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n^{th}-order feature adjoint sensitivity analysis methodology for response-coupled forward/adjoint linear systems: II. Illustrative application to a paradigm energy system

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This work presents a representative application of the newly developed "n^{th}-order feature adjoint sensitivity analysis methodology for response-coupled forward/adjoint linear systems" (abbreviated as "n^{th}-FASAM-L"), which enables the most efficient computation of exactly obtained mathematical expressions of arbitrarily high-order (n^{th}-order) sensitivities of a generic system response with respect to all of the parameters (including boundary and initial conditions) underlying the respective forward/adjoint systems. The n^{th}-FASAM-L has been developed to treat responses of linear systems that simultaneously depend on both the forward and adjoint state functions. Such systems cannot be considered particular cases of nonlinear systems, as illustrated in this work by analyzing an analytically solvable model of the energy distribution of the "contributon flux" of neutrons in a mixture of materials. The unparalleled efficiency and accuracy of the n^{th}-FASAM-L stem from the maximal reduction in the number of adjoint computations (which are "large-scale" computations) for determining the exact expressions of arbitrarily high-order sensitivities since the number of large-scale computations when applying the n^{th}-FASAM-N is proportional to the number of model features as opposed to the number of model parameters (which are considerably more than the number of features). Hence, the higher the order of computed sensitivities, the more efficient the n^{th}-FASAM-N becomes compared to any other methodology. Furthermore, as illustrated in this work, the probability of encountering identically vanishing sensitivities is much higher when using the n^{th}-FASAM-L than other methods.

KEYWORDS

arbitrarily high-order adjoint sensitivity analysis, n^{th}-order feature adjoint sensitivity analysis methodology for response-coupled forward/adjoint linear systems, response-coupled forward/adjoint systems, neutron-slowing down, sensitivity of responses to model features

1 Introduction

The accompanying work ("part I") has presented the newly developed mathematical framework, the "n^{th}-order feature adjoint sensitivity analysis methodology for response-coupled forward/adjoint linear systems" (abbreviated as "n^{th}-FASAM-L"), conceived by Cacuci (2024c). This work illustrates the application of the n^{th}-FASAM-L to a representative energy-dependent neutron-slowing down model of fundamental importance to reactor physics. The physical considerations underlying this model are presented in Section 2, which briefly reviews the concept of "contributon-flux density response" and particularizes this concept within the modeling of neutron slowing down in a mixture of materials. This physical model is of fundamental importance in nuclear reactor physics and enables the derivation of exact closed-form results for the application of the nth-FASAM-L. Section 2 also defines the "features" inherent to this model, which enable the advantageous application of the nth-FASAM-L. By definition, there are considerably fewer "feature functions" of the primary model parameters than there are primary model parameters.

Section 3 presents the first-order adjoint sensitivity analysis of the contributon flux with respect to the features and primary model parameters of the slowing-down model, comparing the application of the 1st-FASAM-L *versus* the first-order comprehensive adjoint sensitivity analysis methodology for response-coupled forward/adjoint linear systems (1st-CASAM-L). Using either the 1st-FASAM-L or 1st-CASAM-L involves solving the same operator equations and boundary conditions within the respective 1st-LASS but with differing source terms. For the computation of the first-order sensitivities, the 1st-FASAM-L enjoys only a slight computational advantage since it requires only one quadrature per component of the feature function, whereas the 1st-CASAM-L requires one quadrature per primary model parameter.

Section 4 presents the second-order adjoint sensitivity analysis of the contributon flux with respect to the features and primary model parameters of the slowing-down model, comparing the application of the 2nd-FASAM-L *versus* the 2nd-CASAM-L. It is shown that the 2nd-FASAM-L requires as many large-scale "adjoint" computations as there are non-vanishing first-order response sensitivities with respect to the components of the feature functions, whereas the 2nd-CASAM-L requires as many large-scale computations as there are non-vanishing first-order response sensitivities with respect to the primary model parameters. Hence, the 2nd-FASAM-L is inherently more efficient than the 2nd-CASAM-L. In particular, one of the three distinct second-order sensitivities with respect to the model's features vanishes identically within the 2nd-FASAM-L but none of the ca. 100 second-order sensitivities with respect to the primary model parameters vanish within the 2nd-CASAM-L.

Section 5 presents the third-order adjoint sensitivity analysis of the contributon flux with respect to the features and primary model parameters of the slowing-down model, comparing the application of the 3rd-FASAM-L *versus* the 3rd-CASAM-L. For computing the exact expressions of the *third-order* contributon-response sensitivities, the 3rd-FASAM-L requires only *two* large-scale computations, whereas the 3rd-CASAM-L would require hundreds of large-scale computations.

The concluding discussion presented in Section 6 emphasizes the fact that the unparalleled efficiency of the nth-FASAM-N increases as the order of computed sensitivities increases, and the probability of encountering vanishing sensitivities is much higher when using the nth-FASAM-L rather than any other methodology. Both the nth-FASAM-L and nth-CASAM-L overcome the limitation of dimensionality in the sensitivity analysis of linear systems, being incomparably more efficient and more accurate than any other method (statistical, finite differences, etc.) for computing exact expressions of response sensitivities (of any order) with respect to the uncertain parameters, boundaries, and internal interfaces of the model.

2 Modeling the contributon flux in a paradigm neutron slowing-down model

Fundamentally important responses of linear models depend *simultaneously* on both the forward and adjoint state functions governing the respective linear model, which makes it necessary to treat linear models/systems in their own right since such responses cannot be treated as particular cases of responses of nonlinear models. Typical examples of such responses arise in the modeling of self-diffusion processes in which the interaction mean free path is independent of the phase-space density. Such processes are modeled by linear equations of the Lorentz–Boltzmann type, and they occur in neutron, electron, and photon transport through media, as well as in certain types of transport processes in gas or plasma dynamics. Numerically solving such time-dependent integro-differential equations, albeit linear, is representative of "large-scale" computations and will be used in the sequel for illustrating the application of the nth-FASAM-L. In particular, the distribution of neutrons in a medium is modeled by the following standard form of the linear Boltzmann equation:

$$L(\mathbf{r},E,\mathbf{\Omega},t)\varphi(\mathbf{r},E,\mathbf{\Omega},t) = Q(\mathbf{r},E,\mathbf{\Omega},t), \tag{1}$$

where the linear integro-differential operator $L(\mathbf{r},E,\mathbf{\Omega},t)$ is defined below:

$$\begin{aligned} L(\mathbf{r},E,\mathbf{\Omega},t)\varphi(\mathbf{r},E,\mathbf{\Omega},t) \triangleq\ & \frac{1}{v}\frac{\partial\varphi(\mathbf{r},E,\mathbf{\Omega},t)}{\partial t} + \mathbf{\Omega}\cdot\nabla\varphi(\mathbf{r},E,\mathbf{\Omega},t) \\ & +\Sigma_t(\mathbf{r},E)\,\varphi(\mathbf{r},E,\mathbf{\Omega},t) \\ & -\int_0^{E_f} dE'\int_{4\pi} d\mathbf{\Omega}'\Sigma_s(\mathbf{r},E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega})\,\varphi(\mathbf{r},E',\mathbf{\Omega}',t) \\ & -\int_0^{E_f} dE'\int_{4\pi}\chi(\mathbf{r},E'\to E)\nu\Sigma(\mathbf{r},E')\,\varphi(\mathbf{r},E',\mathbf{\Omega}',t)d\mathbf{\Omega}'. \end{aligned} \tag{2}$$

The quantities that appear in the standard notation used in Equation 2 are defined as follows:

(i) $\mathbf{r}$ denotes the three-dimensional position vector in space; E denotes the energy-independent variable; the directional vector $\mathbf{\Omega}$ denotes the scattering solid angle; t denotes the time-independent variable; and v denotes the neutron particle speed.
(ii) $\varphi(\mathbf{r},E,\mathbf{\Omega},t)$ denotes the flux of particles (i.e., particle number density multiplied by the particle speed) in the energy range dE about E and volume element $d\mathbf{r}$ about $\mathbf{r}$, with directions of motion in the solid angle element $d\mathbf{\Omega}$ about $\mathbf{\Omega}$.
(iii) $Q(\mathbf{r},E,\mathbf{\Omega},t)$ denotes the rate at which particles are produced in the same element of phase space from sources that are independent of the flux.
(iv) $\Sigma_t(\mathbf{r},E)$ denotes the macroscopic total cross section.

(v) $\Sigma_s(\mathbf{r}, E' \to E, \mathbf{\Omega}' \to \mathbf{\Omega})$ denotes the macroscopic scattering transfer cross section from energy E' to energy E and from a scattering angle through angle $\mathbf{\Omega}' \cdot \mathbf{\Omega}$.
(vi) ν denotes the number of particles emitted isotropically $(1/4\pi)$ per fission.
(vii) $\Sigma_f(\mathbf{r}, E)$ denotes the macroscopic fission cross section.
(viii) $\chi(\mathbf{r}, E' \to E)$ denotes the fraction of fission particles appearing in energy dE about E from fissions in dE' about E'.

The adjoint Boltzmann transport equation is formulated in the Hilbert space denoted as $\mathcal{H}_B$ and is endowed with the following inner product, denoted as $\langle \varphi(\mathbf{r}, E, \mathbf{\Omega}, t), \psi(\mathbf{r}, E, \mathbf{\Omega}, t) \rangle_B$, between two elements $\varphi(\mathbf{r}, E, \mathbf{\Omega}, t) \in \mathcal{H}_B$ and $\psi(\mathbf{r}, E, \mathbf{\Omega}, t) \in \mathcal{H}_B$:

$$\langle \varphi, \psi \rangle_B \triangleq \int_0^{t_f} dt \int_0^{\infty} dE \int_{4\pi} d\mathbf{\Omega} \int_V dV \varphi(\mathbf{r}, E, \mathbf{\Omega}, t) \psi(\mathbf{r}, E, \mathbf{\Omega}, t). \quad (3)$$

In the Hilbert space $\mathcal{H}_B$, the generic adjoint Boltzmann transport equation is as follows:

$$L^*(\mathbf{r}, E, \mathbf{\Omega}, t) \psi(\mathbf{r}, E, \mathbf{\Omega}, t) = Q^*(\mathbf{r}, E, \mathbf{\Omega}, t), \quad (4)$$

where the (adjoint) linear integro-differential operator $L^*(\mathbf{r}, E, \mathbf{\Omega}, t)$ is defined below:

$$\begin{aligned} L^*(\mathbf{r}, E, \mathbf{\Omega}, t) \psi(\mathbf{r}, E, \mathbf{\Omega}, t) \triangleq & -\frac{1}{v} \frac{\partial \psi(\mathbf{r}, E, \mathbf{\Omega}, t)}{\partial t} - \mathbf{\Omega} \cdot \nabla \psi(\mathbf{r}, E, \mathbf{\Omega}, t) \\ & + \Sigma_t(\mathbf{r}, E) \psi(\mathbf{r}, E, \mathbf{\Omega}, t) \\ & - \int_0^{E_f} dE' \int_{4\pi} d\mathbf{\Omega}' \Sigma_s(\mathbf{r}, E \to E', \mathbf{\Omega} \to \mathbf{\Omega}') \psi(\mathbf{r}, E', \mathbf{\Omega}', t) \\ & - \nu \Sigma(\mathbf{r}, E) \int_0^{E_f} dE' \int_{4\pi} \chi(\mathbf{r}, E \to E') \psi(\mathbf{r}, E', \mathbf{\Omega}', t) d\mathbf{\Omega}'. \end{aligned} \quad (5)$$

By construction, the forward and adjoint transport equations satisfy the following relation:

$$\langle \varphi, L^* \psi \rangle_B - \langle \psi, L \varphi \rangle_B = P[\varphi, \psi] = \langle \varphi, Q^* \rangle_B - \langle \psi, Q \rangle_B, \quad (6)$$

where $P[\varphi, \psi]$ denotes the bilinear concomitant evaluated on the boundary of the phase-space domain under consideration. The "generalized reciprocity relation" expressed by Equation 6 relates the bilinear concomitant, which is a functional of the forward and adjoint fluxes at the initial and final times along the incoming and outgoing directions at the surface of the medium, to the fluxes in the interior of the medium comprising fixed sources. This reciprocity relation provides a physical interpretation of the adjoint flux as an "importance function," which quantifies the contribution of a source to a detector and enables transport problems to be posed either in the forward or adjoint descriptions. These reciprocity relations also restrict the combination of forward and adjoint boundary conditions to those that ensure both the forward and adjoint formulations are mathematically "well posed." The reciprocity relation expressed by Equation 6 is extensively used in the so-called "source-detector" problems in steady-state subcritical systems, where $Q^*(\mathbf{r}, E, \mathbf{\Omega})$ models the detector properties (cross section) in the sub-region occupied by the respective detector.

When the boundary conditions for Equation 1 are homogeneous and there is no external source, i.e., when $Q(r, E, \mathbf{\Omega}, t) = 0$, the stationary neutron transport problem becomes an eigenvalue problem. The largest (i.e., fundamental) eigenvalue in such a case is called the "effective multiplication factor" and, depending on its value, corresponds to a critical, subcritical, or supercritical physical system (e.g., nuclear reactor). This eigenvalue (multiplication factor) is an important system (model) response, and its mathematical expression is a functional ("Raleigh quotient") of the forward and the adjoint fluxes. Additional important model responses that are functionals of both the forward and adjoint fluxes include the reactivity, generation time, and lifetime of the system, along with several other Lagrangian functionals used in variational principles for developing efficient Raleigh–Ritz type numerical methods (see, e.g., Lewins, 1965; Stacey, 1974; Stacey, 2001). Perhaps the simplest quantity that depends on both the forward and adjoint fluxes—and has important applications in particle transport (particularly in particle shielding)—is the so-called "*contributon flux*" (Williams and Engle, 1977), which arises as follows:

(i) Multiplying the stationary form of Equation 1 by $\psi(r, E, \mathbf{\Omega})$, multiplying the stationary form of Equation 4 by $\varphi(r, E, \mathbf{\Omega})$, subtracting the resulting equations from each other, and integrating the resulting equation over only the energy- and solid angle-independent variables yield the following relation:

$$\nabla \cdot \mathbf{v}_c R(\mathbf{r}) = S(\mathbf{r}) - S^*(\mathbf{r}), \quad (7)$$

where

$$R_c(\mathbf{r}) \triangleq \frac{1}{v} \int_0^{E_f} dE \int_{4\pi} d\mathbf{\Omega}\, \varphi(r, E, \mathbf{\Omega}) \psi(r, E, \mathbf{\Omega}), \quad (8)$$

$$\mathbf{v}_c \triangleq \frac{\int_0^{E_f} dE \int_{4\pi} d\mathbf{\Omega} \left[\mathbf{\Omega} \varphi(r, E, \mathbf{\Omega}) \psi(r, E, \mathbf{\Omega}) \right]}{\frac{1}{v} \int_0^{E_f} dE \int_{4\pi} d\mathbf{\Omega}\, \varphi(r, E, \mathbf{\Omega}) \psi(r, E, \mathbf{\Omega})}, \quad (9)$$

$$S_c(\mathbf{r}) \triangleq \int_0^{E_f} dE \int_{4\pi} d\mathbf{\Omega} [Q(r, E, \mathbf{\Omega}) \psi(r, E, \mathbf{\Omega})], \quad (10)$$

$$S_c^*(\mathbf{r}) \triangleq \int_0^{E_f} dE \int_{4\pi} d\mathbf{\Omega} [Q^*(r, E, \mathbf{\Omega}) \varphi(r, E, \mathbf{\Omega})]. \quad (11)$$

(ii) The form of Equation 7 is the same as the mass continuity balance/equation for compressible flow, indicating that the "contributon response density" $R_c(\mathbf{r})$ is conserved as it flows from the "contributon response source" $S_c(\mathbf{r})$ toward the "contributon response sink" $S_c^*(\mathbf{r})$, with a "contributon response mean velocity" $\mathbf{v}_c$ corresponding to the neutron speed v.

The application of the nth-FASAM-L is illustrated in this section by considering the simplified model of the distribution in the asymptotic energy range of neutrons produced by a source of neutrons placed in an isotropic medium comprising a homogeneous mixture of "*M*" non-fissionable materials having constant (i.e., energy-independent) properties. For simplicity, but without diminishing the applicability of the nth-FASAM-L, this medium is considered to be infinitely large. The simplified form of the Boltzmann neutron transport equation, as shown in Equation 1, that models the energy distributions of neutrons within a mixture of materials is called the "neutron slowing-down equation." This equation is written using neutron *lethargy* (rather than the neutron energy) as the independent variable. Neutron lethargy is customarily denoted using the variable/letter "u" and is defined as $u \triangleq \ln(E_0/E)$, where E denotes the energy variable and E_0 denotes the highest energy in the system. Thus, the neutron slowing-down model (see, e.g., Meghreblian and Holmes, 1960; Lamarsh, 1966) for the energy distribution of the neutron flux in a homogeneous mixture of non-fissionable materials of infinite extent takes the following simplified form of Equation 1:

$$\frac{d\varphi(u)}{du} + \frac{\Sigma_a}{\bar{\xi}\,\Sigma_t}\varphi(u) = \frac{S(u)}{\bar{\xi}\,\Sigma_t}; \quad 0 < u \le u_{th}; \tag{12}$$

$$\varphi(0) = 0; \;\; at\ u = 0. \tag{13}$$

The quantities that appear in Equation 12 are defined as follows.

