \rightarrow g}(\vec{r}) \phi_{g',l,m}(\vec{r}) Y_{l,m}(\hat{\Omega}_n) \\
&+ \frac{\chi_g(\vec{r})}{4\pi} \sum_{g'=1}^G \nu \sigma_{f,g'} \phi_{g'}(\vec{r}) + \frac{Q_g(\vec{r}, \hat{\Omega}_n)}{4\pi} \\
\phi_{g,l,m} &= \sum_{n=1}^N w_n Y_{l,m}(\hat{\Omega}_n) \psi_{g,n}(\vec{r}) \\
\phi_g &= \sum_{n=1}^N w_n \psi_{g,n}(\vec{r}).
\end{aligned} \tag{5}$$

2.2 The Adjoint Transport Equation

Adapting from Ref. [6], a suitable inner product for the derivation of the multigroup adjoint transport equation is defined by:

$$(\cdot, \cdot) = \sum_{g=1}^G \int_{4\pi} d\hat{\Omega} \int_{\mathcal{D}} dV \cdot . \tag{6}$$

Following [6] the adjoint of the multigroup forward LTE Eq. (1) can then be derived to be:

$$\begin{aligned}
-\hat{\Omega} \cdot \nabla \psi_g^* + \sigma_{t,g} \psi_g^*(\vec{r}, \hat{\Omega}) &= \sum_{g'=1}^G \sum_{l=0}^L \frac{2l+1}{4\pi} \sum_{m=-l}^l \sigma_{s,l}^{g \rightarrow g'}(\vec{r}) \phi_{g',l,m}^*(\vec{r}) Y_{l,m}(\hat{\Omega}) \\
&+ \frac{\nu \sigma_{f,g}}{4\pi} \sum_{g'=1}^G \chi_{g'}(\vec{r}) \phi_{g'}^*(\vec{r}) + \frac{Q_g^*(\vec{r}, \hat{\Omega})}{4\pi},
\end{aligned} \tag{7}$$

An eigenvalue form of Eq. (7) can be defined totally analogous to Eq. (2). Boundary conditions for the adjoint equations are given on the outflow boundary $\partial\mathcal{D}^+$ identified as the fraction of the boundary $\partial\mathcal{D}$ for which the outward normal satisfies $\hat{n} \cdot \hat{\Omega} > 0$. For reasons explained in subsection 2.3 typically vacuum or reflective boundary conditions are used in adjoint calculations.

If we set $G = 1$ in Eq. (1), the resulting one-speed LTE is *almost self-adjoint* in the sense that its solution is the solution of a corresponding forward equation in the reverse direction $-\hat{\Omega}$. Even when allowing G to be arbitrary, the difference between the forward and adjoint equations is small:

- Sign of the direction $\hat{\Omega}$ is flipped.
- The $\sigma_{s,l}^{g' \rightarrow g}$ matrix is transposed.
- $\nu\sigma_{f,g}$ and χ_g change places.

2.3 Properties of the Forward and Adjoint Transport Equations

The adjoint transport problem is always formulated in relation to the forward transport problem of interest and thus the definition of boundary conditions and externally distributed source are purpose-driven. A very important example is the computation of a response of interest under changing distributed forward source and/or forward boundary conditions. If a response of the form:

$$R = (\sigma_d, \psi), \quad (8)$$

is desired, where σ_d is the response cross section, then the adjoint source should be defined as $Q^* = \sigma_d$. Then it holds that:

$$R = (\sigma_d, \psi) = (Q, \psi^*), \quad (9)$$

which enables the computation of R for varying Q without re-solving the forward or adjoint equations. Regarding appropriate boundary conditions, Reference [6] gives two examples both seeking to compute a response as in Eq. (8). These problems

are either driven by a distributed source or driven by a fixed inflow of particles. In both cases, a suitable adjoint operator (i.e. adjoint source and boundary conditions) is constructed to satisfy Eq. (9) and in both cases vacuum boundary conditions for the adjoint equations are appropriate.

Another application, that adjoint fluxes play an important role in, is first order perturbation theory of the multiplication factor[2]. For this application the adjoint eigenvalue problem is solved and the question about the relationship between the forward and adjoint eigenvalues arises. It is easy to show that the forward and adjoint eigenvalues computed from the corresponding continuous equations are identical[6]:

$$k_{\text{eff}} = k_{\text{eff}}^*. \quad (10)$$

The identities Eqs. Eq. (9) and Eq. (10) will be of importance when demonstrating the correctness and advantage of the mathematical adjoint over the physical adjoint of the SAAF- S_N equations.

2.4 Commutability of the Adjoint Operation

The discretization and adjoint operations applied to a linear operator generally do not commute leading to the concept of the mathematical and physical adjoint. For the first order LTE the situation is more complex because several variables need to be discretized increasing the number of permutations of when to discretize and when to apply the adjoint. The order of these operations shall be denoted by a vector with four entries with the position of the entry indicating when the operation is applied. For example the vector $(E, \hat{\Omega}, *, \vec{r})$ describes a situation where first the multigroup formalism is applied, then the S_N discretization is applied, the adjoint of these equations is taken, and finally the spatial variable is discretized. As the order of the discretization operations among each other is fixed, there are four possible

permutations of the order of operations that are listed in Table 1.

The true physical adjoint characterized by $(*, E, S_N, \vec{r})$ requires evaluation of adjoint-weighted multigroup cross sections that are distinct from forward-weighted multigroup cross sections. As long as the forward and (true) adjoint multigroup constants are evaluated using the exact forward or adjoint fluxes, respectively, the multigroup formalism does not incur any approximations. Under these circumstances, the adjoint and multigroup "discretization" operations commute, i.e. $(E, *, S_N, \vec{r})$ and $(*, E, S_N, \vec{r})$ are equivalent. However, in practice, approximate spectra are utilized to evaluate the multigroup constants and under these conditions the said commutativity is, in general, lost. It is noted, that adjoint-weighted multigroup cross sections are not commonly available and thus the true physical adjoint is only of academic interest.

The second and third options in Table 1, permutations $(E, *, S_N, \vec{r})$ and $(E, S_N, *, \vec{r})$, lead to identical sets of adjoint equations. In common production level codes solving the first-order, S_N LTE equations such as TORT [4] and DENOVO [5], the adjoint equations are in general derived by adjoining Eq. (5) and discretizing the resulting equation in space, i.e. the $(E, S_N, *, \vec{r})$ procedure. For the remainder of this work, this adjoint is referred to as physical adjoint of the first order LTE and it is thus distinguished from the true physical adjoint.

Finally, the mathematical adjoint, case four in Table 1, is derived by discretizing Eq. (5) in space and then applying the adjoint operation. Within this work, we present a formalism that allows for a direct derivation of the mathematical adjoint of the SAAF- S_N equations without the detour of full discretization of the forward equations and transposition of the resulting coefficient matrix.

