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A GENERALIZED ADJOINT APPROACH FOR QUANTIFYING REFLECTOR ASSEMBLY DISCONTINUITY FACTOR UNCERTAINTIES*

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ABSTRACT

Sensitivity-based uncertainty analysis of assembly discontinuity factors (ADFs) can be readily performed using adjoint methods for infinite lattice models. However, there is currently no adjoint-based methodology to obtain uncertainties for ADFs along an interface between a fuel and reflector region. To accommodate leakage effects in a reflector region, a 1D approximation is usually made in order to obtain the homogeneous interface flux required to calculate the ADF. Within this 1D framework an adjoint-based method is proposed that is capable of efficiently calculating ADF uncertainties. In the proposed method the sandwich rule is utilized to relate the covariance of the input parameters of 1D diffusion theory in the reflector region to the covariance of the interface ADFs. The input parameters' covariance matrix can be readily obtained using sampling-based codes such as XSUSA or adjoint-based codes such as TSUNAMI. The sensitivity matrix is constructed using a fixed-source adjoint approach for inputs characterizing the reflector region. An analytic approach is then used to determine the sensitivity of the ADFs to fuel parameters using the neutron balance equation. A stochastic approach is used to validate the proposed adjoint-based method.

Key Words: Uncertainty Quantification, Reflector Assembly Discontinuity Factor

1. INTRODUCTION

The utilization of assembly discontinuity factors (ADFs) in reactor simulation codes has become standard practice in nuclear reactor analysis. In a typical reactor simulation the computational burden of calculating ADFs is negligible. However, the use of ADFs is very effective in reducing assembly power error, particularly in highly heterogeneous cores [1]. The motivation for the application of ADFs in full-core reactor analysis can be traced to homogenized cross section

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generation. In diffusion theory, lattice transport solutions are used to generate few-group homogenized cross sections for an infinite assembly. An exact transport solution will produce continuous flux and current profiles across the assembly interface. However, there is no reason to expect that flux continuity at the assembly interface can be preserved while preserving neutron balance, which demands that current continuity be preserved. ADFs attempt to preserve current continuity in the diffusion model by adjusting the flux at the assembly interfaces. The effect of ADF utilization is to produce a more transport-like solution.

The assembly ADF $\mathcal{A}$ can then easily be calculated as the ratio of the heterogeneous surface flux ϕ_i^{het} to the assembly averaged homogenous flux ϕ_i^{hom}:

$$\mathcal{A} = \frac{\phi_i^{\mathrm{het}}}{\phi_i^{\mathrm{hom}}} \tag{1}$$

For a single assembly calculation the surface flux is equal to the assembly-averaged flux because there is no neutron leakage. The situation is complicated when the ADF is to be calculated on the interface of an assembly and reflector region. Due to the non-zero current at the assembly interface, the averaged flux in the region will generally no longer equal the surface flux. The remedy in reactor analysis is to apply a 1D approximation to the reflector region in order to determine the homogenous flux at the assembly/reflector boundary [2].

While it is crucial to be able to produce best-estimate calculations for the ADF, it is equally important to obtain error margins by propagating uncertainty information through the ADF computational process. Because ADF values are strongly correlated to power distribution errors in a full core analysis, uncertainties in the ADF will directly affect solution quality. Generalized Perturbation Theory (GPT) provides a framework in which to propagate cross-section uncertainties to the ADF. The SCALE module TSUNAMI-2D (Tool for Sensitivity and Uncertainty Analysis Methodology Implementation) [2] uses GPT to calculate uncertainties in reaction rate ratios. At the assembly level TSUNAMI can calculate ADF uncertainties approximately by taking the ratio of the average flux of a thin surface at the assembly boundary to the assembly averaged flux. While this methodology is valid for an infinite system, TSUNAMI is currently not capable of accurately quantifying ADF uncertainties at reflector interfaces due to leakage effects.

In this paper an adjoint-based method is proposed for quantifying ADF uncertainties at the interface between assembly and reflector regions. The method utilizes the 1D diffusion approximation generally used to treat reflector interface ADFs. The proposed adjoint-based method is computationally more efficient than a stochastic approach, which would require a substantial amount of full transport solutions.

