SECOND-ORDER SENSITIVITIES OF A GENERAL FUNCTIONAL OF THE
FORWARD AND ADJOINT FLUXES IN A MULTIPLYING NUCLEAR
SYSTEM WITH SOURCE

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Abstract

This work presents an application of the Second-Order Adjoint Sensitivity Analysis Methodology (2nd-ASAM) to compute efficiently and exactly all of the 1st- and 2nd-order functional derivatives (“sensitivities”) of a generic scalar-valued response to parameters for a multiplying subcritical system comprising a non-fission neutron source. The response is defined to be a nonlinear functional of the forward and adjoint particle fluxes while the system parameters include isotopic number densities, microscopic cross sections, fission spectrum, sources, and detector response functions. As indicated by the general theoretical considerations underlying the 2nd-ASAM, the number of computations required to obtain the 1st- and 2nd-order increases linearly in augmented Hilbert spaces as opposed to increasing exponentially in the original Hilbert space. This unique feature provides the fundamental reason for the unmatched efficiency of the 2nd-ASAM for computing exactly all of the 1-st and 2nd-order responses sensitivities to model parameters. The results presented in this work are currently being implemented in several production-oriented three dimensional neutron transport code systems for analyzing specific subcritical systems.
1. INTRODUCTION

The computation of second-order response sensitivities to model parameters is motivated by the need to overcome the linearization limitation which is implicit in the use of first-order sensitivities. During the 1970s, the field of reactor physics has provided pioneering works\textsuperscript{1-5} for computing selected 2\textsuperscript{nd}-order response sensitivities of the system’s effective multiplication factor and reaction rates ratios using the adjoint neutron transport and/or diffusion equations. These works generally indicated that the 2\textsuperscript{nd}-order sensitivities of such responses to cross section perturbations were computationally expensive to obtain, requiring $O(N_a^2)$ large-scale computations per response for a system comprising $N_a$ model parameters, and were smaller than the corresponding 1\textsuperscript{st}-order sensitivities. Such indications may have led to a diminishing interest in developing efficient methods for computing 2\textsuperscript{nd}-order response sensitivities for nuclear engineering systems.

While the interest in computing 2\textsuperscript{nd}-order response sensitivities practically vanished in the nuclear engineering field in the 1990s, interest in this topic became increasingly evident in other fields, driven mostly by the knowledge that 2\textsuperscript{nd}-order (Hessian) sensitivity information accelerates the convergence of optimization algorithms. In structural mechanics\textsuperscript{6}, for example, interest has been focused primarily on the developing adjoint methods for computing 2\textsuperscript{nd}-order sensitivity of structural responses to variations of structural stiffness parameters. In atmospheric sciences\textsuperscript{7,8}, “second-order adjoint models” were used to compute products between the Hessian of the cost functional and a vector (representing a perturbation in sensitivity analysis, a search direction in optimization, an eigenvector, etc.) to perform sensitivity analysis of the cost function with respect to distributed observations, to study the evolution of the condition number (the ratio of the largest to smallest eigenvalues) of the Hessian during minimization, and for sensitivity studies in three-dimensional atmospheric chemical transport models. In the context of parametric circuit analysis and optimization\textsuperscript{9}, second-order sensitivities for linear circuits were also computed, albeit approximately.

The methods used in the works mentioned above were all developed for specific, rather than general, applications for which they usually estimated, rather than computed exactly and exhaustively, 2\textsuperscript{nd}-order response sensitivities to the model’s parameters. Since the availability (or unavailability) of exactly computed 2\textsuperscript{nd}-order sensitivities affects significantly many fields (e.g., optimization, data assimilation/adjustment, model calibration and validation, predictive modeling, convergence of many numerical methods), Cacuci\textsuperscript{10-12} developed the generally applicable “\textbf{Second-Order Adjoint Sensitivity Analysis Methodology (2\textsuperscript{nd}-ASAM)}”. The 2\textsuperscript{nd}-ASAM computes exactly and most efficiently all of the
second-order functional derivatives of model responses to parameters, and simultaneously verifies them intrinsically by computing all of the mixed partial sensitivities twice, using independently derived formulations. The application of the 2nd-ASAM for nonlinear systems\textsuperscript{11} has been illustrated by means of a nonlinear heat conduction benchmark problem\textsuperscript{13}. Furthermore, the 2nd-ASAM for linear systems\textsuperscript{10,12} was applied to an illustrative linear neutron diffusion problem\textsuperscript{14} aimed at highlighting the essential contributions of the 2nd-order sensitivities of a detector response to changes in the underlying neutron cross sections. This illustrative problem\textsuperscript{14} has shown that most of the second-order relative detector sensitivities to cross-sections were actually larger than the corresponding first-order relative sensitivities, contrary to the tacit assumption that “2nd-order sensitivities to cross-sections are negligible in neutron diffusion problems”, which was prevalent in sensitivity analysis works in the 1990s. In particular, the 2nd-order sensitivities were shown\textsuperscript{14} to be responsible for causing: (a) asymmetries in the response distribution; and (b) the “expected value of the response” to differ from the “computed nominal value of the response.” When only the parameters’ mean values and covariance matrices are available, neglecting the second-order sensitivities would nullify the third-order response correlations, and hence would nullify the skewness of the response distribution. Consequently, any events occurring in a response’s long and/or short tails, which are characteristic of rare but decisive events (e.g., major accidents, catastrophes), would likely be missed.

The 2nd-ASAM for linear systems\textsuperscript{10,12} has also been applied\textsuperscript{15,16} to compute the 2nd-order sensitivities of the temperature distributions within a model of a test section comprising a heated rod surrounded by lead-bismuth eutectic coolant. For this model, the six 1st-order and twenty one distinct 2nd-order sensitivities for the temperature distribution at any location within the heated rod (and/or on its surface), and a similar number of 1st- and 2nd-order sensitivity for the temperature distribution at any location within the coolant, were computed using only seven independent 2nd-ASAM-computations. For the thermal-hydraulics parameters used in the test-section benchmark, having mean values and standard deviations typical of the conditions computed in the preliminary conceptual design of the G4M Reactor\textsuperscript{16}, the 2nd-order sensitivities caused the temperature distributions within the rod, on the rod’s surface and in the coolant to become non-Gaussian, asymmetric, and skewed towards temperatures higher than the respective mean temperatures, as all three temperature distributions turned out to have positive skewnesses. In particular, the temperature distribution in the heated rod was skewed significantly towards higher temperatures, indicating that the conventional Gaussian-based metrics are not applicable for performing conventional risk analysis for this important safety-margin indicator.
The 2nd-ASAM for linear systems\textsuperscript{10,12} has also been applied by Cacuci and Favorite\textsuperscript{17} to compute the 2nd-order sensitivities of uncollided particle contributions to radiation detector responses, demonstrating once again its efficiency and accuracy. For a multi-region two-dimensional cylindrical benchmark problem, all of the all of the benchmark’s 18 first-order sensitivities and 224 second-order sensitivities of a detector’s response with respect to the system’s isotopic number densities, microscopic cross sections, source emission rates, and detector response function were obtained exactly by requiring only 12 adjoint large-scale transport computations. In contradistinction, 877 large-scale transport computations would have been needed to compute the respective sensitivities using central finite-differences, and this number does not include the additional calculations that would have been required to find appropriate values of the parameter perturbations to use for the respective central differences expressions.

The present work extends significantly the results presented in Ref 17 by applying the 2nd-ASAM to the neutron transport equation that models a multiplying subcritical system comprising a non-fission neutron source. Section II of this work recalls succinctly the Boltzmann transport equation describing the transport of neutrons within a finite multiplying medium with an internal non-fission neutron source, defining this physical system’s parameters and responses. Section III presents the construction of the First-Level Adjoint Sensitivity System (1st-LASS) for the transport equation. The 1st-LASS is used for the efficient computation of the 1st-order response sensitivities to variations in model parameters, and it serves as the basis for the construction of the Second-Level Adjoint Sensitivity System (2nd-LASS). The actual construction of the 2nd-LASS for the neutron transport equation is presented in Sec. IV, which also presents the specific expressions for computing exactly and efficiently all of the second-order response sensitivities to variations in model parameters. Section V summarizes and concludes this work.
II. SYSTEM RESPONSE: A NONLINEAR FUNCTIONAL OF THE FORWARD AND ADJOINT FLUXES IN A MULTIPLYING NUCLEAR SYSTEM WITH SOURCE

The physical system considered in this work is a finite medium of convex volume $V$ which contains fission and non-fission sources of neutrons. The system’s outer boundary, denoted as $\partial V$, is considered to be perfectly well known and the system is considered to be placed in vacuum, in order to simplify the mathematical treatment by disregarding possible effects of boundary perturbations; such perturbations will be considered in subsequent work. The distribution of neutrons in such a system is modeled using the standard form of the time-independent integro-differential Boltzmann transport equation

$$L(\alpha)\phi(r, \Omega, E) = \Omega \cdot \nabla \phi(r, \Omega, E) + \Sigma_f(t; r, E)\phi(r, \Omega, E)$$

$$- \int_{4\pi} d\Omega' \int_{0}^{E_f} dE' \Sigma_s(s; r, E' \rightarrow E, \Omega' \rightarrow \Omega)\phi(r, \Omega', E')$$

$$- \int_{4\pi} d\Omega' \int_{0}^{E_f} dE' \chi(p; r, E' \rightarrow E)\nu\Sigma_f(f; r, E')\phi(r, \Omega', E') = Q(q; r, \Omega, E),$$

subject to the customary vacuum boundary condition which specifies that there is no incoming flux of particles:

$$\phi(r_x, \Omega, E) = 0, \quad r_x \in \partial V, \quad \Omega \cdot n < 0, \quad 0 < E < \infty,$$

where $n$ denotes the unit outward normal vector at any point $r_x \in \partial V$ on the body’s outer surface $\partial V$, and $E_f$ denotes the highest neutron energy.

The vector $\alpha$, which appears in the definition of the Boltzmann operator $L(\alpha)$, represents generically all of the model’s imprecisely known scalar parameters, and will be defined in Eq. (15), below. The components of $\alpha$ will include all of the components of the vectors of imprecisely known scalar model parameters that enter in the definitions of the various macroscopic cross sections, fission spectrum, forward and adjoint sources, and detector response functions. Thus, the macroscopic cross-sections
The neutron fission spectrum \( \chi(p; r', E \rightarrow E) \), and the source \( Q(q; r, \Omega, E) \) generally depend not only on the spatial variable \( r \), on the energy variable \( E \), and, possibly, solid angle \( \Omega \), but also on imperfectly known scalar-valued model parameters such as atomic number densities, microscopic cross-sections, and weighting functions. Specifically, the macroscopic total cross-section \( \Sigma_i(t; r, E) \) is considered to depend on \( J_t \) imprecisely known scalar-valued model parameters denoted as \( t_i, i = 1, \ldots, J_t \), which are considered to be the components of a vector of model parameters defined as

\[
t = \left[ t_1, \ldots, t_{J_t} \right]^\dagger.
\]

Throughout this work, the “dagger” \((\dagger)\) will be used to denote “transposition.” Similarly, the macroscopic scattering cross section \( \Sigma_s(s; E' \rightarrow E, \Omega' \rightarrow \Omega) \) is considered to depend on \( J_s \) imprecisely known scalar-valued model parameters denoted as \( s_i, i = 1, \ldots, J_s \), while the effective macroscopic fission cross-section \( \nu \Sigma_f(f; r, E') \) is considered to depend on \( J_f \) imprecisely known scalar-valued model parameters denoted as \( f_i, i = 1, \ldots, J_f \), which are considered to be the components of two vectors defined, respectively, as follows:

\[
s = \left[ s_1, \ldots, s_{J_s} \right]^\dagger,
\]

\[
f = \left[ f_1, \ldots, f_{J_f} \right]^\dagger.
\]

Furthermore, the fission spectrum \( \chi(p; r, E' \rightarrow E) \) is considered to depend on \( J_p \) imprecisely known scalar-valued parameters denoted as \( p_i, i = 1, \ldots, J_p \), while the source \( Q(q; r, \Omega, E) \) is considered to depend on \( J_q \) imprecisely known scalar-valued parameters denoted as \( q_i, i = 1, \ldots, J_q \), which are considered to be the components two vectors of model parameters defined, respectively, as follows:

\[
p = \left[ p_1, \ldots, p_{J_p} \right]^\dagger,
\]

\[
q = \left[ q_1, \ldots, q_{J_q} \right]^\dagger.
\]
The customary Hilbert space for defining the customary adjoint neutron transport operator will be denoted as $\mathcal{H}$ and is endowed with the following inner product, denoted as between two square-integrable functions $\varphi_1(r, \Omega, E) \in \mathcal{L}_2(V \times \Omega \times E) \equiv \mathcal{H}$ and $\varphi_2(r, \Omega, E) \in \mathcal{L}_2(V \times \Omega \times E) \equiv \mathcal{H}$:

$$
\langle \varphi_1, \varphi_2 \rangle_h \triangleq \int_{4\pi} \int_{E_1} d\Omega \int_0^{E_2} dE \varphi_1(r, \Omega, E) \varphi_2(r, \Omega, E).
$$

(8)

In the Hilbert space $\mathcal{H}$, the adjoint flux, which will be denoted as $\varphi^+(r, \Omega, E)$, is the solution of the following equation, which is adjoint to Eq. (1):

$$
L^* (\alpha) \varphi^+ = Q^+(k; r, \Omega, E),
$$

(9)

where the adjoint operator $L^* (\alpha)$ is defined as

$$
L^* (\alpha) \varphi^+ \triangleq -\nabla \cdot \mathbf{\Omega} \nabla \varphi^+(r, \Omega, E) + \Sigma_s(t;r,E) \varphi^+(r, \Omega, E)
$$

$$
- \int d\Omega' \int_{0}^{E_1} dE' \Sigma_s(s;r,E \rightarrow E', \Omega \rightarrow \Omega') \varphi^+(r, \Omega', E')
$$

$$
- \nabla \Sigma_f(\mathbf{f}; r, E) \int d\Omega' \int_{0}^{E_1} dE' \chi(p;r,E \rightarrow E') \varphi^+(r, \Omega', E'),
$$

(10)

where the source term $Q^+(k; r, \Omega, E)$ is related to the system’s response, and where the adjoint flux $\varphi^+(r, \Omega, E)$ is subject to the following adjoint boundary condition:

$$
\varphi^+(r_x, \Omega, E) = 0, \quad r_x \in \partial V, \quad \Omega \cdot n > 0,
$$

(11)

The source term $Q^+(k; r, \Omega, E)$ is considered to depend on $J_k$ imprecisely known scalar-valued parameters denoted as $k_i, i = 1, \ldots, J_k$, which are considered to be the components of the vector $\mathbf{k}$ defined as follows:

$$
\mathbf{k} \triangleq [k_1, \ldots, k_{J_k}]^T.
$$

(12)

The system response considered in this work is a scalar-valued nonlinear functional of the adjoint and forward fluxes, denoted as $R(\varphi, \varphi^+; \alpha)$, of the form

$$
R(\varphi, \varphi^+; \alpha) \triangleq \int_{4\pi} \int_0^{E_1} d\Omega dE G(d; \varphi, \varphi^+),
$$

(13)
where \( G(d; \varphi, \varphi^+) \) is a suitably differentiable function of its arguments, and where the vector \( d \) comprises \( J_d \) imprecisely known scalar-valued parameters \( d_i, i = 1, \ldots, J_d \), pertaining to the definition of \( R(\varphi, \varphi^+; \alpha) \), so that

\[
\mathbf{d} \triangleq [d_1, \ldots, d_{J_d}]^T. \tag{14}
\]

Since the response \( R(\varphi, \varphi^+; \alpha) \) defined in Eq. (13) depends explicitly and/or implicitly, through the fluxes \( \varphi^+(\mathbf{r}, \Omega, E) \) and \( \varphi(\mathbf{r}, \Omega, E) \), on all of the imprecisely known model parameters defined in Eqs. (3) through (14), it will be convenient for subsequent mathematical derivations to consider these imprecisely known scalar-valued model parameters as the components of a “vector of model parameters,” denoted as \( \alpha \) and defined as follows:

\[
\alpha \triangleq [\alpha_1, \ldots, \alpha_{J_\alpha}]^T \triangleq [\mathbf{t}, \mathbf{s}, \mathbf{f}, \mathbf{p}, \mathbf{q}, \mathbf{k}, \mathbf{d}], \quad J_\alpha \triangleq J_t + J_s + J_f + J_p + J_q + J_k + J_d, \tag{15}
\]

where \( J_\alpha \) denotes the total number of imprecisely-known scalar model parameters.

The nominal values of the model parameters will be denoted as \( \alpha^0 \triangleq [\alpha^0_1, \ldots, \alpha^0_{J_\alpha}]^T \). Throughout this work, the superscript zero will be used, as needed, to denote “nominal” or “mean” values. The nominal value of the flux, denoted as \( \varphi^0(\mathbf{r}, \Omega, E) \), is obtained by solving Eqs. (1) and (2) using the nominal parameter values \( \alpha^0 \). The nominal value of the detector response, denoted as \( R(\varphi^0, \varphi^{+0}; \alpha^0) \), is obtained by evaluating Eq. (13) at the nominal flux and parameter values.

### III. THE FIRST-LEVEL FORWARD AND ADJOINT SENSITIVITY SYSTEMS FOR COMPUTING FIRST-ORDER RESPONSE SENSITIVITIES TO VARIATIONS IN MODEL PARAMETERS

The total sensitivity, denoted as \( \delta R(\varphi^0, \varphi^{+0}; \alpha^0; \delta \varphi, \delta \varphi^+; \delta \alpha) \), of the detector response defined in Eq. (13) to variations \( \delta \alpha \triangleq [\delta \alpha_1, \ldots, \delta \alpha_{J_\alpha}]^T \) in the model parameters, around the nominal values \( \alpha^0 \), is
obtained by applying the definition of the Gateaux (G-) differential to Eq. (13) at the nominal parameter and flux values, to obtain:

$$\delta R\left(\varphi^0, \varphi^{*0}, a^0; \delta \varphi, \delta \varphi^+; \delta a\right) \triangleq \frac{d}{d \varepsilon} \left\{ \int_{\Omega} \int_0^{E_f} \frac{dV}{4\pi} \int d\Omega \int dE \ G \left[ d^0 + \varepsilon \delta d; \varphi^0 (r, \Omega, E) + \varepsilon \delta \varphi (r, \Omega, E), \varphi^{*0} (r, \Omega, E) + \varepsilon \delta \varphi^+ (r, \Omega, E) \right] \right\}_{\varepsilon=0}$$

(16)

$$= \left\{ \delta R\left(\varphi^0, \varphi^{*0}, a^0; \delta \varphi\right) \right\}_{\text{dir}} + \left\{ \delta R\left(\varphi^0, \varphi^{*0}, a^0; \delta \varphi, \delta \varphi^+\right) \right\}_{\text{ind}} ,$$

where the “direct-effect term” is defined as

$$\left\{ \delta R\left(\varphi^0, \varphi^{*0}, a^0; \delta \varphi\right) \right\}_{\text{dir}} \triangleq \sum_{i=1}^{J_0} \int_{\Omega} \int_0^{E_f} \frac{dV}{4\pi} \int dE \left\{ \frac{\partial G\left(d; \varphi, \varphi^+\right)}{\partial d_i} \right\}_{(a^0, \varphi^0, \varphi^{*0})} \delta d_i ,$$

(17)

and where the “indirect-effect term” is defined as

$$\left\{ \delta R\left(\varphi^0, \varphi^{*0}, a^0; \delta \varphi, \delta \varphi^+\right) \right\}_{\text{ind}} \triangleq \int_{\Omega} \int_0^{E_f} \frac{dV}{4\pi} \int dE \left\{ \frac{\partial G}{\partial \varphi} \delta \varphi (r, \Omega, E) + \frac{\partial G}{\partial \varphi^+} \delta \varphi^+ (r, \Omega, E) \right\}_{(a^0, \varphi^0, \varphi^{*0})} .$$

(18)

Since the nominal values \(\varphi^0(r, \Omega, E)\) and \(\varphi^{*0}(r, \Omega, E)\) of the forward and adjoint fluxes flux are known after having solved Eqs. (1), (2) (9), and (11) using the nominal parameter values \(a^0\), it follows that the direct-effect term defined in Eq. (17) can already be computed at this stage. In contradistinction, however, the indirect-effect term defined in Eq. (18) can be computed only after having determined the flux variations \(\delta \varphi (r, \Omega, E)\) and \(\delta \varphi^* (r, \Omega, E)\), which are the solutions of the equations obtained by G-differentiating the original forward and adjoint transport equations and respective boundary conditions given in Eqs. (1), (2) (9), and (11). Performing these differentiations yields the following 1st-Level Forward Sensitivity System (1st-LFSS)\(^{10-12,18,19}\):

$$F_{11}^{(1)}(a^0) \delta u(r, \Omega, E) = Q^{(1)}(a^0, \varphi^0, \varphi^{*0}; \delta a),$$

(19)

together with the following boundary conditions:

$$\delta \varphi (r_s, \Omega, E) = 0, \quad r_s \in \partial V \ for \ \Omega \cdot n < 0, \quad 0 < E < E_f ,$$

$$\delta \varphi^* (r_s, \Omega, E) = 0, \quad r_s \in \partial V \ for \ \Omega \cdot n > 0, \quad 0 < E < E_f .$$

(20)
The following definitions were used for the matrix $F^{(1)}_{11}(\alpha)$ and the vectors $\delta u(r, \Omega, E)$ and $Q^{(1)}(\alpha^0; \varphi^0, \varphi^0; \delta \alpha)$, which appear in Eq.(19):

$$
F^{(1)}_{11}(\alpha) \triangleq \begin{pmatrix} L(\alpha) & 0 \\ 0 & L'(\alpha) \end{pmatrix}, \quad \delta u \triangleq \begin{pmatrix} \delta \varphi(r, \Omega, E) \\ \delta \varphi'(r, \Omega, E) \end{pmatrix}, \quad Q^{(1)}(\alpha; \varphi, \varphi^*; \delta \alpha) \triangleq \begin{pmatrix} Q^{(1)}_1(\alpha, \varphi; \delta \alpha) \\ Q^{(1)}_2(\alpha, \varphi^*; \delta \alpha) \end{pmatrix}, \quad (21)
$$

where

$$
Q^{(1)}_1(\alpha, \varphi; \delta \alpha) \triangleq \delta Q(q; r, \Omega, E) - \delta \Sigma_t(t; r, E) \varphi(r, \Omega, E)
+ \int_{4\pi}^{E_f} d\Omega' \int_{E_f}^{E_r} E' \varphi(r, \Omega', E') \left[ \delta \Sigma_s(s; r, E' \rightarrow E, \Omega' \rightarrow \Omega) \right]
+ \int_{4\pi}^{E_f} d\Omega' \int_{E_f}^{E_r} E' \delta \chi(p; r, E' \rightarrow E) \varphi(r, \Omega', E') \left[ \nu \Sigma_f(f; r, E') \right]
+ \int_{4\pi}^{E_f} d\Omega' \int_{E_f}^{E_r} E' \delta \chi(p; r, E' \rightarrow E) \varphi(r, \Omega', E') \delta \left[ \nu \Sigma_f(f; r, E') \right].
$$

and

$$
Q^{(1)}_2(\alpha, \varphi^*; \delta \alpha) \triangleq \delta Q^*(k; r, \Omega, E) - \delta \Sigma_t(t; r, E) \varphi^*(r, \Omega, E)
+ \int_{4\pi}^{E_f} d\Omega' \int_{E_f}^{E_r} E' \varphi^*(r, \Omega', E') \left[ \delta \Sigma_s(s; r, E \rightarrow E', \Omega \rightarrow \Omega') \right]
+ \delta \left[ \nu \Sigma_f(f; r, E) \right] \int_{4\pi}^{E_f} d\Omega' \int_{E_f}^{E_r} E' \varphi^*(r, \Omega', E')
+ \nu \Sigma_f(f; r, E) \int_{4\pi}^{E_f} d\Omega' \int_{E_f}^{E_r} E' \delta \chi(p; r, E \rightarrow E') \varphi^*(r, \Omega', E').
$$

The following definitions were used in Eqs. (22) and (23):

$$
\delta \Sigma_t(t; r, E) \triangleq \sum_{j=1}^{J} \frac{\delta \Sigma_t(t; r, E)}{\delta t_j} \delta t_j,
$$

$$
\delta \Sigma_s(s; r, E' \rightarrow E, \Omega' \rightarrow \Omega) \triangleq \sum_{j=1}^{J} \frac{\delta \Sigma_s(s; r, E' \rightarrow E, \Omega' \rightarrow \Omega)}{\delta s_j} \delta s_j,
$$

$$
\delta \chi(p; r, E' \rightarrow E) \triangleq \sum_{j=1}^{J} \frac{\delta \chi(p; r, E' \rightarrow E)}{\delta p_j} \delta p_j.
$$
\[
\delta \left[ v\Sigma_f (f;r,E) \right] \triangleq \sum_{j=1}^{J_f} \delta f_j \delta f_j.
\]

Solving the 1st-LFSS defined by Eqs. (19) and (20) is computationally expensive, since the 1st-LFSS would need to be solved anew for every variation \( \delta \alpha_i, i = 1, \ldots, N_\alpha \) in the model parameters, as each such variation would affect the source term \( Q^{(i)}(\alpha^o; \varphi^{(o)}, \varphi^{(o)}, \delta \alpha) \). The computationally expensive evaluation of the indirect-effect term by using Eq. (18) can be avoided\(^{10-12,18,19} \) by expressing this indirect-effect term in terms of the solution of the 1st-Level Adjoint Sensitivity System (1st-LASS), which is constructed by implementing the following sequence of steps:

(i) Define an inner product \( \left\langle u^{(i)}(r, \Omega, E), v^{(i)}(r, \Omega, E) \right\rangle \) of two vector-valued functions

\[
u^{(i)}(r, \Omega, E) \triangleq \begin{pmatrix} u_1^{(i)}(r, \Omega, E), u_2^{(i)}(r, \Omega, E) \end{pmatrix}^T \quad \text{and} \quad v^{(i)}(r, \Omega, E) \triangleq \begin{pmatrix} v_1^{(i)}(r, \Omega, E), v_2^{(i)}(r, \Omega, E) \end{pmatrix}^T,
\]

with \( u_1^{(i)}(r, \Omega, E) \in \mathcal{L}_2(V \times \Omega \times E), u_2^{(i)}(r, \Omega, E) \in \mathcal{L}_2(V \times \Omega \times E), v_1^{(i)}(r, \Omega, E) \in \mathcal{L}_2(V \times \Omega \times E), \) and \( v_2^{(i)}(r, \Omega, E) \in \mathcal{L}_2(V \times \Omega \times E) \), where \( \mathcal{L}_2(V \times \Omega \times E) \) denotes the customary Lebesgue-space of square-integrable functions, as follows:

\[
\left\langle u^{(i)}(r, \Omega, E), v^{(i)}(r, \Omega, E) \right\rangle \triangleq \sum_{j=1}^{2} \int_{V} \int_{\Omega} \int_{E} dV d\Omega dE u_j^{(i)}(r, \Omega, E) v_j^{(i)}(r, \Omega, E).
\]  \quad (24)

(ii) Denote the Hilbert space endowed with the inner product defined in Eq. (24) as \( \mathcal{H}_{(i)} \) and form the inner product of Eq. (19) with a yet undefined function \( \psi^{(i)}(r, \Omega, E) \triangleq \begin{pmatrix} \psi_1^{(i)}(r, \Omega, E), \psi_2^{(i)}(r, \Omega, E) \end{pmatrix}^T \) to obtain

\[
\left\langle \psi^{(i)}, F_{11}^{(i)}(\alpha^o) \delta u \right\rangle_{(i)} = \left\langle \psi^{(i)}(r, \Omega, E), Q^{(i)}(\alpha^o; \varphi^{(o)}, \varphi^{(o)}, \delta \alpha) \right\rangle_{(i)}.
\]  \quad (25)

(iii) In the Hilbert space \( \mathcal{H}_{(i)} \), define the formal adjoint operator of \( F_{11}^{(i)}(\alpha) \), denoted as \( A_{11}^{(i)}(\alpha) \), through the following relationship:

\[
\left\langle \psi^{(i)}, F_{11}^{(i)}(\alpha^o) \delta u \right\rangle_{(i)} = \left\langle \delta u, A_{11}^{(i)}(\alpha) \psi^{(i)} \right\rangle_{(i)} + P^{(i)} \left[ \delta u, \psi^{(i)} \right],
\]  \quad (26)

where

\[
A_{11}^{(i)}(\alpha) \triangleq \begin{pmatrix} L^*(\alpha) & 0 \\ 0 & L(\alpha) \end{pmatrix}, \quad \psi^{(i)} \triangleq \begin{pmatrix} \psi_1^{(i)}(r, \Omega, E) \\ \psi_2^{(i)}(r, \Omega, E) \end{pmatrix},
\]  \quad (27)
and where the bilinear concomitant, \( P^{(1)}[\delta u, \psi^{(1)}] \), is defined on the phase-space boundary \((\partial V \times \partial \Omega)\) as follows:

\[
P^{(1)}[\delta u, \psi^{(1)}] \equiv \int_{\Omega} dE \int_{\partial V (\partial E \times \partial \Omega)} \delta \varphi (r, \Omega, E) \psi^{(1)}(r, \Omega, E) dA
\]

\[
- \int_{\Omega} dE \int_{\partial V (\partial E \times \partial \Omega)} \Omega \cdot n \delta \varphi (r, \Omega, E) \psi^{(1)}(r, \Omega, E) dA
\]

\[
+ \int_{\Omega} dE \int_{\partial V (\partial E \times \partial \Omega)} \Omega \cdot n \delta \varphi^+ (r, \Omega, E) \psi^{(1)}(r, \Omega, E) dA
\]

\[
- \int_{\Omega} dE \int_{\partial V (\partial E \times \partial \Omega)} \Omega \cdot n \delta \varphi^+ (r, \Omega, E) \psi^{(1)}(r, \Omega, E) dA.
\]

In order to simplify the notation, the superscript “zero” denoting nominal values was omitted in the definitions provided in Eqs.(27) and (28), and will be omitted henceforth. This simplification should not cause any loss of clarity, since it will become clear from the context which quantities are to be evaluated/computed using the nominal values for the model parameters.