(i) The lethargy-dependent neutron flux is denoted as $\varphi(u)$; u_{th} denotes a cut-off lethargy, usually corresponding to the thermal neutron energy (ca. 0.0024 electron volts).

(ii) The macroscopic elastic scattering cross section for the homogeneous mixture of "M" materials is denoted as Σ_s and is defined as follows:

$$\Sigma_s \triangleq \sum_{i=1}^{M} N_m^{(i)}\sigma_s^{(i)}, \tag{14}$$

where $\sigma_s^{(i)}, i = 1, ..., M$ denotes the elastic scattering cross section of material "i," and the atomic or molecular number density of material "i" is denoted as $N_m^{(i)}, i = 1, ..., M$ and is defined as $N_m^{(i)} \triangleq \rho_i N_A/A_i$, where N_A is Avogadro's number $(0.602 \times 10^{24}\ nuclei/mole)$, while A_i and ρ_i denote the mass number and density of the material, respectively.

(iii) The average gain in lethargy of a neutron per collision is denoted as $\bar{\xi}$ and is defined as follows for the homogeneous mixture:

$$\bar{\xi} \triangleq \frac{1}{\Sigma_s}\sum_{i=1}^{M}\xi_i N_m^{(i)}\sigma_s^{(i)}; \quad \xi_i \triangleq 1 + \frac{a_i \ln a_i}{1 - a_i}; \quad a_i \triangleq \left(\frac{A_i - 1}{A_i + 1}\right)^2. \tag{15}$$

(iv) The macroscopic absorption cross section is denoted as Σ_a and is defined as follows for the homogeneous mixture:

$$\Sigma_a \triangleq \sum_{i=1}^{M} N_m^{(i)}\sigma_\gamma^{(i)}, \tag{16}$$

where $\sigma_\gamma^{(i)}, i = 1, ..., M$ denotes the microscopic radiative-capture cross section of material "i."

(v) The macroscopic total cross section is denoted as Σ_t and is defined as follows for the homogeneous mixture:

$$\Sigma_t \triangleq \Sigma_a + \Sigma_s. \tag{17}$$

(vi) The source $S(u)$ is considered to be a simplified "spontaneous fission" source stemming from fissionable actinides, such as ^{239}Pu and ^{240}Pu, emitting monoenergetic neutrons at the highest energy (i.e., zero lethargy). Such a source is comprised within the OECD/NEA polyethylene-reflected plutonium (PERP) OECD/NEA reactor physics benchmark (Valentine, 2006; Cacuci and Fang, 2023), which can be modeled using the following simplified expression:

$$S(u) = S_0\delta(u); \quad S_0 \triangleq \sum_{k=1}^{2}\lambda_k^S N_k^S F_k^S \nu_k^S W_k^S, \tag{18}$$

where the superscript "S" indicates the "source; " the subscript index $k = 1$ indicates material properties pertaining to the isotope ^{239}Pu; the subscript index $k = 2$ indicates material properties pertaining to the isotope ^{240}Pu; λ_k^S denotes the decay constant; N_k^S denotes the atomic density of the respective actinide; F_k^S denotes the spontaneous fission branching ratio; ν_k^S denotes the average number of neutrons per spontaneous fission; and W_k^S denotes a function of parameters used in Watt's fission spectrum to approximate the spontaneous fission neutron spectrum of the respective actinide. The detailed forms of the parameters W_k^S are unimportant for illustrating the application of the nth-FASAM-L. The nominal values for these imprecisely known parameters are available from a library file contained in SOURCES 4C (Wilson et al., 2002).

Mirroring the considerations for the Boltzmann transport equation presented in Equations 1–6, the "adjoint slowing-down model" is constructed in the Hilbert space $\mathcal{H}_B$ of square-integrable functions $\varphi(u) \in \mathcal{H}_B$ and $\psi(u) \in \mathcal{H}_B$ endowed with the following inner product, denoted as $\langle\varphi(u), \psi(u)\rangle_B$:

$$\langle\varphi(u), \psi(u)\rangle_B \triangleq \int_0^{u_{th}} \varphi(u)\psi(u)du. \tag{19}$$

Using the inner product $\langle\varphi(u), \psi(u)\rangle_B$ defined in Equation 19, the adjoint slowing-down model is constructed by the usual procedure, i.e., by (i) constructing the inner product of Equation 12 with a function $\psi(u) \in \mathcal{H}_B$; (ii) integrating by parts the resulting relation so as to transfer the differential operation from the forward function $\varphi(u)$ onto the adjoint function $\psi(u)$; (iii) using the initial condition provided in Equation 13 and eliminating the unknown function $\varphi(u_{th})$ by choosing the final-value condition $\psi(u_{th}) = 0$; and (iv) choosing the source for the resulting adjoint slowing-down model so as to satisfy the generalized reciprocity relation shown in Equation 6. The result of these operations is the following adjoint slowing-down model for the adjoint slowing-down function $\psi(u)$:

$$-\frac{d\psi(u)}{du} + f_1(\boldsymbol{\alpha})\psi(u) = \delta(u - u_d), \tag{20}$$

$$\psi(u_{th}) = 0, at\ u = u_{th}. \tag{21}$$

The "contributon-flux response density" $R_c(\varphi, \psi)$, as generally defined in Equation 8, specialized for the neutron slowing-down model, coincides with the inner product used in this context, i.e.,

$$R_c(\varphi, \psi) \triangleq \int_0^{u_{th}} \varphi(u)\psi(u)\,du \equiv \langle\varphi(u), \psi(u)\rangle_B. \tag{22}$$

It is important to note that $R_c(\varphi, \psi)$ does *not* depend *explicitly* on either the feature function $\mathbf{f}(\boldsymbol{\alpha})$ or any primary model parameter. Therefore, the G-differential of $R_c(\varphi, \psi)$ will not comprise a direct-effect term but will consist entirely of the indirect-effect term.

For this "contributon-flux response density" model, the following *primary model parameters* are subject to experimental uncertainties.

(i) For each material "*i*," $i = 1, ..., M$, included in the homogeneous mixture, the following are primary model parameters: the atomic number densities $N_m^{(i)}$; the microscopic radiative-capture cross section $\sigma_\gamma^{(i)}$; and the scattering cross section $\sigma_s^{(i)}$;

(ii) The source parameters λ_k^S, N_k^S, F_k^S, ν_k^S, and W_k^S, for $k = 1,2$.

The above primary parameters are considered to constitute the components of a "vector of primary model parameters" defined as follows:

$$\boldsymbol{\alpha} \triangleq \left(N_m^{(1)}, \sigma_\gamma^{(1)}, \sigma_s^{(1)}, ..., N_m^{(M)}, \sigma_\gamma^{(M)}, \sigma_s^{(M)}, \lambda_1^S, \lambda_2^S, N_1^S, N_2^S, F_1^S, F_2^S, \nu_1^S, \nu_2^S, W_1^S, W_2^S\right)^\dagger \triangleq (\alpha_1, \ldots, \alpha_{TP})^\dagger; \quad TP \triangleq 3M + 10. \tag{23}$$

The first-level forward/adjoint system (1st-LFAS) for the "first-level forward/adjoint function" $\mathbf{u}^{(1)}(2; u) \triangleq [\varphi(u), \psi(u)]^\dagger$ comprises Equations 12, 13, 20, and 21. The structure of the 1st-LFAS suggests that the components $f_i(\boldsymbol{\alpha})$ of the feature function $\mathbf{f}(\boldsymbol{\alpha})$ can be defined as follows:

$$\mathbf{f}(\boldsymbol{\alpha}) \triangleq [f_1(\boldsymbol{\alpha}), f_2(\boldsymbol{\alpha})]^\dagger; \quad f_1(\boldsymbol{\alpha}) \triangleq \frac{\Sigma_a(\boldsymbol{\alpha})}{\bar{\xi}(\boldsymbol{\alpha})\Sigma_t(\boldsymbol{\alpha})}; \quad f_2(\boldsymbol{\alpha}) \triangleq \frac{S_0(\boldsymbol{\alpha})}{\bar{\xi}(\boldsymbol{\alpha})\Sigma_t(\boldsymbol{\alpha})}. \tag{24}$$

Solving Equations 12, 13 while using the definitions introduced in Equation 24 yields the following expression for the flux $\varphi(u)$ in terms of the components $f_i(\boldsymbol{\alpha})$ of the feature function $\mathbf{f}(\boldsymbol{\alpha})$:

$$\varphi(u) = H(u) f_2(\boldsymbol{\alpha}) \exp[-u f_1(\boldsymbol{\alpha})]; \quad H(0) = 0; \quad H(u) = 1, if\ u > 0. \tag{25}$$

Solving the above adjoint slowing-down model yields the following closed-form expression for the adjoint slowing-down function $\psi(u)$:

$$\psi(u) = H(u_d - u) \exp[(u - u_d) f_1(\boldsymbol{\alpha})]. \tag{26}$$

In terms of the components $f_i(\boldsymbol{\alpha})$ of the feature function $\mathbf{f}(\boldsymbol{\alpha})$, the closed-form expression of the "contributon response density" is obtained by substituting the expressions provided in Equations 25, 26 into Equation 22 and performing the integration over lethargy, which yields

$$R_c(\varphi, \psi) = \int_0^{u_{th}} H(u) f_2(\boldsymbol{\alpha}) \exp[-u f_1(\boldsymbol{\alpha})] H(u_d - u) \exp[(u - u_d) f_1(\boldsymbol{\alpha})]\, du = u_d f_2(\boldsymbol{\alpha}) \exp[-u_d f_1(\boldsymbol{\alpha})]. \tag{27}$$

In terms of the primary model parameters, the closed-form expression of the "contributon response density" is

$$R_c(\varphi, \psi) = u_d \frac{S_0(\boldsymbol{\alpha})}{\bar{\xi}(\boldsymbol{\alpha})\Sigma_t(\boldsymbol{\alpha})} \exp\left[-u_d \frac{\Sigma_a(\boldsymbol{\alpha})}{\bar{\xi}(\boldsymbol{\alpha})\Sigma_t(\boldsymbol{\alpha})}\right]. \tag{28}$$

As Equation 28 indicates, the model response can be considered to depend directly on $TP \triangleq 3M + 10$ primary model parameters. In view of Equation 27, however, the model response can alternatively be considered to depend directly on two feature functions and only indirectly (through the two feature functions) on the primary model parameters. In the former consideration/interpretation, the response sensitivities to the primary model parameters will be obtained by applying the nth-CASAM-L. In the later consideration/interpretation, the response sensitivities to the primary model parameters will be obtained by applying the nth-FASAM-L, which will involve two stages: (a) the response sensitivities with respect to the feature functions will be obtained in the first stage; (b) the subsequent computation of the response sensitivities to the primary model parameters will be performed in the second stage by using the response sensitivities with respect to the feature functions obtained in the first stage. The computational distinctions that stem from these differing considerations/interpretations underlying the nth-CASAM-L *versus* the nth-FASAM-L will become evident in the next section by using a paradigm neutron slowing-down model, which is representative of the general situation for any linear system.

3 First-order adjoint sensitivity analysis of the contributon flux to the slowing-down model's features and parameters

The first-order sensitivities of the response $R_c[\mathbf{u}^{(1)}(2; u)]$, where $\mathbf{u}^{(1)}(2; u) \triangleq [\varphi(u), \psi(u)]^\dagger$, are obtained by determining the first-order Gateaux (G-)- differential, denoted as $\{\delta R_c[\mathbf{u}^{(1)}(2; u), \mathbf{v}^{(1)}(2; u)]\}_{\boldsymbol{\alpha}^0}$, of this response for variations $\mathbf{v}^{(1)}(2; u) \triangleq [\delta\varphi(u), \delta\psi(u)]^\dagger$ around the phase-space point (φ^0, ψ^0). By definition, the first-order G-differential $\{\delta R_c[\mathbf{u}^{(1)}(2; u), \mathbf{v}^{(1)}(2; u)]\}_{\boldsymbol{\alpha}^0}$ is obtained as follows:

$$\{\delta R_c[\mathbf{u}^{(1)}(2; u), \mathbf{v}^{(1)}(2; u)]\}_{\boldsymbol{\alpha}^0} \triangleq \left\{\frac{d}{d\varepsilon} \int_0^{u_{th}} \left[\varphi^0(u) + \varepsilon v^{(1)}(u)\right] \left[\psi^0(u) + \varepsilon \delta\psi(u)\right] du\right\}_{\varepsilon=0} = \left\{\int_0^{u_{th}} \left[v^{(1)}(u)\psi(u) + \varphi(u)\delta\psi(u)\right] du\right\}_{\boldsymbol{\alpha}^0}. \tag{29}$$

The sensitivities of $R_c[\mathbf{u}^{(1)}(2; u)]$ with respect to the feature functions (and subsequently to the primary model parameters) will be determined in Section 3.1 by applying the 1st-FASAM-L. Alternatively, the sensitivities of $R_c[\mathbf{u}^{(1)}(2; u)]$ directly with respect to the primary model parameters will be determined in Section 3.2 by applying the 1st-CASAM-L.

3.1 Application of the 1st-FASAM-L

The first-level variational sensitivity function $\mathbf{v}^{(1)}(2; u) \triangleq [v^{(1)}(u), \delta\psi(u)]^\dagger$ is the solution of the first-level variational sensitivity system (1st-LVSS) obtained by differentiating the 1st-LFAS. The function $v^{(1)}(u)$ is obtained by taking the first-order G-differentials of Equations 12, 13 to obtain

$$\left\{\frac{d}{d\varepsilon}\left[\frac{d(\varphi^0 + \varepsilon v^{(1)})}{du} + \left(f_1^0 + \varepsilon \delta f_1\right)\left(\varphi^0 + \varepsilon v^{(1)}\right)\right]\right\}_{\varepsilon=0} = \delta(u)\left\{\frac{d}{d\varepsilon}\left(f_2^0 + \varepsilon \delta f_2\right)\right\}_{\varepsilon=0}, \tag{30}$$

$$\left\{ \frac{d}{d\varepsilon} \left[\varphi^0(u) + \varepsilon v^{(1)}(u) \right] \right\}_{\varepsilon=0} = 0; \quad at \ u = 0. \tag{31}$$

Carrying out the differentiations with respect to ε in the above equations and setting $\varepsilon = 0$ in the resulting expressions yields the following relations:

$$\frac{dv^{(1)}(u)}{du} + f_1(\boldsymbol{\alpha}^0) v^{(1)}(u) = (\delta f_2)\delta(u) - (\delta f_1)\varphi^0(u), \tag{32}$$

$$v^{(1)}(u) = 0; \quad at \ u = 0. \tag{33}$$

The equations satisfied by the variational function $\delta\psi(u)$ are obtained by G-differentiating Equations 20, 21 to obtain the equations below:

$$-\frac{d}{du}[\delta\psi(u)] + f_1(\boldsymbol{\alpha}^0)[\delta\psi(u)] = -(\delta f_1)\psi(u), \tag{34}$$

$$\delta\psi(u_{th}) = 0, at \ u = u_{th}. \tag{35}$$

Concatenating Equations 32–35 yields the following 1st-LVSS for the first-level variational sensitivity function $\mathbf{v}^{(1)}(2;u) \triangleq [\delta\varphi(u), \delta\psi(u)]^\dagger$:

$$\left\{ \mathbf{V}^{(1)}[2\times 2; u; \mathbf{f}] \mathbf{v}^{(1)}(2;u) \right\}_{\boldsymbol{\alpha}^0} = \left\{ \mathbf{q}_V^{(1)}\left[2; \mathbf{u}^{(1)}(2;u); \mathbf{f}; \delta\mathbf{f}\right] \right\}_{\boldsymbol{\alpha}^0}, \tag{36}$$

$$\left\{ \mathbf{b}_v^{(1)}\left(\mathbf{v}^{(1)}; \mathbf{f}; \delta\mathbf{f}\right) \right\}_{\boldsymbol{\alpha}^0} = \mathbf{0}, \tag{37}$$

where

$$\mathbf{V}^{(1)}[2\times 2; u; \mathbf{f}] \triangleq \begin{pmatrix} d/du + f_1 & 0 \\ 0 & -d/du + f_1 \end{pmatrix}, \mathbf{b}_v^{(1)}\left(\mathbf{v}^{(1)}; \mathbf{f}; \delta\mathbf{f}\right) \triangleq \begin{pmatrix} v^{(1)}(0) \\ \delta\psi(u_{th}) \end{pmatrix}, \tag{38}$$

$$\mathbf{q}_V^{(1)}\left[2; \mathbf{u}^{(1)}; \mathbf{f}; \delta\mathbf{f}\right] \triangleq \begin{pmatrix} (\delta f_2)\delta(u) - (\delta f_1)\varphi(u) \\ -(\delta f_1)\psi(u) \end{pmatrix}. \tag{39}$$

Rather than repeatedly solving the 1st-LVSS for every possible variations δf_i, $i = 1,2$, the appearance of the first-level variational sensitivity function $\mathbf{v}^{(1)}(2;u) \triangleq [\delta\varphi(u), \delta\psi(u)]^\dagger$ will be eliminated from the expression of the G-differential of the response $\{\delta R_c[\mathbf{u}^{(1)}(2;u), \mathbf{v}^{(1)}(2;u)]\}_{\boldsymbol{\alpha}^0}$, defined in Equation 29), by applying the principles of the 1st-FASAM-L outlined in the accompanying "Part I" by Cacuci (2024c). The specific steps are as follows:

1. A Hilbert space, denoted as H_1, is introduced endowed with the following inner product denoted as $\langle \boldsymbol{\chi}^{(1)}(2;u), \boldsymbol{\theta}^{(1)}(2;u) \rangle_1$, between two elements, $\boldsymbol{\chi}^{(1)}(2;u) \triangleq [\chi_1^{(1)}(u), \chi_2^{(1)}(u)]^\dagger \in \mathcal{H}_1$ and $\boldsymbol{\theta}^{(1)}(2;u) \triangleq [\theta_1^{(1)}(u), \theta_2^{(1)}(u)]^\dagger \in \mathcal{H}_1$:

$$\langle \boldsymbol{\chi}^{(1)}(2;u), \boldsymbol{\theta}^{(1)}(2;u) \rangle_1 \triangleq \sum_{i=1}^{2} \int_0^{u_{th}} \chi_i^{(1)}(u) \theta_i^{(1)}(u)\, du. \tag{40}$$

2. In the Hilbert $\mathcal{H}_1$, the inner product of Equation 36 is formed with a yet undefined vector-valued function $\mathbf{a}^{(1)}(2;u) \triangleq [a_1^{(1)}(u), a_2^{(1)}(u)]^\dagger \in \mathcal{H}_1$ to obtain the following relation:

$$\left\{ \langle \mathbf{a}^{(1)}(2;u), \mathbf{V}^{(1)}[2\times 2; u; \mathbf{f}^0] \mathbf{v}^{(1)}(2;u) \rangle_1 \right\}_{\boldsymbol{\alpha}^0} = \left\{ \langle \mathbf{a}^{(1)}(2;u), \mathbf{q}_V^{(1)}\left[2; \mathbf{u}^{(1)}(2;u); \mathbf{f}; \delta\mathbf{f}\right] \rangle_1 \right\}_{\boldsymbol{\alpha}^0}. \tag{41}$$

3. The left-side of Equation 41 is integrated by parts to obtain the following relation, where the specification $\{\}_{\boldsymbol{\alpha}^0}$ is omitted to simplify the notation:

$$\begin{aligned} &\int_0^{u_{th}} a_1^{(1)}(u) \left[\frac{dv^{(1)}}{du} + f_1 v^{(1)} \right] du + \int_0^{u_{th}} a_2^{(1)}(u) \left[-\frac{d}{du}\delta\psi + f_1\delta\psi \right] du \\ &= \int_0^{u_{th}} v^{(1)} \left[-\frac{d}{du} a_1^{(1)}(u) + f_1 a_1^{(1)}(u) \right] du \\ &\quad + \int_0^{u_{th}} \delta\psi(u) \left[\frac{d}{du} a_2^{(1)}(u) + f_1 a_2^{(1)}(u) \right] du + a_1^{(1)}(u_{th}) v^{(1)}(u_{th}) \\ &\quad - a_1^{(1)}(0) v^{(1)}(0) - a_2^{(1)}(u_{th}) \delta\psi(u_{th}) + a_2^{(1)}(0) \delta\psi(0). \end{aligned} \tag{42}$$

4. The first two terms on the right side of Equation 42 are required to represent the G-differentiated response defined in Equation 29, and the unknown boundary values of the function $\mathbf{v}^{(1)}(2;u)$ are eliminated from the bilinear concomitant on the right side of Equation 42 to obtain the following 1st-LASS for the first-level adjoint sensitivity function $\mathbf{a}^{(1)}(2;u) \triangleq [a_1^{(1)}(u), a_2^{(1)}(u)]^\dagger$:

$$\mathbf{A}^{(1)}[2\times 2; \mathbf{x}; \mathbf{f}] \mathbf{a}^{(1)}(2;\mathbf{x}) = \mathbf{q}_A^{(1)}\left[2; \mathbf{u}^{(1)}(2;\mathbf{x}); \mathbf{f}\right], \tag{43}$$

$$\left\{ \mathbf{b}_A^{(1)}\left[\mathbf{u}^{(1)}(2;u); \mathbf{a}^{(1)}(2;u); \mathbf{f} \right] \right\}_{\boldsymbol{\alpha}^0} \triangleq \begin{pmatrix} a_1^{(1)}(u_{th}) \\ a_2^{(1)}(0) \end{pmatrix} = \mathbf{0}, \tag{44}$$

where

$$\mathbf{A}^{(1)}[2\times 2; u; \mathbf{f}] \triangleq \begin{pmatrix} -d/du + f_1 & 0 \\ 0 & d/du + f_1 \end{pmatrix} = \{\mathbf{V}^{(1)}[2\times 2; u; \mathbf{f}]\}^*, \tag{45}$$

$$\mathbf{q}_A^{(1)}\left[2; \mathbf{u}^{(1)}(2;\mathbf{x}); \mathbf{f}\right] \triangleq \begin{pmatrix} \psi(u) \\ \varphi(u) \end{pmatrix}. \tag{46}$$

5. It follows from Equations 29, 41–44 that G-differentiated response defined in Equation 29 takes the following expression in terms of the first-level adjoint sensitivity function $\mathbf{a}^{(1)}(2;u) \triangleq [a_1^{(1)}(u), a_2^{(1)}(u)]^\dagger$:

$$\begin{aligned} &\left\{ \delta R_c\left[\mathbf{u}^{(1)}(2;u), \mathbf{a}^{(1)}(2;u)\right] \right\}_{\boldsymbol{\alpha}^0} \\ &= \left\{ \int_0^{u_{th}} a_1^{(1)}(u) \left[(\delta f_2)\delta(u) - (\delta f_1)\varphi(u) \right] du \right\}_{\boldsymbol{\alpha}^0} \\ &+ \left\{ \int_0^{u_{th}} a_2^{(1)}(u) \left[-(\delta f_1)\psi(u) \right] du \right\}_{\boldsymbol{\alpha}^0}, \end{aligned} \tag{47}$$

The expressions of the sensitivities of the response $R_c(\varphi, \psi)$ with respect to the components of the feature function $\mathbf{f}(\boldsymbol{\alpha})$ are given by the expressions that multiply the respective components of $\mathbf{f}(\boldsymbol{\alpha})$ in Equation 47, i.e.,

$$\frac{\partial R_c(\varphi, \psi)}{\partial f_1} = -\int_0^{u_{th}} \left[a_1^{(1)}(u)\varphi(u) + a_2^{(1)}(u)\psi(u) \right] du, \tag{48}$$

$$\frac{\partial R_c(\varphi, \psi)}{\partial f_2} = \int_0^{u_{th}} a_1^{(1)}(u)\, \delta(u)\, du. \tag{49}$$

The above expressions are to be evaluated at the nominal parameter values $\boldsymbol{\alpha}^0$, but the indication $\{\}_{\boldsymbol{\alpha}^0}$ has been omitted for simplicity.

The first-order sensitivities of the response $R_c(\varphi,\psi)$ with respect to the primary model parameters are obtained by using the results obtained in Equations 48, 49, respectively, in conjunction with the "chain rule" of differentiating the components of the feature function $\mathbf{f}(\boldsymbol{\alpha})$ with respect to the primary model parameters defined in Equation 29 to obtain the following expressions:

$$\frac{\partial R_c(\varphi,\psi)}{\partial\alpha_i}=\frac{\partial R_c(\varphi,\psi)}{\partial f_1}\frac{\partial f_1}{\partial\alpha_i}+\frac{\partial R_c(\varphi,\psi)}{\partial f_2}\frac{\partial f_2}{\partial\alpha_i}$$
$$=-\left(\frac{\partial f_1}{\partial\alpha_i}\right)\int_0^{u_{th}}\left[a_1^{(1)}(u)\varphi(u)+a_2^{(1)}(u)\psi(u)\right]du$$
$$+\left(\frac{\partial f_2}{\partial\alpha_i}\right)\int_0^{u_{th}}a_1^{(1)}(u)\,\delta(u)\,du. \tag{50}$$

Solving the 1^{st}-LASS defined by Equations 43, 44 yields the following closed-form expressions for the components of the first-level adjoint sensitivity function $\mathbf{a}^{(1)}(2;u)\triangleq[a_1^{(1)}(u),a_2^{(1)}(u)]^{\dagger}$:

$$a_1^{(1)}(u)=(u_d-u)H(u_d-u)\exp\left[(u-u_d)f_1(\boldsymbol{\alpha})\right], \tag{51}$$
$$a_2^{(1)}(u)=uf_2(\boldsymbol{\alpha})\exp\left[-uf_1(\boldsymbol{\alpha})\right]. \tag{52}$$

Using the above expressions in Equations 48, 49 yields the following closed-form expressions for the respective sensitivities:

$$\frac{\partial R_c(\varphi,\psi)}{\partial f_1}=-(u_d)^2f_2(\boldsymbol{\alpha})\exp\left[-u_df_1(\boldsymbol{\alpha})\right], \tag{53}$$
$$\frac{\partial R_c(\varphi,\psi)}{\partial f_2}=u_d\exp\left[-u_df_1(\boldsymbol{\alpha})\right]. \tag{54}$$

The correctness of the expressions obtained in Equations 53, 54 can be verified by differentiating accordingly the closed-form expression given in Equation 27.

3.2 Application of the 1^{st}-CASAM-L

The 1^{st}-CASAM-L delivers the first-order sensitivities of the response directly with respect to the primary model parameters. The expression of the G-differentiated response is as shown in Equation 29, but the source term on the right side of the 1^{st}-LVSS takes the following form:

$$\mathbf{q}_V^{(1)}\left[2;\mathbf{u}^{(1)};\mathbf{f};\delta\mathbf{f}\right]\triangleq\begin{pmatrix}\delta(u)\sum_{i=1}^{TP}\frac{\partial f_2}{\partial\alpha_i}\delta\alpha_i-\varphi(u)\sum_{i=1}^{TP}\frac{\partial f_1}{\partial\alpha_i}\delta\alpha_i\\ -\psi(u)\sum_{i=1}^{TP}\frac{\partial f_1}{\partial\alpha_i}\delta\alpha_i\end{pmatrix}. \tag{55}$$

If one were to actually solve the 1^{st}-LVSS to obtain the first-level variational function and subsequently use the respective variational function to compute each sensitivity, one would need to solve the 1^{st}-LVSS *TP-times*, using each time a source that would correspond to the *i*th-primary parameter, of the form $\mathbf{q}_V^{(1)}[i;2;\mathbf{u}^{(1)};\mathbf{f};\delta\mathbf{f}]\mathbf{q}\triangleq[\delta(u)\partial f_2/\partial\alpha_i-\varphi(u)\,\partial f_1/\partial\alpha_i,-\,\psi(u)\partial f_1/\partial\alpha_i]^{\dagger}$, for each primary parameter $i=1,...,TP$.

Since the left side of the 1^{st}-LVSS remains the same as in Equation 36 and the boundary conditions also remain the same as obtained in Equation 37, it follows that the 1^{st}-LASS and its solution $\mathbf{a}^{(1)}(2;u)\triangleq[a_1^{(1)}(u),a_2^{(1)}(u)]^{\dagger}$ remain unchanged. It therefore follows that the counterpart of the expression of the G-differential obtained in Equation 47 takes the following form:

$$\{\delta R_c[\mathbf{u}^{(1)}(2;u),\mathbf{a}^{(1)}(2;u)]\}_{\boldsymbol{\alpha}^0}=$$
$$-\left\{\sum_{i=1}^{TP}\frac{\partial f_1}{\partial\alpha_i}\delta\alpha_i\int_0^{u_{th}}a_2^{(1)}(u)\psi(u)\,du\right\}_{\boldsymbol{\alpha}^0}$$
$$+\left\{\int_0^{u_{th}}a_1^{(1)}(u)\left[\delta(u)\sum_{i=1}^{TP}\frac{\partial f_2}{\partial\alpha_i}\delta\alpha_i-\varphi(u)\sum_{i=1}^{TP}\frac{\partial f_1}{\partial\alpha_i}\delta\alpha_i\right]du\right\}_{\boldsymbol{\alpha}^0}. \tag{56}$$

The first-order sensitivities of the response $R_c(\varphi,\psi)$ with respect to the primary model parameters $\alpha_i, i=1,...,TP$ are obtained by identifying the expressions that multiply the respective variations $\delta\alpha_i$ in Equation 47, which yields the following result:

$$\frac{\partial R_c(\varphi,\psi)}{\partial\alpha_i}=-\left(\frac{\partial f_1}{\partial\alpha_i}\right)\int_0^{u_{th}}\left[a_1^{(1)}(u)\varphi(u)+a_2^{(1)}(u)\psi(u)\right]du$$
$$+\left(\frac{\partial f_2}{\partial\alpha_i}\right)\int_0^{u_{th}}a_1^{(1)}(u)\,\delta(u)\,du. \tag{57}$$

As expected, the result obtained from Equation 57 is identical to the result produced from Equation 50 by using the 1^{st}-FASAM-L. Both the 1^{st}-FASAM-L and 1^{st}-CASAM-L require "one large-scale computation" for solving the 1^{st}-LASS represented by Equations 43, 44.

4 Second-order adjoint sensitivity analysis of the contributon flux to the slowing-down model's features and parameters

In practice, closed-form expressions such as those shown in Equations 53, 54 are unavailable. The 1^{st}-FASAM-L yields the expressions provided in Equations 48, 49, while the 1^{st}-CASAM-L yields the expressions provided in Equation 57. Hence, these expressions will provide the starting points for obtaining the second-order sensitivities that stem from the respective first-order sensitivities. As outlined within the general frameworks of both the n^{th}-FASAM-L and n^{th}-CASAM-L methodologies, the second-order sensitivities are obtained by conceptually considering them to arise as the "first-order sensitivities of the first-order sensitivities."

4.1 Application of the 2^{nd}-FASAM-L

The 2^{nd}-FASAM-L uses the first-order sensitivities obtained from the 1^{st}-CASAM-L, as provided in Equations 48, 49, to obtain the respective second-order sensitivities, as presented in Sections 4.1.1 and 4.1.2.

4.1.1 Second-order sensitivities stemming from the first-order sensitivity $\partial R_c/\partial f_1$

The second-order sensitivities that stem from the first-order sensitivity $\partial R_c/\partial f_1$ are obtained by determining the G-differential of $\partial R_c/\partial f_1$. For subsequent "bookkeeping" purposes, this first-order sensitivity will be denoted as $R^{(1)}[1;\mathbf{u}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})] \triangleq \partial R_c/\partial f_1$, where the superscript "(1)" denotes "*first-order*" (sensitivity) and the argument "1" indicates that this sensitivity is with respect to the *first component*, i.e., $f_1(\boldsymbol{\alpha})$, of the feature function $\mathbf{f}(\boldsymbol{\alpha})$. This sensitivity also depends on the function $\mathbf{u}^{(2)}(2^2;u) \triangleq [\mathbf{u}^{(1)}(2;u),\mathbf{a}^{(1)}(2;u)]^\dagger$, which is the solution of the "second-level forward/adjoint system (2[nd]-LFAS)" obtained by concatenating the 1[st]-LFAS with the 1[st]-LASS, comprising Equations 12, 13, 20, 21, 43, and 44.