For the first-order, multigroup, S_N equations the spatial discretization and adjoint operations commute for linear spatial discretization methods. Under these circumstances, the options 2, 3, and 4 in Table 1 are equivalent. For these methods physical and mathematical adjoint are equivalent and thus Eq. (9) and Eq. (10) hold exactly

even if the adjoint is the discretized physical adjoint,[8] and [9]. For the SAAF- S_N equations considered in this work, these operations do not commute.

3 The Forward and Adjoint SAAF- S_N Equations

The self-adjoint angular flux (SAAF) form of the LTE has been known for almost as long as computational transport theory itself. An early account can be found in [10]. However, it has received little attention by the community until Morel published a comprehensive, algebraic derivation for multi-dimensional geometries [11] facilitating its application for heterogeneous geometries. The SAAF equation belongs to the class of second order forms of the LTE along with the more common even-parity and odd-parity equations, [6]. Multigroup, second-order forms of the LTE can be discretized using the S_N or P_N in angle and continuous finite-element methods in space [11], [12]. Within this work, only the combination of the S_N discretization in angle with continuous finite-elements in space is discussed.

3.1 The Forward SAAF Equations

Within this work, modified SAAF equations are considered that implement a void treatment aimed at circumventing singularities of the standard SAAF equations in regions with vanishing total cross sections $\sigma_{t,g} \rightarrow 0$. The derivation of these equations is described in [7] and [13] and their final form for fixed source and eigenvalue cases are:

$$\text{Fixed source} \quad b(\psi^*, \psi) = l(\psi^*) + F(\psi^*, \psi) \quad (11)$$

$$\text{Eigenvalue} \quad b(\psi^*, \psi) = \frac{1}{k_{\text{eff}}} F(\psi^*, \psi). \quad (12)$$

The bilinear forms contained in Eqs. (11) and (12) are defined as:

$$\begin{aligned}
a(\psi^*, \psi) &= \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \left[\hat{\Omega}_n \cdot \nabla \psi_{g,n}^* \right] \left[\tau_g \hat{\Omega}_n \cdot \nabla \psi_{g,n} - (1 - \tau_g \sigma_{t,g}) \psi_{g,n} \right] \\
&+ \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \sigma_{t,g} \psi_{g,n}^* \psi_{g,n} + \sum_{g=1}^G \int_{\partial\mathcal{D}} d\vec{r} \sum_{\hat{\Omega}_n \cdot \vec{n} > 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{g,n}^* \psi_{g,n}
\end{aligned} \tag{13}$$

$$r(\psi^*, \psi) = \sum_{g=1}^G \int_{\partial\mathcal{D}_r} d\vec{r} \left\{ \sum_{\hat{\Omega}_n \cdot \vec{n} < 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{g,n}^* \psi_{n^r,g} \right\} \tag{14}$$

$$S(\psi^*, \psi) = \sum_{g=1}^G \sum_{g'=1}^G \sum_{l=0}^L \sum_{k=-l}^l \frac{2l+1}{4\pi} \int_{\mathcal{D}} d\vec{r} \left(\phi_{g,l,k}^* + \tau_g \nabla \cdot \vec{X}_{g,l,m}^* \right) \sigma_{s,l}^{g' \rightarrow g} \phi_{g',l,k} \tag{15}$$

$$\begin{aligned}
F(\psi^*, \psi) &= \frac{1}{4\pi} \sum_{g=1}^G \left\{ \int_{\mathcal{D}} d\vec{r} \left[\phi_g^* + \tau_g \nabla \cdot \vec{J}_g^* \right] \chi_g \sum_{g'=1}^G \nu \sigma_{f,g'} \phi_{g'} \right\} \\
&= \frac{1}{4\pi} \sum_{g=1}^G \sum_{g'=1}^G \left\{ \int_{\mathcal{D}} d\vec{r} \left[\phi_g^* + \tau_g \nabla \cdot \vec{J}_g^* \right] \chi_g \nu \sigma_{f,g'} \phi_{g'} \right\}
\end{aligned} \tag{16}$$

$$b(\psi^*, \psi) = a(\psi^*, \psi) - r(\psi^*, \psi) - S(\psi^*, \psi), \tag{17}$$

where $a(\psi^*, \psi)$ represent the streaming and total collision contributions, $r(\psi^*, \psi)$ represents the contributions from reflective boundary conditions, $S(\psi^*, \psi)$ and $F(\psi^*, \psi)$ contain the scattering and fission source terms, respectively.

The following definitions are extensively used in Eqs. (13) through (17) and in

the remainder of this work:

$$\begin{aligned}
\phi_{g,l,k} &= \sum_{n=1}^N w_n Y_{l,k} \left(\hat{\Omega}_n \right) \psi_{g,n} \\
\phi_{g,l,k}^* &= \sum_{n=1}^N w_n Y_{l,k} \left(\hat{\Omega}_n \right) \psi_{g,n}^* \\
\vec{X}_{g,l,k} &= \sum_{n=1}^N w_n \hat{\Omega}_n Y_{l,k} \left(\hat{\Omega}_n \right) \psi_{g,n} \\
\vec{X}_{g,l,k}^* &= \sum_{n=1}^N w_n \hat{\Omega}_n Y_{l,k} \left(\hat{\Omega}_n \right) \psi_{g,n}^*.
\end{aligned} \tag{18}$$

The linear form $l(\psi^*)$ comprises the external, distributed source and the inflow boundary conditions:

$$\begin{aligned}
l(\psi^*) &= \frac{1}{4\pi} \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \left(\psi_{g,n}^*(\vec{r}) + \tau_g \hat{\Omega}_n \cdot \nabla \psi_{g,n}^* \right) Q_{g,n}(\vec{r}) \\
&+ \sum_{g=1}^G \int_{\partial\mathcal{D}} d\vec{r} \sum_{\hat{\Omega}_n \cdot \vec{n} < 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{g,n}^* \psi_{g,n,BC}.
\end{aligned} \tag{19}$$

The stabilization parameter τ is given by the following expression:

$$\tau_g = \begin{cases} \frac{1}{\sigma_{t,g}}, & h\sigma_{t,g} \geq \xi \\ \frac{h}{\xi}, & h\sigma_{t,g} < \xi \end{cases}, \tag{20}$$

Within the framework of the described void treatment, ξ is a free parameter and it is chosen to be 0.5 and h is a measure of the mesh size that is set to the maximum vertex separation in the spatial FEM mesh.