(iv) Identify the term on the left-side of Eq. (26) with the indirect effect term defined in Eq. (18) and use Eq. (26) in conjunction with the boundary conditions given in Eq. (20) to construct the following 1st-Level Adjoint Sensitivity System (1st-LASS) for the 1st-level adjoint function \( \psi^{(1)}(r, \Omega, E) \):

\[
A_{ii}^{(1)}(\alpha) \psi^{(1)}(r, \Omega, E) = \Theta^{(1)}(r, \Omega, E),
\]

where

\[
\Theta^{(1)}(r, \Omega, E) \equiv \left( \frac{\partial G(d; \psi, \varphi^+) / \partial \varphi}{\partial G(d; \psi, \varphi^+) / \partial \varphi^+} \right)
\]

In component form, Eq.(29) reads:

\[
L^* (\alpha) \psi^{(1)}_1 (r, \Omega, E) = \partial G(d; \psi, \varphi^+) / \partial \varphi,
\]

\[
L (\alpha) \psi^{(1)}_2 (r, \Omega, E) = \partial G(d; \psi, \varphi^+) / \partial \varphi^+.
\]

(v) The boundary conditions for \( \psi^{(1)}(r, \Omega, E) \) are now chosen to cause the bilinear concomitant \( P^{(1)}[\delta u, \psi^{(1)}] \) in Eq. (28) to vanish while ensuring that Eq.(29) is well posed. These considerations are fulfilled by imposing the following boundary conditions on the components of \( \psi^{(1)}(r, \Omega, E) \):

\[
\psi^{(1)}_1 (r_1, \Omega, E) = 0, \ r_1 \in \partial V, \ \Omega \cdot n > 0; \ \psi^{(1)}_2 (r_2, \Omega, E) = 0, \ r_2 \in \partial V, \ \Omega \cdot n < 0; \ 0 < E < E_f.
\]

In component form, Eq.(32) reads:

\[
L^* (\alpha) \psi^{(1)}_1 (r, \Omega, E) = \partial G(d; \psi, \varphi^+) / \partial \varphi,
\]

\[
L (\alpha) \psi^{(1)}_2 (r, \Omega, E) = \partial G(d; \psi, \varphi^+) / \partial \varphi^+.
\]
(vi) Use the 1st-LFSS defined by Eqs. (29) and (32) together with Eq. (25) and (26) to obtain the following expression for the indirect-effect term, cf. Eq. (18), in terms of the 1st-level adjoint function \( \psi^{(1)}(r, \Omega, E) \):

\[
\left\{ \delta R \left( \varphi^0, \varphi^{+0}, \alpha^0, \delta \varphi, \delta \varphi^+ \right) \right\}_{\text{ind}} = \left\{ \psi^{(1)}(r, \Omega, E), \ Q^{(1)} \left( \alpha^0; \varphi^0, \varphi^{+0}; \delta \alpha \right) \right\}_{(l)}.
\]

As indicated in Eq. (31), the function \( \psi^{(1)}_1(r, \Omega, E) \) is obtained by applying the adjoint transport solver with the source \( \partial G / \partial \varphi \), while the function \( \psi^{(1)}_2(r, \Omega, E) \) is computed by solving the forward transport equation with the source \( \partial G / \partial \varphi^+ \). Thus, after these two components of the 1st-level adjoint function \( \psi^{(1)}(r, \Omega, E) \) become available, the “indirect-effect term” is computed efficiently and exactly by simply performing the integrations (“quadratures”) indicated by the inner-product on the right-side of Eq. (33).

Replacing Eqs. (33) and (17) in Eq. (16) eliminates the appearance of the functions \( \delta \varphi, \delta \varphi^+ \), and \( \delta \alpha \) in the resulting expression so that the \textit{total 1st-order response sensitivity} in terms of the 1st-level adjoint function \( \psi^{(1)}(r, \Omega, E) \) becomes:

\[
\delta R \left( \varphi, \varphi^+, \alpha; \delta \varphi, \delta \varphi^+ ; \delta \alpha \right) \triangleq \sum_{m=1}^{N_\alpha} \left[ \delta R \left( \varphi, \varphi^+, \alpha; \psi^{(1)} \right) \right]_{\partial \alpha_m},
\]

\[
= \sum_{i=1}^{J_j} \int \int dV \int dE \int_0^{E_j} \left[ \frac{\partial G}{\partial d_i} \left( \varphi, \varphi^+ \right) \right] \delta d_i + \left\{ \psi^{(1)}(r, \Omega, E), \ Q^{(1)} \left( \alpha^0; \varphi^0, \varphi^{+0}; \delta \alpha \right) \right\}_{(l)}.
\]

The \textit{partial 1st-order response sensitivities}, denoted in Eq. (34) as \( \dd{\partial R \left( \varphi, \varphi^+, \alpha; \psi^{(1)} \right)}{\partial \alpha_m} \), \( m = 1, \ldots, N_\alpha \), of the response \( R \left( \varphi, \varphi^+, \alpha \right) \) to a generic parameter \( \alpha_m \) are obtained from Eq. (34) by identifying the quantities that multiply the various parameter variations \( \delta \alpha_m \), and have the following expressions:

\[
\text{For } j = 1, \ldots, J_j : \quad \frac{\partial R \left( \varphi, \varphi^+, \alpha; \psi^{(1)} \right)}{\partial \alpha_j} \triangleq \frac{\partial R \left( \varphi, \varphi^+, \alpha; \psi^{(1)} \right)}{\partial t_j},
\]

\[
= \int \int dV \int dE \left[ \psi^{(1)}_1(r, \Omega, E) \varphi(r, \Omega, E) + \psi^{(1)}_2(r, \Omega, E) \varphi^+(r, \Omega, E) \right] \frac{\partial \Sigma_j(t, r, E)}{\partial t_j}.
\]
The same model parameter could appear in the definitions of more than one macroscopic cross section. For example, the isotopic number density of some element, generically denoted as $N_i$, could be an...
imprecisely known model parameter which might appear in the definitions of the total, scattering, and/or fission macroscopic cross sections, as well as in the forward and/or adjoint source terms. In such a case, the sensitivity of the response to the generic model parameter $N_i$ would be the sum of the corresponding partial sensitivities computed from the above expressions.

IV. THE SECOND-LEVEL FORWARD AND ADJOINT SENSITIVITY SYSTEMS FOR COMPUTING SECOND-ORDER RESPONSE SENSITIVITIES TO VARIATIONS IN MODEL PARAMETERS

The 2nd-order response sensitivities will be obtained by applying the 2nd-ASAM developed by Cacuci\textsuperscript{10-12}, which relies on the construction of a 2nd-Level Adjoint Sensitivity System (2nd-LASS) for each of the 1st-order sensitivities defined by Eqs. (35) through (41).

\textbf{IV.A. Computation of the 2nd-Order Sensitivities $\partial^2 R\left(\phi, \phi^+; \psi^{(1)}; \psi^{(2)}; \alpha\right)$, $j = 1, \ldots, J; m_2 = 1, \ldots, J_\alpha$.}

The 2nd-order sensitivities $\partial^2 R\left(\phi, \phi^+; \psi^{(1)}; \psi^{(2)}; \alpha\right)/\partial t_j \partial \alpha_{m_2}$, $j = 1, \ldots, J; m_2 = 1, \ldots, J_\alpha$, will ultimately depend on a 2nd-level adjoint function (which is denoted as $\psi^{(2)}$) and are obtained by determining the G-differential of the 1st-order sensitivity given in Eq. (35), which yields the following expression:

$$\delta \left[ \frac{\partial R\left(\phi, \phi^+; \alpha; \psi^{(1)}\right)}{\partial t_j} \right] = \left\{ \delta \left[ \frac{\partial R\left(\phi, \phi^+; \alpha; \psi^{(1)}\right)}{\partial t_j} \right] \right\}_{\text{dir}} + \left\{ \delta \left[ \frac{\partial R\left(\phi, \phi^+; \alpha; \psi^{(1)}\right)}{\partial t_j} \right] \right\}_{\text{ind}}, \quad j = 1, \ldots, J_\alpha;$$

where for $j = 1, \ldots, J_\alpha$ :

$$\Delta = \int_{E_i} dV \int_0^1 d\Omega \int_0^{2\pi} dE \left[ \psi^{(1)}_1 \left(\mathbf{r}, \Omega, E\right) \phi\left(\mathbf{r}, \Omega, E\right) + \psi^{(1)}_2 \left(\mathbf{r}, \Omega, E\right) \phi^+\left(\mathbf{r}, \Omega, E\right) \right] \sum_{m_2 = 1}^{J_\alpha} \frac{\partial^2 \Sigma_t}{\partial t_j \partial \alpha_{m_2}} \delta t_m, \quad (43)$$

and
\[
\left\{ \delta \frac{\partial R(\varphi, \varphi^+, \alpha, \psi^{(i)})}{\partial t_j} \right\}_{\text{ind}} \triangleq \\
- \int dV \int d\Omega \int dE \left[ \delta \psi_1^{(i)}(r, \Omega, E) \varphi(r, \Omega, E) + \delta \varphi(r, \Omega, E) \psi_1^{(i)}(r, \Omega, E) \right] \frac{\partial \Sigma_i(t, r, E)}{\partial t_j} \\
- \int dV \int d\Omega \int dE \left[ \delta \psi_2^{(i)}(r, \Omega, E) \varphi^+(r, \Omega, E) + \delta \varphi^+(r, \Omega, E) \psi_2^{(i)}(r, \Omega, E) \right] \frac{\partial \Sigma_i(t, r, E)}{\partial t_j}. 
\]

(44)

The direct-effect term defined in Eq. (43) can be computed immediately. On the other hand, the indirect-effect term defined in Eq. (44) can be computed only after having obtained both the solution \( \delta u(r, \Omega, E) \) of the 1st-LFSS defined by Eq.(19), and the variation \( \delta \psi^{(i)}(r, \Omega, E) \), which is the solution of the system of equations obtained by G-differentiating the 1st-LASS, cf. Eqs. (29) and (32), namely

\[
L' (\alpha) \delta \psi_1^{(i)}(r, \Omega, E) - \frac{\partial^2 G(d: \varphi, \varphi^+)}{\partial \varphi^2} \delta \varphi - \frac{\partial^2 G(d: \varphi, \varphi^+)}{\partial \varphi \partial \varphi^+} \delta \varphi^+ = Q_1^{(2)}(\alpha, \psi^{(i)}; \delta \alpha), \\
L(\alpha) \delta \psi_2^{(i)}(r, \Omega, E) - \frac{\partial^2 G(d: \varphi, \varphi^+)}{\partial \varphi^+ \partial \varphi} \delta \varphi - \frac{\partial^2 G(d: \varphi, \varphi^+)}{\partial \varphi^+ \partial \varphi^+} \delta \varphi^+ = Q_2^{(2)}(\alpha, \psi^{(i)}; \delta \alpha), 
\]

(45)

\[
\delta \psi_1^{(i)}(r, \Omega, E) = 0, \quad r_s \in \partial V, \quad \Omega \cdot \mathbf{n} > 0; \quad \delta \psi_2^{(i)}(r, \Omega, E) = 0, \quad r_s \in \partial V, \quad \Omega \cdot \mathbf{n} < 0; \quad 0 < E < E_f, 
\]

(46)

where

\[
Q_1^{(2)}(\alpha^0, \psi^{(i)}; \delta \alpha) \equiv \int d\Omega' \int dE' [\delta \Sigma_i(r, E \rightarrow E', \Omega \rightarrow \Omega')] \psi_1^{(i)}(r, \Omega', E') \\
+ \delta \left[ \nu \Sigma_j(f; r, E) \right] \int d\Omega' \int dE' \chi(p; r, E \rightarrow E') \psi_1^{(i)}(r, \Omega', E') - \delta \Sigma_i(r, E) \psi_1^{(i)}(r, \Omega, E) \\
+ \left[ \nu \Sigma_j(f; r, E) \right] \int d\Omega' \int dE' \delta \chi(p; r, E \rightarrow E') \psi_1^{(i)}(r, \Omega', E') + \sum_{j=1}^{J_d} \frac{\partial^2 G(d: \varphi, \varphi^+)}{\partial \varphi \partial d_j} \delta d_j. 
\]

(47)

and

\[
Q_2^{(2)}(\alpha^0, \psi^{(i)}; \delta \alpha) \equiv \int d\Omega' \int dE' [\delta \Sigma_i(r, E \rightarrow E, \Omega' \rightarrow \Omega')] \psi_2^{(i)}(r, \Omega', E') \\
+ \int d\Omega' \int dE' \chi(p; r, E' \rightarrow E) \delta \left[ \nu \Sigma_j(f; r, E') \right] \psi_2^{(i)}(r, \Omega', E') - \delta \Sigma_i(r, E) \psi_2^{(i)}(r, \Omega, E) \\
+ \int d\Omega' \int dE' \nu \Sigma_j(f; r, E') \delta \chi(p; r, E' \rightarrow E) \psi_2^{(i)}(r, \Omega', E') + \sum_{j=1}^{J_d} \frac{\partial^2 G(d: \varphi, \varphi^+)}{\partial \varphi^+ \partial d_j} \delta d_j. 
\]

(48)
It has already been discussed in Section III that it is computationally expensive to obtain $\delta u(r, \Omega, E)$, since the 1st-LFSS would need to be solved anew for every variation in the model parameters. It is also evident from Eqs. (45) and (46) that the evaluation of the function $\delta \psi^{(1)}(r, \Omega, E)$ is at least as expensive computationally as determining the variation $\delta u(r, \Omega, E)$. The system comprising Eqs. (45) and (46) is called\textsuperscript{10-12} the 2nd-Level Forward Sensitivity System (2nd-LFSS).

To avoid the need for solving the 2nd-LFSS, the indirect-effect term defined in Eq. (44) will be expressed in terms of a 2nd-Level Adjoint Sensitivity System (2nd-LASS), which will be constructed by following the general principles introduced by Cacuci\textsuperscript{10-12}, comprising the following sequence of steps:

(i) Write the coupled 2nd-LFSS and 1st-LFSS, namely Eqs. (45) and (19), in the following matrix-form:

$$
\begin{pmatrix}
A^{(1)}_{11}(\alpha) & F^{(2)}_{12}(\alpha) \\
0 & F^{(1)}_{11}(\alpha)
\end{pmatrix}
\begin{pmatrix}
\delta \psi^{(1)}(r, \Omega, E) \\
\delta u(r, \Omega, E)
\end{pmatrix}
=
\begin{pmatrix}
Q^{(2)}(\alpha, \psi^{(1)}; \delta \alpha) \\
Q^{(1)}(\alpha; \varphi^*; \delta \alpha)
\end{pmatrix},
$$

(49)

where

$$
F^{(2)}_{12}(\alpha) \equiv \begin{pmatrix}
-\frac{\partial^2 G(d; \varphi, \varphi^*)}{\partial \varphi^2} & -\frac{\partial^2 G(d; \varphi, \varphi^*)}{\partial \varphi \partial \varphi^*} \\
-\frac{\partial^2 G(d; \varphi, \varphi^*)}{\partial \varphi \partial \varphi^*} & -\frac{\partial^2 G(d; \varphi, \varphi^*)}{\partial \varphi^* \partial \varphi^*}
\end{pmatrix},
Q^{(2)}(\alpha, \psi^{(1)}; \delta \alpha) \equiv \begin{pmatrix}
Q^{(2)}_{1}(\alpha, \psi^{(1)}; \delta \alpha) \\
Q^{(2)}_{2}(\alpha, \psi^{(1)}; \delta \alpha)
\end{pmatrix}.
$$

(50)

(ii) Define an inner product $\langle u^{(2)}(r, \Omega, E), v^{(2)}(r, \Omega, E) \rangle_{(2)}$ of two vector-valued functions

$$
\langle u^{(2)}(r, \Omega, E), v^{(2)}(r, \Omega, E) \rangle_{(2)} \equiv \left[u_{11}^{(2)}(r, \Omega, E), u_{12}^{(2)}(r, \Omega, E)\right]^\top \text{ and } v^{(2)}(r, \Omega, E) \equiv \left[v_{11}^{(2)}(r, \Omega, E), v_{12}^{(2)}(r, \Omega, E)\right]^\top,
$$

with

$$
u_{11}^{(2)}(r, \Omega, E) \equiv \left[v_{11}^{(2)}(r, \Omega, E), v_{12}^{(2)}(r, \Omega, E)\right]^\top, \nu_{12}^{(2)}(r, \Omega, E) \equiv \left[u_{11}^{(2)}(r, \Omega, E), u_{12}^{(2)}(r, \Omega, E)\right]^\top,
$$

$$
u_{11}^{(2)}(r, \Omega, E) \in L_{2}((V \times \Omega) \times E), \nu_{12}^{(2)}(r, \Omega, E) \in L_{2}((V \times \Omega) \times E), i, j = 1, 2,
$$

as follows:

$$
\langle u^{(2)}(r, \Omega, E), v^{(2)}(r, \Omega, E) \rangle_{(2)} \equiv \sum_{i=1}^{2} \int dV \int_{\Omega}^{E} \int dE u_{i}^{(2)}(r, \Omega, E) v_{i}^{(2)}(r, \Omega, E)
$$

(51)
(ii) Define a Hilbert space, denoted as \( \mathcal{H}_2 \), which is endowed with the inner product defined in Eq. (51). For a block-matrix-valued linear operator \( L^{(2)} \equiv \begin{pmatrix} L_{11}^{(2)} & L_{12}^{(2)} \\ L_{21}^{(2)} & L_{22}^{(2)} \end{pmatrix} \), having two-by-two dimensional the component matrices \( L_{ij}^{(2)} \), \( i, j = 1, 2 \), define its formal adjoint operator, denoted as

\[
A^{(2)} \equiv \begin{pmatrix} A_{11}^{(2)} & A_{12}^{(2)} \\ A_{21}^{(2)} & A_{22}^{(2)} \end{pmatrix},
\]

through the following relationship:

\[
\left\langle v^{(2)}, L^{(2)} u^{(2)} \right\rangle_{(2)} = \left\langle u^{(2)}, A^{(2)} v^{(2)} \right\rangle_{(2)} + P^{(2)} \left[ u^{(2)}, v^{(2)} \right],
\]

where \( P^{(2)} \left[ u^{(2)}, v^{(2)} \right] \) denotes the corresponding bilinear concomitant on the phase-space boundary \( \partial V \times \partial \Omega \times \partial E \).

(iii) Apply the definition provided in Eq. (51) to form the inner product of Eq. (49) with a yet undefined function \( \psi_j^{(2)} (r, \Omega, E) \equiv \left[ \psi_{21,j}^{(2)} (r, \Omega, E), \psi_{22,j}^{(2)} (r, \Omega, E) \right]^{\dagger} \), where \( \psi_{i,j}^{(2)} \equiv \left[ \psi_{i1,j}^{(2)} (r, \Omega, E), \psi_{i2,j}^{(2)} (r, \Omega, E) \right]^{\dagger} \), \( \psi_{2,j}^{(2)} \equiv \left[ \psi_{21,j}^{(2)} (r, \Omega, E), \psi_{22,j}^{(2)} (r, \Omega, E) \right]^{\dagger} \), with \( \psi_{mn,j}^{(2)} (r, \Omega, E) \in \mathcal{L}_2 (V \times \Omega \times E) \), \( m, n = 1, 2 \), to obtain:

\[
\left\langle \psi_{1,j}^{(2)}, \left( A_{11}^{(2)} (\alpha) \right. \begin{pmatrix} F_{12}^{(2)} (\alpha) \\ 0 \end{pmatrix} \left( \delta \psi^{(1)} (r, \Omega, E) \right) \left. \right| \delta u (r, \Omega, E) \right\rangle_{(2)} = \left\langle \psi_{1,j}^{(2)} \right| \left( Q^{(2)} (\alpha, \psi^{(1)}; \delta \alpha) \right) \right\rangle_{(2)} + \left\langle \psi_{2,j}^{(2)} \right| \left( Q^{(1)} (\alpha; \varphi, \varphi^{+}; \delta \alpha) \right) \right\rangle_{(2)}.
\]

(iv) Use the relation shown in Eq. (52) to recast the left side of Eq. (53) in the following form:

\[
\left\langle \psi_{1,j}^{(2)}, \left( A_{11}^{(2)} (\alpha) \right. \begin{pmatrix} F_{12}^{(2)} (\alpha) \\ 0 \end{pmatrix} \left( \delta \psi^{(1)} \right) \left. \right| \delta u \right\rangle_{(2)} = \left\langle \left( \delta \psi^{(1)} \right)^{\dagger} \left[ \begin{array}{cc} A_{11}^{(2)} (\alpha) & \delta \psi^{(1)} \\ 0 & F_{11}^{(2)} (\alpha) \end{array} \right] \left( \delta u \right) \right\rangle_{(2)} + P^{(2)} \left[ \psi_{j}^{(2)}, \delta \psi^{(1)}, \delta u \right],
\]

where the symbol \( \left[ \quad \right]^{\dagger} \) indicates “adjoint” and where the bilinear concomitant \( P^{(2)} \left[ \psi_{j}^{(2)}, \delta \psi^{(1)}, \delta u \right] \) is defined as follows:
\[ P^{(2)} \left[ \psi_{j}^{(2)}, \delta \psi^{(1)}, \delta u \right] \approx \int_{0}^{E_f} \int_{\Omega \cdot n < 0} d\Omega \int_{\partial V} |\Omega \cdot n| \delta \varphi (r, \Omega, E) \psi_{21,j}^{(2)} (r, \Omega, E) dA \\
- \int_{0}^{E_f} \int_{\Omega \cdot n > 0} d\Omega \int_{\partial V} |\Omega \cdot n| \delta \varphi (r, \Omega, E) \psi_{21,j}^{(2)} (r, \Omega, E) dA \\
- \int_{0}^{E_f} \int_{\Omega \cdot n > 0} d\Omega \int_{\partial V} |\Omega \cdot n| \delta \varphi^+ (r, \Omega, E) \psi_{22,j}^{(2)} (r, \Omega, E) dA \\
- \int_{0}^{E_f} \int_{\Omega \cdot n < 0} d\Omega \int_{\partial V} |\Omega \cdot n| \delta \varphi^+ (r, \Omega, E) \psi_{22,j}^{(2)} (r, \Omega, E) dA \\
- \int_{0}^{E_f} \int_{\Omega \cdot n > 0} d\Omega \int_{\partial V} |\Omega \cdot n| \delta \varphi^{(1)} \psi_{11,j}^{(2)} (r, \Omega, E) dA \\
- \int_{0}^{E_f} \int_{\Omega \cdot n < 0} d\Omega \int_{\partial V} |\Omega \cdot n| \delta \varphi^{(1)} \psi_{11,j}^{(2)} (r, \Omega, E) dA \\
- \int_{0}^{E_f} \int_{\Omega \cdot n > 0} d\Omega \int_{\partial V} |\Omega \cdot n| \delta \varphi^{(1)} \psi_{12,j}^{(2)} (r, \Omega, E) dA \\
- \int_{0}^{E_f} \int_{\Omega \cdot n < 0} d\Omega \int_{\partial V} |\Omega \cdot n| \delta \varphi^{(1)} \psi_{12,j}^{(2)} (r, \Omega, E) dA. \]

(v) Reduce the bilinear concomitant \( P^{(2)} \left[ \psi_{j}^{(2)}, \delta \psi^{(1)}, \delta u \right] \) in Eq. (55) to zero by using the boundary conditions shown in Eqs. (20) and (46), and by imposing on the components of the 2nd-level adjoint function \( \psi_{j}^{(2)} (r, \Omega, E) \) the following boundary conditions:

\[ \psi_{11,j}^{(2)} (r, \Omega, E) = 0, \ r_s \in \partial V, \ \Omega \cdot n < 0; \ \psi_{12,j}^{(2)} (r, \Omega, E) = 0, \ r_s \in \partial V, \ \Omega \cdot n > 0; \ 0 < E < E_f, \]
\[ \psi_{21,j}^{(2)} (r, \Omega, E) = 0, \ r_s \in \partial V, \ \Omega \cdot n > 0; \ \psi_{22,j}^{(2)} (r, \Omega, E) = 0, \ r_s \in \partial V, \ \Omega \cdot n < 0; \ 0 < E < E_f. \]  