Applying the definition of the G-differential to Equation 48 yields the following expression for the G-differential $\{\delta R^{(1)}[1;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$:

$$\begin{aligned}
&\{\delta R^{(1)}[1;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0} \\
&\triangleq -\left\{\tfrac{d}{d\varepsilon}\int_0^{u_{th}}\left[a_1^{(1)}(u)+\varepsilon\delta a_1^{(1)}(u)\right]\left[\varphi(u)+\varepsilon v^{(1)}(u)\right]du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\
&\quad-\left\{\tfrac{d}{d\varepsilon}\int_0^{u_{th}}\left[a_2^{(1)}(u)+\varepsilon\delta a_2^{(1)}(u)\right]\left[\psi(u)+\varepsilon\delta\psi(u)\right]du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\
&= -\int_0^{u_{th}}\varphi(u)\left[\delta a_1^{(1)}(u)\right]du - \int_0^{u_{th}} a_1^{(1)}(u)v^{(1)}(u)\,du - \int_0^{u_{th}}\psi(u)\left[\delta a_2^{(1)}(u)\right]du \\
&\quad-\int_0^{u_{th}} a_2^{(1)}(u)\left[\delta\psi(u)\right]du \equiv \sum_{j=1}^{2}\frac{\partial^2 R(\varphi;\mathbf{f})}{\partial f_j\partial f_1}\left(\delta f_j\right).
\end{aligned} \tag{58}$$

The components $v^{(1)}(u)$, $\delta\psi(u)$, $\delta a_1^{(1)}(u)$, and $\delta a_2^{(1)}(u)$ of the second-level variational sensitivity function $\mathbf{v}^{(2)}(2^2;u) \triangleq [v^{(1)}(u),\delta\psi(u),\delta a_1^{(1)}(u),\delta a_2^{(1)}(u)]^\dagger$ are the solutions of the 2[nd]-LVSS, which is obtained by G-differentiating the 2[nd]-LFAS. Thus, performing the G-differentiation of Equations 12, 13, 20, 21, 43, and 44 yields the following 2[nd]-LVSS for the second-level variational sensitivity function $\mathbf{v}^{(2)}(2^2;u) \triangleq [v^{(1)}(u),\delta\psi(u),\delta a_1^{(1)}(u),\delta a_2^{(1)}(u)]^\dagger$:

$$\left\{\mathbf{V}^{(2)}[2^2\times 2^2;u;\mathbf{f}]\mathbf{v}^{(2)}(2^2;u)\right\}_{\boldsymbol{\alpha}^0} = \left\{\mathbf{q}_V^{(2)}[2^2;u;\mathbf{f};\delta\mathbf{f}]\right\}_{\boldsymbol{\alpha}^0}, \tag{59}$$

$$\left\{\mathbf{b}_v^{(2)}(u;\mathbf{f};\delta\mathbf{f})\right\}_{\boldsymbol{\alpha}^0} = \mathbf{0}, \tag{60}$$

where

$$\mathbf{V}^{(2)}[2^2\times 2^2;u;\mathbf{f}] \triangleq \begin{pmatrix} d\backslash/du+f_1 & 0 & 0 & 0 \\ 0 & -\dfrac{d}{du}+f & 0 & 0 \\ 0 & -1 & -\dfrac{d}{du}+f_1 & 0 \\ -1 & 0 & 0 & \dfrac{d}{du}+f_1 \end{pmatrix}; \tag{61}$$

$$\mathbf{q}_V^{(2)}[2^2;u;\mathbf{f};\delta\mathbf{f}] \triangleq \begin{pmatrix} (\delta f_2)\delta(u)-(\delta f_1)\varphi(u) \\ -(\delta f_1)\psi(u) \\ -(\delta f_1)a_1^{(1)}(u) \\ -(\delta f_1)a_2^{(1)}(u) \end{pmatrix};$$

$$\mathbf{b}_v^{(2)}(u;\mathbf{f};\delta\mathbf{f}) \triangleq \begin{pmatrix} v^{(1)}(0) \\ \delta\psi(u_{th}) \\ \delta a_1^{(1)}(u_{th}) \\ \delta a_2^{(1)}(0) \end{pmatrix}. \tag{62}$$

The second-level variational sensitivity function $\mathbf{v}^{(2)}(2^2;u)$ will be eliminated from the expression of $\{\delta R^{(1)}[1;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$ by constructing the 2[nd]-LASS corresponding to the above 2[nd]-LVSS. The solution of the 2[nd]-LASS will be used in Equation 58 to construct $\{\delta R^{(1)}[1;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$, an alternative expression that will not depend on $\mathbf{v}^{(2)}(2^2;u)$. This 2[nd]-LASS will be constructed in a Hilbert space denoted as H_2, comprising four-component vector-valued functions of the form $\boldsymbol{\chi}^{(2)}(2^2;1;u) \triangleq [\chi_1^{(2)}(1;u),\chi_2^{(2)}(1;u),\chi_3^{(2)}(1;u),\chi_4^{(2)}(1;u)]^\dagger \in \mathcal{H}_2$ as elements, and is endowed with the following inner product between two vectors $\boldsymbol{\chi}^{(2)}(2^2;1;u)$ and $\boldsymbol{\theta}^{(2)}(2^2;1;u)$:

$$\left\langle\boldsymbol{\chi}^{(2)}(2^2;u),\boldsymbol{\theta}^{(2)}(2^2;u)\right\rangle_2 \triangleq \sum_{i=1}^{2^2}\int_0^{u_{th}}\chi_i^{(2)}(1;u)\theta_i^{(2)}(1;u)\,du. \tag{63}$$

The inner product defined in Equation 63 will be used to construct the inner product of Equation 59 with a function denoted as $\mathbf{a}^{(2)}(2^2;1;u) \triangleq [a_1^{(2)}(1;u),a_2^{(2)}(1;u),a_3^{(2)}(1;u),a_4^{(2)}(1;u)]^\dagger \in \mathcal{H}_2$, where the argument "1" of the function $\mathbf{a}^{(2)}(2^2;1;u)$ indicates that this (adjoint) function corresponds to the first-order sensitivity of the response with respect to the "*first*" component, $f_1(\boldsymbol{\alpha})$, of the feature function $\mathbf{f}(\boldsymbol{\alpha})$. Constructing this inner product yields the following relation, where the specification $\{\}_{\boldsymbol{\alpha}^0}$ has been omitted to simplify the notation:

$$\begin{aligned}
&\left\langle\mathbf{a}^{(2)}(2^2;1;\mathbf{x}),\mathbf{V}^{(2)}[2^2\times 2^2;u;\mathbf{f}]\mathbf{v}^{(2)}(2^2;u)\right\rangle_{2^2} \\
&= \int_0^{u_{th}} a_1^{(2)}(1;u)\left[dv^{(1)}/du+f_1v^{(1)}\right]du \\
&\quad+\int_0^{u_{th}} a_2^{(2)}(1;u)\left[-d(\delta\psi)/du+f_1(\delta\psi)\right]du \\
&\quad+\int_0^{u_{th}} a_3^{(2)}(1;u)\left[-\delta\psi-d\left(\delta a_1^{(1)}\right)/du+f_1\left(\delta a_1^{(1)}\right)\right]du \\
&\quad+\int_0^{u_{th}} a_4^{(2)}(1;u)\left[-v^{(1)}(u)+d\left(\delta a_2^{(1)}\right)/du+f_1\left(\delta a_2^{(1)}\right)\right]du \\
&= \int_0^{u_{th}} a_1^{(2)}(1;u)\left[(\delta f_2)\delta(u)-(\delta f_1)\varphi(u)\right]du \\
&\quad+\int_0^{u_{th}} a_2^{(2)}(1;u)\left[-(\delta f_1)\psi(u)\right]du \\
&\quad+\int_0^{u_{th}} a_3^{(2)}(1;u)\left[-(\delta f_1)a_1^{(1)}(u)\right]du \\
&\quad+\int_0^{u_{th}} a_4^{(2)}(1;u)\left[-(\delta f_1)a_2^{(1)}(u)\right]du.
\end{aligned} \tag{64}$$

Integrating by parts the left side of Equation 64 yields the following relation:

$$\int_0^{u_{th}} a_1^{(2)}(1;u)\left[dv^{(1)}/du + f_1 v^{(1)}\right] du$$
$$+ \int_0^{u_{th}} a_2^{(2)}(1;u)\left[-d(\delta\psi)/du + f_1(\delta\psi)\right] du$$
$$+ \int_0^{u_{th}} a_3^{(2)}(1;u)\left[-\delta\psi - d\left(\delta a_1^{(1)}\right)/du + f_1\left(\delta a_1^{(1)}\right)\right] du$$
$$+ \int_0^{u_{th}} a_4^{(2)}(1;u)\left[-v^{(1)}(u) + d\left(\delta a_2^{(1)}\right)/du + f_1\left(\delta a_2^{(1)}\right)\right] du$$
$$= a_1^{(2)}(1;u_{th})v^{(1)}(u_{th}) - a_1^{(2)}(1;0)v^{(1)}(0) + \int_0^{u_{th}} v^{(1)}(u)\left[-da_1^{(2)}(1;u)/du + f_1 a_1^{(2)}(1;u)\right] du$$
$$- a_2^{(2)}(1;u_{th})\delta\psi(u_{th}) + a_2^{(2)}(1;0)\delta\psi(0) + \int_0^{u_{th}} (\delta\psi) \times \left[da_2^{(2)}(1;u)/du + f_1 a_2^{(2)}(1;u)\right] du - a_3^{(2)}(1;u_{th})\delta a_1^{(1)}(u_{th})$$
$$+ a_3^{(2)}(1;0)\delta a_1^{(1)}(0) - \int_0^{u_{th}} (\delta\psi) a_3^{(2)}(1;u)\, du + \int_0^{u_{th}} \delta a_1^{(1)}(u)\left[da_3^{(2)}(1;u)/du + f_1 a_3^{(2)}(1;u)\right] du$$
$$- \int_0^{u_{th}} v^{(1)}(u) a_4^{(2)}(1;u)\, du + a_4^{(2)}(1;u_{th})\delta a_2^{(1)}(u_{th}) - a_4^{(2)}(1;0)\delta a_2^{(1)}(0) + \int_0^{u_{th}} \delta a_2^{(1)}(u)\left[-da_4^{(2)}(1;u)/du + f_1 a_4^{(2)}(1;u)\right] du. \tag{65}$$

The right side of Equation 65 is now tailored to represent the G-differential $\left\{\delta R^{(1)}\left[1;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})\right]\right\}_{\boldsymbol{\alpha}^0}$ expressed by Equation 58 by requiring the second-level adjoint sensitivity function $\mathbf{a}^{(2)}(2^2;1;u)$ to be the solution of the following 2nd-LASS:

$$\mathrm{j}\left\{\mathbf{A}^{(2)}\left[2^2\times 2^2;u;\mathbf{f}\right]\mathbf{a}^{(2)}(2^2;1;u)\right\}_{\boldsymbol{\alpha}^0} = \left\{\mathbf{s}^{(2)}(2^2;1;u;\mathbf{f})\right\}_{\boldsymbol{\alpha}^0}, \tag{66}$$
$$\left\{\mathbf{b}_A^{(2)}(u;\mathbf{f})\right\}_{\boldsymbol{\alpha}^0} = \mathbf{0}, \tag{67}$$

where

$$\mathbf{A}^{(2)}\left[2^2\times 2^2;u;\mathbf{f}\right] \triangleq \begin{pmatrix} -d/du + f_1 & 0 & 0 & -1 \\ 0 & d/du + f_1 & -1 & 0 \\ 0 & 0 & d/du + f_1 & 0 \\ 0 & 0 & 0 & -d/du + f_1 \end{pmatrix}; \tag{68}$$

$$\mathbf{s}^{(2)}(2^2;1;u;\mathbf{f}) \triangleq \begin{pmatrix} -a_1^{(1)}(u) \\ -a_2^{(1)}(u) \\ -\varphi(u) \\ -\psi(u) \end{pmatrix}; \quad \mathbf{b}_A^{(2)}(u;\mathbf{f}) \triangleq \begin{pmatrix} a_1^{(2)}(1;u_{th}) \\ a_2^{(2)}(1;0) \\ a_3^{(2)}(1;0) \\ a_4^{(2)}(1;u_{th}) \end{pmatrix}. \tag{69}$$

Implementing the equations underlying the 2nd-LVSS and the 2nd-LASS and substituting Equation 58 into Equation 64 provide the following alternative expression for the G-differential $\left\{\delta R^{(1)}\left[1;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})\right]\right\}_{\boldsymbol{\alpha}^0}$:

$$\left\{\delta R^{(1)}\left[1;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})\right]\right\}_{\boldsymbol{\alpha}^0} = \left\{\int_0^{u_{th}} a_1^{(2)}(1;u)\left[(\delta f_2)\delta(u) - (\delta f_1)\varphi(u)\right] du\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_0^{u_{th}} a_2^{(2)}(1;u)\left[-(\delta f_1)\psi(u)\right] du\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_0^{u_{th}} a_3^{(2)}(1;u)\left[-(\delta f_1)a_1^{(1)}(u)\right] du\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_0^{u_{th}} a_4^{(2)}(1;u)\left[-(\delta f_1)a_2^{(1)}(u)\right] du\right\}_{\boldsymbol{\alpha}^0}. \tag{70}$$

The expressions that multiply the respective components of $\mathbf{f}(\boldsymbol{\alpha})$ in Equation 70 are the expressions of the second-order sensitivities $\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_j$ (stemming from the first-order sensitivity $\partial R_c/\partial f_1$) of the response $R_c(\varphi,\psi)$, with respect to the components of the feature function $\mathbf{f}(\boldsymbol{\alpha})$. Thus, identifying in Equation 70 the expressions that multiply the respective variations in the components of the feature function $\mathbf{f}(\boldsymbol{\alpha})$ yields the following relations:

$$\frac{\partial^2 R_c(\varphi,\psi)}{\partial f_1 \partial f_1} = -\int_0^{u_{th}} a_1^{(2)}(1;u)\varphi(u)\, du - \int_0^{u_{th}} a_2^{(2)}(1;u)\psi(u)\, du - \int_0^{u_{th}} a_3^{(2)}(1;u)\, a_1^{(1)}(u)\, du - \int_0^{u_{th}} a_4^{(2)}(1;u)\, a_2^{(1)}(u)\, du; \tag{71}$$

$$\frac{\partial R_c(\varphi,\psi)}{\partial f_2 \partial f_1} = \int_0^{u_{th}} a_1^{(2)}(1;u)\delta(u)\, du. \tag{72}$$

Solving the 2nd-LASS represented by Equations 66, 67 yields the following closed-form expressions for the components of the second-level adjoint sensitivity function $\mathbf{a}^{(2)}(2^2;1;u)$:

$$a_1^{(2)}(1;u) = -(u_d - u)^2 H(u_d - u)\exp\left[(u - u_d)f_1(\boldsymbol{\alpha})\right], \tag{73}$$
$$a_2^{(2)}(1;u) = -f_2(\boldsymbol{\alpha})u^2\exp\left[-u f_1(\boldsymbol{\alpha})\right], \tag{74}$$
$$a_3^{(2)}(1;u) = -f_2(\boldsymbol{\alpha})u\exp\left[-u f_1(\boldsymbol{\alpha})\right], \tag{75}$$
$$a_4^{(2)}(1;u) = -(u_d - u)H(u_d - u)\exp\left[(u - u_d)f_1(\boldsymbol{\alpha})\right]. \tag{76}$$

Using the explicit closed-form expressions obtained in Equations 73–76 and substituting them in Equations 71, 72 yield the following closed-form explicit expressions for the respective second-order sensitivities:

$$\frac{\partial^2 R_c(\varphi,\psi)}{\partial f_1 \partial f_1} = (u_d)^3 f_2(\boldsymbol{\alpha})\exp\left[-u_d f_1(\boldsymbol{\alpha})\right], \tag{77}$$
$$\frac{\partial R_c(\varphi,\psi)}{\partial f_2 \partial f_1} = -(u_d)^2\exp\left[-u_d f_1(\boldsymbol{\alpha})\right]. \tag{78}$$

The correctness of the expressions obtained in Equations 77, 78 can be verified by differentiating accordingly the closed-form expression given in Equation 53.

4.1.2 Second-order sensitivities stemming from the first-order sensitivity $\partial R_c/\partial f_2$

The second-order sensitivities that stem from the first-order sensitivity $\partial R_c/\partial f_2$ are obtained by determining the G-differential of $\partial R_c/\partial f_2$. For subsequent "bookkeeping" purposes, this first-order sensitivity will be denoted as $R^{(1)}[2;\mathbf{u}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})]\triangleq\partial R_c/\partial f_2$, where the superscript "(1)" denotes "*first-order*" (sensitivity) and the argument "2" indicates that this sensitivity is with respect to the *second component*, i.e., $f_2(\boldsymbol{\alpha})$, of the feature function $\mathbf{f}(\boldsymbol{\alpha})$. This sensitivity also depends on the function $\mathbf{u}^{(2)}(2^2;u)\triangleq[\mathbf{u}^{(1)}(2;u),\mathbf{a}^{(1)}(2;u)]^{\dagger}$. Applying the definition of the G-differential to the expression provided in Equation 49 yields the result below for the G-differential $\{\delta R^{(1)}[2;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$:

$$\left\{\delta R^{(1)}\left[2;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})\right]\right\}_{\boldsymbol{\alpha}^0} = \int_0^{u_{th}}\delta a_1^{(1)}(u)\delta(u)\,du \equiv \sum_{j=1}^{2}\frac{\partial^2 R(\varphi;\mathbf{f})}{\partial f_j\partial f_2}\left(\delta f_j\right). \quad (79)$$

The function $\delta a_1^{(1)}(u)$, as shown in Equation 79, is the component of the second-level variational sensitivity function $\mathbf{v}^{(2)}(2^2;u)\triangleq[v^{(1)}(u),\delta\psi(u),\delta a_1^{(1)}(u),\delta a_2^{(1)}(u)]^{\dagger}$, which is the solution of the 2nd-LVSS comprising Equations 59, 60. The component $\delta a_1^{(1)}(u)$ will be eliminated from the expression of $\{\delta R^{(1)}[2;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$ by following the same procedure as described in Section 4.1.1 to construct a 2nd-LASS, the solution of which will be denoted as $\mathbf{a}^{(2)}(2^2;2;u)\triangleq[a_1^{(2)}(2;u),a_2^{(2)}(2;u),a_3^{(2)}(2;u),a_4^{(2)}(2;u)]^{\dagger}\in\mathcal{H}_2$ and will be used in Equation 79 to eliminate $\delta a_1^{(1)}(u)$. The argument "2" in $\mathbf{a}^{(2)}(2^2;2;u)$ indicates that this second-level adjoint sensitivity function corresponds to the first-order sensitivity of the response with respect to the "*second*" component, $f_2(\boldsymbol{\alpha})$, of the feature function $\mathbf{f}(\boldsymbol{\alpha})$. The 2nd-LASS for the function $\mathbf{a}^{(2)}(2^2;2;u)$ will have the same left side and boundary conditions as obtained in Equations 66, 67, but the right-side of this 2nd-LASS will correspond to the G-differential obtained in Equation 79, which leads to the following 2nd-LASS:

$$\left\{\mathbf{A}^{(2)}[2^2\times 2^2;u;\mathbf{f}]\mathbf{a}^{(2)}(2^2;2;u)\right\}_{\boldsymbol{\alpha}^0} = \left\{\mathbf{s}^{(2)}(2^2;2;u;\mathbf{f})\right\}_{\boldsymbol{\alpha}^0}, \quad (80)$$

$$\left\{\mathbf{b}_A^{(2)}(u;\mathbf{f})\right\}_{\boldsymbol{\alpha}^0} = \mathbf{0}, \quad (81)$$

where

$$\mathbf{s}^{(2)}(2^2;1;u;\mathbf{f})\triangleq[0,0,\delta(u),0]^{\dagger}. \quad (82)$$

The alternative expression for the G-differential $\{\delta R^{(1)}[2;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$ in terms of the components of $\mathbf{a}^{(2)}(2^2;2;u)$ has the same formal expression as shown in Equation 70 but with the components of the function $\mathbf{a}^{(2)}(2^2;1;u)$ being replaced by the components of $\mathbf{a}^{(2)}(2^2;2;u)$, i.e.,:

$$\begin{aligned}\delta(\partial R_c/\partial f_2) &= \int_0^{u_{th}} a_1^{(2)}(2;u)\left[(\delta f_2)\delta(u)-(\delta f_1)\varphi(u)\right]du \\ &+ \int_0^{u_{th}} a_2^{(2)}(2;u)\left[-(\delta f_1)\psi(u)\right]du \\ &+ \int_0^{u_{th}} a_3^{(2)}(2;u)\left[-(\delta f_1)a_1^{(1)}(u)\right]du \\ &+ \int_0^{u_{th}} a_4^{(2)}(2;u)\left[-(\delta f_1)a_2^{(1)}(u)\right]du.\end{aligned} \quad (83)$$

Solving the 2nd-LASS represented by Equations 80, 81 yields the following expressions:

$$a_1^{(2)}(2;u)=0, \quad (84)$$

$$a_2^{(2)}(2;u)=u\exp[-uf_1(\boldsymbol{\alpha})], \quad (85)$$

$$a_3^{(2)}(2;u)=H(u)\exp[-uf_1(\boldsymbol{\alpha})], \quad (86)$$

$$a_4^{(2)}(2;u)=0. \quad (87)$$

Identifying in Equation 83 the expressions that multiply the respective variations δf_i, $i=1,2$, in the components of the feature function $\mathbf{f}(\boldsymbol{\alpha})$ and using the closed-form expressions obtained in Equations 84–87, 26, 51 yield the following closed-form explicit expressions for the respective second-order sensitivities:

$$\begin{aligned}\frac{\partial^2 R_c(\varphi,\psi)}{\partial f_1\partial f_2} &= -\int_0^{u_{th}} a_2^{(2)}(2;u)\psi(u)\,du - \int_0^{u_{th}} a_3^{(2)}(2;u)a_1^{(1)}(u)\,du \\ &= -(u_d)^2\exp[-u_d f_1(\boldsymbol{\alpha})],\end{aligned} \quad (88)$$

$$\frac{\partial R_c(\varphi,\psi)}{\partial f_2\partial f_2}=0. \quad (89)$$

The correctness of the expressions obtained in Equations 88, 89 can be verified by differentiating accordingly the closed-form expression given in Equation 54.