3.2 Evaluation of the Physical Adjoint of the SAAF- S_N Equations

Within this work the physical adjoint is identified by the $(E, S_N, *, \vec{r})$ order of discretization and adjoint operations. Due to the *almost self-adjoint* property of the transport equation, it is easy to use an existing transport solver, in our case the forward SAAF- S_N system of equations, and trick it into solving the physical adjoint equations. This can be accomplished by applying the following modifications to the forward bilinear forms:

- Transpose the scattering matrix which translates to $\sigma_{s,l}^{g' \rightarrow g} \rightarrow \sigma_{s,l}^{g \rightarrow g'}$ in the bilinear forms.
- Switch the fission production cross section and the fission spectrum, which amounts to setting $\chi_g \rightarrow \chi_{g'}$ and $\nu\sigma_{f,g'} \rightarrow \nu\sigma_{f,g}$ in the bilinear forms.
- As the adjoint is now the primal variable, set $\psi_{g,n}^* \rightarrow \psi_{g,n}$ and $\psi_{g,n} \rightarrow \psi_{g,n}^*$.
- As a post-processing step, reinterpret the solution along $\hat{\Omega}_n$ as the solution along $-\hat{\Omega}_n$.

The bilinear forms of the physical adjoint equations that result from these transformations are (subscript p indicates the physical adjoint):

- Streaming and Collision term:

$$\begin{aligned}
 a_p^*(\psi^*, \psi) &= \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r}' \left[\hat{\Omega}_n \cdot \nabla \psi_{g,n} \right] \left[\tau_g \hat{\Omega}_n \cdot \nabla \psi_{g,n}^* - (1 - \tau_g \sigma_{t,g}) \psi_{g,n}^* \right] \\
 &+ \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \sigma_{t,g} \psi_{g,n} \psi_{g,n}^* + \sum_{g=1}^G \int_{\partial\mathcal{D}} d\vec{r} \sum_{\hat{\Omega}_n \cdot \vec{n} > 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{g,n} \psi_{g,n}^*. \quad (21)
 \end{aligned}$$

- Reflective Boundary Term:

$$r_p^*(\psi^*, \psi) = \sum_{g=1}^G \int_{\partial \mathcal{D}_r} d\vec{r} \left\{ \sum_{\hat{\Omega}_n \vec{n} < 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{n^r, g}^* \psi_{n, g} \right\}. \quad (22)$$

- Fission term:

$$F_p^*(\psi^*, \psi) = \frac{1}{4\pi} \sum_{g=1}^G \sum_{g'=1}^G \left\{ \int_{\mathcal{D}} d\vec{r} \nu \sigma_{f, g} \sum_{n=1}^N w_n \left[\psi_{g, n} + \tau_g \hat{\Omega}_n \cdot \nabla \psi_{g, n} \right] \chi_{g'} \phi_{g'}^* \right\}. \quad (23)$$

- Scattering term:

$$\begin{aligned} S_p^*(\psi^*, \psi) &= \sum_{g=1}^G \sum_{g'=1}^G \sum_{l=0}^L \sum_{k=-l}^l \frac{2l+1}{4\pi} \int_{\mathcal{D}} d\vec{r} \sigma_{s, l}^{g \rightarrow g'} \phi_{g', l, k}^* \\ &\times \sum_{n=1}^N w_n Y_{l, k}^n \left(\psi_{g, n} + \tau_g \hat{\Omega}_n \cdot \nabla \psi_{g, n} \right). \end{aligned} \quad (24)$$

In Eqs. (23) and (24) the angular fluxes are collapsed into angular flux and current moments via Eq. (18) because they constitute the solution space in the physical adjoint weak forms. The presented form is more amenable for implementation into MOOSE.

3.3 Derivation of the Mathematical Adjoint for the SAAF- S_N Equations

In this work, a new approach is presented that derives the weak form of the mathematical adjoint directly from the weak form of the forward equation without the necessity to construct the full system of linear equations.

The derivation of the SAAF forward weak form uses the adjoint angular flux as test functions for the sole purpose of putting the forward weak forms, Eq. (11) and Eq.

(12), into the appropriate form to derive the weak formulation of the mathematical adjoint directly by a transformation and reinterpretation of the test and solution spaces:

- Transformation: The following transformation emulates the solution of the transport equation in the reverse direction:

$$\begin{aligned} \hat{\Omega}_n &\rightarrow -\hat{\Omega}_n \\ \text{Note: } w_n &\rightarrow w_n, \end{aligned} \tag{25}$$

where n is the index of the $-\hat{\Omega}_n$ in the quadrature. Typically, if $\hat{\Omega}_n$ is in the quadrature, then $-\hat{\Omega}_n$ is also in the quadrature.

- Reinterpretation: In the forward weak form the forward flux ψ represents the solution and the adjoint flux ψ^* represents the test space, while for the adjoint equations their roles are reversed: The desired solution is ψ^* and the test function is ψ . Therefore, reinterpretation of ψ^* as the desired solution and ψ as test function complete the derivation of the mathematical adjoint.

In the following section, mostly algebraic transformations are used to derive a suitable formulation of each operator within the framework of the adjoint weak form of the SAAF equations. The derived formulations can directly be implemented into the MOOSE framework as they correspond to kernels that MOOSE is based on [1].

3.3.1 Streaming, Collision and Outflow Term

The streaming and collision term in the forward SAAF- S_N equation Eq. (11) is given by Eq. (13). Applying transformation Eq. (25) results in:

$$\begin{aligned}
a^*(\psi^*, \psi) &= \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \left[\hat{\Omega}_n \cdot \nabla \psi_{g,n}^* \right] \left[\tau_g \hat{\Omega}_n \cdot \nabla \psi_{g,n} + (1 - \tau_g \sigma_{t,g}) \psi_{g,n} \right] \\
&+ \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \sigma_{t,g} \psi_{g,n}^* \psi_{g,n} + \sum_{g=1}^G \int_{\partial \mathcal{D}} d\vec{r} \sum_{\hat{\Omega}_n \cdot \vec{n} < 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{g,n}^* \psi_{g,n}. \quad (26)
\end{aligned}$$

Equation Eq. (26) may be used as adjoint kernel with $\psi_{g,n}^*$ being the primary variable. However, we opt to manipulate Eq. (25) into a more convenient form by applying integration by parts to the $\left[\hat{\Omega}_n \cdot \nabla \psi_{g,n}^* \right] \psi_{g,n}$ term:

$$\begin{aligned}
\sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \left[\hat{\Omega}_n \cdot \nabla \psi_{g,n}^* \right] \psi_{g,n} &= - \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \psi_{g,n}^* \left[\hat{\Omega}_n \cdot \nabla \psi_{g,n} \right] \\
&+ \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\partial \mathcal{D}} d\vec{r} \psi_{g,n}^* \psi_{g,n} \left(\hat{\Omega}_n \cdot \vec{n} \right). \quad (27)
\end{aligned}$$

Separating the integral over the boundary into inflow and outflow parts and substitution into Eq. (26) gives:

$$\begin{aligned}
a^*(\psi^*, \psi) &= \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \left[\hat{\Omega}_n \cdot \nabla \psi_{g,n}^* \right] \tau_g \left[\hat{\Omega}_n \cdot \nabla \psi_{g,n} - \sigma_{t,g} \psi_{g,n} \right] \\
&- \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \psi_{g,n}^* \left[\hat{\Omega}_n \cdot \nabla \psi_{g,n} \right] + \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \sigma_{t,g} \psi_{g,n}^* \psi_{g,n} \\
&+ \sum_{g=1}^G \int_{\partial \mathcal{D}} d\vec{r} \sum_{\hat{\Omega}_n \cdot \vec{n} > 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{g,n}^* \psi_{g,n}. \quad (28)
\end{aligned}$$

Equation (28) has the advantage that less modification to the boundary conditions are necessary because the surface contribution to $a(\psi^*, \psi)$ is an integral over the

outflow boundary that is totally equivalent to the forward bilinear form $a(\psi^*, \psi)$.