(vi) Identify the first term on the right-side of Eq. (54) with the indirect-effect term defined in Eq. (44) and use Eq. (53) to obtain the following expression for the indirect-effect term defined in Eq. (44):
\[
\left\{ \frac{\delta R(\varphi, \varphi^+, \alpha, \psi^{(1)})}{\partial t_f} \right\} \bigg|_{\text{ind}} \leq \left\{ \psi^{(2)}_{1,j} \left( \begin{array}{c} Q^{(2)}(\alpha, \psi^{(1)}; \delta \alpha) \\ Q^{(1)}(\alpha; \varphi, \varphi^+; \delta \alpha) \end{array} \right) \right\}_{(2)}
\]

\[
= \int dV \int_{E_f} d\Omega \int dE \varphi^{(2)}_{11,j}(r, \Omega, E) \left( \int d\Omega' \int_{E_f} dE' \left[ \delta \Sigma_s (r, E \rightarrow E', \Omega \rightarrow \Omega') \right] \psi^{(1)}_1 (r, \Omega', E') \right)
\]

\[
+ \left( \begin{array}{c} \delta \left[ \nu \Sigma_f (f \cdot r, E) \right] \int d\Omega' \int_{E_f} dE' \chi (p \cdot r, E \rightarrow E') \psi^{(1)}_1 (r, \Omega', E') \right) - \delta \Sigma_s (r, E) \psi^{(1)}_1 (r, \Omega, E)
\]

\[
+ \left( \begin{array}{c} \nu \Sigma_j (f \cdot r, E) \int d\Omega' \int_{E_f} dE' \delta \chi (p \cdot r, E \rightarrow E') \psi^{(1)}_1 (r, \Omega', E') \right) + \sum_{i=1}^{J_d} \frac{\delta^2 G (d \cdot \varphi, \varphi^+)}{\partial \varphi \partial \vec{d}_i} \delta d_i
\]

\[
+ \int dV \int_{E_f} d\Omega \int dE \varphi^{(2)}_{12,j}(r, \Omega, E) \left( \int d\Omega' \int_{E_f} dE' \left[ \delta \Sigma_s (r, E \rightarrow E', \Omega \rightarrow \Omega') \right] \psi^{(2)}_2 (r, \Omega', E') \right)
\]

\[
+ \left( \begin{array}{c} \delta \Sigma_s (r, E') \int d\Omega' \int_{E_f} dE' \chi (p \cdot r, E \rightarrow E') \psi^{(1)}_2 (r, \Omega', E') \right) - \delta \Sigma_s (r, E) \psi^{(1)}_2 (r, \Omega, E)
\]

\[
+ \int d\Omega' \int_{E_f} dE' \nu \Sigma_j (f \cdot r, E') \delta \chi (p \cdot r, E \rightarrow E') \psi^{(1)}_2 (r, \Omega', E') + \sum_{i=1}^{J_d} \frac{\delta^2 G (d \cdot \varphi, \varphi^+)}{\partial \varphi^+ \partial \vec{d}_i} \delta d_i
\]

\[
+ \int dV \int_{E_f} d\Omega \int dE \varphi^{(2)}_{21,j}(r, \Omega, E) \left[ \delta Q (q \cdot r, \Omega, E) - \delta \Sigma_s (r, E \rightarrow E', \Omega \rightarrow \Omega') \varphi (r, \Omega, E) \right]
\]

\[
+ \int d\Omega' \int_{E_f} dE' \varphi (r, \Omega', E') \left[ \delta \Sigma_s (s \cdot r, E' \rightarrow E, \Omega' \rightarrow \Omega) \right]
\]

\[
+ \int d\Omega' \int_{E_f} dE' \varphi (r, \Omega', E') \left[ \delta \Sigma_s (s \cdot r, E \rightarrow E', \Omega \rightarrow \Omega') \right]
\]

\[
+ \int d\Omega' \int_{E_f} dE' \varphi (r, \Omega', E') \delta \Sigma_s (s \cdot r, E \rightarrow E', \Omega \rightarrow \Omega') \left[ \nu \Sigma_j (f \cdot r, E') \right]
\]

\[
+ \int dV \int_{E_f} d\Omega \int dE \varphi^{(2)}_{22,j}(r, \Omega, E) \left[ \delta Q^+ (k \cdot r, \Omega, E) - \delta \Sigma_s (t \cdot r, E) \varphi^+ (r, \Omega, E) \right]
\]

\[
+ \int d\Omega' \int_{E_f} dE' \varphi^+ (r, \Omega', E') \left[ \delta \Sigma_s (s \cdot r, E \rightarrow E', \Omega \rightarrow \Omega') \right]
\]

\[
+ \int d\Omega' \int_{E_f} dE' \varphi^+ (r, \Omega', E') \left[ \delta \Sigma_s (s \cdot r, E \rightarrow E', \Omega \rightarrow \Omega') \right]
\]

\[
+ \delta \left[ \nu \Sigma_j (f \cdot r, E) \right] \int d\Omega' \int_{E_f} dE' \chi (p \cdot r, E \rightarrow E') \varphi^+ (r, \Omega', E')
\]

\[
+ \nu \Sigma_j (f \cdot r, E) \int d\Omega' \int_{E_f} dE' \delta \chi (p \cdot r, E \rightarrow E') \varphi^+ (r, \Omega', E')
\]

\[
(57)
\]
where the components of the 2\textsuperscript{nd}-level adjoint function $\psi_j^{(2)}(r,\Omega,E)$ are the solutions of the following system of equations:

$$
\begin{bmatrix}
-A_{11}^{(a)}(a) & 0 \\
F_{12}^{(a)}(a) & F_{11}^{(a)}(a)
\end{bmatrix}
\begin{bmatrix}
\psi_{1_j}^{(2)} \\
\psi_{2_j}^{(2)}
\end{bmatrix}
=
\begin{bmatrix}
-\varphi(r,\Omega,E)\partial\Sigma_r(t;r,E)/\partial t_j \\
-\varphi^+(r,\Omega,E)\partial\Sigma_r(t;r,E)/\partial t_j \\
-\psi_1^{(1)}(r,\Omega,E)\partial\Sigma_r(t;r,E)/\partial t_j \\
\psi_2^{(1)}(r,\Omega,E)\partial\Sigma_r(t;r,E)/\partial t_j
\end{bmatrix},
$$

which, in equivalent component form, reads

$$
L(a)\psi_{1_{j}}^{(2)}(r,\Omega,E) = -\varphi(r,\Omega,E)\frac{\partial\Sigma_r(t;r,E)}{\partial t_j}, \quad j = 1,\ldots,J, \quad (58)
$$

$$
L'(a)\psi_{1_{j}}^{(2)}(r,\Omega,E) = -\varphi^+(r,\Omega,E)\frac{\partial\Sigma_r(t;r,E)}{\partial t_j}, \quad j = 1,\ldots,J, \quad (59)
$$

$$
L'(a)\psi_{1_{j}}^{(2)}(r,\Omega,E) = \frac{\partial^2 G(d;\varphi,\varphi^+)}{\partial \varphi^2}\psi_{1_{j}}^{(2)}(r,\Omega,E) + \frac{\partial^2 G(d;\varphi,\varphi^+)}{\partial \varphi^+ \partial \varphi}\psi_{1_{j}}^{(2)}(r,\Omega,E) \\
-\psi_1^{(1)}(r,\Omega,E)\frac{\partial\Sigma_r(t;r,E)}{\partial t_j}, \quad j = 1,\ldots,J, \quad (60)
$$

$$
L(a)\psi_{2_{j}}^{(2)}(r,\Omega,E) = \frac{\partial^2 G(d;\varphi,\varphi^+)}{\partial \varphi \partial \varphi^+}\psi_{1_{j}}^{(2)}(r,\Omega,E) + \frac{\partial^2 G(d;\varphi,\varphi^+)}{\partial \varphi^+ \partial \varphi}\psi_{1_{j}}^{(2)}(r,\Omega,E) \\
-\psi_2^{(1)}(r,\Omega,E)\frac{\partial\Sigma_r(t;r,E)}{\partial t_j}, \quad j = 1,\ldots,J, \quad (61)
$$

Equations (58) through (61) together with the boundary conditions given in Eq.(56) constitute the 2\textsuperscript{nd}-Level Adjoint Sensitivity System (2\textsuperscript{nd}-LASS) for the 2\textsuperscript{nd}-level adjoint function $\psi_j^{(2)}(r,\Omega,E)$, $j = 1,\ldots,J$. These equations can be solved successively by using a total of two “forward transport” and two “adjoint transport” computations, for each of the imprecisely known scalar model parameters appearing in the definition of the total macroscopic cross section $\Sigma_r(t;r,E)$. Subsequently, the 2\textsuperscript{nd}-level adjoint function $\psi_j^{(2)}(r,\Omega,E)$ is used in Eq.(57), which eliminates the dependence of the 2\textsuperscript{nd}-order sensitivities on parameter variations, directly or indirectly through the variations $\delta u(r,\Omega,E)$ and $\delta \psi^{(1)}(r,\Omega,E)$, to compute efficiently and exactly the indirect-effect term defined in Eq. (44).
(vii) The 2nd-order partial sensitivities \( \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \psi^{(2)}; \alpha)}{\partial t_j \partial t_{m_2}} \), for

\( j = 1, ..., J_j; \) \( m_2 = 1, ..., J_{\alpha} \), can now be determined by replacing in Eq. (42) the expressions of the indirect effect term provided in Eq. (57) together with the expression of the direct-effect term provided in Eq. (43), and subsequently identifying in the resulting expression the quantities multiplying the parameter variations \( \delta \alpha_{m_2} \). This procedure yields the following expressions:

For \( j, m_2 = 1, ..., J_j \):

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \psi^{(2)}; \alpha)}{\partial t_j \partial t_{m_2}} = -\int dV \int_0^{E_f} dE \int_{4\pi}^0 D \left[ \psi^{(1)}_{11,j} (\mathbf{r}, \Omega, E) \varphi (\mathbf{r}, \Omega, E) + \psi^{(1)}_{12,j} (\mathbf{r}, \Omega, E) \varphi^+ (\mathbf{r}, \Omega, E) \right] \frac{\partial^2 \Sigma_j (t; r, \Omega, E)}{\partial t_j \partial t_{m_2}}
\]

\[
+ \int dV \int_0^{E_f} dE \int_{4\pi}^0 \psi^{(2)}_{11,j} (\mathbf{r}, \Omega, E) \psi^{(1)}_{11,j} (\mathbf{r}, \Omega, E) + \psi^{(2)}_{12,j} (\mathbf{r}, \Omega, E) \psi^{(1)}_{12,j} (\mathbf{r}, \Omega, E) \psi^{(2)}_{11,j} (\mathbf{r}, \Omega, E) + \psi^{(2)}_{21,j} (\mathbf{r}, \Omega, E) \varphi (\mathbf{r}, \Omega, E) + \psi^{(2)}_{22,j} (\mathbf{r}, \Omega, E) \varphi^+ (\mathbf{r}, \Omega, E) \right] ;
\]

For \( j = 1, ..., J_j; \) \( m_2 = 1, ..., J_{\alpha} \):

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \psi^{(2)}; \alpha)}{\partial t_j \partial \alpha_{m_2}} = \int dV \int_0^{E_f} dE \int_{4\pi}^0 \psi^{(2)}_{11,j} (\mathbf{r}, \Omega, E) \int dE' \psi^{(1)}_{11,j} (\mathbf{r}, \Omega', E') \frac{\partial \Sigma_j (s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial \alpha_{m_2}}
\]

\[
+ \int dV \int_0^{E_f} dE \int_{4\pi}^0 \psi^{(2)}_{12,j} (\mathbf{r}, \Omega, E) \int dE' \psi^{(1)}_{12,j} (\mathbf{r}, \Omega', E') \frac{\partial \Sigma_j (s; r, E \rightarrow E', \Omega \rightarrow \Omega')} {\partial \alpha_{m_2}}
\]

\[
+ \int dV \int_0^{E_f} dE \int_{4\pi}^0 \psi^{(2)}_{21,j} (\mathbf{r}, \Omega, E) \int dE' \varphi (\mathbf{r}, \Omega', E') \frac{\partial \Sigma_j (s; r, E \rightarrow E', \Omega \rightarrow \Omega')} {\partial \alpha_{m_2}}
\]

\[
+ \int dV \int_0^{E_f} dE \int_{4\pi}^0 \psi^{(2)}_{22,j} (\mathbf{r}, \Omega, E) \int dE' \varphi^+ (\mathbf{r}, \Omega', E') \frac{\partial \Sigma_j (s; r, E \rightarrow E', \Omega \rightarrow \Omega')} {\partial \alpha_{m_2}} ;
\]
For \( j = 1, \ldots, J_f; \ m_2 = 1, \ldots, J_f \):
\[
\frac{\partial^2 R\left(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha\right)}{\partial t_f \partial f_{m_2}} = 
\]
\[= \int dV \int_{4\pi} \int dE \psi^{(2)}_{11,j}(r, \Omega, E) \frac{\partial}{\partial f_{m_2}} \left[ \nu \Sigma_j(f; r, E) \right] \int d\Omega' \int_{4\pi} dE' \chi(p; r, E \to E') \psi^{(1)}_j(r, \Omega', E') \]
\[+ \int dV \int_{4\pi} \int dE \psi^{(2)}_{12,j}(r, \Omega, E) \int d\Omega' \int_{4\pi} dE' \chi(p; r, E \to E') \psi^{(1)}_j(r, \Omega', E') \frac{\partial}{\partial f_{m_2}} \left[ \nu \Sigma_j(f; r, E') \right] \]
\[+ \int dV \int_{4\pi} \int dE \psi^{(2)}_{21,j}(r, \Omega, E) \int d\Omega' \int_{4\pi} dE' \chi(p; r, E \to E') \frac{\partial}{\partial f_{m_2}} \left[ \varphi(r, \Omega', E') \right] \]
\[+ \int dV \int_{4\pi} \int dE \psi^{(2)}_{22,j}(r, \Omega, E) \int d\Omega' \int_{4\pi} dE' \chi(p; r, E \to E') \frac{\partial}{\partial f_{m_2}} \left[ \varphi^+(r, \Omega', E') \right]. \tag{64} \]

For \( j = 1, \ldots, J_f; \ m_2 = 1, \ldots, J_f \):
\[
\frac{\partial^2 R\left(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha\right)}{\partial t_f \partial p_{m_2}} = 
\]
\[= \int dV \int_{4\pi} \int dE \psi^{(2)}_{11,j}(r, \Omega, E) \int d\Omega' \int_{4\pi} dE' \psi^{(1)}_j(r, \Omega', E') \frac{\partial}{\partial p_{m_2}} \chi(p; r, E \to E') \]
\[+ \int dV \int_{4\pi} \int dE \psi^{(2)}_{12,j}(r, \Omega, E) \int d\Omega' \int_{4\pi} dE' \psi^{(1)}_j(r, \Omega', E') \frac{\partial}{\partial p_{m_2}} \chi(p; r, E' \to E) \]
\[+ \int dV \int_{4\pi} \int dE \psi^{(2)}_{21,j}(r, \Omega, E) \int d\Omega' \int_{4\pi} dE' \varphi(r, \Omega', E') \frac{\partial}{\partial p_{m_2}} \chi(p; r, E' \to E') \]
\[+ \int dV \int_{4\pi} \int dE \psi^{(2)}_{22,j}(r, \Omega, E) \varphi(r, \Omega', E') \frac{\partial}{\partial p_{m_2}} \chi(p; r, E \to E'). \tag{65} \]

For \( j = 1, \ldots, J_f; \ m_2 = 1, \ldots, J_f \):
\[
\frac{\partial^2 R\left(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha\right)}{\partial t_f \partial q_{m_2}} = \int dV \int_{4\pi} \int dE \psi^{(2)}_{21,j}(r, \Omega, E) \frac{\partial}{\partial q_{m_2}} Q(q; r, \Omega, E); \tag{66} \]

For \( j = 1, \ldots, J_f; \ m_2 = 1, \ldots, J_f \):
\[
\frac{\partial^2 R\left(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha\right)}{\partial t_f \partial k_{m_2}} = \int dV \int_{4\pi} \int dE \psi^{(2)}_{22,j}(r, \Omega, E) \frac{\partial}{\partial k_{m_2}} Q^+(k; r, \Omega, E); \tag{67} \]

For \( j = 1, \ldots, J_f; \ m_2 = 1, \ldots, J_f \):
\[
\frac{\partial^2 R\left(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha\right)}{\partial t_f \partial d_{m_2}} = \int dV \int_{4\pi} \int dE \left[ \psi^{(2)}_{11,j}(r, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial d_{m_2}} + \psi^{(2)}_{12,j}(r, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ \partial d_{m_2}} \right]. \tag{68} \]
IV.B. Computation of the 2nd-Order Sensitivities \( \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \theta^{(2)}; \alpha)}{\partial s_j \partial \alpha_m}, \ j = 1,...,J_s; \ m = 1,...,J_\alpha. \)

The 2nd-order sensitivities \( \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \theta^{(2)}; \alpha)}{\partial s_j \partial \alpha_m}, \ j = 1,...,J_s; \ m = 1,...,J_\alpha \) will ultimately depend on a 2nd-level adjoint function (which is denoted as \( \theta^{(2)} \)) and are obtained by determining the G-differential of the 1st-order sensitivity defined in Eq. (36), which yields the following expression:

\[
\delta \left[ \frac{\partial R(\varphi, \varphi^+; \alpha; \psi^{(1)})}{\partial s_j} \right] = \left\{ \delta \left[ \frac{\partial R(\varphi, \varphi^+; \alpha; \psi^{(1)})}{\partial s_j} \right] \right\}_{\text{dir}} + \left\{ \delta \left[ \frac{\partial R(\varphi, \varphi^+; \alpha; \psi^{(1)})}{\partial s_j} \right] \right\}_{\text{ind}}, \quad j = 1,...,J_s; \tag{69}
\]

where

\[
\text{For } j = 1,...,J_s: \left\{ \delta \left[ \frac{\partial R(\varphi, \varphi^+; \alpha; \psi^{(1)})}{\partial s_j} \right] \right\}_{\text{dir}} = \int_{4\pi} dV \int_{0}^{E_f} d\varpi \int_{0}^{E_f} d\psi^{(1)} (r, \Omega, E) \int_{0}^{E_f} d\psi^{(2)} (r, \Omega, E') \sum_{m = 1}^{J_\alpha} \frac{\partial^2 \Sigma_s(s; r, E' \rightarrow E, \Omega' \rightarrow \Omega)}{\partial s_j \partial s_m} \delta s_m, \tag{70}
\]

\[
\text{For } j = 1,...,J_s: \left\{ \delta \left[ \frac{\partial R(\varphi, \varphi^+; \alpha; \psi^{(1)})}{\partial s_j} \right] \right\}_{\text{ind}} = \int_{4\pi} dV \int_{0}^{E_f} d\varpi \int_{0}^{E_f} d\psi^{(1)} (r, \Omega, E) \int_{0}^{E_f} d\psi^{(2)} (r, \Omega, E') \sum_{m = 1}^{J_\alpha} \frac{\partial^2 \Sigma_s(s; r, E' \rightarrow E, \Omega' \rightarrow \Omega)}{\partial s_j \partial s_m} \delta s_m, \tag{71}
\]
The direct-effect term defined in Eq. (70) can be computed immediately. On the other hand, the indirect-effect term defined in Eq. (71) can be computed only after having obtained the functions \( \delta \varphi (\mathbf{r}, \Omega, E) \), \( \delta \varphi^* (\mathbf{r}, \Omega', E') \), \( \delta \psi^{(1)} (\mathbf{r}, \Omega, E) \), and \( \delta \psi^{(2)} (\mathbf{r}, \Omega, E) \), which are computationally expensive to obtain. To avoid the need for computing these quantities, the indirect-effect term defined in Eq. (71) will be expressed in terms of a 2nd-Level Adjoint Sensitivity System (2nd-LASS), which will be constructed by following the same sequence of steps as previously outlined in Section IV.A. Thus, applying the definition provided in Eq. (51) to form the inner product of Eqs. (45) and (19) with a yet undefined function \( \theta^{(2)}_j (\mathbf{r}, \Omega, E) \) having the same structure as the function \( \psi^{(2)}_j (\mathbf{r}, \Omega, E) \) that was introduced in Section IV.A, namely

\[
\theta^{(2)}_j (\mathbf{r}, \Omega, E) \triangleq \left[ \theta^{(2)}_{1,j} (\mathbf{r}, \Omega, E), \theta^{(2)}_{2,j} (\mathbf{r}, \Omega, E) \right]^T, \quad \text{where} \quad \theta^{(2)}_{1,j} \triangleq \left[ \theta^{(2)}_{1,j_1} (\mathbf{r}, \Omega, E), \theta^{(2)}_{1,j_2} (\mathbf{r}, \Omega, E) \right]^T,
\]

\[
\theta^{(2)}_{2,j} \triangleq \left[ \theta^{(2)}_{2,j_1} (\mathbf{r}, \Omega, E), \theta^{(2)}_{2,j_2} (\mathbf{r}, \Omega, E) \right]^T, \quad \text{with} \quad \theta^{(2)}_{mn,j} (\mathbf{r}, \Omega, E) \in \mathcal{L}_2 (V \times \Omega \times E), \ m, n = 1, 2, \]

yields a relation that is similar to Eq. (54), except that the components of \( \psi^{(2)}_j \) are replaced by the corresponding components of \( \theta^{(2)}_j (\mathbf{r}, \Omega, E) \), namely:

\[
\left( \begin{bmatrix} \theta^{(2)}_{1,j} \\ \theta^{(2)}_{2,j} \end{bmatrix} \right)^T \begin{bmatrix} A_{11} (\alpha) & F_{12}^{(2)} (\alpha) \\ 0 & F_{11}^{(1)} (\alpha) \end{bmatrix} \begin{bmatrix} \delta \psi^{(1)} \\ \delta \mathbf{u} \end{bmatrix} = 0
\]

\[
= \left( \begin{bmatrix} \delta \psi^{(1)} \\ \delta \mathbf{u} \end{bmatrix} \right)^T \begin{bmatrix} A_{11} (\alpha) \\ F_{12}^{(2)} (\alpha) \end{bmatrix} \begin{bmatrix} 0 \\ F_{11}^{(1)} (\alpha) \end{bmatrix} \begin{bmatrix} \theta^{(2)}_{1,j} \\ \theta^{(2)}_{2,j} \end{bmatrix} + P^{(2)} \left[ \theta^{(2)}_j, \delta \psi^{(1)}, \delta \mathbf{u} \right].
\]

The bilinear concomitant \( P^{(2)} \left[ \theta^{(2)}_j, \delta \psi^{(1)}, \delta \mathbf{u} \right] \) in Eq. (72) will vanish by imposing the same boundary conditions on the components of \( \theta^{(2)}_j (\mathbf{r}, \Omega, E) \) as were imposed in Eq. (56) on the components of \( \psi^{(2)}_j \), namely

\[
\theta^{(2)}_{1,j} (\mathbf{r}, \Omega, E) = 0, \ \mathbf{r} \in \partial V, \ \Omega \cdot \mathbf{n} < 0; \ \theta^{(2)}_{2,j} (\mathbf{r}, \Omega, E) = 0, \ \mathbf{r} \in \partial V, \ \Omega \cdot \mathbf{n} > 0; \ 0 < E < E_f,
\]

\[
\theta^{(2)}_{21,j} (\mathbf{r}, \Omega, E) = 0, \ \mathbf{r} \in \partial V, \ \Omega \cdot \mathbf{n} > 0; \ \theta^{(2)}_{22,j} (\mathbf{r}, \Omega, E) = 0, \ \mathbf{r} \in \partial V, \ \Omega \cdot \mathbf{n} < 0; \ 0 < E < E_f.
\]

Identifying the first term on the right side of Eq. (72) with the indirect-effect term defined in Eq. (71) yields the following 2nd-LASS for the components of the 2nd-level adjoint function \( \theta^{(2)}_j (\mathbf{r}, \Omega, E) \):
The left-side of Eq. (72) is now identified with the indirect-effect term defined in Eq. (71) to obtain the following expression for the indirect-effect term (in which the functions $\delta \varphi (r, \Omega, E)$, $\delta \varphi^* (r, \Omega', E')$, $\delta \psi_1 (r, \Omega, E)$, and $\delta \psi_2^{(1)} (r, \Omega, E)$ have been replaced by terms containing the components of the 2nd-level adjoint function $\theta_j^{(2)} (r, \Omega, E)$):
\[
\int dV \int d\Omega \int dE \left[ \delta \left( \varphi, \varphi^+ ; \psi^{(1)} ; \theta^{(j)} ; \alpha \right) \right] \left\{ \delta \left[ \mathcal{R} \left( \varphi, \varphi^+ ; \psi^{(1)} ; \theta^{(j)} ; \alpha \right) \right] \right\}
\]
Replacing the expressions in Eq. (78) together with the direct-effect term from Eq. (70) into Eq. (69) and subsequently identifying the quantities multiplying the parameter variations \( \delta \alpha_m, m = 1, ..., J \), in Eq. (69) yields the following expressions for the 2nd-order partial sensitivities

\[
\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; \theta^{(2)}; \alpha)}{\partial s \partial \alpha_{m_2}}, \quad j = 1, ..., J, \quad m_2 = 1, ..., J \alpha
\]

For \( j = 1, ..., J \), \( m_2 = 1, ..., J \alpha \):

\[
- \int dV \int_0^{E_f} dE \int_0^{E_f} \frac{\partial \Sigma_s}{\partial m_2} \left[ \theta_{11,j}^{(2)}(r, \Omega, E) \psi_{1}^{(1)}(r, \Omega, E) + \theta_{21,j}^{(2)}(r, \Omega, E) \varphi(r, \Omega, E) + \theta_{22,j}^{(2)}(r, \Omega, E) \varphi^*(r, \Omega, E) \right];
\]

For \( j = 1, ..., J \), \( m_2 = 1, ..., J \alpha \):

\[
\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; \theta^{(2)}; \alpha)}{\partial s \partial \alpha_{m_2}} =
\]

\[
\int dV \int_0^{E_f} dE \int_0^{E_f} \psi_{1}^{(1)}(r, \Omega, E) \int dE' \varphi(r, \Omega', E') \frac{\partial^2 \Sigma_s}{\partial s \partial m_2} \left( s; r, E' \rightarrow E, \Omega' \rightarrow \Omega \right)
\]

\[
+ \int dV \int_0^{E_f} dE \int_0^{E_f} \psi_{1}^{(1)}(r, \Omega, E) \int dE' \varphi^*(r, \Omega', E') \frac{\partial^2 \Sigma_s}{\partial s \partial m_2} \left( s; r, E \rightarrow E', \Omega \rightarrow \Omega' \right)
\]

\[
+ \int dV \int_0^{E_f} dE \int_0^{E_f} \theta_{11,j}^{(2)}(r, \Omega, E) \int dE' \psi_{1}^{(1)}(r, \Omega', E') \frac{\partial^2 \Sigma_s}{\partial s \partial m_2} \left( s; r, E \rightarrow E', \Omega \rightarrow \Omega' \right)
\]

\[
+ \int dV \int_0^{E_f} dE \int_0^{E_f} \theta_{21,j}^{(2)}(r, \Omega, E) \int dE' \psi_{1}^{(1)}(r, \Omega', E') \frac{\partial^2 \Sigma_s}{\partial s \partial m_2} \left( s; r, E' \rightarrow E, \Omega \rightarrow \Omega' \right)
\]

\[
+ \int dV \int_0^{E_f} dE \int_0^{E_f} \theta_{22,j}^{(2)}(r, \Omega, E) \int dE' \varphi(r, \Omega', E') \frac{\partial^2 \Sigma_s}{\partial s \partial m_2} \left( s; r, E \rightarrow E', \Omega \rightarrow \Omega' \right)
\]

\[
+ \int dV \int_0^{E_f} dE \int_0^{E_f} \theta_{22,j}^{(2)}(r, \Omega, E) \int dE' \varphi^*(r, \Omega', E') \frac{\partial^2 \Sigma_s}{\partial s \partial m_2} \left( s; r, E \rightarrow E', \Omega \rightarrow \Omega' \right)
\];
For \( j = 1, \ldots, J_s; m_2 = 1, \ldots, J_f \):
\[
\frac{\partial^2 R \left( \varphi, \varphi^+; \psi^{(1)}; \theta_j^{(2)}; \alpha \right)}{\partial s_j \partial m_2} = \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{11,j}^{(2)} (r, \Omega, E) \frac{\partial}{\partial m_2} \left[ \nu \Sigma_f (f, r, E) \right] \int d\Omega' \int_0^{E_f} dE' \chi (p, r, E \rightarrow E') \psi_1^{(1)} (r, \Omega', E') \]
\[
+ \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{12,j}^{(2)} (r, \Omega, E) \int d\Omega' \int_0^{E_f} dE' \chi (p, r, E \rightarrow E') \psi_2^{(1)} (r, \Omega', E') \frac{\partial}{\partial m_2} \left[ \nu \Sigma_f (f, r, E') \right] \]  
(81)
\[
+ \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{21,j}^{(2)} (r, \Omega, E) \int d\Omega' \int_0^{E_f} dE' \chi (p, r, E' \rightarrow E) \phi (r, \Omega', E') \frac{\partial}{\partial m_2} \left[ \nu \Sigma_f (f, r, E') \right] \]
\[
+ \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{22,j}^{(2)} (r, \Omega, E) \frac{\partial}{\partial m_2} \left[ \nu \Sigma_f (f, r, E) \right] \int d\Omega' \int_0^{E_f} dE' \chi (p, r, E \rightarrow E') \phi^+ (r, \Omega', E') ; \]