Notably, due to the symmetry of the mixed second-order sensitivities, the expressions obtained in Equations 88, 72 provide an intrinsic mutual verification mechanism of the accuracy of the computations of the second-level adjoint sensitivity functions $\mathbf{a}^{(2)}(2^2;1;u)$ and $\mathbf{a}^{(2)}(2^2;2;u)$.

4.2 Application of the 2nd-CASAM-L

The starting point for the application of the 2nd-CASAM-L is to determine the G-differential of the *TP* first-order sensitivities represented by Equation 57. For "bookkeeping" purposes, it is convenient to designate these *TP* first-order sensitivities as follows:

$$\begin{aligned}R_c^{(1)}\left[i;\mathbf{u}^{(2)}(2^2;u);\boldsymbol{\alpha}\right] &\triangleq \partial R_c(\varphi,\psi)/\partial\alpha_i \\ &= -g_1(i;\boldsymbol{\alpha})\int_0^{u_{th}}\left[a_1^{(1)}(u)\varphi(u)+a_2^{(1)}(u)\psi(u)\right]du \\ &+ g_2(i;\boldsymbol{\alpha})\int_0^{u_{th}} a_1^{(1)}(u)\,\delta(u)\,du,\end{aligned} \quad (90)$$

where

$$g_1(i;\boldsymbol{\alpha})\triangleq\partial f_1/\partial\alpha_i;\quad g_2(i;\boldsymbol{\alpha})\triangleq\partial f_2/\partial\alpha_i;\quad i=1,\ldots,TP. \quad (91)$$

The G-differential of the expression in Equation 90 is obtained, by definition, as follows:

$$\begin{aligned}&\{\delta R_c^{(1)}[i;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\}_{\boldsymbol{\alpha}^0} \\ &\triangleq -\left\{\int_0^{u_{th}}\left[a_1^{(1)}(u)\varphi(u)+a_2^{(1)}(u)\psi(u)\right]du\left[\tfrac{d}{d\varepsilon}g_1(i;\boldsymbol{\alpha}+\varepsilon\delta\boldsymbol{\alpha})\right]\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\ &\quad -\left\{g_1(i;\boldsymbol{\alpha})\tfrac{d}{d\varepsilon}\int_0^{u_{th}}\left[\left[a_1^{(1)}(u)+\varepsilon\delta a_1^{(1)}(u)\right]\left[\varphi(u)+\varepsilon v^{(1)}(u)\right]\right]du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\ &\quad -\left\{g_1(i;\boldsymbol{\alpha})\tfrac{d}{d\varepsilon}\int_0^{u_{th}}\left[a_2^{(1)}(u)+\varepsilon\delta a_2^{(1)}(u)\right]\left[\psi(u)+\varepsilon\delta\psi(u)\right]du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\ &\quad +\left\{\int_0^{u_{th}} a_1^{(1)}(u)\,\delta(u)\,du\left[\tfrac{d}{d\varepsilon}g_2(i;\boldsymbol{\alpha}+\varepsilon\delta\boldsymbol{\alpha})\right]\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\ &\quad +\left\{g_2(i;\boldsymbol{\alpha})\tfrac{d}{d\varepsilon}\int_0^{u_{th}}\left[a_1^{(1)}(u)+\varepsilon\delta a_1^{(1)}(u)\right]\delta(u)\,du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\ &\triangleq \{\delta R_c^{(1)}[i;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\boldsymbol{\alpha}]\}_{ind}+\{\delta R_c^{(1)}[i;\mathbf{u}^{(2)}(2^2;u);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\}_{dir},\end{aligned} \quad (92)$$

where the direct-effect and indirect-effect terms are defined, respectively, as follows:

$$\{\delta R_c^{(1)}[i;\mathbf{u}^{(2)}(2^2;u);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\}_{dir} \triangleq \left\{\left[\sum_{j=1}^{TP}\frac{\partial g_2(i;\boldsymbol{\alpha})}{\partial\alpha_j}\delta\alpha_j\right]\int_0^{u_{th}} a_1^{(1)}(u)\,\delta(u)\,du\right\}_{\boldsymbol{\alpha}^0} - \left\{\left[\sum_{j=1}^{TP}\frac{\partial g_1(i;\boldsymbol{\alpha})}{\partial\alpha_j}\delta\alpha_j\right]\int_0^{u_{th}}\left[a_1^{(1)}(u)\varphi(u)+a_2^{(1)}(u)\psi(u)\right]du\right\}_{\boldsymbol{\alpha}^0}, \tag{93}$$

$$\{\delta R_c^{(1)}[i;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\boldsymbol{\alpha}]\}_{ind} \triangleq \left\{g_2(i;\boldsymbol{\alpha})\int_0^{u_{th}}\delta a_1^{(1)}(u)\,\delta(u)\,du\right\}_{\boldsymbol{\alpha}^0} - \left\{g_1(i;\boldsymbol{\alpha})\int_0^{u_{th}}\left[a_1^{(1)}(u)v^{(1)}(u)+\varphi(u)\delta a_1^{(1)}(u)\right]du\right\}_{\boldsymbol{\alpha}^0} - \left\{g_1(i;\boldsymbol{\alpha})\int_0^{u_{th}}\left[a_2^{(1)}(u)\delta\psi(u)+\psi(u)\delta a_2^{(1)}(u)\right]du\right\}_{\boldsymbol{\alpha}^0}. \tag{94}$$

The direct-effect term can be evaluated/computed already at this stage. On the other hand, the indirect-effect depends on the second-level variational function $\mathbf{v}^{(2)}(2^2;u) \triangleq [v^{(1)}(u),\delta\psi(u),\delta a_1^{(1)}(u),\delta a_2^{(1)}(u)]^\dagger$, which is the solution of the counterpart of 2nd-LVSS defined by Equations 59, 60, with the same boundary conditions and right-side but with distinct source terms, each source term involving the quantities $\partial g_1(i;\boldsymbol{\alpha})/\partial\alpha_j$ and $\partial g_2(i;\boldsymbol{\alpha})/\partial\alpha_j$ for $i,j=1,...,TP$. If this path were chosen to compute the second-order sensitivities, the 2nd-LVSS would need to be solved TP^2 times, with TP^2 different sources on the respective right sides, albeit with the same left side and boundary conditions.

The components $v^{(1)}(u),\delta\psi(u),\delta a_1^{(1)}(u),\delta a_2^{(1)}(u)$ are eliminated from the expression of the indirect-effect term $\{\delta R_c^{(1)}[i;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\boldsymbol{\alpha}]\}_{ind}$ defined in Equation 94 by constructing a corresponding 2nd-LASS in the Hilbert space H_2 by following the same sequence of steps as described in Section 4.1. The formal expression of the 2nd-LASS thus obtained will have the same left side and boundary conditions as those described in Section 4.1, but the right side of this formal 2nd-LASS will have a source term that will correspond to the indirect-effect term defined in Equation 94 and, hence, will be different for each $i=1,...,TP$, i.e.,

$$\{\mathbf{A}^{(2)}[2^2\times 2^2;u;\boldsymbol{\alpha}]\mathbf{a}^{(2)}(2^2;i;2;u)\}_{\boldsymbol{\alpha}^0} = \{\mathbf{s}^{(2)}(2^2;i;u;\boldsymbol{\alpha})\}_{\boldsymbol{\alpha}^0},\quad i=1,...,TP; \tag{95}$$

$$\left\{\mathbf{b}_A^{(2)}(u;\boldsymbol{\alpha})\right\}_{\boldsymbol{\alpha}^0} = \mathbf{0};\quad i=1,...,TP; \tag{96}$$

where

$$\mathbf{s}^{(2)}(2^2;i;u;\boldsymbol{\alpha}) \triangleq \left[-g_1(i;\boldsymbol{\alpha})a_1^{(1)},-g_1(i;\boldsymbol{\alpha})a_2^{(1)},\; g_2(i;\boldsymbol{\alpha})\delta(u)-g_1(i;\boldsymbol{\alpha})\varphi,-g_1(i;\boldsymbol{\alpha})\psi\right]^\dagger. \tag{97}$$

In terms of the solution $\mathbf{a}^{(2)}(2^2;i;2;u)$ of the 2nd-LASS represented by Equations 95, 96, the indirect-effect term $\{\delta R_c^{(1)}[i;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\boldsymbol{\alpha}]\}_{ind}$ defined in Equation 94 will have a representation that will formally resemble the expressions provided in Section 4.1, e.g., Equation 83, but with the second-level adjoint function(s) from Section 4.1 being replaced by the second-level adjoint sensitivity function $\mathbf{a}^{(2)}(2^2;i;2;u)$. Finally, the total G-differential $\{\delta R_c^{(1)}[i;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\}_{\boldsymbol{\alpha}^0}$ will be obtained, as shown in Equation 92, by adding the expression of the indirect-effect term obtained in terms of the second-level adjoint sensitivity function $\mathbf{a}^{(2)}(2^2;i;2;u)$ and the expression of the direct-effect term provided in Equation 93. The expression of the individual second-order sensitivities $\partial^2 R_c(\varphi,\psi)/\partial\alpha_i\partial\alpha_j$, $i,j=1,...,TP$ will subsequently be obtained by identifying in the final expression of the total G-differential $\{\delta R_c^{(1)}[i;\mathbf{u}^{(2)}(2^2;u);\mathbf{v}^{(2)}(2^2;u);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\}_{\boldsymbol{\alpha}^0}$ those terms that multiply the parameter variations $\partial\alpha_j$, $j=1,...,TP$.

4.2.1 Comparing the 2nd-FASAM-L *versus* the 2nd-CASAM-L

The computational savings provided by using, whenever possible, the 2nd-FASAM-L rather than the 2nd-CASAM-L are evident by comparing the results obtained in Section 4.1 *versus* the results obtained in Section 4.2. The feature function $\mathbf{f}(\boldsymbol{\alpha})$ comprises two components $f_i(\boldsymbol{\alpha})$, $i=1,2$; consequently, the 2nd-FASAM-L requires two large-scale computations (to solve the corresponding 2nd-LASS) to obtain the second-order response sensitivities with respect to the components of the feature function. Subsequently, the second-order response sensitivities with respect to the primary model parameters are obtained analytically using the chain-rule of differentiation.

In contradistinction, there is $TP \triangleq 3M+10$, where the number (M) of materials in the medium can easily exceed two dozen primary model parameters. Consequently, the 2nd-CASAM-L requires TP large-scale computations (to solve the corresponding 2nd-LASS) to obtain the second-order response sensitivities with respect to the primary model parameters. The boundary conditions and the operators on the left sides for all of the 2nd-LASS, for both the 2nd-FASAM-L and 2nd-CASAM-L, are the same; only the source terms on the left sides of these 2nd-LASS differ from each other. It is therefore computationally advantageous if the inverse operators of the left sides of these 2nd-LASS could be computed just once and stored for subsequent use, in which case the computational advantage of using the 2nd-FASAM-L would not be massive. Such a procedure could be feasible for relatively small models but would be impractical for large-scale problems, for which the advantage of using the 2nd-FASAM-L rather than the 2nd-CASAM-L increases as the number of model parameters increases.

5 Third-order adjoint sensitivity analysis of the contributon flux to the slowing-down model's features and parameters

The 3rd-FASAM-L determines the third-order sensitivities by applying the principles of the 1st-FASAM to the second-order sensitivities, i.e., considering that the third-order sensitivities are "the first-order sensitivities of the second-order sensitivities." The unmixed second-order sensitivity $\partial^2 R_c(\varphi,\psi)/\partial f_2\partial f_2$ is identically zero. The two non-zero second-order sensitivities of the model response with respect to the components of the feature function $\mathbf{f}(\boldsymbol{\alpha})$ are as follows: (i) the unmixed second-order sensitivity $\partial^2 R_c(\varphi,\psi)/\partial f_1\partial f_1$, expressed in Equation 71, and (ii) the mixed second-order sensitivity $\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_2 = \partial^2 R_c(\varphi,\psi)/\partial f_2 \partial f_1$, expressed in either Equation 72 or Equation 88, which are equivalent, in view of the symmetry property of the mixed second-order sensitivities. Therefore, either the expression obtained in Equation 88 or Equation 72 can be used as the starting point for obtaining the third-order sensitivities stemming from this mixed second-order sensitivity. It appears that the expression provided in Equation 72 is the simpler of the two, so it will be used as the starting point for obtaining the corresponding third-order sensitivities.

The second-order sensitivity $\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_1$ expressed in Equation 71 depends on the components of the third-level forward/adjoint function, denoted as $\mathbf{u}^{(3)}(2^3;1;1;u) = [\mathbf{u}^{(2)}(2^2;u), \mathbf{a}^{(2)}(2^2;1;u)]^\dagger$, which is the solution of the third-level forward/adjoint system (3rd-LFAS) obtained by concatenating the 2nd-LFAS with the 2nd-LASS, thus comprising Equations 12, 13, 20, 21, 43, 44, 66 and 67. The argument "1;1" of $\mathbf{u}^{(3)}(2^3;1;1;u)$ indicates that this third-level function corresponds to the (unmixed) second-order sensitivity $\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_1$ of the response with respect to the "first" feature function, f_1. Therefore, the second-order sensitivity $\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_1$ is denoted as follows: $R^{(2)}[1;1;\mathbf{u}^{(3)};\mathbf{f}(\boldsymbol{\alpha})] \triangleq \partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_1$, where the argument "1;1" indicates that this third-level function corresponds to the (unmixed) second-order sensitivity $\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_1$ and the arguments of the function $\mathbf{u}^{(3)}(2^3;1;1;u)$ were omitted, for simplicity. Similarly, the mixed second-order sensitivity $\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_2$ depends on the components of the same function $\mathbf{u}^{(3)}(2^3;1;1;u)$ and will, therefore, be denoted as $R^{(2)}[2;1;\mathbf{u}^{(3)};\mathbf{f}(\boldsymbol{\alpha})] \triangleq \partial^2 R_c(\varphi,\psi)/\partial f_2 \partial f_1$, where the argument "2;1" indicates that this second-order sensitivity is with respect to the components (f_2, f_1) of $\mathbf{f}(\boldsymbol{\alpha})$.