3.3.2 Reflective Boundary Term

The reflective boundary term in the forward weak form Eq. (11) is given by Eq. (14).

In Eq. (14), the modifier r is understood as a map from n to the reflected direction n^r . Reinterpreting direction $\hat{\Omega}_n$ to be along $-\hat{\Omega}_n$ gives:

$$r^*(\psi^*, \psi) = \sum_{g=1}^G \int_{\partial\mathcal{D}_r} d\vec{r} \left\{ \sum_{\hat{\Omega}_n \cdot \vec{n} > 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{g,n}^* \psi_{n^r,g} \right\}, \quad (29)$$

For commonly used angular quadrature rules, it is safe to assume that the following holds:

$$\begin{aligned} w_{n^r} &= w_n \\ \left| \hat{\Omega}_{n^r} \cdot \vec{n} \right| &= \left| \hat{\Omega}_n \cdot \vec{n} \right|. \end{aligned} \quad (30)$$

In addition, the following identities are instrumental for manipulating the reflective boundary term into a convenient form:

$$\begin{aligned} \hat{\Omega}_{(n^r)^r} &= \hat{\Omega}_n \\ \text{sign}(\hat{\Omega}_{n^r} \cdot \vec{n}) &= -\text{sign}(\hat{\Omega}_n \cdot \vec{n}). \end{aligned} \quad (31)$$

Using Eq. (30) and (31) for manipulating Eq. (29) results in:

$$r^*(\psi^*, \psi) = \sum_{g=1}^G \int_{\partial\mathcal{D}_r} d\vec{r} \left\{ \sum_{\hat{\Omega}_n \cdot \vec{n} > 0} w_{n^r} \left| \hat{\Omega}_{n^r} \cdot \vec{n} \right| \psi_{(n^r)^r,g}^* \psi_{n^r,g} \right\}. \quad (32)$$

In the summation over angular directions, n is merely a dummy variable and can be replaced by another suitable summation index. For the derivation of the reflec-

tive boundary term, it is convenient to change the summation index to n^r which entails modifying the condition within the summation to $\hat{\Omega}_{n^r} \cdot \vec{n} < 0$; finally switching notation, $n^r \rightarrow n$, gives the final form of the reflective boundary condition term:

$$r^*(\psi^*, \psi) = \sum_{g=1}^G \int_{\partial \mathcal{D}_r} d\vec{r} \left\{ \sum_{\hat{\Omega}_n \cdot \vec{n} < 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{n^r, g}^* \psi_{n, g} \right\}. \quad (33)$$

3.3.3 Fission Term

The fission term present in the forward SAAF- S_N equations is given by Eq. (16). The currents and scalar fluxes are expanded according to their definition in Eq. (18) leading to:

$$\begin{aligned} F(\psi^*, \psi) &= \frac{1}{4\pi} \sum_{g=1}^G \sum_{g'=1}^G \left\{ \int_{\mathcal{D}} d\vec{r} \left(\sum_{n=1}^N w_n \left[\psi_{g, n}^* + \tau_g \hat{\Omega}_n \cdot \nabla \psi_{g, n}^* \right] \right) \right. \\ &\quad \times \left. \chi_g \left(\nu \sigma_{f, g'} \sum_{m=1}^M w_m \psi_{g', m} \right) \right\}. \end{aligned} \quad (34)$$

Applying the transformation Eq. (25) gives:

$$\begin{aligned} F^*(\psi^*, \psi) &= \frac{1}{4\pi} \sum_{g=1}^G \sum_{g'=1}^G \left\{ \int_{\mathcal{D}} d\vec{r} \left(\sum_{n=1}^N w_n \left[\psi_{g, n}^* - \tau_g \hat{\Omega}_n \cdot \nabla \psi_{g, n}^* \right] \right) \right. \\ &\quad \times \left. \chi_g \left(\nu \sigma_{f, g'} \sum_{m=1}^M w_m \psi_{g', m} \right) \right\}. \end{aligned} \quad (35)$$

Now, terms are reorganized, the definitions Eq. (18) are used to write the equations in terms of ϕ_g^* and $\vec{J}_g^*$, and finally a simple change of notation $g' \rightarrow g$, $g \rightarrow g'$ gives the final form of the mathematical adjoint fission kernel:

$$F^*(\psi^*, \psi) = \frac{1}{4\pi} \sum_{g=1}^G \sum_{m=1}^M w_m \left\{ \int_{\mathcal{D}} d\vec{r} \nu \sigma_{f, g} \left(\sum_{g'=1}^G \chi_{g'} \left[\phi_{g'}^* - \tau_{g'} \nabla \cdot \vec{J}_{g'}^* \right] \right) \psi_{g, m} \right\}. \quad (36)$$

3.3.4 Scattering Term

The consolidated scattering term (up, down and within-group scattering) in the forward SAAF- S_N equations is given by Eq. (15). For convenience let the spherical harmonics evaluated at $\hat{\Omega}_n$ and its conjugate evaluated at $-\hat{\Omega}_n$ be denoted by $Y_{l,k}^n$ and $\bar{Y}_{l,k}^n$, respectively. Using Eq. (18), Eq. (15) can be written as:

$$S(\psi^*, \psi) = \sum_{g=1}^G \dots \int_{\mathcal{D}} d\vec{r} \left\{ \sum_{n=1}^N w_n Y_{l,k}^n \left(\psi_{g,n}^* + \tau_g \hat{\Omega}_n \cdot \nabla \psi_{g,n}^* \right) \right\} \\ \times \left\{ \sigma_{s,l}^{g' \rightarrow g} \sum_{m=1}^M w_m Y_{l,k}^m \psi_{g,m} \right\}, \quad (37)$$

where,

$$\sum_{g=1}^G \dots = \sum_{g=1}^G \sum_{g'=1}^G \sum_{l=0}^L \sum_{k=-l}^l \frac{2l+1}{4\pi}. \quad (38)$$

Performing the transformation Eq. (25), Eq. (37) becomes:

$$S^*(\psi^*, \psi) = \sum_{g=1}^G \dots \int_{\mathcal{D}} d\vec{r} \left\{ \sum_{n=1}^N w_n \bar{Y}_{l,k}^n \left(\psi_{g,n}^* - \tau_g \hat{\Omega}_n \cdot \nabla \psi_{g,n}^* \right) \right\} \\ \times \left\{ \sigma_{s,l}^{g' \rightarrow g} \sum_{m=1}^M w_m \bar{Y}_{l,k}^m \psi_{g,m} \right\}. \quad (39)$$