2. METHODOLOGY

Calculating reflector ADF uncertainties is a specific case of a more general type of problem, which is that of propagating input parameter uncertainties through nonlinear computational models to obtain uncertainties in the model's outputs. If the covariance matrix $\bar{\bar{C}}_i$ of the input

parameters is available along with the sensitivities $\bar{\bar{S}}$ relating the change in outputs with respect to the change in input parameters, the sandwich rule can be applied to obtain a covariance matrix for the outputs $\bar{\bar{C}}_o$. The sandwich rule is expressed as follows [3]:

$$\bar{\bar{C}}_o = \bar{\bar{S}}\bar{\bar{C}}_i\bar{\bar{S}}^T \tag{2}$$

For the problem at hand, the outputs of interest are the ADF values at an assembly/reflector interface. The ADF depends explicitly on the heterogeneous surface flux and implicitly on the few-group homogenized cross sections that determine the homogeneous flux in the reflector region. Defining a proper sensitivity matrix for the ADF at an assembly/reflector interface is necessary to determine a covariance matrix for the ADF.

The sensitivity matrix for the ADF can be decomposed into its implicit and explicit components. In block matrix form, the sensitivity matrix is:

$$\bar{\bar{S}} = \begin{bmatrix} \frac{\partial \mathcal{A}}{\partial \Sigma} & \frac{\partial \mathcal{A}}{\partial \phi_i^{het}} \end{bmatrix} \tag{3}$$

Further, the sensitivity of the ADF can be decomposed into input parameters Σ for the reflector region Σ^R and inputs for the fuel region Σ^F:

$$\frac{\partial \mathcal{A}}{\partial \Sigma} = \begin{bmatrix} \frac{\partial \mathcal{A}}{\partial \Sigma^F} & \frac{\partial \mathcal{A}}{\partial \Sigma^R} \end{bmatrix} \tag{4}$$

Each row of the sensitivity matrix $\bar{\bar{S}}$ represents a single energy group. For a two-group problem composed of a computational model with N inputs the sensitivity matrix has dimensions of $[2 \times N]$. The covariance matrix corresponding to the sensitivity matrix can be written as:

$$\bar{\bar{C}}_i = \begin{bmatrix} \bar{\bar{C}}_{(\Sigma,\Sigma)} & \bar{\bar{C}}_{\left(\phi_i^{het},\Sigma\right)} \\ \bar{\bar{C}}_{\left(\Sigma,\phi_i^{het}\right)} & \bar{\bar{C}}_{\left(\phi_i^{het},\phi_i^{het}\right)} \end{bmatrix} \tag{5}$$

where $\bar{\bar{C}}_{(A,B)}$ corresponds to the covariance matrix for parameters A and B. Expanding the matrix-matrix multiplication in the sandwich rule, the covariance matrix for the ADFs is given by:

$$\begin{aligned} \bar{\bar{C}}_o = \Bigg[& \frac{\partial \mathcal{A}}{\partial \Sigma}\bar{\bar{C}}_{(\Sigma,\Sigma)}\left(\frac{\partial A}{\partial \Sigma}\right)^T + \frac{\partial \mathcal{A}}{\partial \Sigma}\bar{\bar{C}}_{\left(\phi_i^{het},\Sigma\right)}\left(\frac{\partial \mathcal{A}}{\partial \phi_i^{het}}\right)^T + \frac{\partial \mathcal{A}}{\partial \phi_i^{het}}\bar{\bar{C}}_{\left(\Sigma,\phi_i^{het}\right)}\left(\frac{\partial \mathcal{A}}{\partial \Sigma}\right)^T \\ & + \frac{\partial \mathcal{A}}{\partial \phi_i^{het}}\bar{\bar{C}}_{\left(\phi_i^{het},\phi_i^{het}\right)}\left(\frac{\partial \mathcal{A}}{\partial \phi_i^{het}}\right)^T \Bigg] \end{aligned} \tag{6}$$

For a two-group ADF problem, the resulting covariance matrix takes the form:

$$\bar{\bar{C}}_o = \begin{bmatrix} \mathrm{var}(\mathcal{A}_1, \mathcal{A}_1) & \mathrm{cov}(\mathcal{A}_1, \mathcal{A}_2) \\ \mathrm{cov}(\mathcal{A}_1, \mathcal{A}_2) & \mathrm{var}(\mathcal{A}_2, \mathcal{A}_2) \end{bmatrix} \tag{7}$$