5.1 Application of the 3rd-FASAM-L to compute the third-order sensitivities stemming from $\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_1$

The third-order sensitivities stemming from $R^{(2)}[1;1;\mathbf{u}^{(3)};\mathbf{f}(\boldsymbol{\alpha})] \triangleq \partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_1$ are obtained from the G-differential of Equation 71, which will be denoted as $\{\delta R^{(2)}[1;1;\mathbf{u}^{(3)};\mathbf{v}^{(3)};\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0} \triangleq \{\delta[\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_1]\}_{\boldsymbol{\alpha}^0}$, and they are, by definition, determined as follows:

$$\begin{aligned}
&\{\delta R^{(2)}[1;1;\mathbf{u}^{(3)};\mathbf{v}^{(3)};\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0} \\
&\triangleq -\left\{\frac{d}{d\varepsilon}\int_0^{u_{th}}\left[a_1^{(2)}(1;u)+\varepsilon\delta a_1^{(2)}(1;u)\right]\left[\varphi(u)+\varepsilon v^{(1)}(u)\right]du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\
&\quad -\left\{\frac{d}{d\varepsilon}\int_0^{u_{th}}\left[a_2^{(2)}(1;u)+\varepsilon\delta a_2^{(2)}(1;u)\right]\left[\psi(u)+\varepsilon\delta\psi(u)\right]du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\
&\quad -\left\{\frac{d}{d\varepsilon}\int_0^{u_{th}}\left[a_3^{(2)}(1;u)+\varepsilon\delta a_3^{(2)}(1;u)\right]\left[a_1^{(1)}(u)+\varepsilon\delta a_1^{(1)}(u)\right]du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\
&\quad -\left\{\frac{d}{d\varepsilon}\int_0^{u_{th}}\left[a_4^{(2)}(1;u)+\varepsilon\delta a_4^{(2)}(1;u)\right]\left[a_2^{(1)}(u)+\varepsilon\delta a_2^{(1)}(u)\right]du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0}.
\end{aligned} \tag{98}$$

Performing the differentiation with respect to ε in Equation 98 and setting $\varepsilon = 0$ in the resulting expression yield

$$\begin{aligned}
&\left\{\delta R^{(2)}\left[1;1;\mathbf{u}^{(3)};\mathbf{v}^{(3)};\mathbf{f}(\boldsymbol{\alpha})\right]\right\}_{\boldsymbol{\alpha}^0} \\
&= -\left\{\int_0^{u_{th}}\left[a_1^{(2)}(1;u)v^{(1)}(u)+\varphi(u)\delta a_1^{(2)}(1;u)\right]du\right\}_{\boldsymbol{\alpha}^0} \\
&\quad -\left\{\int_0^{u_{th}}\left[a_2^{(2)}(1;u)\delta\psi(u)+\psi(u)\delta a_2^{(2)}(1;u)\right]du\right\}_{\boldsymbol{\alpha}^0} \\
&\quad -\left\{\int_0^{u_{th}}\left[a_3^{(2)}(1;u)\delta a_1^{(1)}(u)+a_1^{(1)}(u)\delta a_3^{(2)}(1;u)\right]du\right\}_{\boldsymbol{\alpha}^0} \\
&\quad -\left\{\int_0^{u_{th}}\left[a_4^{(2)}(1;u)\delta a_2^{(1)}(u)+a_2^{(1)}(u)\delta a_4^{(2)}(1;u)\right]du\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned} \tag{99}$$

The third-level variational function $\mathbf{v}^{(3)} \triangleq \mathbf{v}^{(3)}(2^3;1;1;u) \triangleq [\mathbf{v}^{(2)}(2^2;u), \delta\mathbf{a}^{(2)}(2^2;1;u)]^\dagger$, where $\delta\mathbf{a}^{(2)}(2^2;1;u) \triangleq [\delta a_1^{(2)}(1;u), \delta a_2^{(2)}(1;u), \delta a_3^{(2)}(1;u), \delta a_4^{(2)}(1;u)]^\dagger$, is the solution of the 3rd-LVSS obtained by concatenating the 2nd-LVSS (i.e., Equations 59, 60), with the equations obtained by G-differentiating the 2nd-LASS, represented by Equations 66, 67, for the function $\mathbf{a}^{(2)}(2^2;1;u)$. The resulting 3rd-LVSS for the third-level variational function $\mathbf{v}^{(3)}(2^3;1;1;u)$ comprises the following matrix equation, where the dots are used to denote zero-elements for better visibility of the structure:

$$\begin{pmatrix}
L & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & M & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & -1 & M & \cdot & \cdot & \cdot & \cdot & \cdot \\
-1 & \cdot & \cdot & L & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & M & \cdot & \cdot & -1 \\
\cdot & \cdot & \cdot & 1 & \cdot & L & -1 & \cdot \\
1 & \cdot & \cdot & \cdot & \cdot & \cdot & L & \cdot \\
\cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & M
\end{pmatrix}
\begin{pmatrix}
v^{(1)}(u) \\ \delta\psi(u) \\ \delta a_1^{(1)}(u) \\ \delta a_2^{(1)}(u) \\ \delta a_1^{(2)}(1;u) \\ \delta a_2^{(2)}(1;u) \\ \delta a_3^{(2)}(1;u) \\ \delta a_4^{(2)}(1;u)
\end{pmatrix}
=
\begin{pmatrix}
(\delta f_2)\delta(u) - (\delta f_1)\varphi(u) \\ -(\delta f_1)\psi(u) \\ -(\delta f_1)a_1^{(1)}(u) \\ -(\delta f_1)a_2^{(1)}(u) \\ -(\delta f_1)a_1^{(2)}(1;u) \\ -(\delta f_1)a_2^{(2)}(1;u) \\ -(\delta f_1)a_3^{(2)}(1;u) \\ -(\delta f_1)a_4^{(2)}(1;u)
\end{pmatrix},$$

$$L(u) \triangleq \frac{d}{du} + f_1(\boldsymbol{\alpha}); \quad M(u) \triangleq -\frac{d}{du} + f_1(\boldsymbol{\alpha}); \quad M(u) = L^*(u); \tag{100}$$

$$v^{(1)}(0) = 0;\ \delta\psi(u_{th}) = 0;\ \delta a_1^{(1)}(u_{th}) = 0;\ \delta a_2^{(1)}(0) = 0; \delta a_1^{(2)}(1;u_{th}) = 0;\ \delta a_2^{(2)}(1;0) = 0;\ \delta a_3^{(2)}(1;0) = 0;\ \delta a_4^{(2)}(1;u_{th}) = 0. \tag{101}$$

The 3rd-LVSS comprising Equations 100, 101 can be formally expressed in the following $2^3 \times 2^3$-matrix form:

$$\mathbf{V}^{(3)}[2^3 \times 2^3;u;\mathbf{f}]\mathbf{v}^{(3)}(2^3;1;1;u) = \mathbf{q}_V^{(3)}\left[2^3;\mathbf{u}^{(3)}(2^3;u);\mathbf{f};\delta\mathbf{f}\right], \tag{102}$$

$$\mathbf{b}_v^{(3)}\left[\mathbf{v}^{(3)}(2^3;1;1;u)\right] = \mathbf{0}. \tag{103}$$

The above matrix form of the 3rd-LVSS will be used as a "condensed notation" to construct the 3rd-LASS, the solution of which will be used to derive the alternative expression for the G-differential $\{\delta R^{(2)}[1;1;\mathbf{u}^{(3)}(2^3;1;1;u);\mathbf{v}^{(3)}(2^3;1;1;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$. This 3rd-

LASS will be constructed in a Hilbert space denoted as H_3, comprising as elements eight-component vector-valued functions of the form $\boldsymbol{\chi}^{(3)}(2^3;1;1;u) \triangleq [\chi_1^{(2)}(1;1;u),...,\chi_8^{(2)}(1;1;u)]^\dagger \in \mathcal{H}_3$, and endowed with the following inner product between two vectors $\boldsymbol{\chi}^{(3)}(2^3;1;1;u)$ and $\boldsymbol{\theta}^{(3)}(2^3;1;1;u)$:

$$\langle \boldsymbol{\chi}^{(3)}(2^3;1;1;u), \boldsymbol{\theta}^{(3)}(2^3;1;1;u)\rangle_3 \triangleq \sum_{i=1}^{2^3}\int_0^{u_{th}} \chi_i^{(3)}(1;1;u)\theta_i^{(3)}(1;1;u)\,du\,. \tag{104}$$

The inner product defined in Equation 104 will be used to construct the inner product of Equation 102 with a function denoted as $\mathbf{a}^{(3)}(2^3;1;1;u) \triangleq [a_1^{(3)}(1;1;u),...,a_8^{(3)}(1;1;u)]^\dagger \in \mathcal{H}_3$, where the argument "1,1" of the function indicates that this (third-level adjoint) function corresponds to the unmixed second-order sensitivity of the response with respect to the "*first*" component, $f_1(\boldsymbol{\alpha})$, of the feature function $\mathbf{f}(\boldsymbol{\alpha})$. Constructing this inner product yields the following relation, where the specification $\{\}_{\boldsymbol{\alpha}^0}$ has been omitted to simplify the notation:

$$\begin{aligned}
&\int_0^{u_{th}} a_1^{(3)}(1;1;u)\left[\frac{d}{du}v^{(1)}(u)+f_1v^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_2^{(3)}(1;1;u)\left[-\frac{d}{du}\delta\psi(u)+f_1\delta\psi(u)\right]du \\
&+\int_0^{u_{th}} a_3^{(3)}(1;1;u)\left[-\delta\psi(u)-\frac{d}{du}\delta a_1^{(1)}(u)+f_1\delta a_1^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_4^{(3)}(1;1;u)\left[-v^{(1)}(u)+\frac{d}{du}\delta a_2^{(1)}(u)+f_1\delta a_2^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_5^{(3)}(1;1;u)\left[-\frac{d}{du}\delta a_1^{(2)}(1;u)+f_1\delta a_1^{(2)}(1;u)-\delta a_4^{(2)}(u)+\delta a_1^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_6^{(3)}(1;1;u)\left[\frac{d}{du}\delta a_2^{(2)}(1;u)+f_1\delta a_2^{(2)}(1;u)-\delta a_3^{(2)}(u)+\delta a_2^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_7^{(3)}(1;1;u)\left[\frac{d}{du}\delta a_3^{(2)}(1;u)+f_1\delta a_3^{(2)}(1;u)+v^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_8^{(3)}(1;1;u)\left[-\frac{d}{du}\delta a_4^{(2)}(1;u)+f_1\delta a_4^{(2)}(1;u)+\delta\psi(u)\right]du \\
=&\int_0^{u_{th}} a_1^{(3)}(1;1;u)[(\delta f_2)\delta(u)-(\delta f_1)\varphi(u)]du \\
&+\int_0^{u_{th}} a_2^{(3)}(1;1;u)[-(\delta f_1)\psi(u)]du \\
&+\int_0^{u_{th}} a_3^{(3)}(1;1;u)\left[-(\delta f_1)a_1^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_4^{(3)}(1;1;u)\left[-(\delta f_1)a_2^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_5^{(3)}(1;1;u)\left[-(\delta f_1)a_1^{(2)}(1;u)\right]du \\
&+\int_0^{u_{th}} a_6^{(3)}(1;1;u)\left[-(\delta f_1)a_2^{(2)}(1;u)\right]du \\
&+\int_0^{u_{th}} a_7^{(3)}(1;1;u)\left[-(\delta f_1)a_3^{(2)}(1;u)\right]du \\
&+\int_0^{u_{th}} a_8^{(3)}(1;1;u)\left[-(\delta f_1)a_4^{(2)}(1;u)\right]du\,.
\end{aligned} \tag{105}$$

The component for Equation 105 can be written as follows:

$$\begin{aligned}
&\langle \mathbf{a}^{(3)}(2^3;1;1;u), \mathbf{V}^{(3)}[2^3\times 2^3;u;\mathbf{f}]\mathbf{v}^{(3)}(2^3;1;1;u)\rangle_3 \\
&= \langle \mathbf{a}^{(3)}(2^3;1;1;u), \mathbf{q}_V^{(3)}[2^3;\mathbf{u}^{(3)}(2^3;u);\mathbf{f};\delta\mathbf{f}]\rangle_3.
\end{aligned} \tag{106}$$

The left side of Equation 106 is integrated by parts to obtain the relation given below, in which the argument "1;1" has been omitted when writing the components $a_i^{(3)}(1;1;u), i=1,...,8$ to simplify the notation:

$$\begin{aligned}
&\int_0^{u_{th}} a_1^{(3)}(u)\left[\frac{d}{du}v^{(1)}(u)+f_1v^{(1)}(u)\right]du+\int_0^{u_{th}} a_2^{(3)}(u)\left[-\frac{d}{du}\delta\psi(u)+f_1\delta\psi(u)\right]du \\
&+\int_0^{u_{th}} a_3^{(3)}(u)\left[-\delta\psi(u)-\frac{d}{du}\delta a_1^{(1)}(u)+f_1\delta a_1^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_4^{(3)}(u)\left[-v^{(1)}(u)+\frac{d}{du}\delta a_2^{(1)}(u)+f_1\delta a_2^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_5^{(3)}(u)\left[-\frac{d}{du}\delta a_1^{(2)}(1;u)+f_1\delta a_1^{(2)}(1;u)-\delta a_4^{(2)}(u)+\delta a_1^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_6^{(3)}(u)\left[\frac{d}{du}\delta a_2^{(2)}(1;u)+f_1\delta a_2^{(2)}(1;u)-\delta a_3^{(2)}(u)+\delta a_2^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_7^{(3)}(u)\left[\frac{d}{du}\delta a_3^{(2)}(1;u)+f_1\delta a_3^{(2)}(1;u)+v^{(1)}(u)\right]du \\
&+\int_0^{u_{th}} a_8^{(3)}(u)\left[-\frac{d}{du}\delta a_4^{(2)}(1;u)+f_1\delta a_4^{(2)}(1;u)+\delta\psi(u)\right]du \\
=& a_1^{(3)}(u_{th})v^{(1)}(u_{th})-a_1^{(3)}(0)v^{(1)}(0)+\int_0^{u_{th}} v^{(1)}(u)\left[-\frac{d}{du}a_1^{(3)}(u)+f_1a_1^{(3)}(u)\right]du \\
&-a_2^{(3)}(u_{th})\delta\psi(u_{th})+a_2^{(3)}(0)\delta\psi(0)+\int_0^{u_{th}}\delta\psi(u)\left[\frac{d}{du}a_2^{(3)}(u)+f_1a_2^{(3)}(u)\right]du \\
&-a_3^{(3)}(u_{th})\delta a_1^{(1)}(u_{th})+a_3^{(3)}(0)\delta a_1^{(1)}(0)+\int_0^{u_{th}}\delta a_1^{(1)}(u)\left[\frac{d}{du}a_3^{(3)}(u)+f_1a_3^{(3)}(u)\right]du \\
&-\int_0^{u_{th}} a_3^{(3)}(u)\delta\psi(u)\,du-\int_0^{u_{th}} a_4^{(3)}(u)v^{(1)}(u)\,du \\
&+a_4^{(3)}(u_{th})\delta a_2^{(1)}(u_{th})-a_4^{(3)}(0)\delta a_2^{(1)}(0)+\int_0^{u_{th}}\delta a_2^{(1)}(u)\left[-\frac{d}{du}a_4^{(3)}(u)+f_1a_4^{(3)}(u)\right]du \\
&-a_5^{(3)}(u_{th})\delta a_1^{(2)}(1;u_{th})+a_5^{(3)}(0)\delta a_1^{(2)}(1;0)+\int_0^{u_{th}}\delta a_1^{(2)}(1;u)\left[\frac{d}{du}a_5^{(3)}(u)+f_1a_5^{(3)}(u)\right]du \\
&+\int_0^{u_{th}} a_5^{(3)}(u)\left[-\delta a_4^{(2)}(u)+\delta a_1^{(1)}(u)\right]du+a_6^{(3)}(u_{th})\delta a_2^{(2)}(1;u_{th})-a_6^{(3)}(0)\delta a_2^{(2)}(1;0) \\
&+\int_0^{u_{th}}\delta a_2^{(2)}(1;u)\left[\frac{d}{du}a_6^{(3)}(u)+f_1a_6^{(3)}(u)\right]du+\int_0^{u_{th}} a_6^{(3)}(u)\left[-\delta a_3^{(2)}(u)+\delta a_2^{(1)}(u)\right]du \\
&+a_7^{(3)}(u_{th})\delta a_3^{(2)}(1;u_{th})-a_7^{(3)}(0)\delta a_3^{(2)}(1;0)+\int_0^{u_{th}}\delta a_3^{(2)}(1;u)\left[-\frac{d}{du}a_7^{(3)}(u)+f_1a_7^{(3)}(u)\right]du \\
&+\int_0^{u_{th}} a_7^{(3)}(u)v^{(1)}(u)\,du-a_8^{(3)}(u_{th})\delta a_4^{(2)}(1;u_{th})+a_8^{(3)}(0)\delta a_4^{(2)}(1;0) \\
&+\int_0^{u_{th}}\delta a_4^{(2)}(1;u)\left[\frac{d}{du}a_8^{(3)}(u)+f_1a_8^{(3)}(u)\right]du+\int_0^{u_{th}} a_8^{(3)}(1;1;u)\delta\psi(u)\,du\,.
\end{aligned} \tag{107}$$

The boundary terms that appear in Equation 107 will vanish by using Equation 101 and imposing the following boundary conditions on the components $a_i^{(3)}(1;1;u), i=1,...,8$ of the third-level adjoint sensitivity function $\mathbf{a}^{(3)}(2^3;1;1;u)$:

$$a_1^{(3)}(1;1;u_{th})=0;\ a_2^{(3)}(1;1;0)=0;\quad a_3^{(3)}(1;1;0)=0;$$
$$a_4^{(3)}(1;1;u_{th})=0; a_5^{(3)}(1;1;0)=0;\ a_6^{(3)}(1;1;u_{th})=0; \tag{108}$$
$$a_7^{(3)}(1;1;u_{th})=0;\quad a_8^{(3)}(1;1;0)=0.$$

