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# Introducing the $n^{th}$-Order Features Adjoint Sensitivity Analysis Methodology for Nonlinear Systems ($n^{th}$-FASAM-N): II. Illustrative Example

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## Abstract

This work highlights the unparalleled efficiency of the "$n^{th}$-Order Function/ Feature Adjoint Sensitivity Analysis Methodology for Nonlinear Systems" ($n^{th}$-FASAM-N) by considering the well-known Nordheim-Fuchs reactor dynamics/safety model. This model describes a short-time self-limiting power excursion in a nuclear reactor system having a negative temperature coefficient in which a large amount of reactivity is suddenly inserted, either intentionally or by accident. This nonlinear paradigm model is sufficiently complex to model realistically self-limiting power excursions for short times yet admits closed-form exact expressions for the time-dependent neutron flux, temperature distribution and energy released during the transient power burst. The $n^{th}$-FASAM-N methodology is compared to the extant "$n^{th}$-Order Comprehensive Adjoint Sensitivity Analysis Methodology for Nonlinear Systems" ($n^{th}$-CASAM-N) showing that: (i) the $1^{st}$-FASAM-N and the $1^{st}$-CASAM-N methodologies are equally efficient for computing the first-order sensitivities; each methodology requires a single large-scale computation for solving the "First-Level Adjoint Sensitivity System" ($1^{st}$-LASS); (ii) the $2^{nd}$-FASAM-N methodology is considerably more efficient than the $2^{nd}$-CASAM-N methodology for computing the second-order sensitivities since the number of feature-functions is much smaller than the number of primary parameters; specifically for the Nordheim-Fuchs model, the $2^{nd}$-FASAM-N methodology requires 2 large-scale computations to obtain all of the exact expressions of the 28 distinct second-order response sensitivities with respect to the model parameters while the $2^{nd}$-CASAM-N methodology requires 7 large-scale computations for obtaining these 28 second-order sensitivities; (iii) the $3^{rd}$-FASAM-N methodology is even more efficient than the $3^{rd}$-CASAM-N methodology: only 2 large-scale computations are needed to obtain the exact expressions of the 84 distinct third-order response sensitivities with respect to the Nordheim-Fuchs model's parameters when applying the 3rd-FASAM-N methodology, while the application of the 3rd-CASAM-N methodology requires at least 22 large-scale computations for computing the same 84 distinct third-order sensitivities. Together, the nth-FASAM-N and the nth-CASAM-N methodologies are the most practical methodologies for computing response sensitivities of any order comprehensively and accurately, overcoming the curse of dimensionality in sensitivity analysis.

## Keywords

Nordheim-Fuchs Reactor Safety Model, Feature Functions of Model Parameters, High-Order Response Sensitivities to Parameters, Adjoint Sensitivity Systems

## 1. Introduction

As presented in the accompanying work by Cacuci [1], the "nth-Order Function/Feature Adjoint Sensitivity Analysis Methodology for Nonlinear Systems" (abbreviated as "nth-FASAM-N") enables the most efficient computation of exactly-determined expressions of arbitrarily high-order sensitivities of generic nonlinear system responses with respect to functions (features) of model parameters, which enables, in turn, the most efficient computation of the corresponding high-order sensitivities to primary model parameters, uncertain boundaries and internal interfaces in the model's phase-space. It was shown in [1] that the nth-FASAM-N methodology requires the fewest possible number of large-scale computations of any method for determining exactly the respective high-order sensitivities, being even more efficient than the well-known "nth-Order Comprehensive Adjoint Sensitivity Analysis Methodology for Nonlinear Systems" (nth-CASAM-N) [2]. The unparalleled efficiency of the nth-FASAM-N methodology stems from its formulation in the phase-space of "feature-functions," which is always smaller than the phase-space of model parameters. The application of the nth-FASAM-N is illustrated in this work by considering a well-known paradigm model that describes a short-time self-limiting power excursion in a nuclear reactor system having a negative temperature coefficient in which a large amount of reactivity is suddenly inserted, either intentionally or by accident. In the textbook by Lamarsh [3], this model is called the "Fuchs model" while in the textbook by Hetrick [4] this model is called the "Nordheim-Fuchs model." This nonlinear paradigm model is sufficiently complex to realistically model self-limiting power excursions for short times while admitting closed-form exact expressions for the time-dependent neutron flux, temperature distribution and energy released during the transient power burst.