For \( j = 1, \ldots, J_s; m_2 = 1, \ldots, J_f \):
\[
\frac{\partial^2 R \left( \varphi, \varphi^+; \psi^{(1)}; \theta_j^{(2)}; \alpha \right)}{\partial s_j \partial p_{m_2}} = \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{11,j}^{(2)} (r, \Omega, E) \frac{\partial}{\partial p_{m_2}} \left[ \chi (p, r, E \rightarrow E') \right] \]
\[
+ \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{12,j}^{(2)} (r, \Omega, E) \int d\Omega' \int_0^{E_f} dE' \chi (p, r, E \rightarrow E') \psi_1^{(1)} (r, \Omega', E') \frac{\partial}{\partial p_{m_2}} \left[ \chi (p, r, E' \rightarrow E) \right] \]  
(82)
\[
+ \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{21,j}^{(2)} (r, \Omega, E) \int d\Omega' \int_0^{E_f} dE' \chi (p, r, E \rightarrow E') \phi (r, \Omega', E') \frac{\partial}{\partial p_{m_2}} \left[ \chi (p, r, E' \rightarrow E) \right] \]
\[
+ \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{22,j}^{(2)} (r, \Omega, E) \chi (p, r, E) \int d\Omega' \int_0^{E_f} dE' \phi^+ (r, \Omega', E') \frac{\partial}{\partial p_{m_2}} \left[ \chi (p, r, E \rightarrow E') \right] ; \]

For \( j = 1, \ldots, J_s; m_2 = 1, \ldots, J_q \):
\[
\frac{\partial^2 R \left( \varphi, \varphi^+; \psi^{(1)}; \theta_j^{(2)}; \alpha \right)}{\partial s_j \partial q_{m_2}} = \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{11,j}^{(2)} (r, \Omega, E) \frac{\partial}{\partial q_{m_2}} \left[ Q (r, \Omega, E) \right] ; \]

For \( j = 1, \ldots, J_s; m_2 = 1, \ldots, J_k \):
\[
\frac{\partial^2 R \left( \varphi, \varphi^+; \psi^{(1)}; \theta_j^{(2)}; \alpha \right)}{\partial s_j \partial k_{m_2}} = \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{11,j}^{(2)} (r, \Omega, E) \frac{\partial}{\partial k_{m_2}} \left[ Q^+ (r, \Omega, E) \right] ; \]

For \( j = 1, \ldots, J_s; m_2 = 1, \ldots, J_d \):
\[
\frac{\partial^2 R \left( \varphi, \varphi^+; \psi^{(1)}; \theta_j^{(2)}; \alpha \right)}{\partial s_j \partial d_{m_2}} = \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{11,j}^{(2)} (r, \Omega, E) \frac{\partial}{\partial d_{m_2}} \left[ G (d, \varphi, \varphi^+) \right] + \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \theta_{12,j}^{(2)} (r, \Omega, E) \frac{\partial}{\partial d_{m_2}} \left[ G (d, \varphi, \varphi^+) \right] . \]

(85)
It is important to note that the forward and adjoint operators appearing on the left-side of the 2nd-LASS defined by Eqs.(74) through (77) for the 2nd-level adjoint function $\theta_j^{(2)}$ are the same operators as appearing on the left-side of the 2nd-LASS defined by Eqs.(58) through (61) for the 2nd-level adjoint function $\psi_j^{(2)}$, the forward operator being the same as on the left side of the original forward transport Eq. (1), while the adjoint operator is the same as that appearing in the original adjoint transport namely Eq.(10). Furthermore, the forward and, respectively, adjoint functions are subject to the same forward and, respectively, adjoint (vacuum) boundary conditions. Only the source-terms on the left sides of the respective forward, 1st-LASS and 2nd-LASS differ from each other. Therefore, the same “forward” and “adjoint” software packages can be used for solving numerically the various equations underlying the 1st-LASS and the 2nd-LASS. Furthermore, the formal expression in terms of 2nd-level adjoint functions of the indirect-effect term defined in Eq.(57), involving the function $\psi_j^{(2)}$, has the same formal expression in terms of 2nd-level adjoint functions as the indirect-effect term defined in Eq. (78), involving the function $\theta_j^{(2)}$. Therefore, these indirect-effect terms can by evaluated numerically (quantitatively) using the same software package, while inputting the corresponding 2nd-level adjoint functions $\psi_j^{(2)}$ and $\theta_j^{(2)}$. Consequently, the 2nd-order sensitivities shown in Eqs.(79) through (85) have formally the same expressions as the 2nd-order sensitivities shown in Eqs.(62) through (68), respectively, except that the 2nd-level adjoint function $\theta_j^{(2)}$ in Eqs.(79) through (85) plays the role of the 2nd-level adjoint function $\psi_j^{(2)}$ in Eqs.(62) through (68). Thus, the software package used for computing the sensitivities shown in Eqs.(62) through (68) can also be used for computing the sensitivities shown in Eqs.(79) through (85).

The expressions of the 2nd-order sensitivities computed using Eq. (79) must be identical to those computed using Eq.(63), i.e.
For $j = 1,...,J_s$; $k = 1,...,J_f$:
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j, \theta_j^{(2)}; \alpha)}{\partial t_k \partial t_j} =
\]
\[
= -\int dV \int_{4\pi} d\Omega \int_0 dE \frac{\partial^2 \Sigma_j(t; \mathbf{r}, \Omega, E)}{\partial t_k} \left[ \theta_{11,j}^{(2)}(\mathbf{r}, \Omega, E) \psi_1^{(1)}(\mathbf{r}, \Omega, E) + \theta_{12,j}^{(2)}(\mathbf{r}, \Omega, E) \varphi(\mathbf{r}, \Omega, E) \right] + \theta_{21,j}^{(2)}(\mathbf{r}, \Omega, E) \varphi(\mathbf{r}, \Omega, E) + \theta_{22,j}^{(2)}(\mathbf{r}, \Omega, E) \varphi^+(\mathbf{r}, \Omega, E)
\]
\[
= \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; u_j^{(2)}; \alpha)}{\partial t_k \partial t_j} =
\]
\[
= \int dV \int_{4\pi} d\Omega \int_0 dE \psi^{(2)}_{11,k}(\mathbf{r}, \Omega, E) \int_{4\pi} d\Omega' \int_0 dE' \psi^{(1)}_1(\mathbf{r}, \Omega', E') \frac{\partial \Sigma_j(s; \mathbf{r}, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_j}
\]
\[
+ \int dV \int_{4\pi} d\Omega \int_0 dE \psi^{(2)}_{12,k}(\mathbf{r}, \Omega, E) \int_{4\pi} d\Omega' \int_0 dE' \psi^{(1)}_2(\mathbf{r}, \Omega', E') \frac{\partial \Sigma_j(s; \mathbf{r}, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_j}
\]
\[
+ \int dV \int_{4\pi} d\Omega \int_0 dE \psi^{(2)}_{21,k}(\mathbf{r}, \Omega, E) \int_{4\pi} d\Omega' \int_0 dE' \varphi(\mathbf{r}, \Omega', E') \frac{\partial \Sigma_j(s; \mathbf{r}, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_j}
\]
\[
+ \int dV \int_{4\pi} d\Omega \int_0 dE \psi^{(2)}_{22,k}(\mathbf{r}, \Omega, E) \int_{4\pi} d\Omega' \int_0 dE' \varphi^+(\mathbf{r}, \Omega', E') \frac{\partial \Sigma_j(s; \mathbf{r}, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_j}.
\]

The relation shown in Eq. (86) provides an independent path for the mutual verification of the solutions $\theta_j^{(2)}$ and $\psi_j^{(2)}$, $j = 1,...,J_s$, of the respective 2nd-LASS.

\textit{IV.C. Computation of the 2nd-Order Sensitivities} \[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; u_j^{(2)}; \alpha)}{\partial f_j \partial \alpha_{m_j}}, \quad j = 1,...,J_f; \quad m_j = 1,...,J_{\alpha}.
\]

The 2nd-order sensitivities $\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; u_j^{(2)}; \alpha)}{\partial f_j \partial \alpha_{m_j}}$, $j = 1,...,J_f; \quad m_j = 1,...,J_{\alpha}$ will ultimately depend on a 2nd-level adjoint function (which is denoted as $u_j^{(2)}$) and are obtained by determining the G-differential of the 1st-order sensitivity defined in Eq. (37), which yields the following expression:
\[
\delta \left[ \frac{\partial R(\varphi, \alpha; \psi^{(1)}_j)}{\partial f_j} \right] = \left\{ \delta \left[ \frac{\partial R(\varphi, \alpha; \psi^{(1)}_j)}{\partial f_j} \right] \right\}_{\text{dir}} + \left\{ \delta \left[ \frac{\partial R(\varphi, \alpha; \psi^{(1)}_j)}{\partial f_j} \right] \right\}_{\text{ind}}, \quad j = 1,...,J_f;
\]
where
For \( j = 1, \ldots, J_f \):
\[
\left\{ \delta \left[ \frac{\partial R(\varphi, \varphi^+; \psi^{(1)})}{\partial f_j} \right] \right\}_{dir} \triangleq \\
= \int dV \int_0^{E_f} \int_{4\pi} dE' \varphi(\mathbf{r}, \Omega, E) \int_0^{E_f} dE' \chi(p; r, E' \rightarrow E) \sum_{m_2=1}^{J_f} \frac{\partial^2 \left[ \nu \Sigma_f(\mathbf{r}, \Omega, E') \right]}{\partial f_j \partial f_m^2} \delta f_m^2 \\
+ \int dV \int_0^{E_f} \int_{4\pi} dE' \varphi(\mathbf{r}, \Omega, E) \int_0^{E_f} dE' \sum_{m_2=1}^{J_f} \frac{\partial \chi(p; r, E' \rightarrow E)}{\partial p_{m_2}} \delta p_{m_2} \int d\Omega' \int dE' \chi(p; r, E' \rightarrow E') \varphi^+(\mathbf{r}, \Omega', E') \\
+ \int dV \int_0^{E_f} \int_{4\pi} dE' \varphi(\mathbf{r}, \Omega, E) \int_0^{E_f} dE' \varphi^+(\mathbf{r}, \Omega', E') \sum_{m_2=1}^{J_f} \frac{\partial \chi(p; r, E \rightarrow E')}{\partial p_{m_2}} \delta p_{m_2}.
\]

For \( j = 1, \ldots, J_f \):
\[
\left\{ \delta \left[ \frac{\partial R(\varphi, \varphi^+; \psi^{(1)})}{\partial f_j} \right] \right\}_{ind} \triangleq \\
= \int dV \int_0^{E_f} \int_{4\pi} dE' \left[ \delta \varphi^{(1)}(\mathbf{r}, \Omega, E) \right] \int_0^{E_f} dE' \varphi(\mathbf{r}, \Omega', E') \chi(p; r, E' \rightarrow E) \frac{\partial \left[ \nu \Sigma_f(\mathbf{r}, \Omega, E') \right]}{\partial f_j} \\
+ \int dV \int_0^{E_f} \int_{4\pi} dE' \left[ \delta \varphi^{(1)}(\mathbf{r}, \Omega, E) \right] \int_0^{E_f} dE' \chi(p; r, E' \rightarrow E') \frac{\partial \left[ \nu \Sigma_f(\mathbf{r}, \Omega, E') \right]}{\partial f_j} \\
+ \int dV \int_0^{E_f} \int_{4\pi} dE' \left[ \delta \varphi^{(1)}(\mathbf{r}, \Omega, E) \right] \int_0^{E_f} dE' \chi(p; r, E' \rightarrow E') \frac{\partial \left[ \nu \Sigma_f(\mathbf{r}, \Omega, E') \right]}{\partial f_j} \\
+ \int dV \int_0^{E_f} \int_{4\pi} dE' \left[ \delta \varphi^{(1)}(\mathbf{r}, \Omega, E) \right] \int_0^{E_f} dE' \chi(p; r, E' \rightarrow E') \left[ \delta \varphi^+(\mathbf{r}, \Omega, E') \right].
\]

The direct-effect term defined in Eq. (88) can be computed immediately. On the other hand, as before, the indirect-effect term defined in Eq. (89) can be computed only after having obtained the variations \( \delta \varphi^{(1)}(\mathbf{r}, \Omega, E) \), \( \delta \varphi^{(1)}(\mathbf{r}, \Omega, E) \), \( \delta \varphi(\mathbf{r}, \Omega, E) \) and \( \delta \varphi^+(\mathbf{r}, \Omega, E) \), which are computational expensive to determine. To avoid the need for computing these variations, the indirect-effect term defined in Eq. (89) will be expressed in terms of the solution of a 2nd-Level Adjoint Sensitivity System (2nd-LASS), which will be constructed by following the same sequence of steps as previously outlined in Sections IV.A and B. Thus, applying the definition provided in Eq. (51) to form the inner product of Eqs. (45) and (19) with a yet undefined function \( u_j^{(2)}(\mathbf{r}, \Omega, E) \) which has the same structure as the
functions $\psi_j^{(2)}(r, \Omega, E)$ and $\theta_j^{(2)}(r, \Omega, E)$, namely: $u_j^{(2)}(r, \Omega, E) = \left[u_{1,j}^{(2)}(r, \Omega, E), u_{2,j}^{(2)}(r, \Omega, E)\right]'$, where $u_{1,j}^{(2)} = \left[u_{1,j}^{(2)}(r, \Omega, E), u_{1,j}^{(2)}(r, \Omega, E)\right]'$, $u_{2,j}^{(2)} = \left[u_{2,j}^{(2)}(r, \Omega, E), u_{2,j}^{(2)}(r, \Omega, E)\right]'$, with

$u_{mn,j}^{(2)}(r, \Omega, E) \in \mathbb{L}_2(V \times \Omega \times E)$, $m, n = 1, 2$, yields a relation that is similar to Eq. (54), except that the components of $\psi_j^{(2)}$ are replaced by the corresponding components of $u_j^{(2)}(r, \Omega, E)$, namely:

$$
\begin{align*}
&\left\langle \left(u_{1,j}^{(2)}\right)' \begin{bmatrix} A_{11}^{(1)}(\alpha) & F_{12}^{(2)}(\alpha) \\ 0 & F_{11}^{(1)}(\alpha) \end{bmatrix} \begin{bmatrix} \delta\psi_1^{(1)} \\ \delta u \end{bmatrix} \right\rangle_{(2)} = \\
&= \left\langle \left(\delta\psi_1^{(1)}\right)' \begin{bmatrix} A_{11}^{(1)}(\alpha) \\ F_{12}^{(2)}(\alpha) \end{bmatrix}' \begin{bmatrix} 0 \\ F_{11}^{(1)}(\alpha) \end{bmatrix}' \begin{bmatrix} u_{1,j}^{(2)} \\ u_{2,j}^{(2)} \end{bmatrix} \right\rangle_{(2)} + P^{(2)} \begin{bmatrix} u_{1,j}^{(2)} \delta\psi_1^{(1)} \delta u \end{bmatrix}.
\end{align*}
$$

The bilinear concomitant $P^{(2)} \begin{bmatrix} u_{j}^{(2)} \delta\psi_1^{(1)} \delta u \end{bmatrix}$ in Eq. (90) will vanish by imposing the same boundary conditions on the components of $u_j^{(2)}(r, \Omega, E)$ as were imposed in Eq. (56) on the components of $\psi_j^{(2)}$, namely

$$
\begin{align*}
&u_{11,j}(r, \Omega, E) = 0, \quad r \in \partial V, \quad \Omega \cdot n < 0; \quad u_{12,j}(r, \Omega, E) = 0, \quad r \in \partial V, \quad \Omega \cdot n > 0; \quad 0 < E < E_f, \\
&u_{21,j}(r, \Omega, E) = 0, \quad r \in \partial V, \quad \Omega \cdot n > 0; \quad u_{22,j}(r, \Omega, E) = 0, \quad r \in \partial V, \quad \Omega \cdot n < 0; \quad 0 < E < E_f.
\end{align*}
$$

Identifying the first term on the right side of Eq. (90) with the indirect-effect term defined in Eq. (89) yields the following $2^{nd}$-LASS for the components of the $2^{nd}$-level adjoint function $u_j^{(2)}(r, \Omega, E)$:

$$
\begin{align*}
&L(\alpha)u_{11,j}(r, \Omega, E) = \int_{4\pi} d\Omega' \int_{E_f}^E dE' \chi(p, r, E' \rightarrow E) \varphi(r, \Omega', E') \frac{\partial \left[v\Sigma_f \begin{bmatrix} f(r, E') \end{bmatrix}\right]}{\partial f_j}, \quad j = 1, \ldots, J_f, \\
&L^+(\alpha)u_{12,j}(r, \Omega, E) = \frac{\partial \left[v\Sigma_f \begin{bmatrix} f(r, E) \end{bmatrix}\right]}{\partial f_j} \int_{4\pi} d\Omega' \int_{E_0}^{E_f} dE' \chi(p, r, E \rightarrow E') \varphi^+(r, \Omega', E'), \quad j = 1, \ldots, J_f, \\
&L^+(\alpha)u_{21,j}(r, \Omega, E) = \frac{\partial^2 G(d, \varphi^+, \varphi^+)}{\partial \varphi^2} u_{11,j}^{(2)}(r, \Omega, E) + \frac{\partial^2 G(d, \varphi, \varphi^+)}{\partial \varphi^2 \partial \varphi} u_{12,j}^{(2)}(r, \Omega, E) \\
&+ \frac{\partial \left[v\Sigma_f \begin{bmatrix} f(r, E) \end{bmatrix}\right]}{\partial f_j} \int_{4\pi} d\Omega' \int_{E_0}^{E_f} dE' \chi(p, r, E \rightarrow E') \varphi_1^{(1)}(r, \Omega', E'), \quad j = 1, \ldots, J_f.
\end{align*}
$$
Identifying the term on the left-side of Eq.(90) with the indirect-effect term defined in Eq.(89) leads to the following expression for the indirect-effect term, in which the terms containing the functions
\[ \delta \phi (r, \Omega, E) \], \[ \delta \phi^* (r, \Omega', E') \], \[ \delta \psi_1^{(i)} (r, \Omega, E) \], and \[ \delta \psi_2^{(i)} (r, \Omega, E) \] have been replaced by terms containing the components of the 2\textsuperscript{nd}-level adjoint function \( u^{(2)}_j (r, \Omega, E) \):

\[
L(a)u^{(2)}_j (r, \Omega, E) = \frac{\partial^2 G(d, \varphi, \varphi^*)}{\partial \varphi \partial \varphi^*} u^{(2)}_{11,j} (r, \Omega, E) + \frac{\partial^2 G(d, \varphi, \varphi^*)}{\partial \varphi^* \partial \varphi^*} u^{(2)}_{12,j} (r, \Omega, E)
\]

\[
+ \int_{4\pi} \int_{d \Omega'} dE' \chi(p, r, E' \rightarrow E) \psi_2^{(i)} (r, \Omega', E') \frac{\partial [\nu \Sigma_f (f, r', E')]}{\partial f_j}, \quad j = 1, \ldots, J_f,
\]
\[
\delta \left[ \frac{\partial R(\varphi, \varphi^+; \psi^{(1)}; \mathbf{u}_f^{(2)}; \mathbf{a})}{\partial f_j} \right]_{\text{ind}} \triangleq \left\langle \left( \mathbf{u}_{i,f}^{(2)} \right)^\dagger \left( \mathbf{Q}^{(2)}(\mathbf{a}, \psi^{(1)}; \delta \mathbf{a}) \right) \right\rangle_{(2)}
\]

\[
= \int dV \int d\Omega \int_0^{E_f} dE \mathbf{u}_{11,j}^{(2)}(\mathbf{r}, \Omega, E) \left\{ \int d\Omega' \int_0^{E_f} dE' [\delta\Sigma_s(\mathbf{r}, E \rightarrow E', \Omega \rightarrow \Omega')] \psi^{(1)}(\mathbf{r}, \Omega', E') \right.
\]

\[
+ \delta \left[ \nu \Sigma_f(\mathbf{f}; \mathbf{r}, E) \right] \int d\Omega' \int_0^{E_f} dE' \chi(\mathbf{p}; \mathbf{r}, E \rightarrow E') \psi^{(1)}(\mathbf{r}, \Omega', E') - \delta\Sigma_s(\mathbf{r}, E) \psi^{(1)}(\mathbf{r}, \Omega, E)
\]

\[
+ \left\{ \int d\Omega' \int_0^{E_f} dE' \delta\chi(\mathbf{p}; \mathbf{r}, E \rightarrow E') \psi^{(1)}(\mathbf{r}, \Omega', E') + \sum_{i=1}^{J_d} \frac{\delta^2 G(\mathbf{d}; \varphi, \varphi^+)}{\delta \phi \delta d_i} \delta d_i \right\}
\]

\[
+ \int dV \int d\Omega \int_0^{E_f} dE \mathbf{u}_{12,j}^{(2)}(\mathbf{r}, \Omega, E) \left\{ \int d\Omega' \int_0^{E_f} dE' [\delta\Sigma_s(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega)] \psi^{(1)}(\mathbf{r}, \Omega', E') \right.
\]

\[
+ \left\{ \int d\Omega' \int_0^{E_f} dE' \chi(\mathbf{p}; \mathbf{r}, E' \rightarrow E) \delta \left[ \nu \Sigma_f(\mathbf{f}; \mathbf{r}, E') \right] \psi^{(1)}(\mathbf{r}, \Omega', E') - \delta\Sigma_s(\mathbf{r}, E) \psi^{(1)}(\mathbf{r}, \Omega, E)
\]

\[
+ \left\{ \int d\Omega' \int_0^{E_f} dE' \nu \Sigma_f(\mathbf{f}; \mathbf{r}, E') \delta\chi(\mathbf{p}; \mathbf{r}, E' \rightarrow E) \psi^{(1)}(\mathbf{r}, \Omega', E') + \sum_{i=1}^{J_d} \frac{\delta^2 G(\mathbf{d}; \varphi, \varphi^+)}{\delta \varphi \delta d_i} \delta d_i \right\}
\]

\[
+ \int dV \int d\Omega \int_0^{E_f} dE \mathbf{u}_{21,j}^{(2)}(\mathbf{r}, \Omega, E) \left\{ \delta Q(\mathbf{q}; \mathbf{r}, \Omega, E) - \delta\Sigma_s(\mathbf{t}; \mathbf{r}, E) \varphi(\mathbf{r}, \Omega, E)
\right.
\]

\[
+ \left\{ \int d\Omega' \int_0^{E_f} dE' \delta\varphi(\mathbf{r}, \Omega', E') [\delta\Sigma_s(\mathbf{s}; \mathbf{r}, E \rightarrow E, \Omega' \rightarrow \Omega)] \right.
\]

\[
+ \left\{ \int d\Omega' \int_0^{E_f} dE' \delta\chi(\mathbf{p}; \mathbf{r}, E' \rightarrow E) \varphi(\mathbf{r}, \Omega', E') \nu \Sigma_f(\mathbf{f}; \mathbf{r}, E') \right.
\]

\[
+ \left\{ \int d\Omega' \int_0^{E_f} dE' \chi(\mathbf{p}; \mathbf{r}, E' \rightarrow E) \varphi(\mathbf{r}, \Omega', E') \delta \left[ \nu \Sigma_f(\mathbf{f}; \mathbf{r}, E') \right] \right.
\]

\[
+ \left\{ \int d\Omega' \int_0^{E_f} dE' \mathbf{u}_{22,j}^{(2)}(\mathbf{r}, \Omega, E) \left\{ \delta Q^+(\mathbf{k}; \mathbf{r}, \Omega, E) - \delta\Sigma_s(\mathbf{t}; \mathbf{r}, E) \varphi^+(\mathbf{r}, \Omega, E)
\right.
\]

\[
+ \left\{ \int d\Omega' \int_0^{E_f} dE' \delta\varphi^+(\mathbf{r}, \Omega', E') [\delta\Sigma_s(\mathbf{s}; \mathbf{r}, E \rightarrow E, \Omega' \rightarrow \Omega')] \right.
\]

\[
+ \delta \left[ \nu \Sigma_f(\mathbf{f}; \mathbf{r}, E) \right] \int d\Omega' \int_0^{E_f} dE' \chi(\mathbf{p}; \mathbf{r}, E \rightarrow E') \varphi^+(\mathbf{r}, \Omega', E')
\]

\[
+ \nu \Sigma_f(\mathbf{f}; \mathbf{r}, E) \int d\Omega' \int_0^{E_f} dE' \delta\chi(\mathbf{p}; \mathbf{r}, E \rightarrow E') \varphi^+(\mathbf{r}, \Omega', E') \right\},
\]

(96)
Replacing Eq. (96) together with the direct-effect term from Eq. (88) into Eq. (87) and subsequently identifying the quantities multiplying the parameter variations $\delta \alpha_{m_2}, m_2 = 1, \ldots, J_\alpha$, in Eq. (87) yields the following expressions:

For $j = 1, \ldots, J_f$; $m_2 = 1, \ldots, J_f$:

$$
\frac{\partial^2 R \left( \varphi, \varphi^+; \psi^{(1)}; u^{(2)}_j; \alpha \right)}{\partial f_j \partial t_{m_2}} 
$$

$$
= -\int dV \int_{4\pi}^{E_f} d\Omega \int_0^E dE \frac{\partial \Sigma_t \left( t; \mathbf{r}, \Omega, E \right)}{\partial t_{m_2}} \left[ u^{(2)}_{11,j} \left( \mathbf{r}, \Omega, E \right) \varphi^{(1)}_1 \left( \mathbf{r}, \Omega, E \right) 
+ u^{(2)}_{12,j} \left( \mathbf{r}, \Omega, E \right) \varphi^{(1)}_2 \left( \mathbf{r}, \Omega, E \right) + u^{(2)}_{21,j} \left( \mathbf{r}, \Omega, E \right) \varphi \left( \mathbf{r}, \Omega, E \right) + u^{(2)}_{22,j} \left( \mathbf{r}, \Omega, E \right) \varphi^+ \left( \mathbf{r}, \Omega, E \right) \right] ;
$$

(97)

For $j = 1, \ldots, J_f$; $m_2 = 1, \ldots, J_s$:

$$
\frac{\partial^2 R \left( \varphi, \varphi^+; \psi^{(1)}; u^{(2)}_j; \alpha \right)}{\partial f_j \partial s_{m_2}} 
$$

$$
= \int dV \int_{4\pi}^{E_f} d\Omega \int_0^E dE \ u^{(2)}_{11,j} \left( \mathbf{r}, \Omega, E \right) \int_{4\pi}^{E_f} d\Omega' \int_0^{E_f} dE' \varphi^{(1)}_1 \left( \mathbf{r}, \Omega', E' \right) \frac{\partial \Sigma_s \left( s; \mathbf{r}, E \rightarrow E', \Omega \rightarrow \Omega' \right)}{\partial s_{m_2}} 
+ \int dV \int_{4\pi}^{E_f} d\Omega \int_0^E dE \ u^{(2)}_{12,j} \left( \mathbf{r}, \Omega, E \right) \int_{4\pi}^{E_f} d\Omega' \int_0^{E_f} dE' \varphi^{(1)}_2 \left( \mathbf{r}, \Omega', E' \right) \frac{\partial \Sigma_s \left( s; \mathbf{r}, E \rightarrow E', \Omega \rightarrow \Omega' \right)}{\partial s_{m_2}} 
+ \int dV \int_{4\pi}^{E_f} d\Omega \int_0^E dE \ u^{(2)}_{21,j} \left( \mathbf{r}, \Omega, E \right) \int_{4\pi}^{E_f} d\Omega' \int_0^{E_f} dE' \varphi \left( \mathbf{r}, \Omega', E' \right) \frac{\partial \Sigma_s \left( s; \mathbf{r}, E \rightarrow E', \Omega \rightarrow \Omega' \right)}{\partial s_{m_2}} 
+ \int dV \int_{4\pi}^{E_f} d\Omega \int_0^E dE \ u^{(2)}_{22,j} \left( \mathbf{r}, \Omega, E \right) \int_{4\pi}^{E_f} d\Omega' \int_0^{E_f} dE' \varphi^+ \left( \mathbf{r}, \Omega', E' \right) \frac{\partial \Sigma_s \left( s; \mathbf{r}, E \rightarrow E', \Omega \rightarrow \Omega' \right)}{\partial s_{m_2}} ;
$$