The input parameters' covariance matrix in Eq. (5) can be obtained through either sampling-based techniques or adjoint-based techniques. For this work, the XSUSA code was chosen to generate $\bar{\bar{C}}_i$ in order to be able to consistently compare ADF uncertainties obtained using the proposed approach with a pure sampling-based approach. To generate $\bar{\bar{C}}_i$ using XSUSA, the "super assembly" model in Fig. 1, composed of a fuel assembly and reflector region, can be simulated using SCALE. Uncertainty-based perturbations are introduced into the SCALE cross-section libraries through XSUSA. The input parameters' covariance matrix can then be determined by post-processing the set of perturbed values of fuel and reflector parameters that comprise $\bar{\bar{C}}_i$. Once $\bar{\bar{C}}_i$ is computed, the problem is reduced to determining the reflector ADF sensitivities to fuel and reflector parameters. In the proposed method, these sensitivities will be determined by applying a 1D diffusion model to the reflector.

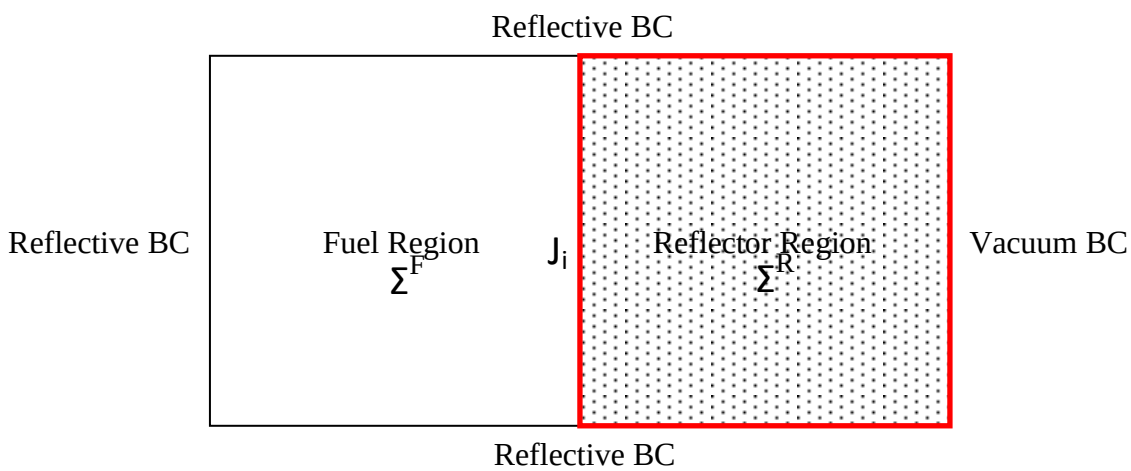

Figure 1. A typical geometric layout for a problem where ADFs are of interest. The arrangement is called a "super assembly."

First, an adjoint-based method will be proposed for calculating the ADF sensitivity to reflector inputs. Since the ADF depends implicitly on reflector model inputs, the chain rule must be applied. Perturbations in the reflector inputs will perturb the homogeneous flux, which will in turn perturb the ADF:

$$\frac{\partial \mathcal{A}}{\partial \Sigma^R} = \frac{\partial \mathcal{A}}{\partial \phi_i^{hom}} \frac{\partial \phi_i^{hom}}{\partial \Sigma^R} = -\frac{\phi_i^{het}}{\left(\phi_i^{hom}\right)^2} \frac{\partial \phi_i^{hom}}{\partial \Sigma^R} \tag{8}$$

The values for ϕ_i^{het} can be determined using a lattice transport code like NEWT[2] while ϕ_i^{hom} is determined using a 1D diffusion model for the reflector. The energy group g forward diffusion equation in the reflector region is as follows:

$$-\frac{d}{dx}\left(D_g \frac{d\phi_g}{dx}\right) + \Sigma_{tg}\phi_g - \sum_{g'=1}^{G} \Sigma_{sg'g}\,\phi_{g'} = 0 \tag{9}$$