This work is structured as follows: Section 2 presents the balance equations which underly the Nordheim-Fuchs phenomenological model describing a prompt-critical reactor transient. Section 3 illustrates the computation of first-order sensitivities of the Nordheim-Fuchs model's response (which is chosen to be the total energy released during the modeled power-burst) with respect to the parameters underlying this model by applying the well-known 1st-CASAM-N methodology (in Subsection 3.1) and subsequently comparing (in Subsection 3.2) this methodology with the 1st-FASAM-N methodology. Both methodologies require just one large-scale adjoint computation to obtain the exact analytical expressions of the first-order sensitivities of the model's response with respect to the model's parameters.

Section 4 illustrates the computation of the second-order response sensitivities with respect to the Nordheim-Fuchs model's parameters by first showing that applying the 2nd-FASAM-N (in Subsection 4.1) requires just 2 large-scale computations, while applying the 2nd-CASAM-N (in Subsection 4.2) requires 7 large-scale computations, to obtain all of the 7 distinct second-order sensitivities.

Section 5 illustrates the computation of the third-order response sensitivities with respect to the Nordheim-Fuchs model's parameters by applying the 3rd-FASAM-N versus applying the 3rd-CASAM-N. It is shown (in Subsection 5.1) that the 3rd-FASAM-N requires just 2 large-scale computations to obtain all of the 84 distinct third-order sensitivities. By comparison, applying the 3rd-CASAM-N (in Subsection 5.2) requires at least 22 computations large-scale for determining the 84 distinct third-order sensitivities. Evidently, the 3rd-FASAM methodology is significantly more efficient for computing the second-and higher-order sensitivities than the 3rd-CASAM-N methodology. Both the 3rd-FASAM-N and the 3rd-CASAM-N methodologies yield exact values for the expressions of the third-order sensitivities

The concluding discussion presented in Section 6 commences by noting that when no feature functions of parameters can be identified, the mathematical frameworks of the nth-FASAM-N and the nth-CASAM-N methodologies coincide. When feature-functions of parameters can be identified within the model, the nth-FASAM-N methodology requires the least number of large-scale computations of any practical methodology for computing exact expressions of second- and higher-order sensitivities. In general, the number of large-scale computations required when applying the nth-FASAM-N is proportional to the number of feature-functions underlying the model being analyzed, while the number of large-scale computations required when applying the nth-CASAM-N is proportional to the number of the parameters underlying the respective model. Since the number of feature-functions is necessarily smaller than the number of model parameters, it follows that the nth-FASAM-N is computationally more efficient than the nth-CASAM-N. Both the nth-FASAM-N and the nth-CASAM-N are vastly more efficient computationally than finite-difference schemes, particularly for computing sensitivities of order higher than first for large-scale models with many parameters. Furthermore, the finite difference-schemes are approximate, while the nth-FASAM-N and the nth-CASAM-N accurately compute exact expressions of the arbitrarily-high order sensitivities of model responses with respect to model's parameters. Altogether, the n$^{th}$-FASAM-N and the n$^{th}$-CASAM-N methodologies remain the most practical methodologies for computing response sensitivities comprehensively and accurately, overcoming the curse of dimensionality in sensitivity analysis of nonlinear systems.

## 2. The Nordheim-Fuchs Phenomenological Reactor Dynamics/Safety Model

The Nordheim-Fuchs phenomenological model (Lamarsh, 1966; Hetrick, 1993) describes a short-time self-limiting power transient in a nuclear reactor system having a negative temperature coefficient in which a large amount of reactivity is suddenly inserted, either intentionally or by accident. The response of such a reactor system can be estimated by considering that the reactivity insertion is sufficiently large and the time-span of the transient phenomena under consideration is of the order of the life-time of prompt-neutrons, which is sufficiently small to neglect the effects of delayed neutrons. For such short times, the local spatial variations of the neutron distribution in the reactor are negligible, and the heat generated during the transient remains within the reactor.

Using the notation of Lamarsh (1966), the Nordheim-Fuchs paradigm model describing the aforementioned self-limiting power transient comprises the following balance equations:

1) The time-dependent neutron balance (point kinetics) equation for the neutron flux $\varphi(t)$:

$$\frac{\mathrm{d}\varphi(t)}{\mathrm{d}t}=\frac{k(t)-1}{l_p}\varphi(t),\ t>0, \tag{1}$$

$$\varphi(0)=\varphi_0,\ t=0, \tag{2}$$

where $l_p$ denotes the prompt-neutron lifetime, $k(t)$ denotes the reactor's multiplication factor, and $\varphi_0$ denotes the initial (*i.e.*, extant flux) prior to initiating the transient at time $t=0$.