(98)
For $j = 1, \ldots, J_f$; $m_2 = 1, \ldots, J_f$:

$$
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \mathbf{u}_j^{(2)}; \mathbf{u})}{\partial f_j \partial f_{m_2}} =
$$

$$
= \int dV \int_{4\pi}^E d\Omega \int dE \psi_1^{(1)}(r, \Omega, E) \int d\Omega' \int dE' \varphi(r, \Omega', E') \chi(p, r, E' \rightarrow E) \frac{\partial^2 [v \Sigma_f(f, r, E')]}{\partial f_j \partial f_{m_2}}
$$

$$
+ \int dV \int_{4\pi}^E d\Omega \int dE \psi_2^{(1)}(r, \Omega, E) \frac{\partial^2 [v \Sigma_f(f, r, E')]}{\partial f_j \partial f_{m_2}} \int d\Omega' \int dE' \chi(p, r, E' \rightarrow E') \varphi^+ (r, \Omega', E')
$$

$$
+ \int dV \int_{4\pi}^E d\Omega \int dE \psi_2^{(2)}(r, \Omega, E) \frac{\partial^2 [v \Sigma_f(f, r, E')]}{\partial f_j \partial f_{m_2}} \int d\Omega' \int dE' \chi(p, r, E' \rightarrow E') \varphi^+(r, \Omega', E')\psi_1^{(1)}(r, \Omega', E')
$$

$$
+ \int dV \int_{4\pi}^E d\Omega \int dE \psi_2^{(2)}(r, \Omega, E) \frac{\partial^2 [v \Sigma_f(f, r, E')]}{\partial f_j \partial f_{m_2}} \int d\Omega' \int dE' \chi(p, r, E' \rightarrow E') \varphi^+(r, \Omega', E')\psi_2^{(2)}(r, \Omega', E')\psi_1^{(1)}(r, \Omega', E') \quad (99)
$$

For $j = 1, \ldots, J_f$; $m_2 = 1, \ldots, J_f$:

$$
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \mathbf{u}_j^{(2)}; \mathbf{u})}{\partial f_j \partial p_{m_2}} =
$$

$$
= \int dV \int_{4\pi}^E d\Omega \int dE \psi_1^{(1)}(r, \Omega, E) \int d\Omega' \int dE' \varphi(r, \Omega', E') \frac{\partial \chi(p, r, E' \rightarrow E)}{\partial p_{m_2}} \frac{\partial [v \Sigma_f(f, r, E')]}{\partial f_j}
$$

$$
+ \int dV \int_{4\pi}^E d\Omega \int dE \psi_2^{(1)}(r, \Omega, E) \frac{\partial [v \Sigma_f(f, r, E')]}{\partial f_j} \int d\Omega' \int dE' \varphi^+ (r, \Omega', E') \frac{\partial \chi(p, r, E' \rightarrow E)}{\partial p_{m_2}}
$$

$$
+ \int dV \int_{4\pi}^E d\Omega \int dE \psi_2^{(2)}(r, \Omega, E) \frac{\partial [v \Sigma_f(f, r, E')]}{\partial f_j} \int d\Omega' \int dE' \chi(p, r, E' \rightarrow E') \varphi^+(r, \Omega', E') \frac{\partial \chi(p, r, E' \rightarrow E)}{\partial p_{m_2}}
$$

$$
+ \int dV \int_{4\pi}^E d\Omega \int dE \psi_2^{(2)}(r, \Omega, E) \frac{\partial [v \Sigma_f(f, r, E')]}{\partial f_j} \int d\Omega' \int dE' \chi(p, r, E' \rightarrow E') \varphi^+(r, \Omega', E') \frac{\partial \chi(p, r, E' \rightarrow E')}{\partial p_{m_2}}
$$

$$
\int dV \int_{4\pi}^E d\Omega \int dE \psi_2^{(2)}(r, \Omega, E) \frac{\partial [v \Sigma_f(f, r, E')]}{\partial f_j} \int d\Omega' \int dE' \varphi^+(r, \Omega', E') \frac{\partial \chi(p, r, E' \rightarrow E')}{\partial p_{m_2}} \quad (100)
$$
For \( j = 1, \ldots, J_f \); \( m_2 = 1, \ldots, J_q \):

\[
\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; \mathbf{u}^{(2)}; \alpha)}{\partial f_j \partial q_{m_2}} = \int dV \int d\Omega \int_0^{E_f} dE \mathbf{u}^{(2)}_{21,j}(\mathbf{r}, \Omega, E) \frac{\partial Q(q; \mathbf{r}, \Omega, E)}{\partial q_{m_2}};
\]

Equation (101)

For \( j = 1, \ldots, J_f \); \( m_2 = 1, \ldots, J_k \):

\[
\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; \mathbf{u}^{(2)}; \alpha)}{\partial f_j \partial k_{m_2}} = \int dV \int d\Omega \int_0^{E_f} dE \mathbf{u}^{(2)}_{22,j}(\mathbf{r}, \Omega, E) \frac{\partial Q^*(k; \mathbf{r}, \Omega, E)}{\partial k_{m_2}};
\]

Equation (102)

For \( j = 1, \ldots, J_f \); \( m_2 = 1, \ldots, J_d \):

\[
\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; \mathbf{u}^{(2)}; \alpha)}{\partial f_j \partial d_{m_2}} = \int dV \int d\Omega \int_0^{E_f} dE \mathbf{u}^{(2)}_{1,j}(\mathbf{r}, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^*)}{\partial \varphi \partial d_{m_2}} + \int dV \int d\Omega \int_0^{E_f} dE \mathbf{u}^{(2)}_{12,j}(\mathbf{r}, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^*)}{\partial \varphi^* \partial d_{m_2}}.
\]

Equation (103)

As discussed in the previous Sections, it is important to note that the forward and adjoint operators appearing on the left-side of the 2nd-LASS defined by Eqs. (92) through (95) for the 2nd-level adjoint function \( \psi_j^{(2)} \) are the same operators as appearing on the left-side of the corresponding 2nd-LASS for the 2nd-level adjoint function \( \psi_j^{(2)} \) and \( \theta_j^{(2)} \), respectively. Furthermore, all of these the 2nd-level adjoint functions are subject to the same respective boundary conditions. Only the source-terms on the left sides of the respective 2nd-LASS differ from each other. Therefore, the same “forward” and “adjoint” software packages can be used for solving numerically the various forward and adjoint equations underlying the 1st-LASS and the 2nd-LASS. Furthermore, as has already been noted, the various indirect-effect terms all have equivalent formal expression in terms of 2nd-level adjoint functions. Therefore, these indirect-effect terms can by evaluated numerically (quantitatively) using the same software package, while inputting the corresponding 2nd-level adjoint functions. Consequently, most of the 2nd-order sensitivities can also be computing using the same basic software package.

The expressions of the 2nd-order sensitivities computed using Eq. (97) must be identical to those computed using Eq. (64), i.e.
For $j = 1, \ldots, J_f$, $k = 1, \ldots, J_i$, 
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \alpha)}{\partial f \partial t_k} = -\int dV \int_{4\pi} d\Omega \int_0^E dE \frac{\partial \Sigma_f}{\partial t_k} \left[ u^{(2)}_{11} (\mathbf{r}, \Omega, E) \psi^{(1)}_i (\mathbf{r}, \Omega, E) \right. \\
+ u^{(2)}_{12} (\mathbf{r}, \Omega, E) \psi^{(2)}_2 (\mathbf{r}, \Omega, E) + u^{(2)}_{21} (\mathbf{r}, \Omega, E) \varphi (\mathbf{r}, \Omega, E) + u^{(2)}_{22} (\mathbf{r}, \Omega, E) \varphi^+ (\mathbf{r}, \Omega, E) \left. \right] \\
= \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha)}{\partial t_k \partial f_j} = \\
= \int dV \int_{4\pi} d\Omega \int_0^E dE \psi^{(2)}_{11} (\mathbf{r}, \Omega, E) \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}; \mathbf{r}, E) \right]}{\partial f_j} \int_{4\pi} d\Omega' \int_0^{E'} dE' \chi (p; \mathbf{r}, E \rightarrow E') \psi^{(1)}_i (\mathbf{r}, \Omega', E') \\
+ \int dV \int_{4\pi} d\Omega \int_0^E dE \psi^{(2)}_{12} (\mathbf{r}, \Omega, E) \int_{4\pi} d\Omega' \int_0^{E'} dE' \chi (p; \mathbf{r}, E \rightarrow E') \psi^{(2)}_2 (\mathbf{r}, \Omega', E') \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}; \mathbf{r}, E') \right]}{\partial f_j} \\
+ \int dV \int_{4\pi} d\Omega \int_0^E dE \psi^{(2)}_{21} (\mathbf{r}, \Omega, E) \int_{4\pi} d\Omega' \int_0^{E'} dE' \chi (p; \mathbf{r}, E \rightarrow E') \varphi (\mathbf{r}, \Omega', E') \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}; \mathbf{r}, E') \right]}{\partial f_j} \\
+ \int dV \int_{4\pi} d\Omega \int_0^E dE \psi^{(2)}_{22} (\mathbf{r}, \Omega, E) \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}; \mathbf{r}, E) \right]}{\partial f_j} \int_{4\pi} d\Omega' \int_0^{E'} dE' \chi (p; \mathbf{r}, E \rightarrow E') \varphi^+ (\mathbf{r}, \Omega', E').
\]

Also, expressions of the 2\textsuperscript{nd}-order sensitivities computed using Eq. (98) must be identical to those computed using Eq. (81), i.e.
\[ \frac{\partial^2 R(\psi^{(1)}, \psi^{(2)}; u_j^{(2)}, \alpha)}{\partial f_j \partial s_k} = \]

\[ = \int dV \int_{E_f} d\Omega \int_0^{4\pi} dE \ u_{1,j}^{(2)} (r, \Omega, E) \int_{E_f} d\Omega' \int_0^{4\pi} dE' \psi_1^{(1)} (r, \Omega', E') \frac{\partial \Sigma_s (s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_k} \]

\[ + \int dV \int_{E_f} d\Omega \int_0^{4\pi} dE \ u_{12,j}^{(2)} (r, \Omega, E) \int_{E_f} d\Omega' \int_0^{4\pi} dE' \psi_2^{(1)} (r, \Omega', E') \frac{\partial \Sigma_s (s; r, E' \rightarrow E, \Omega' \rightarrow \Omega)}{\partial s_k} \]

\[ + \int dV \int_{E_f} d\Omega \int_0^{4\pi} dE \ u_{21,j}^{(2)} (r, \Omega, E) \int_{E_f} d\Omega' \int_0^{4\pi} dE' \varphi (r, \Omega', E') \frac{\partial \Sigma_s (s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_k} \]

\[ + \int dV \int_{E_f} d\Omega \int_0^{4\pi} dE \ u_{22,j}^{(2)} (r, \Omega, E) \int_{E_f} d\Omega' \int_0^{4\pi} dE' \varphi^+ (r, \Omega', E') \frac{\partial \Sigma_s (s; r, E \rightarrow E', \Omega \rightarrow \Omega)}{\partial s_k} \]

\[ = \frac{\partial^2 R(\psi^{(1)}, \psi^{(2)}; u_j^{(2)}, \alpha)}{\partial f_j \partial s_k} = \]

\[ = \int dV \int_{E_f} d\Omega \int_0^{4\pi} dE \ \theta_{1,k}^{(2)} (r, \Omega, E) \frac{\partial [\nu \Sigma_f (\alpha; r, E)]}{\partial f_j} \int_{E_f} d\Omega' \int_0^{4\pi} dE' \chi (p; r, E \rightarrow E') \psi_1^{(1)} (r, \Omega', E') \]

\[ + \int dV \int_{E_f} d\Omega \int_0^{4\pi} dE \ \theta_{12,k}^{(2)} (r, \Omega, E) \int_{E_f} d\Omega' \int_0^{4\pi} dE' \chi (p; r, E' \rightarrow E) \psi_2^{(1)} (r, \Omega', E') \frac{\partial [\nu \Sigma_f (\alpha; r, E')]}{\partial f_j} \]

\[ + \int dV \int_{E_f} d\Omega \int_0^{4\pi} dE \ \theta_{21,k}^{(2)} (r, \Omega, E) \int_{E_f} d\Omega' \int_0^{4\pi} dE' \chi (p; r, E' \rightarrow E) \varphi (r, \Omega', E') \frac{\partial [\nu \Sigma_f (\alpha; r, E')]}{\partial f_j} \]

\[ + \int dV \int_{E_f} d\Omega \int_0^{4\pi} dE \ \theta_{22,k}^{(2)} (r, \Omega, E) \frac{\partial [\nu \Sigma_f (\alpha; r, E)]}{\partial f_j} \int_{E_f} d\Omega' \int_0^{4\pi} dE' \chi (p; r, E \rightarrow E') \varphi^+ (r, \Omega', E'). \]
IV.D. Computation of the 2nd-Order Sensitivities

\[ \frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; w_j^{(2)}; \alpha)}{\partial p_j \partial \alpha_{m_2}} , \quad j = 1, \ldots, J_p ; \quad m_2 = 1, \ldots, J_a \]

The 2nd-order sensitivities \( \partial^2 R(\varphi, \varphi^*; \psi^{(1)}; w_j^{(2)}; \alpha) \) will ultimately depend on a 2nd-level adjoint function which is denoted as \( w_j^{(2)} \), and are obtained by computing the G-differential of the 1st-order sensitivities defined in Eq. (38), which yields the following expression:

\[
\delta \left[ \frac{\partial R(\mathbf{a}, \varphi; \psi^{(1)})}{\partial p_j} \right] = \left\{ \delta \left[ \frac{\partial R(\mathbf{a}, \varphi; \psi^{(1)})}{\partial p_j} \right] \right\}_{\text{dir}} + \left\{ \delta \left[ \frac{\partial R(\mathbf{a}, \varphi; \psi^{(1)})}{\partial p_j} \right] \right\}_{\text{ind}} , \quad j = 1, \ldots, J_p ;
\]

where

\[
\frac{\partial^2 R(\mathbf{a}, \varphi; \psi^{(1)})}{\partial \alpha_{m_2}} = \int dV \int d\Omega \int dE \psi_1 \left( \mathbf{r}, \Omega, E \right) \int d\Omega' \int dE' \nu \Sigma_f \left( \mathbf{f}, \mathbf{r}, \Omega', E' \right) \varphi \left( \mathbf{r}, \Omega', E' \right) \sum_{m_2=1}^{J_1} \frac{\partial^2 \chi \left( \mathbf{p}, \mathbf{r}, E' \to E \right)}{\partial p_j \partial \alpha_{m_2}} \delta \alpha_{m_2}
\]

\[
+ \int dV \int d\Omega \int dE \psi_1 \left( \mathbf{r}, \Omega, E \right) \int d\Omega' \int dE' \varphi \left( \mathbf{r}, \Omega', E' \right) \frac{\partial \chi \left( \mathbf{p}, \mathbf{r}, E' \to E \right)}{\partial p_j} \sum_{m_2=1}^{J_1} \frac{\partial \nu \Sigma_f \left( \mathbf{f}, \mathbf{r}, E' \right)}{\partial \alpha_{m_2}} \delta \alpha_{m_2} \int d\Omega' \int dE' \nu \Sigma_f \left( \mathbf{f}, \mathbf{r}, E' \right) \varphi \left( \mathbf{r}, \Omega', E' \right)
\]

\[
+ \int dV \int d\Omega \int dE \psi_2 \left( \mathbf{r}, \Omega, E \right) \nu \Sigma_f \left( \mathbf{f}, \mathbf{r}, E \right) \int d\Omega' \int dE' \varphi^* \left( \mathbf{r}, \Omega', E' \right) \sum_{m_2=1}^{J_1} \frac{\partial^2 \chi \left( \mathbf{p}, \mathbf{r}, E' \to E \right)}{\partial p_j \partial \alpha_{m_2}} \delta \alpha_{m_2} \int d\Omega' \int dE' \nu \Sigma_f \left( \mathbf{f}, \mathbf{r}, E' \right) \varphi \left( \mathbf{r}, \Omega', E' \right)
\]

\[
+ \int dV \int d\Omega \int dE \psi_3 \left( \mathbf{r}, \Omega, E \right) \nu \Sigma_f \left( \mathbf{f}, \mathbf{r}, E \right) \int d\Omega' \int dE' \varphi^* \left( \mathbf{r}, \Omega', E' \right) \sum_{m_2=1}^{J_1} \frac{\partial \chi \left( \mathbf{p}, \mathbf{r}, E' \to E \right)}{\partial p_j \partial \alpha_{m_2}} \delta \alpha_{m_2} \int d\Omega' \int dE' \nu \Sigma_f \left( \mathbf{f}, \mathbf{r}, E' \right) \varphi \left( \mathbf{r}, \Omega', E' \right)
\]

\[ \bigg( \bigg) \]
For \( j = 1, \ldots, J_p \):
\[
\left\{ \delta \left[ \frac{\partial R(a, \varphi; \psi^{(1)})}{\partial p_j} \right] \right\}_{\text{ind}} \triangleq \Delta \int_{\frac{4\pi}{2}} dV \int_{\frac{4\pi}{2}} d\Omega \int_{\frac{4\pi}{2}} dE \left[ \delta \psi_1^{(i)}(r, \Omega, E) \right] \int_{\frac{4\pi}{2}} d\Omega' \int_{\frac{4\pi}{2}} dE' \frac{\partial \chi'(p; r, E' \rightarrow E)}{\partial p_j} \nu_{\Sigma_j}(f; r, E') \phi(r, \Omega', E')
\]
\[
+ \int_{\frac{4\pi}{2}} dV \int_{\frac{4\pi}{2}} d\Omega \int_{\frac{4\pi}{2}} dE \psi_1^{(i)}(r, \Omega, E) \int_{\frac{4\pi}{2}} d\Omega' \int_{\frac{4\pi}{2}} dE' \left[ \delta \varphi(r, \Omega', E') \right] \frac{\partial \chi'(p; r, E' \rightarrow E)}{\partial p_j} \nu_{\Sigma_j}(f; r, E')
\]
\[
+ \int_{\frac{4\pi}{2}} dV \int_{\frac{4\pi}{2}} d\Omega \int_{\frac{4\pi}{2}} dE \psi_2^{(i)}(r, \Omega, E) \nu_{\Sigma_j}(f; r, E) \int_{\frac{4\pi}{2}} d\Omega' \int_{\frac{4\pi}{2}} dE' \left[ \delta \varphi'(r, \Omega', E') \right] \frac{\partial \chi'(p; r, E' \rightarrow E)}{\partial p_j}.
\]

The direct-effect term defined in Eq. (107) can be computed immediately but the indirect-effect term defined in Eq. (108) can be computed only after having obtained the functions \( \delta \psi_1^{(i)}(r, \Omega, E) \), \( \delta \psi_2^{(i)}(r, \Omega, E) \), \( \delta \varphi(r, \Omega, E) \) and \( \delta \varphi'(r, \Omega', E') \), which are computationally expensive to obtain. To avoid the need for computing these variations, the indirect-effect term defined in Eq. (108) will be expressed in terms of the solution of a 2nd-Level Adjoint Sensitivity System (2nd-LASS), which will be constructed by following the same sequence of steps as outlined in the previous Sections, namely by applying the definition provided in Eq. (51) to form the inner product of Eqs. (45) and (19) with a yet undefined function \( w_j^{(2)}(r, \Omega, E) \) which has the same structure as the 2nd-level adjoint functions that were introduced in previous sections, i.e., \( w_j^{(2)}(r, \Omega, E) \triangleq \left[ w_{1,j}^{(2)}(r, \Omega, E) , w_{2,j}^{(2)}(r, \Omega, E) \right] \), with
\[
w_{1,j}^{(2)} = \left[ w_{11,j}^{(2)}(r, \Omega, E) , w_{12,j}^{(2)}(r, \Omega, E) \right] , \quad w_{2,j}^{(2)} = \left[ w_{21,j}^{(2)}(r, \Omega, E) , w_{22,j}^{(2)}(r, \Omega, E) \right] ,
\]
with
\[
w_{mn,j}^{(2)}(r, \Omega, E) \in \mathcal{L}_2(J \times \Omega \times E) , \quad m, n = 1, 2 .
\]
This procedure yields the following relation:
\[
\left[ \begin{array}{c}
\delta \psi_1^{(i)} \\
\delta \psi_2^{(i)} \\
\delta \varphi^{(i)} \\
\delta \varphi'^{(i)}
\end{array} \right] =
\left[ \begin{array}{c}
A_{11}^{(i)}(\alpha) & F_{12}^{(i)}(\alpha) \\
0 & F_{11}^{(i)}(\alpha)
\end{array} \right] \left[ \begin{array}{c}
\delta \psi_1^{(i)} \\
\delta \psi_2^{(i)} \\
\delta \varphi^{(i)} \\
\delta \varphi'^{(i)}
\end{array} \right] =
\left[ \begin{array}{c}
\delta \psi_1^{(i)} \\
\delta \psi_2^{(i)} \\
\delta \varphi^{(i)} \\
\delta \varphi'^{(i)}
\end{array} \right] \left[ \begin{array}{c}
A_{11}^{(i)}(\alpha) & F_{12}^{(i)}(\alpha) \\
0 & F_{11}^{(i)}(\alpha)
\end{array} \right] \left[ \begin{array}{c}
\delta \psi_1^{(i)} \\
\delta \psi_2^{(i)} \\
\delta \varphi^{(i)} \\
\delta \varphi'^{(i)}
\end{array} \right] + P^{(2)} \left[ w_j^{(2)} , \delta \psi_1^{(i)} , \delta \varphi^{(i)} \right].
\]
The bilinear concomitant $P^{(2)}\left[w_j^{(2)}, \delta \psi^{(1)}, \delta u\right]$ in Eq. (109) will vanish by imposing on the components of $w_j^{(2)}(r, \Omega, E)$ the following boundary conditions:

\begin{align*}
w_{11,j}(r, \Omega, E) & = 0, \quad r_s \in \partial V, \quad \Omega \cdot n < 0; \quad w_{12,j}(r, \Omega, E) = 0, \quad r_s \in \partial V, \quad \Omega \cdot n > 0; \quad 0 < E < E_f, \\
w_{21,j}(r, \Omega, E) & = 0, \quad r_s \in \partial V, \quad \Omega \cdot n > 0; \quad w_{22,j}(r, \Omega, E) = 0, \quad r_s \in \partial V, \quad \Omega \cdot n < 0; \quad 0 < E < E_f. \tag{110}
\end{align*}

Identifying the first term on the right side of Eq. (109) with the indirect-effect term defined in Eq. (108) yields the following 2nd-LASS for the components of the 2nd-level adjoint function $w_j^{(2)}(r, \Omega, E)$:

\begin{align*}
L(a)w_{11,j}(r, \Omega, E) & = \int_{4\pi} d\Omega' \int_0^{E_f} dE' \frac{\partial \chi(p_r, r, E' \to E)}{\partial p_j} \nu \Sigma_f (f; r, E') \phi(r, \Omega', E'), \quad j = 1, \ldots, J_p, \tag{111}
\end{align*}

\begin{align*}
L'(a)w_{12,j}(r, \Omega, E) & = \nu \Sigma_f (f; r, E) \int_{4\pi} d\Omega' \int_0^{E_f} dE' \frac{\partial \chi(p_r, r, E \to E')}{\partial p_j} \phi^+(r, \Omega', E'), \quad j = 1, \ldots, J_f, \tag{112}
\end{align*}

\begin{align*}
L'(a)w_{21,j}(r, \Omega, E) & = \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^2} w_{11,j}(r, \Omega, E) + \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ \partial \varphi} w_{12,j}(r, \Omega, E) \\
& + \nu \Sigma_f (f; r, E) \int_{4\pi} d\Omega' \int_0^{E_f} dE' \frac{\partial \chi(p_r, r, E' \to E')}{\partial p_j} \psi^{(1)}_1(r, \Omega', E'), \quad j = 1, \ldots, J_p, \tag{113}
\end{align*}

\begin{align*}
L(a)w_{22,j}(r, \Omega, E) & = \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial \varphi^+} w_{11,j}(r, \Omega, E) + \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ \partial \varphi^+} w_{12,j}(r, \Omega, E) \\
& + \int_{4\pi} d\Omega' \int_0^{E_f} dE' \left[\nu \Sigma_f (f; r, E')\right] \psi^{(1)}_2(r, \Omega', E') \frac{\partial \chi(p_r, r, E' \to E)}{\partial p_j}, \quad j = 1, \ldots, J_p. \tag{114}
\end{align*}

As in the previous Sections, the operators appearing on the left-side of the 2nd-LASS defined by Eqs. (111) through (114) for the 2nd-level adjoint function $w_j^{(2)}(r, \Omega, E)$ are the same operators as appearing on the respective left-sides of the 2nd-LASS for the 2nd-level adjoint function $\theta_j^{(2)}$, $\psi_j^{(2)}$, and $u_j^{(2)}$; all of these the 2nd-level adjoint functions are subject to similar boundary conditions. Only the source-terms on the left sides of the respective 2nd-LASS differ from each other. Therefore, the same “forward” and “adjoint” software packages can be used for solving numerically the various forward and adjoint equations underlying the 1st-LASS and the 2nd-LASS.
Using the 2\textsuperscript{nd}-LASS defined by Eqs. (111) through (114) together with the term on the left-side of Eq.(109) leads to an expression for the indirect-effect term defined in Eq.(108) in which the terms containing the functions $\delta \varphi \left( r, \Omega, E \right)$, $\delta \varphi^+ \left( r, \Omega', E' \right)$, $\delta \psi_1^{(i)} \left( r, \Omega, E \right)$, and $\delta \psi_2^{(i)} \left( r, \Omega, E \right)$ have been replaced by terms containing the components of the 2\textsuperscript{nd}-level adjoint function $w_j^{(2)} \left( r, \Omega, E \right)$, as follows:
\[
\left\{ \left[ \frac{\partial R(\varphi, \varphi^+; \psi^{(1)}; w^{(2)}_{j}; a)}{\partial f_j} \right] \right\}_{\text{ind}} \triangleq \left\langle \left( w^{(2)}_{1,j} \right)^{\dagger} \left( Q^{(2)}(a, \psi^{(1)}; \delta a) \right) \right\rangle_{\text{(2)}}
\]

\[
= \int dV \int d\Omega \int dE \, w^{(2)}_{11,j}(r, \Omega, E) \left\{ \int d\Omega' \int dE' \left[ \delta \Sigma_s(\varpi, \varpi' \rightarrow E', \Omega' \rightarrow \Omega') \right] \psi^{(1)}_1(r', \Omega', E') - \delta \Sigma_s(\varpi, \varpi') \psi^{(1)}_1(r', \Omega, E') \right\} + \delta \left[ \nu \Sigma_j(\varpi, \varpi', E) \right] \int d\Omega' \int dE' \Delta \chi(\varpi', \varpi' \rightarrow E') \psi^{(1)}_2(r, \Omega', E') - \delta \Sigma_s(\varpi, \varpi') \psi^{(1)}_2(r, \Omega, E') \right\} + \frac{J_d}{\partial \varphi^+ \partial \varphi^{-}} \delta d_i \right\}
\]

\[
+ \int dV \int d\Omega \int dE \, w^{(2)}_{12,j}(r, \Omega, E) \left\{ \int d\Omega' \int dE' \left[ \delta \Sigma_s(\varpi, \varpi' \rightarrow E', \Omega' \rightarrow \Omega') \right] \psi^{(1)}_2(r', \Omega', E') - \delta \Sigma_s(\varpi, \varpi') \psi^{(1)}_2(r', \Omega, E') \right\} + \frac{J_d}{\partial \varphi^+ \partial \varphi^{-}} \delta d_i \right\}
\]

\[
+ \int dV \int d\Omega \int dE \, w^{(2)}_{21,j}(r, \Omega, E) \{ \delta Q(q, r, \Omega, E) - \delta \Sigma_s(\varpi, \varpi', E) \varphi(r, \Omega, E) \}
\]

\[
+ \int d\Omega' \int dE' \varphi(r', \Omega', E') \left[ \delta \Sigma_s(\varpi, \varpi', \varpi', \varpi' \rightarrow E, \Omega' \rightarrow \Omega) \right] \]

\[
+ \int d\Omega' \int dE' \Delta \chi(\varpi, \varpi' \rightarrow E) \varphi(r, \Omega', E') \left[ \nu \Sigma_j(\varpi', \varpi' \rightarrow E') \right] \]

\[
+ \int d\Omega' \int dE' \Delta \chi(\varpi', \varpi' \rightarrow E) \varphi(r, \Omega', E') \left[ \nu \Sigma_j(\varpi', \varpi' \rightarrow E') \right] \}
\]

\[
+ \int dV \int d\Omega \int dE \, w^{(2)}_{22,j}(r, \Omega, E) \{ \delta Q^+(k, r, \Omega, E) - \delta \Sigma_s(\varpi, \varpi', E) \varphi^+(r, \Omega, E) \}
\]

\[
+ \int d\Omega' \int dE' \varphi^+(r', \Omega', E') \left[ \delta \Sigma_s(\varpi, \varpi', \varpi', \varpi' \rightarrow E', \Omega \rightarrow \Omega') \right] \]

\[
+ \delta \left[ \nu \Sigma_j(\varpi, \varpi', E) \right] \int d\Omega' \int dE' \Delta \chi(\varpi, \varpi', \varpi', \varpi' \rightarrow E') \varphi^+(r, \Omega', E') \}
\]

\[
+ \nu \Sigma_j(\varpi, \varpi', E) \int d\Omega' \int dE' \Delta \chi(\varpi, \varpi', \varpi', \varpi' \rightarrow E') \varphi^+(r, \Omega', E') \}
\]