Reorganizing Eq. (39), using the definitions Eq. (18), noting that $Y_{l,k}^n = (-1)^l \bar{Y}_{l,k}^n$, and finally changing notation $g' \rightarrow g$, $g \rightarrow g'$ results in the final expression for the adjoint scattering term:

$$S^*(\psi^*, \psi) = \sum_{g=1}^G \sum_{g'=1}^G \sum_{l=0}^L \sum_{k=-l}^l \frac{2l+1}{4\pi} \int_{\mathcal{D}} d\vec{r} \left\{ \sigma_{s,l}^{g \rightarrow g'} (-1)^l \left(\phi_{g',l,k}^* - \tau_{g'} \nabla \cdot \vec{X}_{g',l,k}^* \right) \right\} \\ \times \left\{ \sum_{m=1}^M w_m \bar{Y}_{l,k}^m \psi_{g,m} \right\}. \quad (40)$$

3.3.5 Computation of $\vec{X}_{g,l,k}^*$

The angular current-moment $\vec{X}_{g,l,k}^*$ is defined as:

$$\vec{X}_{g,l,k}^* = \sum_{n=1}^N w_n \hat{\Omega}_n Y_{l,k}^n \psi_{g,n}^*. \quad (41)$$

The adjoint angular fluxes can be represented as a series of spherical harmonics:

$$\psi_{g,n}^* = \sum_{l=0}^{\infty} \sum_{k=-l}^l \frac{2l+1}{4\pi} Y_{l,k}^n \phi_{g,l,k}^* = \vec{R}^T \vec{\phi}_g^*, \quad (42)$$

where, for the last expressions, we think of the indices l, k to be ordered along a single index p and the entries $Y_{l,k}^n$ and $\phi_{g,l,k}^*$ are collected in the vectors $\vec{R}$ and $\vec{\phi}_g^*$, respectively. Note, that the length of the vectors is $(L+1)^2$ with $L \rightarrow \infty$. Now for the element $u = x, y, z$ of the three-vector $\vec{X}_{g,l,k}^*$ we get:

$$\left(\vec{X}_{g,l,k}^* \right)_u = \sum_{n=1}^N w_n \left(\hat{\Omega}_n \right)_u Y_{l,k}^n \vec{R}^T \vec{\phi}_g^*. \quad (43)$$

Assembling the $\left(\vec{X}_{g,l,k}^* \right)_u$ for all l, k ordered along a single index p into the vector $\overrightarrow{\left(\vec{X}_g^* \right)_u} = \vec{X}_{g,u}^*$ leads to:

$$\vec{X}_{g,u}^* = \sum_{n=1}^N w_n \left(\hat{\Omega}_n \right)_u \vec{Y} \vec{R}^T \vec{\phi}_g^*, \quad (44)$$

where $\vec{Y}$ collects all $Y_{l,k}^n$. Let us now define the matrix $\mathbf{D}_u^*$:

$$\mathbf{D}_u^* = \sum_{n=1}^N w_n \left(\hat{\Omega}_n \right)_u \vec{Y} \vec{R}^T, \quad (45)$$

such that Eq. (44) becomes:

$$\vec{X}_{g,u}^* = \mathbf{D}_u^* \vec{\phi}_g^*, \quad (46)$$

Without further insight $\mathbf{D}_u^*$ has infinite dimensions. However, we do not need infinitely many rows of $\mathbf{D}_u^*$, just $(L + 1)^2$, where L is the scattering order. Furthermore, the matrix $\mathbf{D}_u^*$ is banded with finite bandwidth so only a finite number of columns features non-zero entries. Therefore, it is possible to store $\mathbf{D}_u^*$ exactly using a finite amount of memory. As a consequence $\vec{X}_{g,l,k}^*$ can be computed from the angular flux moments without additional approximation.

3.3.6 Definition of the Linear Form $l^*(\psi)$

In contrast to the other operators that are formally derived from the respective forward operators, the linear form of the mathematical adjoint equations $l^*(\psi)$ is selected such that the adjoint equations serve a particular purpose. We select the volumetric source term to be:

$$l^*(\psi) = \frac{1}{4\pi} \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} Q_{g,n}^*(\vec{r}) \psi_{g,n}(\vec{r}) + \sum_{g=1}^G \int_{\partial\mathcal{D}} d\vec{r} \sum_{\hat{\Omega}_n \cdot \vec{n} < 0} w_n \left| \hat{\Omega}_n \cdot \vec{n} \right| \psi_{g,n,BC}^* \psi_{g,n}. \quad (47)$$

The integration over the boundary is performed for all angular directions satisfying $\hat{\Omega}_n \cdot \vec{n} < 0$ because due to the transformation Eq. (25) these are the outflow direction of the forward equation. As pointed out in [6], the boundary conditions of the adjoint equations are often selected to be vacuum even if the forward equations feature non-zero inflow boundary conditions. Therefore, we shall focus on describing how the mathematical adjoint volumetric source term can be used in the framework of the described SAAF- S_N equations.

It is instructive to review how the adjoint of the SAAF- S_N equations can be used for fixed source problems. In the described case the subject of interest is the response R :

$$R = (\sigma_d, \psi) = \frac{1}{4\pi} \sum_{g=1}^G \sum_{n=1}^N w_n \int_{\mathcal{D}} d\vec{r} \psi_{g,n}(\vec{r}) \sigma_d(\vec{r}). \quad (48)$$

The modified bilinear forward and adjoint forms $\tilde{b}(\psi^*, \psi)$ and $\tilde{b}^*(\psi^*, \psi)$ are defined as:

$$\begin{aligned}\tilde{b}(\psi^*, \psi) &= b(\psi^*, \psi) - F(\psi^*, \psi) \\ \tilde{b}^*(\psi^*, \psi) &= b^*(\psi^*, \psi) - F^*(\psi^*, \psi).\end{aligned}\tag{49}$$

Then the adjoint problem is set up using $Q_{g,n}^* = \sigma_d$ resulting in the following expression:

$$\tilde{b}^*(\psi^*, \psi) = R.\tag{50}$$

Because of the equality of the bilinear forms $\tilde{b}(\psi^*, \psi) = \tilde{b}^*(\psi^*, \psi)$, it is easy to show that

$$R = (\sigma_d, \psi) = \tilde{b}^*(\psi^*, \psi) = \tilde{b}(\psi^*, \psi) = l(\psi^*).\tag{51}$$

Thus, the desired response can be obtained by an inner product of the adjoint function and the forward source.