Discretization of the 1D diffusion equation with known-current boundary conditions on the reflector boundary and on the fuel/reflector interface is sufficient for determining the homogeneous interface flux. To determine the homogeneous flux sensitivity, perturbation theory can be applied. The reflector problem is a fixed source problem where the source is determined entirely by the neutron current at the interface of the reflector and fuel assembly. Discretization of the forward 1D diffusion equation will lead to the following linear system:

$$B\phi(x) = Q(x) \tag{10}$$

In this formulation B is the migration and loss matrix, $Q(x)$ is the fixed source vector and $\phi(x)$ is the space-dependent homogeneous flux solution in the reflector. A perturbation in any element of the linear system will result in a new perturbed system:

$$B'\phi'(x) = Q'(x) \tag{11}$$

Responses of interest (R and R') are considered for the reference and perturbed states, respectively. The variational approach is applied with the Lagrangian multiplier λ to determine the perturbation (ΔR) in the response of interest. The variational approach calls for the creation of an auxiliary functional K, which uses the forward diffusion equation as a constraint. The auxiliary functional K is a function of the flux ϕ, input data Σ and the Lagrangian multiplier[4].

$$K[\phi, \Sigma, \lambda] = R - < \lambda(B\phi - Q) > \tag{12}$$

To first-order, the perturbed auxiliary function is expanded about the reference state[5]:

$$K' = K + < \frac{\partial K}{\partial \Sigma}\Delta\Sigma > + < \frac{\partial K}{\partial \phi}\Delta\phi > + < \frac{\partial K}{\partial \lambda}\Delta\lambda > \tag{13}$$

To gauge the effect of perturbations in the input parameters only, it is desirable to have the auxiliary functional be invariant to changes in ϕ:

$$\begin{aligned} &< \frac{\partial K}{\partial \phi}\Delta\phi > = 0 \\ \Rightarrow &< \frac{\partial R}{\partial \phi}\Delta\phi > - < \lambda B \Delta\phi > = < \frac{\partial R}{\partial \phi}\Delta\phi > - < \Delta\phi B^{*}\lambda > = 0 \\ &= < \left(\frac{\partial R}{\partial \phi} - B^{*}\lambda\right)\Delta\phi > = 0 \end{aligned} \tag{14}$$

$$\Rightarrow\ B^{*}\lambda = \frac{\partial R}{\partial \phi}$$

Equation (14) is satisfied if the Lagrangian multiplier λ is equal to the adjoint vector ϕ^{*}. The adjoint vector ϕ^{*} is found by solving the adjoint system to the discretization of the 1D diffusion equation in the reflector region:

$$B^{*}\phi^{*}(x) = \frac{\partial R}{\partial \phi} \tag{15}$$

The auxiliary functional should also be invariant to changes in the Lagrangian multiplier λ:

$$\begin{gathered} < \frac{\partial K}{\partial \lambda} > = < B\phi - Q > = 0 \\ \Rightarrow\ B\phi = Q,\ \ B'\phi' = Q' \end{gathered} \tag{16}$$

If the exact solution to the perturbed and unperturbed forward equations is available then $K' = R'$ and $K = R$, respectively since $B\phi - Q = 0$ and $B'\phi' - Q' = 0$. Using this fact, the response perturbation is obtained[4]:

$$\begin{gathered} K' - K = R' - R = < \frac{\partial K}{\partial \Sigma}\Delta\Sigma > = < \frac{\partial K}{\partial B}\Delta B\ +\ \frac{\partial K}{\partial Q}\Delta Q > \\ \Rightarrow\ \Delta R = < \left(\frac{\partial R}{\partial B}\Delta B -\ \lambda\Delta B\phi\right) + \left(\frac{\partial R}{\partial Q}\Delta Q +\ \lambda\Delta Q\right) > \\ = < \phi^{*}\Delta Q - \phi^{*}\Delta B\phi > \\ \Delta R = < \phi^{*}(\Delta Q - \Delta B\phi) > \end{gathered} \tag{17}$$

The sensitivity of the response perturbation to some input parameter perturbation $\Delta\Sigma$ is then:

$$\frac{\Delta R}{\Delta \Sigma} = \frac{< \phi^{*}(\Delta Q - \Delta B\phi) >}{\Delta \Sigma} \tag{18}$$

If the response is defined as $R = \delta(x - x_i)\phi(x)$, which is the homogeneous interface flux, then Eq. (18) can be used to determine the sensitivity of the homogeneous interface flux to reflector input parameters.