(115)
Replacing Eq. (115) together with the direct-effect term from Eq. (107) into Eq. (106) and subsequently identifying the quantities multiplying the parameter variations $\delta\alpha_{m}, m_2 = 1, \ldots, J_\alpha$, in the resulting expression yields the following results:

For $j = 1, \ldots, J_p ; \ m_2 = 1, \ldots, J_r$:

\[
\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; w^{(2)}_j; \alpha)}{\partial p_j \partial t_{m_2}} =
\]

\[
-\int dV \int_0^{E_f} dE \int w^{(2)}_{11,j}(r, \Omega, E) \psi_1^{(1)}(r, \Omega, E) + w^{(2)}_{12,j}(r, \Omega, E) \psi_2^{(1)}(r, \Omega, E)
\]

\[
+ w^{(2)}_{21,j}(r, \Omega, E) \varphi(r, \Omega, E) + w^{(2)}_{22,j}(r, \Omega, E) \varphi^*(r, \Omega, E) \frac{\partial \Sigma_s(t; r, \Omega, E)}{\partial t_k};
\]

For $j = 1, \ldots, J_p ; \ m_2 = 1, \ldots, J_s$:

\[
\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; w^{(2)}_j; \alpha)}{\partial p_j \partial \Sigma_{m_2}} =
\]

\[
= \int dV \int_0^{E_f} dE \int w^{(2)}_{11,j}(r, \Omega, E) \int dE' \psi_1^{(1)}(r, \Omega', E') \frac{\partial \Sigma_s(s; r, E \to E', \Omega \to \Omega')}{\partial \Sigma_{m_2}}
\]

\[
+ \int dV \int_0^{E_f} dE \int w^{(2)}_{12,j}(r, \Omega, E) \int dE' \psi_2^{(1)}(r, \Omega', E') \frac{\partial \Sigma_s(s; r, E \to E', \Omega \to \Omega')}{\partial \Sigma_{m_2}}
\]

\[
+ \int dV \int_0^{E_f} dE \int w^{(2)}_{21,j}(r, \Omega, E) \int dE' \varphi(r, \Omega', E') \frac{\partial \Sigma_s(s; r, E \to E', \Omega \to \Omega')}{\partial \Sigma_{m_2}}
\]

\[
+ \int dV \int_0^{E_f} dE \int w^{(2)}_{22,j}(r, \Omega, E) \int dE' \varphi^*(r, \Omega', E') \frac{\partial \Sigma_s(s; r, E \to E', \Omega \to \Omega')}{\partial \Sigma_{m_2}};
\]
For $j = 1, \ldots, J_p$; $m_2 = 1, \ldots, J_p$:

\[ \frac{\partial^2 R\left( \varphi, \varphi^+ ; \psi^{(1)} ; w^{(2)} ; \alpha \right)}{\partial p_j \partial f_{m_2}} = \]

\[ = \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(1)}_1 (r, \omega, E) \int dE' \varphi (r, \omega', E') \frac{\partial \chi (p, r, E' \rightarrow E)}{\partial p_j} \frac{\partial \left[ \nu \Sigma_f (f ; r, E) \right]}{\partial f_{m_2}} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(2)}_2 (r, \omega, E) \frac{\partial \left[ \nu \Sigma_f (f ; r, E) \right]}{\partial f_{m_2}} \int dE' \varphi^+ (r, \omega', E') \frac{\partial \chi (p, r, E \rightarrow E')}{{\partial p_j}} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(1)}_1 (r, \omega, E) \frac{\partial \left[ \nu \Sigma_f (f ; r, E) \right]}{\partial f_{m_2}} \int dE' \varphi (r, \omega', E') \frac{\partial \chi (p, r, E' \rightarrow E)}{\partial p_j} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(2)}_2 (r, \omega, E) \frac{\partial \left[ \nu \Sigma_f (f ; r, E) \right]}{\partial f_{m_2}} \int dE' \varphi^+ (r, \omega', E') \frac{\partial \chi (p, r, E \rightarrow E')}{{\partial p_j}} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(1)}_1 (r, \omega, E) \frac{\partial \left[ \nu \Sigma_f (f ; r, E) \right]}{\partial f_{m_2}} \int dE' \varphi (r, \omega', E') \frac{\partial \chi (p, r, E' \rightarrow E)}{\partial p_j} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(2)}_2 (r, \omega, E) \frac{\partial \left[ \nu \Sigma_f (f ; r, E) \right]}{\partial f_{m_2}} \int dE' \varphi^+ (r, \omega', E') \frac{\partial \chi (p, r, E \rightarrow E')}{{\partial p_j}} ; \quad (118) \]

For $j = 1, \ldots, J_p$; $m_2 = 1, \ldots, J_p$:

\[ \frac{\partial^2 R\left( \varphi, \varphi^+ ; \psi^{(1)} ; w^{(2)} ; \alpha \right)}{\partial p_j \partial p_{m_2}} = \]

\[ = \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(1)}_1 (r, \omega, E) \int dE' \nu \Sigma_f (f ; r, E') \varphi (r, \omega', E') \frac{\partial \chi (p, r, E' \rightarrow E)}{\partial p_j \partial p_{m_2}} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(2)}_2 (r, \omega, E) \nu \Sigma_f (f ; r, E) \int dE' \varphi^+ (r, \omega', E') \frac{\partial^2 \chi (p, r, E \rightarrow E')}{{\partial p_j} \partial p_{m_2}} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(1)}_1 (r, \omega, E) \int dE' \nu \Sigma_f (f ; r, E') \varphi^+ (r, \omega', E') \frac{\partial \chi (p, r, E' \rightarrow E)}{\partial p_j} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(2)}_2 (r, \omega, E) \int dE' \nu \Sigma_f (f ; r, E') \varphi^+ (r, \omega', E') \frac{\partial \chi (p, r, E \rightarrow E')}{{\partial p_j}} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(1)}_1 (r, \omega, E) \int dE' \nu \Sigma_f (f ; r, E') \varphi^+ (r, \omega', E') \frac{\partial \chi (p, r, E' \rightarrow E)}{\partial p_j} \]

\[ + \int dV \int_{E_f}^{E_i} dE \int_{0}^{E_f} dE' \psi^{(2)}_2 (r, \omega, E) \int dE' \nu \Sigma_f (f ; r, E') \varphi^+ (r, \omega', E') \frac{\partial \chi (p, r, E \rightarrow E')}{\partial p_{m_2}} ; \quad (119) \]
\[
\frac{\partial^2 R \left( \varphi, \varphi^* ; w^{(1)}_j, \alpha \right)}{\partial p_j \partial q_{m_2}} = \int \int d\Omega \int dE \, w^{(2)}_{21,j} \left( r, \Omega, E \right) \frac{\partial Q \left( q; r, \Omega, E \right)}{\partial q_{m_2}} ; \\
\frac{\partial^2 R \left( \varphi, \varphi^* ; w^{(1)}_j, \alpha \right)}{\partial p_j \partial k_{m_2}} = \int \int d\Omega \int dE \, w^{(2)}_{22,j} \left( r, \Omega, E \right) \frac{\partial Q^* \left( k; r, \Omega, E \right)}{\partial k_{m_2}} ; \\
\frac{\partial^2 R \left( \varphi, \varphi^* ; w^{(1)}_j, \alpha \right)}{\partial p_j \partial \Omega} = \int \int d\Omega \int dE \, \left[ w^{(2)}_{11,j} \left( r, \Omega, E \right) \frac{\partial^2 G \left( d; \varphi, \varphi^* \right)}{\partial \varphi \partial \Omega} + w^{(2)}_{12,j} \left( r, \Omega, E \right) \frac{\partial^2 G \left( d; \varphi, \varphi^* \right)}{\partial \varphi^* \partial \Omega} \right] .
\]

The expressions of the 2nd-order sensitivities computed using Eq. (116) must be identical to those computed using Eq. (65), i.e.

\[
\frac{\partial^2 R \left( \varphi, \varphi^* ; w^{(1)}_j, \alpha \right)}{\partial p_j \partial t_k} = -\int \int d\Omega \int dE \left[ w^{(2)}_{11,j} \left( r, \Omega, E \right) \psi^{(1)}_1 \left( r, \Omega, E \right) + w^{(2)}_{12,j} \left( r, \Omega, E \right) \psi^{(1)}_2 \left( r, \Omega, E \right) \right] \frac{\partial \Sigma \left( t; r, \Omega, E \right)}{\partial t_k} = \\
\frac{\partial^2 R \left( \varphi, \varphi^* ; w^{(1)}_j, \alpha \right)}{\partial t_k \partial p_j} = \\
\int \int d\Omega \int dE \psi^{(1)}_{11,j} \left( r, \Omega, E \right) \psi^{(1)}_1 \left( r, \Omega', E' \right) \frac{\partial \chi \left( p; r, E \rightarrow E' \right)}{\partial p_j} + \\
\int \int d\Omega \int dE \psi^{(1)}_{12,j} \left( r, \Omega, E \right) \psi^{(1)}_2 \left( r, \Omega', E' \right) \frac{\partial \chi \left( p; r, E \rightarrow E' \right)}{\partial p_j} + \\
\int \int d\Omega \int dE \psi^{(1)}_{21,j} \left( r, \Omega, E \right) \psi^{(1)}_1 \left( r, \Omega', E' \right) \frac{\partial \chi \left( p; r, E \rightarrow E' \right)}{\partial p_j} + \\
\int \int d\Omega \int dE \psi^{(1)}_{22,j} \left( r, \Omega, E \right) \psi^{(1)}_2 \left( r, \Omega', E' \right) \frac{\partial \chi \left( p; r, E \rightarrow E' \right)}{\partial p_j} ;
\]
The relation expressed by Eq. (123) provides an independent mutual verification of the 2nd-level adjoint functions $w_j^{(2)}$ and $\psi_j^{(2)}$.

Furthermore, the expressions of the 2nd-order sensitivities computed using Eq. (117) must be identical to those computed using Eq. (82), i.e.

$$
\frac{\partial^2 R\left(\varphi, \varphi^+; \psi_1^{(1)}; w_j^{(2)}; \alpha\right)}{\partial p_j \partial s_k} = \int dV \int_{E_f} d\Omega \int_{0} dE \psi_{1, j}^{(1)}(r, \Omega, E) \int dE' \psi_1^{(1)}(r, \Omega', E') \frac{\partial \Sigma_s (s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_k} \\
+ \int dV \int_{E_f} d\Omega \int_{0} dE \psi_{2, j}^{(1)}(r, \Omega, E) \int dE' \psi_2^{(1)}(r, \Omega', E') \frac{\partial \Sigma_s (s; r, E' \rightarrow E, \Omega \rightarrow \Omega')}{\partial s_k} \\
+ \int dV \int_{E_f} d\Omega \int_{0} dE \phi(r, \Omega, E) \int dE' \varphi(r, \Omega', E') \frac{\partial \Sigma_s (s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_k} \\
+ \int dV \int_{E_f} d\Omega \int_{0} dE \psi_j^{(2)}(r, \Omega, E) \int dE' \varphi^+(r, \Omega', E') \frac{\partial \Sigma_s (s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_k};
$$

$$
= \frac{\partial^2 R\left(\varphi, \varphi^+; \psi_1^{(1)}; \theta_j^{(2)}; \alpha\right)}{\partial s_k \partial p_j} = \int dV \int_{E_f} d\Omega \int_{0} dE \theta_{1, j}^{(2)}(r, \Omega, E) \int dE' \psi_1^{(1)}(r, \Omega', E') \frac{\partial \chi(p; r, E \rightarrow E')}{\partial p_j} \\
+ \int dV \int_{E_f} d\Omega \int_{0} dE \theta_{1, j}^{(2)}(r, \Omega, E) \int dE' \nu \Sigma_f (f; r, E') \psi_2^{(1)}(r, \Omega', E') \frac{\partial \chi(p; r, E' \rightarrow E)}{\partial p_j} \\
+ \int dV \int_{E_f} d\Omega \int_{0} dE \theta_{2, j}^{(2)}(r, \Omega, E) \int dE' \varphi(r, \Omega, E') \frac{\partial \chi(p; r, E \rightarrow E')}{\partial p_j} \\
+ \int dV \int_{E_f} d\Omega \int_{0} dE \theta_{2, j}^{(2)}(r, \Omega, E) \nu \Sigma_f (f; r, E') \int dE' \varphi^+(r, \Omega', E') \frac{\partial \chi(p; r, E \rightarrow E')}{\partial p_j}.
$$

The relation expressed by Eq. (124) provides an independent mutual verification of the 2nd-level adjoint functions $w_j^{(2)}$ and $\theta_j^{(2)}$.

Finally, the expressions of the 2nd-order sensitivities computed using Eq. (118) must be identical to those computed using Eq. (100), i.e.
For \( j = 1, \ldots, J_p; \ k = 1, \ldots, J_f \):

\[
\frac{\partial^2 R \left( \phi, \phi^*; \psi^{(1)}; \mathbf{w}^{(2)}_j; \mathbf{u} \right)}{\partial p_j \partial f_k} = \\
= \int dV \int_{4\pi}^E d\Omega \int_{0}^E dE \psi^{(1)}_j (\mathbf{r}, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \varphi (\mathbf{r}, \Omega', E') \frac{\partial \chi (\mathbf{p}, \mathbf{r}, E' \to E)}{\partial p_j} \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}, \mathbf{r}, E') \right]}{\partial \mathbf{f_k}} \\
+ \int dV \int_{4\pi}^E d\Omega \int_{0}^E dE \psi^{(2)}_j (\mathbf{r}, \Omega, E) \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}, \mathbf{r}, E) \right]}{\partial \mathbf{f_k}} \int d\Omega' \int_{0}^{E_f} dE' \varphi^* (\mathbf{r}, \Omega', E') \frac{\partial \chi (\mathbf{p}, \mathbf{r}, E \to E')}{\partial p_j} \\
+ \int dV \int_{4\pi}^E d\Omega \int_{0}^E dE \psi_{11,j} \psi^{(2)}_j (\mathbf{r}, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \chi (\mathbf{p}, \mathbf{r}, E' \to E) \psi^{(1)}_j (\mathbf{r}, \Omega', E') \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}, \mathbf{r}, E') \right]}{\partial \mathbf{f_k}} \\
+ \int dV \int_{4\pi}^E d\Omega \int_{0}^E dE \psi_{21,j} \psi^{(2)}_j (\mathbf{r}, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \chi (\mathbf{p}, \mathbf{r}, E' \to E) \varphi (\mathbf{r}, \Omega', E') \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}, \mathbf{r}, E') \right]}{\partial \mathbf{f_k}} \\
+ \int dV \int_{4\pi}^E d\Omega \int_{0}^E dE \psi_{21,j} \psi^{(2)}_j (\mathbf{r}, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \chi (\mathbf{p}, \mathbf{r}, E' \to E) \varphi^* (\mathbf{r}, \Omega', E') \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}, \mathbf{r}, E') \right]}{\partial \mathbf{f_k}} \\
+ \int dV \int_{4\pi}^E d\Omega \int_{0}^E dE \psi_{22,j} \psi^{(2)}_j (\mathbf{r}, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \chi (\mathbf{p}, \mathbf{r}, E' \to E) \varphi (\mathbf{r}, \Omega', E') \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}, \mathbf{r}, E') \right]}{\partial \mathbf{f_k}} \\
+ \int dV \int_{4\pi}^E d\Omega \int_{0}^E dE \psi_{22,j} \psi^{(2)}_j (\mathbf{r}, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \chi (\mathbf{p}, \mathbf{r}, E' \to E) \varphi^* (\mathbf{r}, \Omega', E') \frac{\partial \left[ \nu \Sigma_f (\mathbf{f}, \mathbf{r}, E') \right]}{\partial \mathbf{f_k}} \\
\text{for } j = 1, \ldots, J_p; \ k = 1, \ldots, J_f ; \quad (125)
\]

The relation shown in Eq. (125) provides an independent path for the mutual verification of the solutions \( \mathbf{w}_j^{(2)} \) and \( \mathbf{u}_j^{(2)} \).
IV.E. Computation of the 2nd-Order Sensitivities $\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; g^{(2)}; \alpha)}{\partial q_j \partial \alpha_m^2}, \ j = 1, \ldots, J_q, \ m_2 = 1, \ldots, J_\alpha$

The 2nd-order sensitivities $\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; g^{(2)}; \alpha)}{\partial q_j \partial \alpha_m^2}, \ j = 1, \ldots, J_q, \ m_2 = 1, \ldots, J_\alpha$ will ultimately depend on a 2nd-level adjoint function which is denoted as $g^{(2)}_j$, and are obtained by computing the G-differential of the 1st-order sensitivities defined in Eq. (39), which yields the following expression:

$$
\delta \left[ \frac{\partial R(\varphi, \varphi^*, \alpha; \psi^{(1)})}{\partial q_j} \right] = \left[ \delta \left[ \frac{\partial R(\varphi, \varphi^*, \alpha; \psi^{(1)})}{\partial q_j} \right] \right]_{\text{dir}} + \left[ \delta \left[ \frac{\partial R(\varphi, \varphi^*, \alpha; \psi^{(1)})}{\partial q_j} \right] \right]_{\text{ind}}, \ j = 1, \ldots, J_q, \ (126)
$$

where

For $j = 1, \ldots, J_q : \left[ \delta \left[ \frac{\partial R(\varphi, \varphi^*, \alpha; \psi^{(1)})}{\partial q_j} \right] \right]_{\text{dir}} \triangleq \int dV \int d\Omega \int_0^{E_f} dE \psi^{(1)}_j(r, \Omega, E) \sum_{m_1=1}^{J_\alpha} \frac{\partial^2 Q(q, r, \Omega, E)}{\partial q_j \partial q_{m_2}} \delta q_{m_2}, \ (127)

For $j = 1, \ldots, J_q : \left[ \delta \left[ \frac{\partial R(\varphi, \varphi^*, \alpha; \psi^{(1)})}{\partial q_j} \right] \right]_{\text{ind}} \triangleq \int dV \int d\Omega \int_0^{E_f} dE \left. \delta \psi^{(1)}_j(r, \Omega, E) \frac{\partial Q(q, r, \Omega, E)}{\partial q_j} \right|, \ (128)

The direct-effect term defined in Eq. (127) can be computed immediately. On the other hand, the indirect-effect term defined in Eq. (128) can be computed only after having obtained the function $\delta \psi^{(1)}_j(r, \Omega, E)$, which is computationally expensive to obtain. To avoid the need for computing this function, the indirect-effect term defined in Eq. (128) will be expressed in terms of the solution, denoted as $g^{(2)}_j(r, \Omega, E) \triangleq \left[ g^{(2)}_{1,j}(r, \Omega, E), g^{(2)}_{2,j}(r, \Omega, E) \right]^{\top}$ of a 2nd-Level Adjoint Sensitivity System (2nd-LASS) which will turn out to have the same structure as in the previous sections. The 2nd-level adjoint function $g^{(2)}_j(r, \Omega, E) \triangleq \left[ g^{(2)}_{1,j}(r, \Omega, E), g^{(2)}_{2,j}(r, \Omega, E) \right]^{\top}$ has the same structure as the 2nd-level adjoint functions that were introduced in previous sections, having components $g^{(2)}_{1,j} \triangleq \left[ g^{(2)}_{11,j}(r, \Omega, E), g^{(2)}_{12,j}(r, \Omega, E) \right]^{\top}$,
The bilinear concomitant \( P^{(2)} \left[ g^{(2)}_j, \delta \psi^{(1)}_j, \delta u_j \right] \) in Eq.(129) will vanish by imposing on the components of \( g^{(2)}_j (r, \Omega, E) \) the following boundary conditions:

\[
g^{(2)}_{11, j} (r_s, \Omega, E) = 0, \; r_s \in \partial V, \; \nabla \cdot n < 0; \quad g^{(2)}_{22, j} (r_s, \Omega, E) = 0, \; r_s \in \partial V, \; \nabla \cdot n > 0; \quad 0 < E < E_f, \quad g^{(2)}_{21, j} (r_s, \Omega, E) = 0, \; r_s \in \partial V, \; \nabla \cdot n < 0; \quad g^{(2)}_{22, j} (r_s, \Omega, E) = 0, \; r_s \in \partial V, \; \nabla \cdot n > 0; \quad 0 < E < E_f. \tag{130}
\]

Identifying the first term on the right side of Eq. (129) with the indirect-effect term defined in Eq. (128) yields the following 2nd-LASS for the components of the 2nd-level adjoint function \( g^{(2)}_j (r, \Omega, E) \):

\[
L (\alpha) g^{(2)}_{11, j} (r, \Omega, E) = \frac{\partial Q (q \cdot r, \Omega, E)}{\partial q_j}, \quad j = 1, \ldots, J_q, \tag{131}
\]

\[
L^* (\alpha) g^{(2)}_{12, j} (r, \Omega, E) = 0, \quad j = 1, \ldots, J_q, \tag{132}
\]

\[
L^* (\alpha) g^{(2)}_{21, j} (r, \Omega, E) = \frac{\partial^2 G (d : \varphi, \varphi^*)}{\partial \varphi^2} g^{(2)}_{11, j} (r, \Omega, E) + \frac{\partial^2 G (d : \varphi, \varphi^*)}{\partial \varphi^* \partial \varphi} g^{(2)}_{12, j} (r, \Omega, E), \quad j = 1, \ldots, J_q, \tag{133}
\]

\[
L (\alpha) g^{(2)}_{22, j} (r, \Omega, E) = \frac{\partial^2 G (d : \varphi, \varphi^*)}{\partial \varphi^2} g^{(2)}_{11, j} (r, \Omega, E) + \frac{\partial^2 G (d : \varphi, \varphi^*)}{\partial \varphi^* \partial \varphi^*} g^{(2)}_{12, j} (r, \Omega, E), \quad j = 1, \ldots, J_q. \tag{134}
\]

It follows from Eqs.(132) and (130) that

\[
g^{(2)}_{12, j} (r, \Omega, E) \equiv 0, \quad j = 1, \ldots, J_q, \tag{135}
\]

which implies, in turn, that Eqs. (133) and (134) reduce to the following decoupled equations for determining the components \( g^{(2)}_{21, j} (r, \Omega, E) \) and \( g^{(2)}_{22, j} (r, \Omega, E) \):

\[
L^* (\alpha) g^{(2)}_{21, j} (r, \Omega, E) = \frac{\partial^2 G (d : \varphi, \varphi^*)}{\partial \varphi^2} g^{(2)}_{11, j} (r, \Omega, E), \quad j = 1, \ldots, J_q, \tag{136}
\]
Using the 2nd-LASS defined by Eqs. (131), and (135) through (137) together with the term on the left-side of Eq.(129) leads to the following expression for the indirect-effect term defined in Eq.(128):

\[
\left\{ \frac{\partial R(\varphi, \varphi^+; \psi^{(1)}; g_j^{(2)}; \alpha)}{\partial q_j} \right\}_{\text{ind}} = \left\{ \left( g_0^{(2)} \right)^\dagger \left( Q^{(2)}(\alpha; \psi^{(1)}; \delta \alpha) \right) \right\}_{(2)}
\]

\[
\begin{align*}
&= \int_{4\pi}^{E_f} dV \int_{4\pi}^{E_f} dE \ g_{21,j}^{(2)}(r, \Omega, E) \int_{4\pi}^{E_f} dE' \left[ \delta \Sigma_j(r, E \rightarrow E', \Omega \rightarrow \Omega') \right] \psi_i^{(1)}(r, \Omega', E') \\
&\quad + \delta \left[ \nu \Sigma_j(f; r, E) \right] \int_{4\pi}^{E_f} dE' \chi(p; r, E \rightarrow E') \psi_i^{(1)}(r, \Omega', E') - \delta \Sigma_j(r, E) \psi_i^{(1)}(r, \Omega, E) \\
&\quad + \left[ \nu \Sigma_j(f; r, E) \right] \int_{4\pi}^{E_f} dE' \delta \chi(p; r, E \rightarrow E') \psi_i^{(1)}(r, \Omega', E') + \sum_{i=1}^{J_q} \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial d_i} \delta d_i \\
&\quad + \int_{4\pi}^{E_f} dV \int_{4\pi}^{E_f} dE \ g_{21,j}^{(2)}(r, \Omega, E) \left\{ \delta Q(q, r, \Omega, E) - \delta \Sigma_j(t; r, E) \varphi(r, \Omega, E) \right\} \\
&\quad + \int_{4\pi}^{E_f} dE' \left[ \delta \Sigma_j(s; r, E' \rightarrow E, \Omega \rightarrow \Omega') \right] \\
&\quad + \int_{4\pi}^{E_f} dE' \delta \chi(p; r, E \rightarrow E) \varphi(r, \Omega', E') \left[ \nu \Sigma_j(f; r, E') \right] \\
&\quad + \int_{4\pi}^{E_f} dE' \chi(p; r, E \rightarrow E) \varphi(r, \Omega', E') \delta \left[ \nu \Sigma_j(f; r, E') \right] \\
&\quad + \int_{4\pi}^{E_f} dV \int_{4\pi}^{E_f} dE \ g_{22,j}^{(2)}(r, \Omega, E) \left\{ \delta Q^+(k; r, \Omega, E) - \delta \Sigma_j(t; r, E) \varphi^+(r, \Omega, E) \right\} \\
&\quad + \int_{4\pi}^{E_f} dE' \left[ \delta \Sigma_j(s; r, E \rightarrow E', \Omega \rightarrow \Omega') \right] \\
&\quad + \delta \left[ \nu \Sigma_j(f; r, E) \right] \int_{4\pi}^{E_f} dE' \chi(p; r, E \rightarrow E') \varphi^+(r, \Omega', E') \\
&\quad + \left[ \nu \Sigma_j(f; r, E) \right] \int_{4\pi}^{E_f} dE' \delta \chi(p; r, E \rightarrow E') \varphi^+(r, \Omega', E'),
\end{align*}
\]
Replacing Eqs.(138) and (127) into Eq. (126) and subsequently identifying the quantities multiplying the parameter variations $\delta \alpha_{m_z}$, $m_z = 1, ..., J \alpha$, in the resulting expression yields the following results:

For $j = 1, ..., J_q$; $m_z = 1, ..., J_\ell$:

$$
\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; g^{(2)}; \alpha)}{\partial q_j \partial t_{m_z}} = 
$$

$$
= -\int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \frac{\partial \Sigma}{\partial t_{m_z}} \left[ g_{11,j}(r, \Omega, E) \psi_1^{(1)}(r, \Omega, E) 
+ g_{21,j}(r, \Omega, E) \varphi(r, \Omega, E) + g_{22,j}(r, \Omega, E) \varphi^*(r, \Omega, E) \right];
$$

(139)

(140)

For $j = 1, ..., J_q$; $m_z = 1, ..., J_\ell$:

$$
\frac{\partial^2 R(\varphi, \varphi^*; \psi^{(1)}; g^{(2)}; \alpha)}{\partial q_j \partial s_{m_z}} = 
$$

$$
= \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \frac{\partial \Sigma}{\partial s_{m_z}} \left( s; r \rightarrow E', \Omega \rightarrow \Omega' \right)
$$

$$
+ \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \frac{\partial \Sigma}{\partial s_{m_z}} \left( s; r, E \rightarrow E', \Omega' \rightarrow \Omega \right)
$$

$$
+ \int dV \int_{4\pi} d\Omega \int_0^{E_f} dE \frac{\partial \Sigma}{\partial s_{m_z}} \left( s; r, E \rightarrow E', \Omega' \rightarrow \Omega \right);
$$

(141)
For \( j = 1, \ldots, J_q \); \( m_2 = 1, \ldots, J_p \) :

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}, g^{(2)}; \alpha)}{\partial q_j \partial p_{m_2}} = \\
\int dV \int_{4\pi}^E d\Omega' \int dE' \psi^{(1)}_1\left( \mathbf{r}, \mathbf{r}', E' \right) \frac{\partial \chi\left( \mathbf{p} : E \rightarrow E' \right)}{\partial p_{m_2}} \\
+ \int dV \int_{4\pi}^E d\Omega' \int dE'\left[ \nu \Sigma_f\left( \mathbf{f} : \mathbf{r}', E' \right) \right] \varphi\left( \mathbf{r}, \mathbf{r}', E' \right) \frac{\partial \chi\left( \mathbf{p} : E' \rightarrow E \right)}{\partial p_{m_2}} \\
+ \int dV \int_{4\pi}^E d\Omega' \int dE' \varphi^\dagger\left( \mathbf{r}, \mathbf{r}', E' \right) \frac{\partial \chi\left( \mathbf{p} : E \rightarrow E' \right)}{\partial p_{m_2}};
\]

(142)

For \( j = 1, \ldots, J_q \); \( m_2 = 1, \ldots, J_q \) :

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}, g^{(2)}; \alpha)}{\partial q_j \partial q_{m_2}} = \\
\int dV \int_{4\pi}^E d\Omega' \int dE' \psi^{(1)}_1\left( \mathbf{r}, \mathbf{r}', E' \right) \frac{\partial^2 Q\left( \mathbf{q} \cdot \mathbf{r}, \mathbf{r}, E \right)}{\partial q_j \partial q_{m_2}} + \int dV \int_{4\pi}^E d\Omega' \int dE \ g^{(2)}_{21,j}\left( \mathbf{r}, \mathbf{r}, E \right) \frac{\partial Q\left( \mathbf{q} \cdot \mathbf{r}, \mathbf{r}, E \right)}{\partial q_{m_2}};
\]

(143)

For \( j = 1, \ldots, J_q \); \( m_2 = 1, \ldots, J_k \) :

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}, g^{(2)}; \alpha)}{\partial q_j \partial k_{m_2}} = \\
\int dV \int_{4\pi}^E d\Omega' \int dE \ g^{(2)}_{21,j}\left( \mathbf{r}, \mathbf{r}, E \right) \frac{\partial Q^+\left( \mathbf{k} \cdot \mathbf{r}, \mathbf{r}, E \right)}{\partial k_{m_2}};
\]

(144)

For \( j = 1, \ldots, J_q \); \( m_2 = 1, \ldots, J_d \) :

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}, g^{(2)}; \alpha)}{\partial q_j \partial d_{m_2}} = \\
\int dV \int_{4\pi}^E d\Omega' \int dE \ g^{(2)}_{11,j}\left( \mathbf{r}, \mathbf{r}, E \right) \frac{\partial G\left( \mathbf{d} \cdot \varphi, \varphi^+ \right)}{\partial \varphi \partial d_{m_2}}.
\]

(145)

The expressions of the 2nd-order sensitivities computed using Eq. (139) must be identical to those computed using Eq. (66), i.e.

For \( j = 1, \ldots, J_q \); \( k = 1, \ldots, J_j \) :

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}, g^{(2)}; \alpha)}{\partial q_j \partial t_k} = \\
-\int dV \int_{4\pi}^E d\Omega' \int dE \ \frac{\partial \Sigma\left( \mathbf{t} \cdot \mathbf{r}, \mathbf{r}, E \right)}{\partial t_k} \left[ g^{(2)}_{11,j}\left( \mathbf{r}, \mathbf{r}, E \right) \psi^{(1)}_1\left( \mathbf{r}, \mathbf{r}, E \right) + g^{(2)}_{21,j}\left( \mathbf{r}, \mathbf{r}, E \right) \varphi\left( \mathbf{r}, \mathbf{r}, E \right) \right]
\]

(146)

\[
= \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}, g^{(2)}; \alpha)}{\partial t_k \partial q_j} = \int dV \int_{4\pi}^E d\Omega' \int dE \ \psi^{(2)}_{21,k}\left( \mathbf{r}, \mathbf{r}, E \right) \frac{\partial Q\left( \mathbf{q} \cdot \mathbf{r}, \mathbf{r}, E \right)}{\partial q_j}.
\]
The relation expressed by Eq. (146) provides an independent mutual verification of the 2nd-level adjoint functions $g_j^{(2)}$ and $\psi_j^{(2)}$.

The expressions of the 2nd-order sensitivities computed using Eq. (140) must be identical to those computed using Eq. (83), i.e.

$$\frac{\partial^2 R\left(\phi, \phi^+; \psi_1^{(1)}; g_j^{(2)}; \alpha\right)}{\partial q_j \partial s_k} =$$

$$= \int dV \int_{4\pi}^{E_f} d\Omega \int_{0}^{E_f} dE \ g_{11,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \psi_1^{(1)}(r, \Omega', E') \frac{\partial \Sigma_s(s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_k}$$

$$+ \int dV \int_{4\pi}^{E_f} d\Omega \int_{0}^{E_f} dE \ g_{21,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \varphi(r, \Omega', E') \frac{\partial \Sigma_s(s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_k}$$

$$+ \int dV \int_{4\pi}^{E_f} d\Omega \int_{0}^{E_f} dE \ g_{22,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \varphi^+(r, \Omega', E') \frac{\partial \Sigma_s(s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial s_k}$$

$$\partial^2 R\left(\phi, \phi^+; \psi_1^{(1)}; g_j^{(2)}; \alpha\right) = \int dV \int_{4\pi}^{E_f} d\Omega \int_{0}^{E_f} dE \ \theta_{21,k}^{(2)}(r, \Omega, E) \frac{\partial Q(q; r, \Omega, E)}{\partial q_j}. \tag{147}$$

The relation expressed by Eq. (147) provides an independent mutual verification of the 2nd-level adjoint functions $g_j^{(2)}$ and $\theta_j^{(2)}$.

The expressions of the 2nd-order sensitivities computed using Eq. (141) must be identical to those computed using Eq. (101), i.e.

$$\frac{\partial^2 R\left(\phi, \phi^+; \psi_1^{(1)}; g_j^{(2)}; \alpha\right)}{\partial q_j \partial f_k} =$$

$$= \int dV \int_{4\pi}^{E_f} d\Omega \int_{0}^{E_f} dE \ g_{11,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \chi(p; r, E \rightarrow E') \psi_1^{(1)}(r, \Omega', E')$$

$$+ \int dV \int_{4\pi}^{E_f} d\Omega \int_{0}^{E_f} dE \ g_{21,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \chi(p; r, E \rightarrow E') \varphi(r, \Omega', E') \frac{\partial \psi_1^{(1)}(r, \Omega', E')}{\partial f_k}$$

$$+ \int dV \int_{4\pi}^{E_f} d\Omega \int_{0}^{E_f} dE \ g_{22,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_{0}^{E_f} dE' \chi(p; r, E \rightarrow E') \varphi^+(r, \Omega', E')$$

$$\partial^2 R\left(\phi, \phi^+; \psi_1^{(1)}; u_j^{(2)}; \alpha\right) = \int dV \int_{4\pi}^{E_f} d\Omega \int_{0}^{E_f} dE \ u_{21,k}^{(2)}(r, \Omega, E) \frac{\partial Q(q; r, \Omega, E)}{\partial q_j}. \tag{148}$$

The relation shown in Eq. (148) provides an independent path for the mutual verification of the solutions $g_j^{(2)}$ and $u_j^{(2)}$. 
The expressions of the 2nd-order sensitivities computed using Eq. (142) must be identical to those computed using Eq. (120), i.e.

\[
\frac{\partial^2 R(\varphi,\varphi^*;\psi^{(1)};g_j^{(2)};\alpha)}{\partial q_j \partial p_k} = \\
\int dV \int d\Omega \int dE \ g_{11,j}^{(2)}(r,\Omega,E) \int d\Omega' \int dE' \psi_1^{(1)}(r,\Omega',E') \frac{\partial \chi(p;r,E \to E')}{\partial p_k} \\
+ \int dV \int d\Omega \int dE \ g_{21,j}^{(2)}(r,\Omega,E) \int d\Omega' \int dE' \varphi_2(\Omega,E',E') \frac{\partial \chi(p;r,E \to E')}{\partial p_k} \\
+ \int dV \int d\Omega \int dE \ g_{22,j}^{(2)}(r,\Omega,E) \int d\Omega' \int dE' \varphi^+_2(\Omega,E',E') \frac{\partial \chi(p;r,E \to E')}{\partial p_k} \\
= \frac{\partial^2 R(\varphi,\varphi^*;\psi^{(1)};w_j^{(2)};\alpha)}{\partial p_k \partial q_j} = \int dV \int d\Omega \int dE \ w_{21,k}^{(2)}(r,\Omega,E) \frac{\partial Q(q;r,\Omega,E)}{\partial q_j}.
\]

The relation shown in Eq. (149) provides an independent path for the mutual verification of the solutions \(g_j^{(2)}\) and \(w_j^{(2)}\).

\[
IV.F. \text{ Computation of the 2nd-Order Sensitivities} \ \frac{\partial^2 R(\varphi,\varphi^*;\psi^{(1)};\gamma_j^{(2)};\alpha)}{\partial k_j \partial \alpha_{m_2}}, \ j = 1,...,J_k, \ m_2 = 1,...,J_\alpha
\]

The 2nd-order sensitivities \(\partial^2 R(\varphi,\varphi^*;\psi^{(1)};\gamma_j^{(2)};\alpha)/\partial k_j \partial \alpha_{m_2}\), \(j = 1,...,J_k, \ m_2 = 1,...,J_\alpha\) will ultimately depend on a 2nd-level adjoint function which is denoted as \(\gamma_j^{(2)}\), and are obtained by computing the G-differential of the 1st-order sensitivities defined in Eq.(40), which yields the following expression:

\[
\delta \left[ \frac{\partial R(\varphi,\varphi^*;\alpha;\psi^{(1)})}{\partial k_j} \right] = \delta \left[ \frac{\partial R(\varphi,\varphi^*;\alpha;\psi^{(1)})}{\partial k_j} \right]_{dir} + \delta \left[ \frac{\partial R(\varphi,\varphi^*;\alpha;\psi^{(1)})}{\partial k_j} \right]_{ind}, \ j = 1,...,J_k, \quad (150)
\]

where

\[
For \ j = 1,...,J_k : \ \left\{ \delta \left[ \frac{\partial R(\varphi,\varphi^*;\alpha;\psi^{(1)})}{\partial k_j} \right] \right\}_{dir} \triangleq \int dV \int d\Omega \int dE \ \psi_2^{(1)}(r,\Omega,E) \sum_{m_2=1}^{J_{\alpha}} \frac{\partial^2 Q^+(k;r,\Omega,E)}{\partial k_j \partial \alpha_{m_2}} \delta k_{m_2}, \quad (151)
\]
For $j = 1, \ldots, J_k$:

$$
\delta \left[ \frac{\partial R(\varphi, \varphi^+, \alpha, \psi^{(1)})}{\partial k_j} \right]_{\text{ind}} \triangleq \int dV \int d\Omega \int_0^{E_f} dE \ \delta \psi_2^{(1)}(\mathbf{r}, \Omega, E) \frac{\partial Q^+ (\mathbf{k} : \mathbf{r}, \Omega, E)}{\partial k_j}.
$$

(152)

The direct-effect term defined in Eq. (151) can be computed immediately. On the other hand, the indirect-effect term defined in Eq. (152) can be computed only after having obtained the function $\delta \psi_2^{(1)}(\mathbf{r}, \Omega, E)$, which is computationally expensive to obtain. To avoid the need for computing this function, the indirect-effect term defined in Eq. (152) will be expressed in terms of the solution, denoted as $\gamma_j^{(2)}(\mathbf{r}, \Omega, E) \triangleq \left[ \gamma_{1,j}^{(2)}(\mathbf{r}, \Omega, E) , \gamma_{2,j}^{(2)}(\mathbf{r}, \Omega, E) \right]^T$ of a 2nd-Level Adjoint Sensitivity System (2nd-LASS) which will turn out to have the same structure as in the previous sections. The 2nd-level adjoint function $\gamma_j^{(2)}(\mathbf{r}, \Omega, E) \triangleq \left[ \gamma_{1,j}^{(2)}(\mathbf{r}, \Omega, E) , \gamma_{2,j}^{(2)}(\mathbf{r}, \Omega, E) \right]^T$ has the same structure as the 2nd-level adjoint functions that were introduced in previous sections, having components $\gamma_{1,j}^{(2)} \triangleq \left[ \gamma_{1,j}^{(2)}(\mathbf{r}, \Omega, E) , \gamma_{12,j}^{(2)}(\mathbf{r}, \Omega, E) \right]^T$, $\gamma_{2,j}^{(2)} \triangleq \left[ \gamma_{21,j}^{(2)}(\mathbf{r}, \Omega, E) , \gamma_{22,j}^{(2)}(\mathbf{r}, \Omega, E) \right]^T$, with $\gamma_{mn,j}^{(2)}(\mathbf{r}, \Omega, E) \in \mathcal{L}_2(V \times \Omega \times E)$, $m,n = 1,2$. Forming the inner product of $\gamma_j^{(2)}(\mathbf{r}, \Omega, E)$ with Eqs. (45) and (19) leads to the following relation:

$$
\left\langle \left[ \begin{array}{cc} \gamma_{1,j}^{(2)}(\mathbf{r}, \Omega, E) \\ \gamma_{2,j}^{(2)}(\mathbf{r}, \Omega, E) \end{array} \right] , \left[ \begin{array}{cc} A^{(1)}(\mathbf{r}, \Omega, E) & F^{(2)}(\mathbf{r}, \Omega, E) \\ 0 & F^{(1)}(\mathbf{r}, \Omega, E) \end{array} \right] \delta \psi^{(1)}(\mathbf{r}, \Omega, E) \right\rangle = \left[ \left[ \begin{array}{cc} \gamma_{1,j}^{(2)}(\mathbf{r}, \Omega, E) \\ \gamma_{2,j}^{(2)}(\mathbf{r}, \Omega, E) \end{array} \right] , \left[ \begin{array}{cc} \delta \psi^{(1)}(\mathbf{r}, \Omega, E) \\ \delta \mathbf{u} \end{array} \right] \right] + P^{(2)}[\gamma_j^{(2)} , \delta \psi^{(1)} , \delta \mathbf{u}] .
$$

(153)

The bilinear concomitant $P^{(2)}[\gamma_j^{(2)} , \delta \psi^{(1)} , \delta \mathbf{u}]$ in Eq. (153) will vanish by imposing on the components of $\gamma_j^{(2)}(\mathbf{r}, \Omega, E)$ the following boundary conditions:

$$
\gamma_{1,j}^{(2)}(\mathbf{r}, \Omega, E) = 0, \mathbf{r}_s \in \partial V, \Omega \cdot \mathbf{n} < 0; \gamma_{12,j}^{(2)}(\mathbf{r}, \Omega, E) = 0, \mathbf{r}_s \in \partial V, \Omega \cdot \mathbf{n} > 0; 0 < E < E_f,
$$

$$
\gamma_{21,j}^{(2)}(\mathbf{r}, \Omega, E) = 0, \mathbf{r}_s \in \partial V, \Omega \cdot \mathbf{n} > 0; \gamma_{22,j}^{(2)}(\mathbf{r}, \Omega, E) = 0, \mathbf{r}_s \in \partial V, \Omega \cdot \mathbf{n} < 0; 0 < E < E_f.
$$

(154)

Identifying the first term on the right side of Eq. (153) with the indirect-effect term defined in Eq. (152) yields the following 2nd-LASS for the components of the 2nd-level adjoint function $\gamma_j^{(2)}(\mathbf{r}, \Omega, E)$:

$$
L(\alpha) \gamma_{1,j}^{(2)}(\mathbf{r}, \Omega, E) = 0, \ j = 1, \ldots, J_k .
$$

(155)
\[ L^j(a)\gamma^{(2)}_{12,j}(r,\Omega,E) = \frac{\partial Q^j}{\partial k_j}, \quad j = 1,\ldots,J_k, \]  

\[ L^j(a)\gamma^{(2)}_{21,j}(r,\Omega,E) = \frac{\partial^2 G(d,\varphi^+,\varphi^+)}{\partial \varphi^+ \partial \varphi^+} \gamma^{(2)}_{11,j}(r,\Omega,E) + \frac{\partial^2 G(d,\varphi^+,\varphi^+)}{\partial \varphi^+ \partial \varphi^+} \gamma^{(2)}_{12,j}(r,\Omega,E), \quad j = 1,\ldots,J_k, \]  

\[ L(a)\gamma^{(2)}_{22,j}(r,\Omega,E) = \frac{\partial^2 G(d,\varphi^+,\varphi^+)}{\partial \varphi^+ \partial \varphi^+} \gamma^{(2)}_{11,j}(r,\Omega,E) + \frac{\partial^2 G(d,\varphi^+,\varphi^+)}{\partial \varphi^+ \partial \varphi^+} \gamma^{(2)}_{12,j}(r,\Omega,E), \quad j = 1,\ldots,J_k. \]  

It follows from Eqs. (155) and (154) that  

\[ \gamma^{(2)}_{11,j}(r,\Omega,E) \equiv 0, \quad j = 1,\ldots,J_k, \]  

which implies, in turn, that Eqs. (157) and (158) reduce to the following decoupled equations for determining the components \( \gamma^{(2)}_{21,j}(r,\Omega,E) \) and \( \gamma^{(2)}_{22,j}(r,\Omega,E) \):  

\[ L^j(a)\gamma^{(2)}_{21,j}(r,\Omega,E) = \frac{\partial^2 G(d,\varphi^+,\varphi^+)}{\partial \varphi^+ \partial \varphi^+} \gamma^{(2)}_{12,j}(r,\Omega,E), \quad j = 1,\ldots,J_k, \]  

\[ L(a)\gamma^{(2)}_{22,j}(r,\Omega,E) = \frac{\partial^2 G(d,\varphi^+,\varphi^+)}{\partial \varphi^+ \partial \varphi^+} \gamma^{(2)}_{12,j}(r,\Omega,E), \quad j = 1,\ldots,J_k. \]  

Using the 2\textsuperscript{nd}-LASS defined by Eqs. (156), and (159) through (161) together with the term on the left-side of Eq. (153) leads to the following expression for the indirect-effect term defined in Eq. (152):
Replacing Eqs. (162) and (151) into Eq. (150) and subsequently identifying the quantities multiplying the parameter variations \( \delta \alpha_{m_2} \), \( m_2 = 1, \ldots, J_\alpha \), in the resulting expression yields the following results:
For $j = 1, \ldots, J_k$; $m_2 = 1, \ldots, J_s$, 
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \gamma_j^{(2)}; \alpha)}{\partial k_j \partial s_{m_2}} = 
\]
\[
= -\int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{12,j}^{(2)}(r, \sigma, \Omega, E) \psi_2^{(1)}(r, \sigma, \Omega, E) \right] + \gamma_{21,j}^{(2)}(r, \Omega, E) \varphi(r, \Omega, E) + \gamma_{22,j}^{(2)}(r, \Omega, E) \varphi^+ (r, \Omega, E) \bigg] ; 
\]
(163)

For $j = 1, \ldots, J_k$; $m_2 = 1, \ldots, J_s$,
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \gamma_j^{(2)}; \alpha)}{\partial k_j \partial s_{m_2}} = 
\]
\[
= -\int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{12,j}^{(2)}(r, \sigma, \Omega, E) \psi_2^{(1)}(r, \sigma, \Omega, E) \right] \frac{\partial \Sigma}{\partial s_{m_2}} \left( s; r, E' \rightarrow E, \Omega' \rightarrow \Omega \right) 
\]
+ \int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{21,j}^{(2)}(r, \Omega, E) \varphi(r, \Omega, E') \right] \frac{\partial \Sigma}{\partial s_{m_2}} \left( s; r, E' \rightarrow E, \Omega' \rightarrow \Omega \right) 
\]
+ \int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{22,j}^{(2)}(r, \Omega, E) \varphi^+ (r, \Omega', E') \right] \frac{\partial \Sigma}{\partial s_{m_2}} \left( s; r, E' \rightarrow E', \Omega' \rightarrow \Omega \right) ; 
\]
(164)

For $j = 1, \ldots, J_k$; $m_2 = 1, \ldots, J_f$,
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \gamma_j^{(2)}; \alpha)}{\partial k_j \partial f_{m_2}} = 
\]
\[
= \int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{12,j}^{(2)}(r, \sigma, \Omega, E) \psi_2^{(1)}(r, \sigma, \Omega, E) \right] \frac{\partial \Sigma}{\partial f_{m_2}} \left( f; r, E' \rightarrow E \right) 
\]
+ \int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{21,j}^{(2)}(r, \Omega, E) \varphi(r, \Omega, E') \right] \frac{\partial \Sigma}{\partial f_{m_2}} \left( f; r, E' \rightarrow E \right) 
\]
+ \int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{22,j}^{(2)}(r, \Omega, E) \varphi^+ (r, \Omega', E') \right] \frac{\partial \Sigma}{\partial f_{m_2}} \left( f; r, E' \rightarrow E' \right) ; 
\]
(165)

For $j = 1, \ldots, J_k$; $m_2 = 1, \ldots, J_p$,
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; \gamma_j^{(2)}; \alpha)}{\partial k_j \partial p_{m_2}} = 
\]
\[
= \int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{12,j}^{(2)}(r, \sigma, \Omega, E) \psi_2^{(1)}(r, \sigma, \Omega, E) \right] \frac{\partial \Sigma}{\partial p_{m_2}} \left( p; r, E' \rightarrow E \right) 
\]
+ \int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{21,j}^{(2)}(r, \Omega, E) \varphi(r, \Omega, E') \right] \frac{\partial \Sigma}{\partial p_{m_2}} \left( p; r, E' \rightarrow E \right) 
\]
+ \int dV \int \frac{E_f}{4\pi} d\Omega \int_0 dE \frac{\partial \Sigma}{\partial t_{m_2}} \left( t; r, \Omega, E \right) \left[ \gamma_{22,j}^{(2)}(r, \Omega, E) \varphi^+ (r, \Omega', E') \right] \frac{\partial \Sigma}{\partial p_{m_2}} \left( p; r, E' \rightarrow E' \right) ; 
\]
(166)
For $j = 1,...,J_k; m_2 = 1,...,J_q$:

$$\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; \gamma_j^{(2)}; \alpha \right)}{\partial k_j \partial q_{m_2}} = \gamma_j^{(2)} (r, \Omega, E) \frac{\partial R (q, r, \Omega, E)}{\partial q_{m_2}};$$

(167)

For $j = 1,...,J_k; m_2 = 1,...,J_k$:

$$\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; \gamma_j^{(2)}; \alpha \right)}{\partial k_j \partial k_{m_2}} = \gamma_j^{(2)} (r, \Omega, E) \frac{\partial R (q, r, \Omega, E)}{\partial k_{m_2}};$$

(168)

For $j = 1,...,J_k; m_2 = 1,...,J_d$:

$$\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; \gamma_j^{(2)}; \alpha \right)}{\partial k_j \partial d_{m_2}} = \gamma_j^{(2)} (r, \Omega, E) \frac{\partial R (q, r, \Omega, E)}{\partial d_{m_2}};$$

(169)

The expressions of the 2nd-order sensitivities computed using Eq. (163) must be identical to those computed using Eq.(67), i.e.

$$\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; \gamma_j^{(2)}; \alpha \right)}{\partial k_j \partial t_m} = \gamma_j^{(2)} (r, \Omega, E) \frac{\partial R (q, r, \Omega, E)}{\partial t_m};$$

(170)

The relation expressed by Eq.(170) provides an independent mutual verification of the 2nd-level adjoint functions $\gamma_j^{(2)}$ and $\psi_j^{(2)}$.

The expressions of the 2nd-order sensitivities computed using Eq.(164) must be identical to those computed using Eq.(84), i.e.
For \( j = 1, \ldots, J_k \), \( m = 1, \ldots, J_x \):
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha)}{\partial k_j \partial s_m} = \\
= \int dV \int d\Omega \int_0^E dE \gamma_{12,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_0^{E'} dE' \psi_2^{(1)}(r, \Omega', E') \frac{\partial \Sigma_j (s, \Omega, E' \rightarrow \Omega, \Omega' \rightarrow \Omega)}{\partial s_m} \\
+ \int dV \int d\Omega \int_0^E dE \gamma_{21,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_0^{E'} dE' \varphi (r, \Omega', E') \frac{\partial \Sigma_j (s, r, E' \rightarrow \Omega, \Omega' \rightarrow \Omega)}{\partial s_m} \\
+ \int dV \int d\Omega \int_0^E dE \gamma_{22,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_0^{E'} dE' \varphi^+ (r, \Omega', E') \frac{\partial \Sigma_j (s, r, E \rightarrow \Omega', \Omega \rightarrow \Omega')}{\partial s_m};
\]
\[
= \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha)}{\partial s_m \partial k_j} = \int dV \int d\Omega \int_0^E dE \theta_{22,m}^{(2)}(r, \Omega, E) \frac{\partial Q^+ (k, r, \Omega, E)}{\partial k_j}.
\]

The relation expressed by Eq. (171) provides an independent mutual verification of the 2nd-level adjoint functions \( \gamma_j^{(2)} \) and \( \theta_j^{(2)} \).

The expressions of the 2nd-order sensitivities computed using Eq.(165) must be identical to those computed using Eq.(102), i.e.