4 Consistency of the Mathematical and Physical Adjoint SAAF- S_N Eigenvalue Equations

Within this section, the behavior of the physical and mathematical adjoint eigenvalue and eigenfunctions in the limit of vanishing mesh size is examined. Both the discretized forward and physical adjoint equations approximate physically meaningful equations, the forward and adjoint multigroup S_N equations. The mathematical adjoint does not discretize any physically meaningful equation, but it is a useful mathematical construct as it satisfies e.g. Eq. 51 exactly, regardless of the truncation error. Even though it is true for first order linear S_N transport methods with upwind

DGFEM, that the physical and mathematical adjoint eigenvalues and eigenfunctions are identical, the same does not necessarily hold for the SAAF- S_N equations. Within this section, we will explore under which conditions the mathematical and physical adjoint eigenvalues and eigenfunctions are consistent.

4.1 Consistency of the Mathematical and Physical Adjoint Eigenvalues

Within this section, it will be proved that for the SAAF- S_N the physical adjoint eigenvalue is consistent with the mathematical eigenvalue:

$$|k_m^{*,h} - k_p^*| \rightarrow 0 \text{ as } h \rightarrow 0, \quad (52)$$

where the superscript h indicates an approximate quantity obtained on a mesh characterized by the mesh parameter h , the superscript $*$ indicates the adjoint quantity and the subscripts m and p denote the mathematical and physical adjoints, respectively. In order to prove Eq. 52, we need to require that the forward equations are discretized consistently, implying that:

$$|k^h - k| \rightarrow 0 \text{ as } h \rightarrow 0. \quad (53)$$

Remember that, by design, the mathematical adjoint eigenvalue is equal to the forward eigenvalue at each mesh refinement level

$$k^h = k_m^{*,h}, \quad (54)$$

and that the exact physical eigenvalue is equal to the exact forward eigenvalue:

$$k = k_p^*. \quad (55)$$

Using Eqs. 53 to 55, it follows that:

$$\begin{aligned}
|k_m^{*,h} - k_p^*| &= |k^h - k_p^*| = |k_p^* - k^h| = |(k_p^* - k) - (k^h - k)| \\
&\leq \underbrace{|k_p^* - k|}_{=0} + \underbrace{|k^h - k|}_{\rightarrow 0},
\end{aligned} \tag{56}$$

which proves Eq. 52. In addition to Eq. 52, it shall be shown that with mesh refinement, the approximate physical eigenvalue and the mathematical eigenvalue converge to the same value:

$$|k_m^{*,h} - k_p^{*,h}| \rightarrow 0 \text{ as } h \rightarrow 0, \tag{57}$$

under the condition that the physical adjoint equations are discretized consistently:

$$|k_p^* - k_p^{*,h}| \rightarrow 0 \text{ as } h \rightarrow 0. \tag{58}$$

Starting from Eq. 52, add a "smart" zero and apply the reverse triangle inequality:

$$\begin{aligned}
|k_m^{*,h} - k_p^*| &\geq \left| |k_m^{*,h} - k_p^{*,h}| - \underbrace{|k_p^* - k_p^{*,h}|}_{\rightarrow 0} \right| \\
&\Rightarrow |k_m^{*,h} - k_p^{*,h}| \leq |k_m^{*,h} - k_p^*|,
\end{aligned} \tag{59}$$

On the other hand we could start from Eq. 57 and repeat the process described in Eq. 59:

$$\begin{aligned}
|k_m^{*,h} - k_p^{*,h}| &\geq \left| |k_m^{*,h} - k_p^*| - \underbrace{|k_p^* - k_p^{*,h}|}_{\rightarrow 0} \right| \\
&\Rightarrow |k_m^{*,h} - k_p^*| \leq |k_m^{*,h} - k_p^{*,h}|,
\end{aligned} \tag{60}$$

From Eqs. 59 and 60 it is concluded that in the limit of $h \rightarrow 0$:

$$|k_m^{*,h} - k_p^{*,h}| \rightarrow 0 \Leftrightarrow |k_m^{*,h} - k_p^*| \rightarrow 0. \quad (61)$$

In conclusion, in the limit of $h \rightarrow 0$, the mathematical adjoint eigenvalue becomes identical to the physical eigenvalue.

4.2 Consistency of the Mathematical and Physical Adjoint

Even though the physical and mathematical eigenvalues are consistent regardless of the SAAF- S_N method's free parameter ξ comprised in Eq. 20, the same does not generally hold true for the physical and mathematical adjoint eigenfunctions. It will be shown in this subsection that the mathematical and physical adjoint eigenvalues are only consistent for $\xi > 0$.

Similar to subsection 4.1, the proposition of this subsection is to prove or disprove:

$$\|\psi_m^{*,h} - \psi_p^*\| \rightarrow 0 \text{ as } h \rightarrow 0, \quad (62)$$

where $\psi_m^{*,h}$ is an approximation of the mathematical adjoint and ψ_p^* is the exact solution of the physical adjoint equation. For most transport methods Eq. 62 holds true.

Totally equivalent to the derivation of Eq. 61 it can be shown that

$$\|\psi_m^{*,h} - \psi_p^*\| \rightarrow 0 \Leftrightarrow \|\psi_m^{*,h} - \psi_p^{*,h}\| \rightarrow 0, \quad (63)$$

if the physical adjoint equations are discretized consistently.

First, the case $\xi > 0$ shall be discussed. Under this condition, the stabilization

parameter τ_g converges to zero as the mesh is refined:

$$\tau_g \rightarrow 0 \text{ as } h \rightarrow 0 \forall g = 1, \dots, G. \quad (64)$$

Setting $\tau_g = 0$, $g = 1, \dots, G$ leads to bilinear forms a_p^* , r_p^* , F_p^* , and S_p^* that are identical to their mathematical adjoint counterparts. Moreover, the resulting bilinear forms are equal to the first order S_N weak forms reported in [14]. Under the condition that we (1) exclude the trivial solution of the eigenvalue equations ($\psi = 0$), (2) looking for the fundamental mode, and (3) select a suitable normalization, for example:

$$(\nu \sigma_{f,g} \psi_{g,n}^*, \nu \sigma_{f,g} \psi_{g,n}^*) = 1,$$

the solution of the eigenvalue S_N weak form is unique. Therefore, it must hold that:

$$\psi_m^* = \psi_p^*. \quad (65)$$

In case of $\xi = 0$ the stabilization parameter is equal to $\tau_g = \frac{1}{\sigma_{t,g}} \neq f(h)$ and thus the bilinear forms contained in the mathematical and physical adjoint equations are different even at $h \rightarrow 0$. Therefore, in the general case, the solution obtained in the limit $h \rightarrow 0$ from the mathematical and physical adjoint equations will not be identical.

In summary, the eigenvalues computed from the mathematical and physical adjoint equations are consistent, while the eigenfunctions computed from the mathematical and physical adjoint equations are only consistent if $\xi > 0$. In Sec. 5 numerical examples are presented demonstrating these findings.

5 Numerical Results

Within this section numerical results for three test problems are presented that illustrate the correct implementation and the utility of the new mathematical adjoint functionality in RattleSnake/Yak. In subsections 5.1 through 5.3 results for a simple two-dimensional well-logging fixed source problem, a simplified two-dimensional pin cell problem, and a simplified variation of the two-dimensional IAEA PWR eigenvalue problem are presented, respectively.