Equation 107 can be written in matrix form as follows:

$$\langle \mathbf{a}^{(3)}(2^3;1;1;u), \mathbf{V}^{(3)}[2^3\times 2^3;u;\mathbf{f}]\mathbf{v}^{(3)}(2^3;1;1;u)\rangle_3 = \langle \mathbf{v}^{(3)}(2^3;1;1;u), \mathbf{A}^{(3)}[2^3\times 2^3;u;\mathbf{f}]\mathbf{a}^{(3)}(2^3;1;1;u)\rangle_3, \tag{109}$$

where $\mathbf{A}^{(3)}[2^3\times 2^3;u;\mathbf{f}] \triangleq \{\mathbf{V}^{(3)}[2^3\times 2^3;u;\mathbf{f}]\}^*$ denotes the formal adjoint of $\mathbf{V}^{(3)}[2^3\times 2^3;u;\mathbf{f}]$. The right side of Equation 109 is now required to represent the G-differential $\{\delta R^{(2)}[1;1;\mathbf{u}^{(3)}(2^3;1;1;u);\mathbf{v}^{(3)}(2^3;1;1;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$ by imposing the following relation:

$$\mathbf{A}^{(3)}[2^3\times 2^3;u;\mathbf{f}]\mathbf{a}^{(3)}(2^3;1;1;u) = \mathbf{s}_A^{(3)}(2^3;1;1;\mathbf{f}), \tag{110}$$

where

$$\mathbf{s}_A^{(3)}(2^3;1;1;\mathbf{f}) \triangleq [a_1^{(2)}(1;u), a_2^{(2)}(1;u), a_3^{(2)}(1;u), a_4^{(2)}(1;u); \varphi(u), \psi(u), a_1^{(1)}(u), a_2^{(1)}(u)]^\dagger. \tag{111}$$

The relations provided in Equations 108, 110 constitute the 3rd-LASS for the third-level adjoint sensitivity function $\mathbf{a}^{(3)}(2^3;1;1;u)$. In component form, Equation 110 has the following expression, where the dots are used to denote zero-elements for better visibility of the structure:

$$\begin{pmatrix} M & \cdot & \cdot & -1 & \cdot & \cdot & 1 & \cdot \\ \cdot & L & -1 & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & L & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & M & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & L & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & M & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -1 & M & \cdot \\ \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & L \end{pmatrix} \begin{pmatrix} a_1^{(3)}(1;1;u) \\ a_2^{(3)}(1;1;u) \\ a_3^{(3)}(1;1;u) \\ a_4^{(3)}(1;1;u) \\ a_5^{(3)}(1;1;u) \\ a_6^{(3)}(1;1;u) \\ a_7^{(3)}(1;1;u) \\ a_8^{(3)}(1;1;u) \end{pmatrix} = \begin{pmatrix} -a_1^{(2)}(1;u) \\ -a_2^{(2)}(1;u) \\ -a_3^{(2)}(1;u) \\ -a_4^{(2)}(1;u) \\ -\varphi(u) \\ -\psi(u) \\ -a_1^{(1)}(u) \\ -a_2^{(1)}(u) \end{pmatrix}. \tag{112}$$

Using the relations in Equations 99, 102, 103, 108, 110 yields the following alternative expression for $\{\delta R^{(2)}[1;1;\mathbf{u}^{(3)}(2^3;1;1;u);\mathbf{v}^{(3)}(2^3;1;1;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$:

$$\begin{aligned}
&\{\delta R^{(2)}[1;1;\mathbf{u}^{(3)}(2^3;1;1;u);\mathbf{v}^{(3)}(2^3;1;1;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0} \\
&= \left\{\int_0^{u_{th}} a_1^{(3)}(1;1;u)[(\delta f_2)\delta(u)-(\delta f_1)\varphi(u)]\,du\right\}_{\boldsymbol{\alpha}^0} \\
&- \left\{\int_0^{u_{th}} a_2^{(3)}(1;1;u)(\delta f_1)\psi(u)\,du\right\}_{\boldsymbol{\alpha}^0} \\
&- \left\{\int_0^{u_{th}} a_3^{(3)}(1;1;u)(\delta f_1)a_1^{(1)}(u)\,du\right\}_{\boldsymbol{\alpha}^0} \\
&- \left\{\int_0^{u_{th}} a_4^{(3)}(1;1;u)(\delta f_1)a_2^{(1)}(u)\,du\right\}_{\boldsymbol{\alpha}^0} \\
&- \left\{\int_0^{u_{th}} a_5^{(3)}(1;1;u)(\delta f_1)a_1^{(2)}(1;u)\,du\right\}_{\boldsymbol{\alpha}^0} \\
&- \left\{\int_0^{u_{th}} a_6^{(3)}(1;1;u)(\delta f_1)a_2^{(2)}(1;u)\,du\right\}_{\boldsymbol{\alpha}^0} \\
&- \left\{\int_0^{u_{th}} a_7^{(3)}(1;1;u)(\delta f_1)a_3^{(2)}(1;u)\,du\right\}_{\boldsymbol{\alpha}^0} \\
&- \left\{\int_0^{u_{th}} a_8^{(3)}(1;1;u)(\delta f_1)a_4^{(2)}(1;u)\,du\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned} \tag{113}$$

The third-order sensitivities stemming from the relation obtained in Equation 113 are the expressions that multiply the respective variations δf_1 and δf_2 and are as follows:

$$\begin{aligned}
\partial^3 R_c(\varphi,\psi)/\partial f_1\partial f_1\partial f_1 = &-\int_0^{u_{th}} a_1^{(3)}(1;1;u)\varphi(u)\,du \\
&-\int_0^{u_{th}} a_2^{(3)}(1;1;u)\psi(u)\,du \\
&-\int_0^{u_{th}} a_3^{(3)}(1;1;u)a_1^{(1)}(u)\,du \\
&-\int_0^{u_{th}} a_4^{(3)}(1;1;u)a_2^{(1)}(u)\,du \\
&-\int_0^{u_{th}} a_5^{(3)}(1;1;u)a_1^{(2)}(1;u)\,du \\
&-\int_0^{u_{th}} a_6^{(3)}(1;1;u)a_2^{(2)}(1;u)\,du \\
&-\int_0^{u_{th}} a_7^{(3)}(1;1;u)a_3^{(2)}(1;u)\,du \\
&-\int_0^{u_{th}} a_8^{(3)}(1;1;u)a_4^{(2)}(1;u)\,du;
\end{aligned} \tag{114}$$

$$\partial^3 R_c(\varphi,\psi)/\partial f_1\partial f_1\partial f_2 = \int_0^{u_{th}} a_1^{(3)}(1;1;u)\delta(u)\,du. \tag{115}$$

The expressions obtained in Equations 114, 115 are to be evaluated at the nominal values of parameters and state functions, but the notation $\{\}_{\boldsymbol{\alpha}^0}$ has been omitted for simplicity.

Solving Equations 112, 108 yields the following expressions for the components of the third-level adjoint sensitivity function $\mathbf{a}^{(3)}(2^3;1;1;u)$:

$$a_1^{(3)}(1;1;u) = (u_d-u)^3 H(u_d-u)\exp[(u-u_d)f_1(\boldsymbol{\alpha})], \tag{116}$$
$$a_2^{(3)}(1;1;u) = f_2(\boldsymbol{\alpha})u^3\exp[-uf_1(\boldsymbol{\alpha})], \tag{117}$$
$$a_3^{(3)}(1;1;u) = f_2(\boldsymbol{\alpha})u^2\exp[-uf_1(\boldsymbol{\alpha})], \tag{118}$$
$$a_4^{(3)}(1;1;u) = (u_d-u)^2 H(u_d-u)\exp[(u-u_d)f_1(\boldsymbol{\alpha})], \tag{119}$$
$$a_5^{(3)}(1;1;u) = -f_2(\boldsymbol{\alpha})u\exp[-uf_1(\boldsymbol{\alpha})], \tag{120}$$
$$a_6^{(3)}(1;1;u) = -(u_d-u)H(u_d-u)\exp[(u-u_d)f_1(\boldsymbol{\alpha})], \tag{121}$$
$$a_7^{(3)}(1;1;u) = -(u_d-u)^2 H(u_d-u)\exp[(u-u_d)f_1(\boldsymbol{\alpha})], \tag{122}$$
$$a_8^{(3)}(1;1;u) = -f_2(\boldsymbol{\alpha})u^2\exp[-uf_1(\boldsymbol{\alpha})]. \tag{123}$$

Using the expressions obtained in in Equations 132, 133 and performing the respective operations yield the following results:

$$\partial^3 R_c(\varphi,\psi)/\partial f_1\partial f_1\partial f_1 = -u_d^4 f_2(\boldsymbol{\alpha})\exp[-u_d f_1(\boldsymbol{\alpha})], \tag{124}$$
$$\partial^3 R_c(\varphi,\psi)/\partial f_1\partial f_1\partial f_2 = u_d^3\exp[-u_d f_1(\boldsymbol{\alpha})]. \tag{125}$$

5.2 Application of the 3rd-FASAM-L to compute the 3rd-order sensitivities stemming from $\partial^2 R_c(\varphi,\psi)/\partial f_1 \partial f_2 = \partial^2 R_c(\varphi,\psi)/\partial f_2 \partial f_1$

The third-order sensitivities stemming from $R^{(2)}[2;1;\mathbf{u}^{(3)};\mathbf{f}(\boldsymbol{\alpha})] \triangleq \partial^2 R_c(\varphi,\psi)/\partial f_2 \partial f_1$ will be obtained from the G-differential of (Equation 72), which will be denoted as $\{\delta R^{(2)}[2;1;\mathbf{u}^{(3)};\mathbf{v}^{(3)};\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0} \triangleq \{\delta[\partial^2 R_c(\varphi,\psi)/\partial f_2 \partial f_1]\}_{\boldsymbol{\alpha}^0}$, and which is by definition determined as follows:

$$\begin{aligned}\{\delta R^{(2)}[2;1;\mathbf{u}^{(3)};\mathbf{v}^{(3)};\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0} &\triangleq \{\delta[\partial^2 R_c(\varphi,\psi)/\partial f_2 \partial f_1]\}_{\boldsymbol{\alpha}^0} \\ &\triangleq \left\{\frac{d}{d\varepsilon}\int_0^{u_{th}}\left[a_1^{(2)}(1;u)+\varepsilon\delta a_1^{(2)}(1;u)\right]\delta(u)\,du\right\}_{\boldsymbol{\alpha}^0,\varepsilon=0} \\ &= \int_0^{u_{th}} \delta a_1^{(2)}(1;u)\delta(u)\,du. \end{aligned} \tag{126}$$

The function $\delta a_1^{(2)}(1;u)$ is one of the components of the third-level variational function $\mathbf{v}^{(3)}(2^3;1;1;u)$, which is the solution of the 3rd-LVSS represented by Equations 101, 102. To avoid the need for solving the 3rd-LVSS, the appearance of this function will be eliminated from Equation 126 by deriving an alternative expression for the G-differential $\{\delta R^{(2)}[2;1;\mathbf{u}^{(3)};\mathbf{v}^{(3)};\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$ in terms of a third-level adjoint sensitivity function, denoted as $\mathbf{a}^{(3)}(2^3;2;1;u) \triangleq [a_1^{(3)}(2;1;u),...,a_8^{(3)}(2;1;u)]^\dagger \in \mathcal{H}_3$. The argument "2,1" of the function $\mathbf{a}^{(3)}(2^3;2;1;u)$ indicates that this (third-level adjoint) function corresponds to the mixed second-order sensitivity of the response with respect to the "*second and first*" components, (f_2,f_1), of the feature function $\mathbf{f}(\boldsymbol{\alpha})$.

The third-level adjoint sensitivity function $\mathbf{a}^{(3)}(2^3;2;1;u)$ will be the solution of 3rd-LASS to be constructed in the Hilbert space $\mathcal{H}_3$ using Equation 104 to construct the inner product of $\mathbf{a}^{(3)}(2^3;2;1;u)$ with Equation 102. Constructing this inner product yields the following relation, where the specification $\{\}_{\boldsymbol{\alpha}^0}$ has been omitted to simplify the notation:

$$\begin{aligned}&\langle \mathbf{a}^{(3)}(2^3;2;1;u), \mathbf{V}^{(3)}[2^3\times 2^3;u;\mathbf{f}]\mathbf{v}^{(3)}(2^3;1;1;u)\rangle_3 \\ &= \langle \mathbf{a}^{(3)}(2^3;2;1;u), \mathbf{q}_V^{(3)}[2^3;\mathbf{u}^{(3)}(2^3;u);\mathbf{f};\delta\mathbf{f}]\rangle_3.\end{aligned} \tag{127}$$

The left side of Equation 127 is integrated by parts to obtain the following relation:

$$\begin{aligned}&\langle \mathbf{a}^{(3)}(2^3;2;1;u), \mathbf{V}^{(3)}[2^3\times 2^3;u;\mathbf{f}]\mathbf{v}^{(3)}(2^3;1;1;u)\rangle_3 \\ &= \langle \mathbf{v}^{(3)}(2^3;1;1;u), \mathbf{A}^{(3)}[2^3\times 2^3;u;\mathbf{f}]\mathbf{a}^{(3)}(2^3;2;1;u)\rangle_3,\end{aligned} \tag{128}$$

where the following boundary conditions were imposed on the components $a_i^{(3)}(2;1;u)$, $i=1,...,8$, of the third-level adjoint sensitivity function $\mathbf{a}^{(3)}(2^3;2;1;u)$:

$$\begin{aligned}&a_1^{(3)}(2;1;u_{th})=0;\; a_2^{(3)}(2;1;0)=0;\quad a_3^{(3)}(2;1;0)=0; \\ &a_4^{(3)}(2;1;u_{th})=0;\, a_5^{(3)}(2;1;0)=0;\; a_6^{(3)}(2;1;u_{th})=0; \\ &a_7^{(3)}(2;1;u_{th})=0;\quad a_8^{(3)}(2;1;0)=0.\end{aligned} \tag{129}$$

The right side of Equation 109 is now required to represent the G-differential $\{\delta R^{(2)}[2;1;\mathbf{u}^{(3)}(2^3;1;1;u);\mathbf{v}^{(3)}(2^3;1;1;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$ by imposing the following relation:

$$\mathbf{A}^{(3)}[2^3\times 2^3;u;\mathbf{f}]\mathbf{a}^{(3)}(2^3;2;1;u) = \mathbf{s}_A^{(3)}(2^3;2;1;\mathbf{f}) \triangleq [0,0,0,0,0,\delta(u),0,0]^\dagger. \tag{130}$$

The relations provided in Equations 108, 110 constitute the 3rd-LASS for the third-level adjoint sensitivity function $\mathbf{a}^{(3)}(2^3;1;1;u)$. Using the relations in Equations 99, 102, 103, 108, and 110 yields the following alternative expression for $\{\delta R^{(2)}[2;1;\mathbf{u}^{(3)}(2^3;1;1;u);\mathbf{a}^{(3)}(2^3;2;1;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0}$, in which the function $\mathbf{v}^{(3)}(2^3;1;1;u)$ has been replaced by the function $\mathbf{a}^{(3)}(2^3;2;1;u)$:

$$\begin{aligned}&\{\delta R^{(2)}[2;1;\mathbf{u}^{(3)}(2^3;1;1;u);\mathbf{a}^{(3)}(2^3;2;1;u);\mathbf{f}(\boldsymbol{\alpha})]\}_{\boldsymbol{\alpha}^0} \\ &= \left\{\int_0^{u_{th}} a_1^{(3)}(2;1;u)[(\delta f_2)\delta(u)-(\delta f_1)\varphi(u)]\,du\right\}_{\boldsymbol{\alpha}^0} \\ &- \left\{\int_0^{u_{th}} a_2^{(3)}(2;1;u)(\delta f_1)\psi(u)\,du\right\}_{\boldsymbol{\alpha}^0} \\ &- \left\{\int_0^{u_{th}} a_3^{(3)}(2;1;u)(\delta f_1)a_1^{(1)}(u)\,du\right\}_{\boldsymbol{\alpha}^0} \\ &- \left\{\int_0^{u_{th}} a_4^{(3)}(2;1;u)(\delta f_1)a_2^{(1)}(u)\,du\right\}_{\boldsymbol{\alpha}^0} \\ &- \left\{\int_0^{u_{th}} a_5^{(3)}(2;1;u)(\delta f_1)a_1^{(2)}(1;u)\,du\right\}_{\boldsymbol{\alpha}^0} \\ &- \left\{\int_0^{u_{th}} a_6^{(3)}(2;1;u)(\delta f_1)a_2^{(2)}(1;u)\,du\right\}_{\boldsymbol{\alpha}^0} \\ &- \left\{\int_0^{u_{th}} a_7^{(3)}(2;1;u)(\delta f_1)a_3^{(2)}(1;u)\,du\right\}_{\boldsymbol{\alpha}^0} \\ &- \left\{\int_0^{u_{th}} a_8^{(3)}(2;1;u)(\delta f_1)a_4^{(2)}(1;u)\,du\right\}_{\boldsymbol{\alpha}^0}.\end{aligned} \tag{131}$$

The third-order sensitivities stemming from the relation obtained in Equation 131 are the expressions that multiply the respective variations δf_1 and δf_2 and are as follows:

$$\begin{aligned}\partial^3 R_c(\varphi,\psi)/\partial f_1 \partial f_2 \partial f_1 = &-\int_0^{u_{th}} a_1^{(3)}(2;1;u)\varphi(u)\,du \\ &-\int_0^{u_{th}} a_2^{(3)}(2;1;u)\psi(u)\,du \\ &-\int_0^{u_{th}} a_3^{(3)}(2;1;u)a_1^{(1)}(u)\,du \\ &-\int_0^{u_{th}} a_4^{(3)}(2;1;u)a_2^{(1)}(u)\,du \\ &-\int_0^{u_{th}} a_5^{(3)}(2;1;u)a_1^{(2)}(1;u)\,du \\ &-\int_0^{u_{th}} a_6^{(3)}(2;1;u)a_2^{(2)}(1;u)\,du \\ &-\int_0^{u_{th}} a_7^{(3)}(2;1;u)a_3^{(2)}(1;u)\,du \\ &-\int_0^{u_{th}} a_8^{(3)}(2;1;u)a_4^{(2)}(1;u)\,du;\end{aligned} \tag{132}$$

$$\partial^3 R_c(\varphi,\psi)/\partial f_2 \partial f_2 \partial f_1 = \int_0^{u_{th}} a_1^{(3)}(2;1;u)\delta(u)\,du. \tag{133}$$

The expressions obtained in Equations 132, 133 are to be evaluated at the nominal values of parameters and state functions, but the notation $\{\}_{\alpha^0}$ has been omitted for simplicity.