2) The energy conservation equation:

$$c_p\left[T(t)-T_0\right]=E(t), \tag{3}$$

where $E(t)$ denotes the total energy released (per cm$^3$) at time $t$ in the reactor since the onset of reactivity change; $c_p$ denotes the specific heat (per cm3) of the reactor.

3) The energy production equation:

$$E(t)=\gamma\Sigma_f\int_0^t\varphi(x)\mathrm{d}x, \tag{4}$$

where $\gamma$ denotes the recoverable energy per fission; $\Sigma_f \triangleq \sigma_f N_f$ denotes the reactor's effective macroscopic fission cross section, where $\sigma_f$ denotes the reactor's equivalent microscopic fission cross section while $N_f$ denotes the reactor's equivalent atomic number density.

4) The reactivity-temperature feedback equation: $k(t)=k_0-\alpha_T k_0\left[T(t)-T_0\right]$,

where $k_0 \triangleq k(0) \geq 1$ denotes the changed multiplication factor following the reactivity insertion at $t = 0$, $\alpha_T$ denotes the magnitude of the negative temperature coefficient, $T(t)$ denotes the reactor's temperature, and $T_0$ denotes the reactor's initial temperature at time $t = 0$. For illustrating the application of the 1st-FASAM methodology, it suffices to consider the special case of a "prompt critical transient", when the reactor becomes prompt critical after the reactivity insertion, *i.e.*, when $k_0 = 1$, so that the reactivity-temperature feedback equation takes on the following particular form:

$$k(t) = 1 - \alpha_T \left[ T(t) - T_0 \right]. \tag{5}$$

The Nordheim-Fuchs model, comprising Equations (1)-(5), is representative of the types of equations that underly large-scale computational models, including a combination of algebraic, differential, and integral equations. Typically, such equations are discretized into systems of nonlinear algebraic and/or differential equations, which are then solved numerically by using standard solvers for such systems of equations. Equations (1)-(5) can be transformed into the following system of nonlinear differential equations:

$$\frac{\mathrm{d}\varphi(t)}{\mathrm{d}t} = -\frac{\alpha_T}{l_p c_p} E(t) \varphi(t), \; t > 0. \quad \varphi(0) = \varphi_0, \; t = 0 \tag{6}$$

$$\frac{\mathrm{d}E(t)}{\mathrm{d}t} = \gamma \sigma_f N_f \varphi(t), \; E(0) = 0, \tag{7}$$

$$\frac{\mathrm{d}T(t)}{\mathrm{d}t} = \frac{\gamma \sigma_f N_f}{c_p} \varphi(t); \; T(0) = T_0. \tag{8}$$

The Nordheim-Fuchs model described by Equations (6)-(8) can be solved analytically to obtain closed-form expression for the state functions $\varphi(t)$, $E(t)$, and $T(t)$. Thus, eliminating the function $\varphi(t)$ from Equations (6) and (7) yields a nonlinear equation that can be integrated directly to obtain the following relation:

$$\varphi(t) = -\frac{\alpha_T}{2 l_p c_p \gamma \sigma_f N_f} E^2(t) + \varphi_0. \tag{9}$$

Using Equation (9) in Equation (7) yields the following nonlinear equation for the released energy $E(t)$:

$$\frac{\mathrm{d}E(t)}{\mathrm{d}t} = -\frac{\alpha_T}{2 l_p c_p} E^2(t) + \varphi_0 \gamma \sigma_f N_f, \; E(0) = 0. \tag{10}$$

The most important quantity of interest (*i.e.*, "model response") for the Nordheim-Fuchs model is the total energy per cm$^3$, $E(\tau)$, released at a user-chosen "final time" instance denoted as $t = \tau$, after the initiation at $t = 0$ of the prompt-critical power transient. This response can be defined mathematically in several equivalent ways, the simplest of which is as follows:

$$E(\tau) = \int_0^\tau E(t) \delta(t - \tau) \mathrm{d}t, \tag{11}$$

where $\delta(t-\tau)$ denotes the Dirac-delta functional.