The problem of calculating the sensitivity of the interface ADF to fuel input parameters is more complicated than that of the reflector inputs since the effect is implicit. The physical effects of the fuel can be transferred to the ADF through the neutron current at the fuel assembly/reflector interface. Applying the chain rule, the sensitivity of the ADF to fuel parameters can be calculated as follows:

$$\frac{\partial \mathcal{A}}{\partial \Sigma^{F}} = \frac{\partial \mathcal{A}}{\partial \phi_i^{hom}}\frac{\partial \phi_i^{hom}}{\partial \Sigma^{F}} = -\frac{\phi_i^{het}}{\left(\phi_i^{hom}\right)^2}\left(\frac{\partial \phi_i^{hom}}{\partial J_1}\frac{\partial J_1}{\partial \Sigma^{F}} + \frac{\partial \phi_i^{hom}}{\partial J_2}\frac{\partial J_2}{\partial \Sigma^{F}}\right) \tag{19}$$

The sensitivity of the homogeneous flux to the interface current $\partial\phi_i^{hom}/\partial J$ can be obtained using Eq. (18). The neutron balance equation is utilized to obtain the sensitivity of the neutron current to fuel parameters. The two-group neutron balance equations in the fuel region are:

$$J_1 = \frac{h}{k}\left(\nu\Sigma_{f1}^F\bar{\phi}_1^F + \nu\Sigma_{f2}^F\bar{\phi}_2^F\right) + h\Sigma_{s21}^F\bar{\phi}_2^F + h\Sigma_{s11}^F\bar{\phi}_1^F - h\Sigma_{t1}^F\bar{\phi}_1^F \tag{20}$$

and

$$J_2 = h\Sigma_{s12}^F\bar{\phi}_1^F + h\Sigma_{s22}^F\bar{\phi}_2^F - h\Sigma_{t2}^F\bar{\phi}_2^F \tag{21}$$

where
h is the fuel assembly width,
$\bar{\phi}_1^F$ is the fuel-avereraged fast flux,
$\bar{\phi}_2^F$ is the fuel-averaged thermal flux,
k is the multiplication factor,
$\nu\Sigma_{f1}^F$ is fast group nu-fission cross section,
$\nu\Sigma_{f2}^F$ is the thermal group nu-fission cross section,
Σ_{t1}^F is the fast group total cross section,
Σ_{t2}^F is the thermal group total cross section,
Σ_{s11}^F is the fast self-scatter cross section,
Σ_{s22}^F is the thermal self-scatter cross section,
Σ_{s12}^F is the downscatter cross section,
Σ_{s21}^F is the upscatter cross section.

Since neutrons are only able to leak from the fuel assembly to the reflector region through the interface the neutron current will be nonzero only at the interface. Consequently, the interface current sensitivities can be found analytically.

To complete the sensitivity matrix $\bar{\bar{S}}$ the only term now needed is the sensitivity of the ADF to the heterogeneous flux. This sensitivity can be calculated analytically from the definition of the ADF:

$$\frac{\partial\mathcal{A}}{\partial\phi_i^{het}} = \frac{1}{\phi_i^{hom}} \tag{22}$$

Note that the proposed method for calculating ADF uncertainties has been demonstrated here for a two-group problem. However, the method can be easily generalized to any number of groups.

3. RESULTS

A representative model based on a pressurized water reactor was chosen to demonstrate the validity of the proposed method to quantify uncertainties in the ADF along fuel/reflector interfaces. The problem consists of seven UO_2 pin cells enriched to 4.85% followed by a reflector region whose width matches that of the pin cells. The problem geometry is shown in Fig. 2.

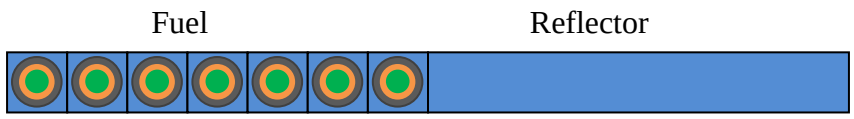

Figure 2. The geometric layout for the representative problem used to test the proposed method. The fuel pin cells are typical for a pressurized light water reactor.

Using the sampling-based uncertainty analysis software XSUSA, 100 perturbed homogenized two-group cross-section sets are obtained for the problem at hand [6]. First, a stochastic approach is employed to obtain ADF uncertainties. For each set of cross-section data the interface currents; transport, absorption, and scattering cross sections; and interface heterogeneous fluxes are input into a MATLAB code that solves the 1D diffusion equation in the reflector region. Each input data set yields two-group ADF values. Once all 100 data samples are processed, statistics are taken to analyze the uncertainty in the two-group interface ADFs. The uncertainty calculated using the stochastic method will be used to compare the results obtained using the proposed adjoint-based method.