5.1 Well-Logging Fixed Source Problem

The simplified two-dimensional well-logging test problem depicted in Fig. 1 comprises two material regions, a steel tool body and a formation region which for simplicity is composed of water. Vacuum boundaries are applied on all boundary edges. Two-group cross sections listed in Table 2 are used. The isotropic source is uniformly distributed in the source region with a strength of unity in the fast group and zero in the thermal group. A detector response is sought within the detector region with the response cross section $\sigma_d = (1/3, 1)$. The problem is meshed with a structured, uniform quadrilateral mesh with an initial mesh size of $h = 5$ cm. Four additional uniform refinement levels are considered with a minimum mesh size of $h = 0.3125$ cm. The S_4 level symmetric quadrature is utilized for all considered cases and the iterative convergence criterion is set to 10^{-12} throughout.

The exercise is to show that Eq. 51 holds, i.e. that the response can be computed using the mathematical adjoint function and the forward source under the condition that the adjoint linear form has been set up appropriately. For the given mesh-refinement levels the response computed by solving the forward equation and evaluating (σ_d, ψ) and the response computed using the adjoint function match to all printed digits. Therefore, we conclude that the (isotropic) fixed source portion is

implemented correctly.

5.2 Pin-Cell Eigenvalue Problem

The second test problem depicted in Fig. 2 is a two-dimensional eigenvalue problem with a geometry resembling a simplified fuel pin. A fuel lump (red) is positioned in the center of the geometry and is surrounded by the moderator (water). Reflective boundary conditions are applied on all four boundary edges and the overall size of the quadratic domain is 1.3 cm.

Two group cross section data listed in Table 3 is used for the fuel and moderator regions. Within this work the problem is considered for two different cases: (1) Isotropic scattering with the cross sections listed in Table 3 and (2) linearly anisotropic scattering with $\sigma_{s,1}^{g' \rightarrow g} = 0.6\sigma_{s,0}^{g' \rightarrow g}$. The computed difference of the eigenvalues for the P_0 and P_1 is small (10^{-3}) but it is large enough to detect errors in the implementation of the higher order scattering treatment.

The problem is initially meshed using a uniform 4×4 quadrilateral mesh (i.e. squares) with $h = 0.325$ cm. Seven additional uniform mesh refinement steps are conducted reducing the mesh size h to $h \approx 0.0027$ cm. The iterative convergence of the eigenvalue is checked and the simulation is terminated if the difference of two successive eigenvalues in the power iteration is less than ϵ , where four different $\epsilon = 10^{-6}, 10^{-8}, 10^{-10}, 10^{-12}$ are tested in order to distinguish significant differences in the computed forward and adjoint eigenvalues from iterative convergence error. The relative difference of two eigenvalues denoted by $\delta_{x,y}k$ is defined as:

$$\delta_{x,y}k = \left| 1 - \frac{k_{\text{eff}}^{x,h}}{k_{\text{eff}}^{y,h}} \right|, \quad (66)$$

where x and y take values f, m, and p referring to the forward, mathematical adjoint, and physical adjoint eigenvalues, respectively. If the error $\delta_{x,y}k$ remains almost

constant when tightening ϵ and is consistently above the noise level set by ϵ , the difference is significant and is caused by a truncation error. The same reasoning is applied to the difference of the mathematical and physical eigenfunctions measured in the relative L_2 norm:

$$\|\phi_m^{*,h} - \phi_p^{*,h}\|_2 = \sqrt{\frac{\sum_{g=1}^G \int_{\mathcal{D}} d\vec{r} \left(\phi_{g,m}^{*,h}(\vec{r}) - \phi_{g,p}^{*,h}(\vec{r}) \right)^2}{\sum_{g=1}^G \int_{\mathcal{D}} d\vec{r} \phi_{g,m}^{*,h}(\vec{r})^2}}, \quad (67)$$

5.2.1 Isotropic Scattering Results

First, the consistency results of the mathematical and physical adjoints with respect to the eigenvalue and eigenfunctions discussed in sections 4.1 and 4.2, respectively, are checked numerically. In Fig. 3, $\delta_{m,p}k$ (upper plot) and the difference of the forward and adjoint eigenfunctions measured in the relative L_2 norm Eq. 67 (lower plot) are plotted versus the mesh refinement level for $\xi = 0, 0.5$ and $\epsilon = 10^{-6}, 10^{-12}$. For both plots the results are independent of ϵ meaning that the observed difference between the mathematical and physical adjoint results are driven by a truncation error rather than iterative convergence.

According to the results in Sections 4.1 and 4.2 the difference of physical and mathematical adjoint eigenvalues should converge to zero with mesh refinement regardless of ξ , while the L_2 difference will only converge to zero for $\xi > 0$. These predictions are corroborated by the numerical evidence presented in Fig. 3. The difference of the eigenvalues converges to zero with mesh refinement for both $\xi = 0$ and $\xi = 0.5$ even though onset of convergence for the $\xi = 0$ case occurs for a finer mesh than for $\xi = 0.5$. In contrast, an $\mathcal{O}(h)$ convergence of the L_2 norm difference of the eigenfunctions is only observed for $\xi = 0.5$, while the L_2 norm difference levels out for $\xi = 0$. In addition to these integral results, the spatial distribution of the difference between the mathematical and physical adjoint fluxes for groups 1 and 2

are plotted in Fig. 4 and 5 for $\xi = 0$ and $\xi = 0.5$, respectively. It can be clearly seen that the difference decreases for the latter case, while it levels out when $\xi = 0$.

In Fig. 6 the relative difference of the forward and mathematical eigenvalues, $\delta_{f,m}k$, is examined for various values of the convergence criterion ϵ . According to Eq. 10, the approximate mathematical adjoint and forward eigenvalues are identical at each mesh refinement level h . However, Eq. 10 assumes that the underlying equations are solved without iterative convergence error which is often impossible, and thus it holds only up to the iterative convergence error. The results presented in Fig. 6 demonstrate that the implemented mathematical adjoint satisfies Eq. 10. The relative difference of the eigenvalues $\delta_{f,m}k$ is controlled by the iterative convergence error because $\delta_{f,m}k$ exhibits great sensitivity with respect to ϵ and no general trend with respect to mesh refinement. Moreover, tightening ϵ leads to a decrease in $\delta_{f,m}k$ until the mathematical adjoint and forward eigenvalue agree to all printed digits. As the log-log plot Fig. 6 does not support plotting $\delta_{f,m}k = 0$, this situation is handled by setting $\delta_{f,m}k \leftarrow \min(\delta_{f,m}k, 10^{-12})$.

In order to put these results into perspective, the discretization error present in the forward eigenvalue is also plotted on Fig. 6. The discretization error is estimated by extrapolating the computed forward eigenvalues using Richardson extrapolation. The discretization error in the forward eigenvalue is significantly above the difference of the forward and mathematical eigenvalues underlining that regardless of discretization errors, the forward and mathematical adjoints are identical up to iterative convergence error.