The response $E(\tau)$ defined in Equation (11) is an implicit function of seven uncertain parameters $i=1,\cdots,7=TP$ primary model parameters (where "TP" denotes the "total number of primary model parameters") which are considered to be the components of a "vector of model parameters" denoted as $\boldsymbol{\alpha}$ and defined as follows:

$$\boldsymbol{\alpha} \triangleq (\alpha_1,\cdots,\alpha_7)^\dagger \triangleq (\alpha_T, l_p, c_p, \varphi_0, \gamma, \sigma_f, N_f)^\dagger . \tag{12}$$

In this work, all vectors are considered to be column vectors and the dagger symbol ($\dagger$) will be used to denote "transposition." The model parameters are considered to be uncertain (*i.e.*, imprecisely known), but have known nominal values which will be denoted using a superscript "zero," as follows:

$$\boldsymbol{\alpha}^0 \triangleq (\alpha_1^0,\cdots,\alpha_7^0)^\dagger \triangleq (\alpha_T^0, l_p^0, c_p^0, \varphi_0^0, \gamma^0, \sigma_f^0, N_f^0)^\dagger . \tag{13}$$

For further reference, the closed-form solution of Equation (10) has the following form:

$$E(t) = K(\boldsymbol{\alpha})\tanh\left[t\theta(\boldsymbol{\alpha})\right], \tag{14}$$

where:

$$K(\boldsymbol{\alpha}) \triangleq \left[\frac{2\varphi_0\gamma\sigma_f N_f l_p c_p}{\alpha_T}\right]^{1/2}; \quad \theta(\boldsymbol{\alpha}) \triangleq \left[\frac{\alpha_T\varphi_0\gamma\sigma_f N_f}{2 l_p c_p}\right]^{1/2}. \tag{15}$$

The closed-form expression of $\varphi(t)$ is obtained by replacing Equation (15) into Equation (9) to obtain:

$$\varphi(t) = \varphi_0\left\{1-\tanh^2\left[t\theta(\boldsymbol{\alpha})\right]\right\} = \frac{\varphi_0}{\cosh^2\left[t\theta(\boldsymbol{\alpha})\right]}. \tag{16}$$

The closed-form expression of $T(t)$ is obtained by replacing Equation (15) into Equation (3) to obtain:

$$T(t) = T_0 + \frac{K(\boldsymbol{\alpha})}{c_p}\tanh\left[t\theta(\boldsymbol{\alpha})\right]. \tag{17}$$

The remainder of this work will use the model response $E(\tau)$ to illustrate the advantages of applying the nth-FASAM-N versus the nth-CASAM-N for the higher-order sensitivity analysis of this response to the underlying model parameters.

## 3. Computation of First-Order Sensitivities of the Model Response to Model Parameters: Application of the Conventional 1st-CASAM-N Versus the 1st-FASAM-N Methodology

This Section presents the computation of the first-order sensitivities of the selected model response by following two alternative pathways. Thus, Subsection 3.1 presents the application of the conventional 1st-CASAM methodology, while Subsection 3.2 presents the application of the novel 1st-FASAM methodology;

the advantages of applying the 1st-FASAM methodology versus the conventional 1st-CASAM methodology are summarized in Subsection 3.1

### 3.1. Application of the 1st-CASAM-N to Obtain the First-Order Sensitivities of the Response $E(\tau)$ Directly with Respect to the Model Parameters

The first-order sensitivities of $E(\tau)$ with respect to variations in the model parameters are obtained by determining the first-order Gateaux (G)-differential $\delta E(\tau)$ of $E(\tau)$ for known parameter variations $\delta\boldsymbol{\alpha} \triangleq \boldsymbol{\alpha} - \boldsymbol{\alpha}^0$ around the nominal values $\left(E^0;\boldsymbol{\alpha}^0\right)$. Considering that the final observation time is perfectly well known, the first-order Gateaux (G)-differential $\delta E(\tau)$ is obtained, by definition, as follows:

$$\delta E(\tau) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\int_0^\tau \left[E^0 + \varepsilon\delta E(t)\right]\delta(t-\tau)\right\}_{\varepsilon=0}\mathrm{d}t = \int_0^\tau \delta E(t)\delta(t-\tau)\mathrm{d}t\,. \tag{18}$$

The variational function $\delta E(t)$ is the solution of the first-order G-differential of Equation (10), which is obtained, by definition, as follows:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\frac{\mathrm{d}\left[E(t)+\varepsilon\delta E(t)\right]}{\mathrm{d}t}\right\}_{\varepsilon=0}\\ &=\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{-\frac{\left(\alpha_T+\varepsilon\delta\alpha_T\right)}{2\left(l_p+\varepsilon\delta l_p\right)\left(c_p+\varepsilon\delta c_p\right)}\left[E(t)+\varepsilon\delta E(t)\right]^2\right.\\ &\quad\left.+\left(\varphi_0+\varepsilon\delta\varphi_0\right)\left(\gamma+\varepsilon\delta\gamma\right)\left(\sigma_f+\varepsilon\delta\sigma_f\right)\left(N_f+\varepsilon\delta N_f\right)\right\}_{\varepsilon=0},\end{aligned} \tag{19}$$