The first step in the adjoint-based method is to build a covariance matrix for the model input parameters. In order to best reproduce the error attributable to the interface current, all parameters appearing in the neutron balance of the fuel assembly are input into the model. All parameters required for the reflector diffusion equation along with the interface heterogeneous fluxes are also inputs. To summarize, the model inputs are k, Σ_{tg}^{F}, $\nu\Sigma_{fg}^{F}$, Σ_{s11}^{F}, Σ_{s12}^{F}, Σ_{s21}^{F}, Σ_{s22}^{F}, $\bar{\phi}_{g}^{F}$, Σ_{trg}^{R}, Σ_{ag}^{R}, Σ_{s12}^{R}, Σ_{s21}^{R} and ϕ_{i}^{het}. A statistically-based covariance matrix is constructed for these inputs using the 100 samples generated by XSUSA. The size of the covariance matrix is $[19 \times 19]$ while the sensitivity matrix has size $[2 \times 19]$. Alternatively, a GPT-based covariance matrix could be generated using TSUNAMI. However a statistically-based covariance matrix ensures complete consistency among the parameter data for this demonstration.

Once the sensitivity matrix is constructed using the method outlined in the previous section the sandwich rule is applied to obtain two-group ADF uncertainties. The sensitivities of the reflector ADFs to input parameters obtained using the proposed adjoint method can be verified by performing a central differencing routine. Reflector input parameters are perturbed ± 1%with the few-group ADFs being calculated for each perturbation. The central difference formula is then used to estimate the derivative of the ADFs with respect to the input parameters. A comparison of the sensitivities obtained using adjoints and central differencing is presented in Table I.

Table I. A comparison of ADF sensitivities to reflector input parameters

Input parameter	Reflector ADF, group 1		Reflector ADF, group 2	
	Adjoint method	Central differencing	Adjoint method	Central differencing
Σ_{tr1}^{R}	-4.35E-01	-4.41E-01	-5.79E-01	-5.86E-01
Σ_{tr2}^{R}	-2.05E-04	-2.08E-04	3.35E-01	3.43E-01
Σ_{a1}^{R}	4.93E-03	4.98E-03	2.95E-02	2.98E-02
Σ_{a2}^{R}	6.33E-03	6.33E-03	1.34E+00	1.35E+00
Σ_{s12}^{R}	5.56E-01	5.60E-01	-6.14E-01	-6.15E-01
Σ_{s21}^{R}	-6.54E-03	-6.60E-03	2.90E-03	2.93E-03

The adjoint-based sensitivities are completely consistent with the central differencing results. The stochastic and adjoint approaches to calculating reflector ADF uncertainties are summarized in Table II.

Table II. A comparison of ADF uncertainty values using the proposed adjoint method and a stochastic approach

Input parameter	Mean			Standard deviation		
	Adjoint method	Stochastic method	Absolute error	Adjoint method	Stochastic method	Absolute error
$\mathcal{A}_1$	1.17207	1.17201	0.00006	0.00443	0.00440	0.00003
$\mathcal{A}_2$	0.95852	0.95947	0.00095	0.03001	0.02946	0.00055
$\mathrm{cov}(\mathcal{A}_1, \mathcal{A}_2)$	0.00012	0.00012	0.00000			

Comparisons between the stochastic approach and the proposed adjoint-based approach indicate that the two methods are consistent. Discrepancies in the thermal ADF calculations can likely be minimized by using more perturbed cross section sets. Some of the discrepancies can also be attributed to non-linear effects in the scattering-dominant reflector problem.

4. CONCLUSIONS

Although GPT provides an efficient framework for calculating assembly ADF uncertainties there has previously been no method to calculate ADF uncertainties on the interface of a fuel assembly and reflector region. The proposed adjoint-based method, which is fully consistent with GPT, can efficiently calculate reflector ADF uncertainties using the pre-existing 1D diffusion framework for calculating ADFs. In the proposed method the sandwich rule is utilized to relate the covariance of the input parameters of 1D diffusion theory in the reflector region to the covariance of the interface ADFs. The covariance matrix can be readily obtained using

TSUNAMI or a similar code. The sensitivity matrix is constructed using a fixed-source adjoint approach for inputs characterizing the reflector region. An analytic approach is then used to determine the sensitivity of the ADFs to fuel parameters using the neutron balance equation.

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