In component form, the 3rd-LASS for the third-level adjoint sensitivity function $\mathbf{a}^{(3)}(2^3;2;1;u)$ has the following expression, where dots are used to denote zero-elements for better visibility of the structure:

$$\begin{pmatrix} M & \cdot & \cdot & -1 & \cdot & \cdot & 1 & \cdot \\ \cdot & L & -1 & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & L & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & M & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & L & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & M & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -1 & M & \cdot \\ \cdot & \cdot & \cdot & \cdot & -1 & \cdot & \cdot & L \end{pmatrix} \begin{pmatrix} a_1^{(3)}(2;1;u) \\ a_2^{(3)}(2;1;u) \\ a_3^{(3)}(2;1;u) \\ a_4^{(3)}(2;1;u) \\ a_5^{(3)}(2;1;u) \\ a_6^{(3)}(2;1;u) \\ a_7^{(3)}(2;1;u) \\ a_8^{(3)}(2;1;u) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \delta(u) \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{134}$$

Solving Equation 134 yields the following expressions for the components of the third-level adjoint sensitivity function $\mathbf{a}^{(3)}(2^3;2;1;u)$:

$$\begin{aligned} &a_1^{(3)}(2;1;u) = a_4^{(3)}(2;1;u) = a_6^{(3)}(2;1;u) = a_7^{(3)}(2;1;u) = 0\,; \\ &a_5^{(3)}(2;1;u) = H(u)\exp[-uf_1(\boldsymbol{\alpha})];\, a_2^{(3)}(2;1;u) \\ &\qquad\qquad = -u^2\exp[-uf_1(\boldsymbol{\alpha})]\,; \\ &a_3^{(3)}(2;1;u) = -u\exp[-uf_1(\boldsymbol{\alpha})] = -a_8^{(3)}(2;1;u). \end{aligned} \tag{135}$$

Using the expressions obtained in Equation 135, substituting them into Equations 132, 133 and performing the respective operations yield the following results:

$$\begin{aligned} \partial^3 R_c(\varphi,\psi)\Big/\partial f_1\partial f_2\partial f_1 &= -\int_0^{u_{th}} a_2^{(3)}(2;1;u)\psi(u)\,du \\ &- \int_0^{u_{th}} a_3^{(3)}(2;1;u)a_1^{(1)}(u)\,du - \int_0^{u_{th}} a_5^{(3)}(2;1;u)a_1^{(2)}(1;u)\,du \\ &- \int_0^{u_{th}} a_8^{(3)}(2;1;u)a_4^{(2)}(1;u)\,du \\ &= u_d^3\exp[-u_d f_1(\boldsymbol{\alpha})] \end{aligned} \tag{136}$$

$$\partial^3 R_c(\varphi,\psi)\Big/\partial f_2\partial f_2\partial f_1 = 0. \tag{137}$$

6 Concluding discussion

This work has presented illustrative applications of the "nth-FASAM-L," which has been specifically developed to be the most efficient methodology for computing exact expressions of sensitivities of responses (of such unique linear models) to features of model parameters and, subsequently, to the model parameters themselves. The efficiency of the nth-FASAM-L stems from the maximal reduction of the number of adjoint computations (which are "large-scale" computations) compared to the extant conventional high-order adjoint sensitivity analysis methodology nth-CASAM-L (Cacuci, 2022). The unique characteristics of the nth-FASAM-L have been illustrated in this work using a paradigm model of a "contributon-flux density response" that occurs in the energy distribution of neutrons stemming from a fission source in a homogeneous mixture of materials. This analytically solvable illustrative paradigm model has been used to demonstrate the following general conclusions regarding the characteristics and applicability of the nth-FASAM-L.

(i) Comparing the mathematical framework of the nth-FASAM-L to that of the nth-CASAM-L indicates that the components $f_i(\boldsymbol{\alpha}), i = 1,...,TF$ of the "feature function" $\mathbf{f}(\boldsymbol{\alpha}) \triangleq [f_1(\boldsymbol{\alpha}),...,f_{TF}(\boldsymbol{\alpha})]^\dagger$ play within the nth-FASAM-L the same role as played by the components $\alpha_j, j = 1,...,TP$ of the "vector of primary model parameters" $\boldsymbol{\alpha} \triangleq (\alpha_1,\ldots,\alpha_{TP})^\dagger$ within the framework of the nth-CASAM-L. It is paramount to underscore, at the outset, that the total number of model parameters is always larger (usually by a wide margin) than the total number of components of the feature function $\mathbf{f}(\boldsymbol{\alpha})$, i.e., $TP \gg TF$. The illustrative paradigm model of "neutron slowing down in a homogeneous mixture of materials" presented in this work comprised a feature function with two components (i.e., $TF = 2$) denoted as $f_1(\boldsymbol{\alpha})$ and $f_2(\boldsymbol{\alpha})$, which were, in turn, functions of $TP \triangleq 3M + 10$ imprecisely known model parameters (where M denotes the number of materials and/or isotopes in the mixture, which is of the order of 20–50 in a nuclear reactor, depending on its service in operation).

(ii) For computing the exact expressions of the *first-order* sensitivities of a model response to the uncertain parameters, boundaries, and internal interfaces of the model, both the 1st-FASAM-L and 1st-CASAM-L require a *single* large-scale "adjoint" computation. This "large-scale" computation using either the 1st-FASAM-L or 1st-CASAM-L involves solving the same operator equations and boundary conditions within the respective 1st-LASS; only the sources for the respective 1st-LASS differ from each other. The 1st-FASAM-L enjoys a slight computational advantage since it requires only TF quadratures (one quadrature per component of the feature function), while the 1st-CASAM-L requires TP quadratures (one quadrature per model parameter). For the illustrative "contributon response of the neutron slowing-down" paradigm model, the computation of the first-order response sensitivities with respect to the model parameters required two quadratures using the 1st-FASAM-L, while the 1st-CASAM-L required TP-quadratures. Within the 1st-FASAM-L, the sensitivities with respect to the primary model parameters are obtained by using the first-order sensitivities $\partial R_c/\partial f_1$ and $\partial R_c/\partial f_2$ (with respect to the components of the feature function) in conjunction with the chain rule of differentiation of the exactly known expressions of the components $f_1(\boldsymbol{\alpha})$ and $f_2(\boldsymbol{\alpha})$ in terms of the primary model parameters.

(iii) Both the 2nd-FASAM-L and 2nd-CASAM-L conceptually determine the *second-order* sensitivities by using the fundamental concept that "the second-order sensitivities are the first-order sensitivities of the first-order sensitivities." For computing the exact expressions of the second-order response sensitivities with respect to the primary model's parameters, the fundamental difference between the 2nd-FASAM-L and 2nd-CASAM-L is obtained as follows: the 2nd-FASAM-L requires as many large-scale "adjoint" computations as there are "feature functions of parameters" $f_i(\boldsymbol{\alpha}), i = 1, ..., TF$ (where TF denotes the total number of feature functions) for solving the left side of the 2nd-LASS with TF distinct sources on its right side. In contradistinction, the 2nd-CASAM-L requires TP (where TP denotes the total number of model parameters or non-zero first-order sensitivities) large-scale computations for solving the same left side of the 2nd-LASS but with TP distinct sources. Remarkably, the types of "large-scale" computations are the same in both the 2nd-FASAM-L and 2nd-CASAM-L since they both solve the same operator equations and boundary conditions within the respective 2nd-LASS systems; only the sources for these adjoint systems differ from each other. Since $TF \ll TP$, the 2nd-FASAM-L is considerably more efficient than the 2nd-CASAM-L for computing the exact expressions of the second-order sensitivities of a model response to the uncertain parameters, boundaries, and internal interfaces of the model. For the illustrative contributon-response paradigm model, the computation of the second-order response sensitivities with respect to the model parameters using the 2nd-FASAM-L requires just two large-scale computations, for solving the two 2nd-LASS that correspond to the first-order sensitivities, $\partial R_c/\partial f_1$ and $\partial R_c/\partial f_2$, of the contributon response with respect to the respective components, $f_1(\boldsymbol{\alpha})$ and $f_2(\boldsymbol{\alpha})$, of the model's "feature function" $f(\boldsymbol{\alpha})$. In contradistinction, computing the second-order sensitivities to the model parameters using the 2nd-CASAM-L requires TP large-scale computations, one for solving each of the 2nd-LASS that corresponds to each one of the distinct first-order sensitivities $\partial R_c/\partial \alpha_i$, $i = 1, ..., TP$, of the response with respect to the TP model parameters. Remarkably, only the unmixed second-order sensitivity $\partial^2 R_c(\varphi, \psi)/\partial f_1 \partial f_1$ and the mixed second-order sensitivity $\partial^2 R_c(\varphi, \psi)/\partial f_1 \partial f_2 = \partial^2 R_c(\varphi, \psi)/\partial f_2 \partial f_1$ are non-zero. The unmixed second-order sensitivity is identically zero, i.e., $\partial^2 R_c(\varphi, \psi)/\partial f_2 \partial f_2 \equiv 0$. In contradistinction, computing the second-order sensitivities to the model parameters using the 2nd-CASAM-L requires TP large-scale computations, one for solving each of the 2nd-LASS that corresponds to one of the distinct TP model parameters. None of the second-order sensitivities with respect to the primary model parameters vanish.

(iv) For computing the exact expressions of the *third-order* response sensitivities with respect to the primary model's parameters, the 3rd-FASAM-L requires at most $TF(TF+1)/2$ large-scale "adjoint" computations for solving the 3rd-LASS with $TF(TF+1)/2$ distinct sources, while the 3rd-CASAM-L requires at most $TP(TP+1)/2$ large-scale computations for solving the 3rd-LASS with $TP(TP+1)/2$ distinct sources. For the illustrative "contributon response of the neutron slowing-down" paradigm model, the computation of the third-order response sensitivities with respect to the model parameters using the 3rd-FASAM-L requires only *two* large-scale computations for solving the two 3rd-LASS that correspond to the respective non-zero second-order sensitivities $\partial^2 R_c(\varphi, \psi)/\partial f_1 \partial f_1$ and $\partial^2 R_c(\varphi, \psi)/\partial f_1 \partial f_2 = \partial^2 R_c(\varphi, \psi)/\partial f_2 \partial f_1$. Only the unmixed third-order sensitivity $\partial^3 R_c(\varphi, \psi)/\partial f_1 \partial f_1 \partial f_1$ and the mixed third-order sensitivity $\partial^3 R_c(\varphi, \psi)/\partial f_1 \partial f_1 \partial f_2$ are non-zero; all other third-order sensitivities vanish identically. In contradistinction, the 3rd-CASAM-L requires all $TP(TP+1)/2$ large-scale computations for solving the 3rd-LASS since all of the second-order sensitivities with respect to the primary model parameters are non-zero. Furthermore, all of the third-order response sensitivities with respect to the primary model parameters are non-zero.

(v) The same computational count of "large-scale computations" caries over when computing the fourth- and higher-order sensitivities, i.e., the formula for calculating the "number of large-scale adjoint computations" is formally the same for both the nth-FASAM-N (Cacuci, 2024a, 2024b) and nth-CASAM-N (Cacuci, 2023a), but the "variable" in the formula for determining the number of adjoint computations for the nth-FASAM-N is TF (i.e., total number of feature functions), while the counterpart for the formula for determining the number of adjoint computations for the nth-CASAM-N is TP (i.e., total number of model parameters). Since $TF \ll TP$, it follows that the higher the order of computed sensitivities, the more efficient the nth-FASAM-N (Cacuci, 2024a, 2024b) becomes compared to the nth-CASAM-N (Cacuci, 2023a).

(vi) The probability of encountering vanishing sensitivities is much higher when using the nth-FASAM-L than when using the nth-CASAM-L. For the illustrative "contributon response of the neutron slowing-down" paradigm model, it is evident that the only a few of the response sensitivities of fourth order (and higher order) with respect to the components of the feature function $\mathbf{f}(\boldsymbol{\alpha})$ will *not* vanish, and the non-vanishing sensitivities will all involve the component $f_1(\boldsymbol{\alpha})$ of the feature function since this component appears in an exponential, whereas the other component appears just as a multiplicative factor. In contradistinction, none of the higher-order response sensitivities with respect to the primary model parameters will vanish using the 2nd-CASAM-L.

(vii) When a model has no "feature" functions of parameters, but only comprises primary parameters, the nth-FASAM-L becomes identical to the nth-CASAM-L.

(viii) Both the nth-FASAM-L and nth-CASAM-L are formulated in linearly increasing higher-dimensional Hilbert spaces—as opposed to exponentially increasing parameter-dimensional spaces—thus overcoming the limitation of dimensionality in the sensitivity analysis of linear systems. Both the nth-FASAM-L and nth-

CASAM-L are incomparably more efficient and more accurate than any other method (statistical, finite differences, etc.) for computing the exact expressions of response sensitivities (of any order) with respect to the uncertain parameters, boundaries, and internal interfaces of the model.

Data availability statement

The original contributions presented in the study are included in the article/Supplementary Material; further inquiries can be directed to the corresponding author.

Author contributions

DC: conceptualization, data curation, formal analysis, investigation, methodology, project administration, resources, software, supervision, validation, visualization, writing–original draft, and writing–review and editing.

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References

Cacuci, D. G. (2022). "The n^{th}-order comprehensive adjoint sensitivity analysis methodology (n^{th}-CASAM): overcoming the curse of dimensionality in sensitivity and uncertainty analysis," in *Volume I: Linear systems* (Cham, Switzerland: Springer Nature), 362. doi:10.1007/978-3-030-96364-4

Cacuci, D. G. (2023a). "The n^{th}-order comprehensive adjoint sensitivity analysis methodology (nth-CASAM): overcoming the curse of dimensionality in sensitivity and uncertainty analysis," in *Volume III: Nonlinear Systems* (Cham, Switzerland: Springer Nature), 369. doi:10.1007/978-3-031-22757-8

Cacuci, D. G. (2024a). Introducing the n^{th}-order features adjoint sensitivity analysis methodology for nonlinear systems (n^{th}-FASAM-N): I. Mathematical framework. *Am. J. Comput. Math.* 14, 11–42. doi:10.4236/ajcm.2024.141002

Cacuci, D. G. (2024b). Introducing the n^{th}-order features adjoint sensitivity analysis methodology for nonlinear systems (n^{th}-FASAM-N): II. Illustrative example. *Am. J. Comput. Math.* 14, 43–95. doi:10.4236/ajcm.2024.141003

Cacuci, D. G. (2024c). The n^{th}-order features adjoint sensitivity analysis methodology for response-coupled forward/adjoint linear systems (n^{th}-FASAM-L):I. I. Mathematical framework. *Front. Energy Res.* 12, 1417594. doi:10.3389/fenrg.2024.1417594

Cacuci, D. G., and Fang, R. (2023). "The n^{th}-order comprehensive adjoint sensitivity analysis methodology (nth-CASAM): overcoming the curse of dimensionality in sensitivity and uncertainty analysis," in *Application to a large-scale system* (Nature Switzerland, Cham: Springer), 463. doi:10.1007/978-3-031-19635-5

Lamarsh, J. R. (1966). *Introduction to nuclear reactor theory*. Reading MA, USA: Adison-Wesley Publishing Co., 491–492.

Lewins, J. (1965). *IMPORTANCE: the adjoint function*. Oxford, UK: Pergamon Press Ltd.

Meghreblian, R. V., and Holmes, D. K. (1960). *Reactor analysis*. New York, USA: McGraw-Hill.

Stacey, W. M. (1974). *Variational methods in nuclear reactor physics*. New York, USA: Academic Press.

Stacey, W. M. (2001). *Nuclear reactor physics*. New York. USA: John Wiley and Sons.

Valentine, T. E. (2006). "Polyethylene-reflected plutonium metal sphere subcritical noise measurements, SUB-PU-METMIXED-001," in *International handbook of evaluated criticality safety benchmark experiments, NEA/NSC/DOC(95)03/I-ix, organization for economic Co-operation and development (OECD)*. Paris, France: Nuclear Energy Agency.

Williams, M. L., and Engle, W. W. (1977). The concept of spatial channel theory applied to reactor shielding analysis. *Nucl. Sci. Eng.* 62, 92–104. doi:10.13182/nse77-a26941

Wilson, W. B., Perry, R. T., Shores, E. F., Charlton, W. S., Parish, T. A., Estes, G. P., et al. (2002). "SOURCES4C: a code for calculating (α, n), spontaneous fission, and delayed neutron sources and spectra," in *Proceedings of the American nuclear society/radiation protection and shielding division 12th biennial topical meeting* (Santa Fe, NM, USA), 14–18.