For \( j = 1, \ldots, J_k \), \( m = 1, \ldots, J_x \):
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha)}{\partial k_j \partial f_m} = \\
= \int dV \int d\Omega \int_0^E dE \gamma_{12,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_0^{E'} dE' \chi (p; r, E' \rightarrow E) \psi_2^{(1)}(r, \Omega', E') \frac{\partial \Sigma_j (f, r, E')}{\partial f_m} \\
+ \int dV \int d\Omega \int_0^E dE \gamma_{21,j}^{(2)}(r, \Omega, E) \int d\Omega' \int_0^{E'} dE' \chi (p; r, E' \rightarrow E) \varphi (r, \Omega', E') \frac{\partial \Sigma_j (f, r, E')}{\partial f_m} \\
+ \int dV \int d\Omega \int_0^E dE \gamma_{22,j}^{(2)}(r, \Omega, E) \frac{\partial \Sigma_j (f, r, E')}{\partial f_m} \int d\Omega' \int_0^{E'} dE' \chi (p; r, E \rightarrow E') \varphi^+ (r, \Omega', E') \\
= \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha)}{\partial f_m \partial k_j} = \int dV \int d\Omega \int_0^E dE \theta_{22,m}^{(2)}(r, \Omega, E) \frac{\partial Q^+ (k, r, \Omega, E)}{\partial k_j}.
\]

The relation shown in Eq. (172) provides an independent path for the mutual verification of the solutions \( \gamma_j^{(2)} \) and \( \psi_j^{(2)} \).

The expressions of the 2nd-order sensitivities computed using Eq.(166) must be identical to those computed using Eq.(121), i.e.
For \( j = 1,...,J_k; \ m = 1,...,J_p \):

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \gamma^{(2)}_j; \alpha)}{\partial k_j \partial p_m} = \\
\int dV \int_{4\pi}^{E_i} d\Omega \int_0^{E_f} dE \ \gamma^{(2)}_{12,j} (r, \Omega, E) \int d\Omega' \int_0^{E_f} dE' \nu \Sigma_j (f; r, E') \varphi_1(r, \Omega', E') \frac{\partial \chi(p; r, E' \rightarrow E)}{\partial p_m}
\]

\[
= \int dV \int_{4\pi}^{E_i} d\Omega \int_0^{E_f} dE \ \gamma^{(2)}_{21,j} (r, \Omega, E) \int d\Omega' \int_0^{E_f} dE' \left[ \nu \Sigma_j (f; r, E') \right] \varphi(r, \Omega', E') \frac{\partial \chi(p; r, E' \rightarrow E)}{\partial p_m}
\] (173)

\[
= \int dV \int_{4\pi}^{E_i} d\Omega \int_0^{E_f} dE \ \gamma^{(2)}_{22,j} (r, \Omega, E) \left[ \nu \Sigma_j (f; r, E) \right] \int d\Omega' \int_0^{E_f} dE' \varphi^+ (r, \Omega', E') \frac{\partial \chi(p; r, E \rightarrow E')}{\partial p_m}.
\]

The relation shown in Eq.(173) provides an independent path for the mutual verification of the solutions \( \gamma^{(2)}_j \) and \( \psi^{(2)}_j \).

The expressions of the 2nd-order sensitivities computed using Eq.(167) must be identical to those computed using Eq.(144), i.e.

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \gamma^{(2)}_j; \alpha)}{\partial p_m \partial k_j} = \\
\int dV \int_{4\pi}^{E_i} d\Omega \int_0^{E_f} dE \ \psi^{(2)}_{22,m} (r, \Omega, E) \frac{\partial Q^+(k; r, \Omega, E)}{\partial k_j}.
\]

The relation shown in Eq.(174) provides an independent path for the mutual verification of the solutions \( \gamma^{(2)}_j \) and \( g^{(2)}_j \).

IV.G. Computation of the 2nd-Order Sensitivities

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \gamma^{(2)}_j; \alpha)}{\partial d_j \partial \alpha_{m_2}} , \ j = 1,...,J_d; \ m_2 = 1,...,J_{\alpha}
\]

The 2nd-order sensitivities \( \partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \gamma^{(2)}_j; \alpha) / (\partial d_j)(\partial \alpha_{m_2}) \), \( j = 1,...,J_d; \ m_2 = 1,...,J_{\alpha} \) will ultimately depend on a 2nd-level adjoint function which is denoted as \( h^{(2)}_j \), and are obtained by computing the G-differential of the 1st-order sensitivities defined in of Eq. (41), which yields the following expression:
\[
\frac{\partial R(\varphi, \varphi^+; \psi^{(1)}; \alpha)}{\partial d_j} = \left\{ \frac{\partial R(\varphi, \varphi^+; \psi^{(1)}; \alpha)}{\partial d_j} \right\}_{\text{dir}} + \left\{ \frac{\partial R(\varphi, \varphi^+; \psi^{(1)}; \alpha)}{\partial d_j} \right\}_{\text{ind}}, \quad j = 1, \ldots, J_d; \quad (175)
\]

where

\[
\text{For } j = 1, \ldots, J_d : \quad \left\{ \frac{\partial R(\varphi, \varphi^+; \psi^{(1)}; \alpha)}{\partial d_j} \right\}_{\text{dir}} = \int dV \int d\Omega \sum_{m_2=1}^{J_d} \int_{0}^{d} \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial d_{m_2} d_{j}} \delta d_{m_2}, \quad (176)
\]

\[
\text{For } j = 1, \ldots, J_d : \quad \left\{ \frac{\partial R(\varphi, \varphi^+; \psi^{(1)}; \alpha)}{\partial d_j} \right\}_{\text{ind}} = \int dV \int d\Omega \int_{0}^{d} \left[ \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi d_{j}} \delta \varphi(r, \Omega, E) + \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ d_{j}} \delta \varphi^+(r, \Omega, E) \right]. \quad (177)
\]

The direct-effect term defined in Eq. (176) can be computed immediately. On the other hand, the indirect-effect term defined in Eq. (177) can be computed only after having obtained the functions \( \delta \varphi(r, \Omega, E) \) and \( \delta \varphi^+(r, \Omega, E) \), which are computationally expensive to obtain. To avoid the need for computing these functions, the indirect-effect term defined in Eq. (177) will be expressed in terms of the solution, denoted as \( h^{(2)}(r, \Omega, E) \equiv [h^{(2)}_{1,j}(r, \Omega, E), h^{(2)}_{2,j}(r, \Omega, E)]^T \) of a 2nd-Level Adjoint Sensitivity System (2nd-LASS) which will turn out to have the same structure as the 2nd-LASS in the previous sections. Thus, the 2nd-level adjoint function \( h^{(2)}(r, \Omega, E) \equiv [h^{(2)}_{1,j}(r, \Omega, E), h^{(2)}_{2,j}(r, \Omega, E)]^T \) has the same structure as the 2nd-level adjoint functions that were introduced in previous sections, having components \( h^{(2)}_{1,j} \equiv [h^{(2)}_{1,1,j}(r, \Omega, E), h^{(2)}_{1,2,j}(r, \Omega, E)]^T \), \( h^{(2)}_{2,j} \equiv [h^{(2)}_{2,1,j}(r, \Omega, E), h^{(2)}_{2,2,j}(r, \Omega, E)]^T \), with \( h^{(2)}_{m,n,j}(r, \Omega, E) \in \mathcal{L}_2(V \times \Omega \times E) \), \( m, n = 1, 2 \). Forming the inner product of \( h^{(2)}(r, \Omega, E) \) with Eqs. (45) and (19) leads to the following relation:

\[
\begin{aligned}
\left\langle \begin{pmatrix} h^{(2)}_{1,j} \\ h^{(2)}_{2,j} \end{pmatrix} \right| \begin{pmatrix} A^{(1)}_{11}(\alpha) & F^{(2)}_{12}(\alpha) \\ 0 & F^{(1)}_{11}(\alpha) \end{pmatrix} \begin{pmatrix} \delta \psi^{(1)} \\ \delta u \end{pmatrix} \right\rangle &= \left\langle \begin{pmatrix} \delta \psi^{(1)} \\ \delta u \end{pmatrix} \right| \begin{pmatrix} A^{(1)}_{11}(\alpha)^T & 0 \\ F^{(2)}_{12}(\alpha)^T & F^{(1)}_{11}(\alpha)^T \end{pmatrix} \begin{pmatrix} h^{(2)}_{1,j} \\ h^{(2)}_{2,j} \end{pmatrix} \right\rangle + P^{(2)} \begin{pmatrix} h^{(2)}_j, \delta \psi^{(1)}, \delta u \end{pmatrix}.
\end{aligned} \quad (178)
\]
The bilinear concomitant $P^{(2)}[h_j^{(2)}, \delta \psi^{(1)}, \delta u]$ in Eq.(178) will vanish by imposing on the components of $h_j^{(2)}(r, \Omega, E)$ the following boundary conditions:

\[
\begin{align*}
    h_{11,j}^{(2)}(r, \Omega, E) &= 0, \quad r_s \in \partial V, \quad \Omega \cdot n < 0; \quad h_{12,j}^{(2)}(r, \Omega, E) = 0, \quad r_s \in \partial V, \quad \Omega \cdot n > 0; \quad 0 < E < E_f, \\
    h_{21,j}^{(2)}(r, \Omega, E) &= 0, \quad r_s \in \partial V, \quad \Omega \cdot n > 0; \quad h_{22,j}^{(2)}(r, \Omega, E) = 0, \quad r_s \in \partial V, \quad \Omega \cdot n < 0; \quad 0 < E < E_f.
\end{align*}
\]  

Identifying the first term on the right side of Eq.(178) with the indirect-effect term defined in Eq.(177) yields the following 2nd-LASS for the components of the 2nd-level adjoint function $h_j^{(2)}(r, \Omega, E)$:

\[
\begin{align*}
    L(a)h_{11,j}^{(2)}(r, \Omega, E) &= 0, \quad j = 1, \ldots, J_d, \\
    L'(a)h_{12,j}^{(2)}(r, \Omega, E) &= 0, \quad j = 1, \ldots, J_d, \\
    L'(a)h_{21,j}^{(2)}(r, \Omega, E) &= \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^2}h_{11,j}^{(2)}(r, \Omega, E) \\
    &\quad + \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ \partial \varphi}h_{12,j}^{(2)}(r, \Omega, E) + \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial d_j}, \quad j = 1, \ldots, J_d, \\
    L(a)h_{22,j}^{(2)}(r, \Omega, E) &= \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial \varphi^+}h_{11,j}^{(2)}(r, \Omega, E) \\
    &\quad + \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ \partial \varphi}h_{12,j}^{(2)}(r, \Omega, E) + \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ \partial d_j}, \quad j = 1, \ldots, J_d.
\end{align*}
\]

It follows from Eqs. (179) through (183) that

\[
\begin{align*}
    h_{11,j}^{(2)}(r, \Omega, E) \equiv 0, \quad h_{12,j}^{(2)}(r, \Omega, E) \equiv 0, \quad j = 1, \ldots, J_d, \\
    L'(a)h_{21,j}^{(2)}(r, \Omega, E) &= \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial d_j}, \quad j = 1, \ldots, J_d, \\
    L(a)h_{22,j}^{(2)}(r, \Omega, E) &= \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ \partial d_j}, \quad j = 1, \ldots, J_d.
\end{align*}
\]

Using the 2nd-LASS defined by Eqs. (184) through (186) together with the term on the left-side of Eq.(178) leads to the following expression for the indirect-effect term defined in Eq.(177):
Replacing Eq. (187) together with the direct-effect term from Eq. (176) into Eq. (175) and subsequently identifying the quantities multiplying the parameter variations \( \delta \alpha_{m_2}, m_2 = 1, \ldots, J, \) in the resulting expression yields the following results:

\[
\delta \left[ \frac{\partial R \left( \varphi, \varphi^\dagger, \psi^{(1)}; h^{(2)}_j; \alpha \right)}{\partial d_j} \right]_{\text{ind}} = \left\langle \left( \begin{array}{c}
\mathbf{h}^{(2)}_{1j} \\
\mathbf{h}^{(2)}_{2j}
\end{array} \right) \right| \left( \begin{array}{c}
Q^{(2)}(\alpha, \psi^{(1)}; \delta \alpha) \\
Q^{(1)}(\alpha, \varphi^\dagger; \delta \alpha)
\end{array} \right) \right\rangle_{\text{(2)}}
\]

\[
= \int_{4\pi}^E \int_{d\Omega}^E dE \int_{d\Omega, j}^E dE' \varphi \left( \mathbf{r}, \Omega, E \right) \left[ \delta Q \left( \mathbf{q}, \mathbf{r}, \Omega, E \right) - \delta \Sigma \left( \mathbf{t}, \mathbf{r}, E \right) \right] \varphi \left( \mathbf{r}, \Omega, E \right)
\]

\[
+ \int_{4\pi}^E \int_{d\Omega'}^E dE' \varphi \left( \mathbf{r}, \Omega', E' \right) \left[ \delta \Sigma \left( \mathbf{s}, \mathbf{r}, E \right) \varphi \left( \mathbf{r}, \Omega, E \right) \right] \varphi \left( \mathbf{r}, \Omega', E' \right)
\]

\[
+ \int_{4\pi}^E \int_{d\Omega'}^E dE' \varphi \left( \mathbf{r}, \Omega', E' \right) \left[ \delta \Sigma \left( \mathbf{s}, \mathbf{r}, E, \Omega \right) \varphi \left( \mathbf{r}, \Omega, E \right) \right] \varphi \left( \mathbf{r}, \Omega', E' \right) \right\rangle.
\]

For \( j = 1, \ldots, J_d; \) \( m_2 = 1, \ldots, J_f, \)

\[
\frac{\partial^2 R \left( \varphi, \varphi^\dagger; \psi^{(1)}; h^{(2)}_j; \alpha \right)}{\partial d_j \partial t_{m_2}} = -\int_{4\pi}^E \int_{d\Omega}^E dE \frac{\partial \Sigma \left( \mathbf{t}, \mathbf{r}, \Omega, E \right)}{\partial t_{m_2}} \left[ h^{(2)}_{11j} \left( \mathbf{r}, \Omega, E \right) \varphi \left( \mathbf{r}, \Omega, E \right) + h^{(2)}_{21j} \left( \mathbf{r}, \Omega, E \right) \varphi^\dagger \left( \mathbf{r}, \Omega, E \right) \right]
\]
For $j = 1, \ldots, J_d; \ m_2 = 1, \ldots, J_s$:
\[
\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; h^{(2)}_j; \alpha \right)}{\partial d_j \partial s_{m_2}} = \int dV \int_{4\pi} d\Omega \int_{0}^{E_j} dE \ h^{(2)}_{21,j} (r, \Omega, E) \int_{4\pi} d\Omega' \int_{0}^{E_j} dE' \varphi(r, \Omega', E') \frac{\partial \Sigma_s (s; r, E' \to E, \Omega' \to \Omega)}{\partial s_{m_2}}
\]
(189)

\[
+ \int dV \int_{4\pi} d\Omega \int_{0}^{E_j} dE \ h^{(2)}_{22,j} (r, \Omega, E) \int_{4\pi} d\Omega' \int_{0}^{E_j} dE' \varphi^*(r, \Omega', E') \frac{\partial \Sigma_s (s; r, E \to E', \Omega \to \Omega')}{\partial s_{m_2}};
\]

For $j = 1, \ldots, J_d; \ m_2 = 1, \ldots, J_f$:
\[
\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; h^{(2)}_j; \alpha \right)}{\partial d_j \partial f_{m_2}} = \int dV \int_{4\pi} d\Omega \int_{0}^{E_f} dE \ h^{(2)}_{21,j} (r, \Omega, E) \int_{4\pi} d\Omega' \int_{0}^{E_f} dE' \chi(p; r, E' \to E) \varphi(r, \Omega', E') \frac{\partial \nu \Sigma_f (f; r, E')}{\partial f_{m_2}}
\]
(190)

\[
+ \int dV \int_{4\pi} d\Omega \int_{0}^{E_f} dE \ h^{(2)}_{22,j} (r, \Omega, E) \nu \Sigma_f (f; r, E) \int_{4\pi} d\Omega' \int_{0}^{E_f} dE' \varphi^*(r, \Omega', E') \frac{\partial \chi (p; r, E \to E')}{\partial f_{m_2}};
\]

For $j = 1, \ldots, J_d; \ m_2 = 1, \ldots, J_p$:
\[
\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; h^{(2)}_j; \alpha \right)}{\partial d_j \partial p_{m_2}} = \int dV \int_{4\pi} d\Omega \int_{0}^{E_p} dE \ h^{(2)}_{21,j} (r, \Omega, E) \int_{4\pi} d\Omega' \int_{0}^{E_p} dE' \varphi (r, \Omega', E') \frac{\partial \chi (p; r, E')}{\partial p_{m_2}}
\]
(191)

\[
+ \int dV \int_{4\pi} d\Omega \int_{0}^{E_p} dE \ h^{(2)}_{22,j} (r, \Omega, E) \nu \Sigma_j (f; r, E) \int_{4\pi} d\Omega' \int_{0}^{E_p} dE' \varphi^*(r, \Omega', E') \frac{\partial \chi (p; r, E \to E')}{\partial p_{m_2}};
\]

For $j = 1, \ldots, J_d; \ m_2 = 1, \ldots, J_q$:
\[
\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; h^{(2)}_j; \alpha \right)}{\partial d_j \partial q_{m_2}} = \int dV \int_{4\pi} d\Omega \int_{0}^{\infty} dE \ h^{(2)}_{21,j} (r, \Omega, E) \frac{\partial Q (q; r, \Omega, E)}{\partial q_{m_2}};
\]
(192)

For $j = 1, \ldots, J_d; \ m_2 = 1, \ldots, J_q$:
\[
\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; h^{(2)}_j; \alpha \right)}{\partial d_j \partial k_{m_2}} = \int dV \int_{4\pi} d\Omega \int_{0}^{\infty} dE \ h^{(2)}_{22,j} (r, \Omega, E) \frac{\partial Q^* (k; r, \Omega, E)}{\partial k_{m_2}};
\]
(193)

For $j = 1, \ldots, J_d; \ m_2 = 1, \ldots, J_d$:
\[
\frac{\partial^2 R \left( \varphi, \varphi^*; \psi^{(1)}; h^{(2)}_j; \alpha \right)}{\partial d_j \partial d_{m_2}} = \int dV \int_{4\pi} d\Omega \int_{0}^{\infty} dE \frac{\partial^2 G (d; \varphi, \varphi^*)}{\partial d_j \partial d_{m_2}}.
\]
(194)

The expressions of the 2nd-order sensitivities computed using Eq. (188) must be identical to those computed using Eq. (68), i.e.
For \( j = 1,\ldots,J_d; \ m = 1,\ldots,J_s \),
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; h^{(2)}_j; \alpha)}{\partial d_j \partial t_m} =
\]
\[
= -\int dV \int_{4\pi}^{E_j} d\Omega \int_0^{E_j} dE \frac{\partial \Sigma_s(t; r, \Omega, E)}{\partial t_m} \left[ h^{(2)}_{21,j}(r, \Omega, E) \varphi(r, \Omega, E) + h^{(2)}_{22,j}(r, \Omega, E) \varphi^+(r, \Omega, E) \right]
\]
\[
= \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \psi^{(2)}_j; \alpha)}{\partial t_j \partial d_j} =
\]
\[
= \int dV \int_{4\pi}^{E_j} d\Omega \int_0^{E_j} dE \left[ \psi^{(2)}_{11,m}(r, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial d_j} + \psi^{(2)}_{12,m}(r, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ \partial d_j} \right].
\]

The relation expressed by Eq. (195) provides an independent mutual verification of the 2nd-level adjoint functions \( h^{(2)}_j \) and \( \psi^{(2)}_j \).

The expressions of the 2nd-order sensitivities computed using Eq. (189) must be identical to those computed using Eq. (85), i.e.,
\[
\]
\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; h^{(2)}_j; \alpha)}{\partial d_j \partial \tilde{s}_m} =
\]
\[
= \int dV \int_{4\pi}^{E_j} d\Omega \int_0^{E_j} dE \ h^{(2)}_{21,j}(r, \Omega, E) \int dE' \ \varphi(r, \Omega', E') \frac{\partial \Sigma_s(s; r, E' \rightarrow E, \Omega' \rightarrow \Omega)}{\partial \tilde{s}_m}
\]
\[
+ \int dV \int_{4\pi}^{E_j} d\Omega \int_0^{E_j} dE \ h^{(2)}_{22,j}(r, \Omega, E) \int dE' \ \varphi^+(r, \Omega', E') \frac{\partial \Sigma_s(s; r, E \rightarrow E', \Omega \rightarrow \Omega')}{\partial \tilde{s}_m}
\]
\[
\]
\[
= \frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}_j; \theta^{(2)}_j; \alpha)}{\partial \tilde{s}_m \partial d_j} =
\]
\[
= \int dV \int_{4\pi}^{E_j} d\Omega \int_0^{E_j} dE \ \theta^{(2)}_{11,m}(r, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial d_j} + \int dV \int_{4\pi}^{E_j} d\Omega \int_0^{E_j} dE \ \theta^{(2)}_{12,j}(r, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi^+ \partial d_j}.
\]

The relation expressed by Eq. (196) provides an independent mutual verification of the 2nd-level adjoint functions \( h^{(2)}_j \) and \( \theta^{(2)}_j \).

The expressions of the 2nd-order sensitivities computed using Eq. (190) must be identical to those computed using Eq. (103), i.e.
The relation shown in Eq. (197) provides an independent path for the mutual verification of the solutions \( h_j^{(2)} \) and \( u_j^{(2)} \).

The expressions of the 2nd-order sensitivities computed using Eq. (191) must be identical to those computed using Eq. (122), i.e.

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}, h_j^{(2)}; \alpha)}{\partial d_j \partial \hat{f}_m} = \int dV \int_{\Omega} dE \int_{\Omega'} dE' \chi(p; r, E' \rightarrow E) \varphi(r, \Omega', E') \frac{\partial \nu \Sigma_f (f; r, E)}{\partial f_m} \\
+ \int dV \int_{\Omega} dE \int_{\Omega'} dE' \chi(p; r, E' \rightarrow E) \varphi^+ (r, \Omega', E') \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial \varphi d_j}.
\]

(197)

The relation shown in Eq. (198) provides an independent path for the mutual verification of the solutions \( h_j^{(2)} \) and \( w_j^{(2)} \).

The expressions of the 2nd-order sensitivities computed using Eq. (192) must be identical to those computed using Eq.(145), i.e.

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}, w_j^{(2)}; \alpha)}{\partial d_j \partial \hat{p}_m} = \int dV \int_{\Omega} dE \int_{\Omega'} dE' \chi(p; r, E' \rightarrow E) \varphi(r, \Omega', E') \frac{\partial \nu \Sigma_f (f; r, E)}{\partial p_m} \\
+ \int dV \int_{\Omega} dE \int_{\Omega'} dE' \varphi^+ (r, \Omega', E') \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi \partial \varphi d_j}.
\]

(198)
For \( j = 1, \ldots, J_d; \ m = 1, \ldots, J_q \):

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; h^{(2)}; \alpha)}{\partial d_j \partial q_m} = \int dV \int d\Omega \int dE h^{(2)}_{21,j}(r, \Omega, E) \frac{\partial Q(q; r, \Omega, E)}{\partial q_m} = \int dV \int d\Omega \int dE g^{(2)}_{11,m}(r, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi d_j}.
\]

(199)

The relation shown in Eq. (199) provides an independent path for the mutual verification of the solutions \( h^{(2)}_j \) and \( g^{(2)}_j \).

The expressions of the 2nd-order sensitivities computed using Eq. (193) must be identical to those computed using Eq. (169), i.e.

For \( j = 1, \ldots, J_d; \ m = 1, \ldots, J_q \):

\[
\frac{\partial^2 R(\varphi, \varphi^+; \psi^{(1)}; g^{(2)}; \alpha)}{\partial q_m \partial d_j} = \int dV \int d\Omega \int dE h^{(2)}_{22,j}(r, \Omega, E) \frac{\partial Q^+(k; r, \Omega, E)}{\partial k_m} = \int dV \int d\Omega \int dE g^{(2)}_{11,m}(r, \Omega, E) \frac{\partial^2 G(d; \varphi, \varphi^+)}{\partial \varphi d_j}.
\]

(200)

The relation shown in Eq. (200) provides an independent path for the mutual verification of the solutions \( h^{(2)}_j \) and \( \gamma^{(2)}_j \).

IV.H. Impact of Second-Order Sensitivities on Response Expected Value, Variance, and Skewness

Knowledge of the first- and second-order sensitivities is required to compute the following moments of the response distribution:

(i) The expected value of a response \( R \): \( E(R) = R(\alpha^0) + \frac{1}{2} \sum_{i=1}^{N_a} \frac{\partial^2 R}{\partial \alpha_i^2} s_i^2 \), where \( s_i \) denotes the standard deviation of the model parameter \( \alpha_i \).

(ii) The variance of response: \( \text{var}(R) = \sum_{i=1}^{N_a} \left( \frac{\partial R}{\partial \alpha_i} \right)^2 s_i^2 + \frac{1}{2} \sum_{i=1}^{N_a} \left( \frac{\partial^2 R}{\partial \alpha_i^2} \right)^2 s_i^4. \)

(iii) The skewness \( \gamma_1 \) of response: \( \gamma_1(R) = \frac{\mu_3(R)}{[\text{var}(R)]^{\frac{3}{2}}} \), where \( \mu_3(R) = 3 \sum_{i=1}^{N_a} \left( \frac{\partial R}{\partial \alpha_i} \right)^2 \frac{\partial^2 R}{\partial \alpha_i^2} s_i^4. \)

denoted the third central moment of the response distribution.
V. CONCLUSIONS

The following conclusions can be drawn based on the results that have been presented in this work:

(i) As is well-known\textsuperscript{10-12,18,19}, a single 1\textsuperscript{st}-LASS needs to be solved in order to compute all 1\textsuperscript{st}-order response sensitivities, to all $N_\alpha$ model parameters.

(ii) For each model parameter, a single 2\textsuperscript{nd}-LASS needs to be solved for computing the corresponding mixed 2\textsuperscript{nd}-order sensitivities. Hence, computing all of the $N_\alpha(N_\alpha+1)/2$ second-order sensitivities could theoretically require solving at most $N_\alpha$ 2\textsuperscript{nd}-LASSs. In practice, however, the number of computation is much less, as has been shown in Refs. 11, 13-17. In particular, the results in Ref 17 showed that only 12 large-scale adjoint particle transport computations were required by using the 2\textsuperscript{nd}-ASAM to compute all of the detector’s response to the flux of uncollided particles for the 18 first-order sensitivities and 224 second-order sensitivities, in contrast to the 877 large-scale forward particle transport calculations needed to compute the respective sensitivities using central finite-differences, and this number did not include the additional calculations that were required to find appropriate values of the perturbations to use for the central differences.

(iii) For a scalar-values response that depends nonlinearly on both the forward and adjoint particle fluxes, as considered in this work, the solution of each of the 2\textsuperscript{nd}-LASS is, in general, a two-component vector-valued 2\textsuperscript{nd}-level adjoint function.

(iv) Solving each of the 2\textsuperscript{nd}-LASSs involves the inversion of the same operators as are needed to be inverted for solving the original transport equation and/or the 1\textsuperscript{st}-LASS. Only the various source terms on the right sides of the 2\textsuperscript{nd}-LASSs may differ from each other. Therefore, the same software can be used to solve both the 1\textsuperscript{st}-LASS and the 2\textsuperscript{nd}-LASS.

(v) The computation of the 2\textsuperscript{nd}-order sensitivities involves the evaluations of integrals of the same form as those needed for computing the 1\textsuperscript{st}-order sensitivities. Therefore, the same software can be used for computing both the 1\textsuperscript{st}-order and 2\textsuperscript{nd}-order sensitivities.

(vi) Each of the mixed 2\textsuperscript{nd}-order sensitivities is computed twice, using two distinct 2\textsuperscript{nd}-level adjoint functions. Consequently the 2\textsuperscript{nd}-ASAM possesses an inherent solution verification mechanism that enables and ensures the accuracy verification of the solutions of all of the 2\textsuperscript{nd}-LASS.
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REFERENCES