5.2.2 Linearly Anisotropic Results

Consistency results for the mathematical and physical adjoints with respect to the eigenvalue and eigenfunctions are plotted in Fig. 7 for $\xi = 0.5$ and linearly anisotropic scattering. As for isotropic scattering, the implemented mathematical adjoint behaves

as expected. The difference of the mathematical and physical eigenvalues converges to zero with mesh refinement until its behavior is either governed by ϵ (only for the $\epsilon = 10^{-6}$ case) or until the eigenvalues agree to all printed digits (in which case the difference is set to 10^{-12}). These results substantiate that the mathematical adjoint's anisotropic scattering capabilities are implemented correctly.

5.3 Simplified IAEA Test Case

The two-dimensional IAEA benchmark described in [15] is an assembly-homogenized two energy-group representation of a PWR core model. Within the described work, the IAEA problem is simplified into a two-group, two-region (fuel and reflector) problem as depicted in Fig. 8. The utilized cross sections are listed in Table 3. Vacuum boundary conditions are applied on all four domain boundaries and scattering is limited to isotropic contribution ($L = 0$). The main difference of the previous pin cell problem and the IAEA test case is the significantly larger domain of the latter and the vacuum boundary conditions that apply on all four domain boundaries.

Initially, a uniform, rectangular 10 by 10 mesh is applied with inadequately large cell sizes of $h = 10$ cm. Five mesh refinement steps are applied, whereby in each step the mesh size is cut in half such that the final mesh features $h = 0.3125$ cm. For the computation of the multiplication factor, RattleSnake's SAAF- S_N solver is utilized with linear finite elements and an S_2 level symmetric quadrature. The solution is performed using the forward and mathematical adjoint modes.

In Fig. 9 the eigenvalue computed using the RattleSnake forward mode is plotted using the scale on the left edge of the plot. Further, using the right edge scale, the relative difference of the forward eigenvalue and the mathematical and physical eigenvalues $\delta_{f,m}k$ are plotted versus the mesh refinement level for different values of the convergence tolerance ϵ . The results obtained for the IAEA test problem confirm the results previously presented for the pin cell test problem. The difference $\delta_{f,m}k$

is controlled by the convergence tolerance ϵ rather than by the truncation error. In addition to the results presented for the pin cell problem, the reduction of $\delta_{f,m}k$ with ϵ is very pronounced in Fig. 9.

6 Conclusions

This work describes the development and implementation of mathematical adjoint equations for the modified SAAF- S_N discretization scheme.

In contrast to first-order method S_N transport equation, the physical and the mathematical adjoints of the modified (and original) SAAF- S_N equations are never equal for a finite mesh size h . In the presented work it is proved that the eigenvalues of the physical adjoints of the SAAF- S_N equations are consistent, i.e. converge to the same value with mesh refinement. However, the mathematical and physical eigenfunctions are only consistent for a suitable choice of the stabilization parameter.

The mathematical adjoint is to be preferred over the physical adjoint because it satisfies common identities of the continuous forward and adjoint transport equations exactly regardless of the discretization error. Thus the implemented mathematical adjoint will be essential for future development efforts related to the Rattle S_N ake code, e.g. sensitivity analysis and uncertainty quantification and generation of consistent transient parameters for the point kinetics equations. Numerical results demonstrate correct implementation and utility of the mathematical adjoint.

7 Acknowledgment

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Order	Description
1. $(*, E, \hat{\Omega}, \vec{r})$	True physical adjoint. Missing cross section data.
2. $(E, *, \hat{\Omega}, \vec{r})$	Practical physical adjoint. Implemented in TORT [4] and DENOVO [5].
3. $(E, \hat{\Omega}, *, \vec{r})$	Equivalent to 2. since $*$ and $\hat{\Omega}$ operations commute.
4. $(E, \hat{\Omega}, \vec{r}, *)$	Mathematical adjoint.

Table 1: Possible permutations of the order of discretizing and applying the adjoint for the first order LTE.

Figure 1: Geometry of the two-dimensional well-logging fixed source problem.

	Fuel		Water		Steel	
	Group 1	Group 2	Group 1	Group 2	Group 1	Group 2
$\sigma_{t,g}$	0.22	0.8	0.7	2.0	0.53	0.94
$\sigma_{s,0}^{g \rightarrow 1}$	0.193	0.0	0.65	0.0	0.526	0.0
$\sigma_{s,0}^{g \rightarrow 2}$	0.017	0.73	0.05	1.97	0.001	0.83
κ_g	1.0	0.0	0	0	0	0
$\nu \Sigma_{f,g}$	0.006	0.1	0	0	0	0

Table 2: Cross sections used in the Well Logging and Wagner eigenvalue test case.

Figure 2: Geometry of the two-dimensional pin-cell eigenvalue problem.

	Fuel		Water/Reflector	
	Group 1	Group 2	Group 1	Group 2
$\sigma_{t,g}$	0.22222	0.83333	0.16666	1.11111
$\sigma_{s,0}^{g \rightarrow 1}$	0.192102	0.00001	0.126506	0.00001
$\sigma_{s,0}^{g \rightarrow 2}$	0.02	0.7483013	0.04	1.1010871
χ_g	0.99999	0.00001	0	0
$\nu \Sigma_{f,g}$	0.00001	0.135	0	0

Table 3: Cross sections used in the pin-cell and modified IAEA-2D eigenvalue test case.

Figure 3: Difference of the mathematical and physical eigenvalue for the pin-cell test problem (upper plot) with isotropic scattering. L_2 Difference of the mathematical and physical eigenfunctions for the pin-cell test problem (lower plot) with isotropic scattering.

Figure 4: Spatial distribution of the difference of the mathematical and adjoint eigenfunctions for $\xi = 0.0$ and the fuel pin test case. The left column corresponds to group $g = 1$ and the right column corresponds to group $g = 2$.

Figure 5: Spatial distribution of the difference of the mathematical and adjoint eigenfunctions for $\xi = 0.5$ and the fuel pin test case. The left column corresponds to group $g = 1$ and the right column corresponds to group $g = 2$.

Figure 6: Convergence of the forward eigenvalue with mesh refinement (left axis) and $\delta_{f,m}k$ plotted versus mesh refinement for various values of ϵ .

Figure 7: Difference of the mathematical and physical eigenvalue for the pin-cell test problem (upper plot) with linearly anisotropic scattering. L_2 Difference of the mathematical and physical eigenfunctions for the pin-cell test problem (lower plot) with linearly anisotropic scattering.

Figure 8: Layout of the simplified IAEA-2D benchmark. Red denotes the fuel and blue denotes the reflector regions.

Figure 9: Rattle S_N ake computed eigenvalues using forward mode (left axis) and $\delta_{f,m}k$ (right axis) versus mesh refinement .