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\left[E(t)+\varepsilon\delta E(t)\right]_{t=0}\right\}_{\varepsilon=0} = 0\,. \tag{20}$$

Performing the operations indicated in Equations (19) and (20) yields the following differential equation, which constitutes the 1st-Level Variational Sensitivity System (1st-LVSS) for the 1st-level variational function $\delta E(t)$:

$$\begin{aligned}&\left\{\left[\frac{\mathrm{d}}{\mathrm{d}t}+\frac{\alpha_T}{l_p c_p}E(t)\right]\delta E(t)\right\}_{\boldsymbol{\alpha}^0}\\ &=\left\{-\frac{\delta\alpha_T}{2l_p c_p}+\frac{\alpha_T}{2l_p\left(c_p\right)^2}\delta c_p+\frac{\alpha_T}{2\left(l_p\right)^2 c_p}\delta l_p\right\}_{\boldsymbol{\alpha}^0}E^2(t)\\ &\quad+\left\{\varphi_0\sigma_f N_f(\delta\gamma)+\varphi_0\gamma N_f\left(\delta\sigma_f\right)+\varphi_0\gamma\sigma_f\left(\delta N_f\right)+\gamma\sigma_f N_f\left(\delta\varphi_0\right)\right\}_{\boldsymbol{\alpha}^0},\ t>0,\end{aligned} \tag{21}$$

$$\delta E(0) = 0,\ t = 0. \tag{22}$$

In Equation (21), the parameter variations are known and the notation $\{\ \}_{\boldsymbol{\alpha}^0}$ indicates that the quantity enclosed within the braces is to be evaluated at the nominal parameter values $\boldsymbol{\alpha}^0$. For every parameter variation, the 1st-LVSS would need to be solved anew. This need for repeatedly solving the 1st-LVSS can be avoided by constructing the corresponding 1st-Level Adjoint Sensitivity System (1st-LASS), by applying the 1st-CASAM-N methodology. Thus, the Hilbert space appropriate for the construction of the 1st-LASS corresponding to the above 1st-LVSS is endowed with the following inner product, denoted as $\langle u(t), v(t)\rangle$, between two square integrable functions $u(t)$ and $v(t)$:

$$\langle u(t), v(t)\rangle \triangleq \int_0^\tau u(t)v(t)\mathrm{d}t . \tag{23}$$

Forming the inner product of Equation (21) with a yet undefined function $a^{(1)}(t)$ yields the following relation:

$$\begin{aligned}&\left\{\int_0^\tau a^{(1)}(t)\left[\frac{\mathrm{d}}{\mathrm{d}t} + \frac{\alpha_T}{l_p c_p}E(t)\right]\delta E(t)\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0} \\ &= \left\{\varphi_0\sigma_f N_f(\delta\gamma) + \varphi_0\gamma N_f(\delta\sigma_f) + \varphi_0\gamma\sigma_f(\delta N_f) + \gamma\sigma_f N_f(\delta\varphi_0)\right\}_{\boldsymbol{\alpha}^0}\int_0^\tau a^{(1)}(t)\mathrm{d}t \\ &\quad + \left\{-\frac{\delta\alpha_T}{2l_p c_p} + \frac{\alpha_T}{2l_p(c_p)^2}\delta c_p + \frac{\alpha_T}{2(l_p)^2 c_p}\delta l_p\right\}_{\boldsymbol{\alpha}^0}\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t.\end{aligned} \tag{24}$$

Integrating by parts the left side of Equation (24) yields the following relation:

$$\begin{aligned}&\left\{\int_0^\tau a^{(1)}(t)\left[\frac{\mathrm{d}}{\mathrm{d}t} + \frac{\alpha_T}{l_p c_p}E(t)\right]\delta E(t)\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0} \\ &= a^{(1)}(\tau)\delta E(\tau) - a^{(1)}(0)\delta E(0) \\ &\quad + \left\{\int_0^\tau \delta E(t)\left[-\frac{\mathrm{d}a^{(1)}(t)}{\mathrm{d}t} + \frac{\alpha_T}{l_p c_p}E(t)a^{(1)}(t)\right]\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}.\end{aligned} \tag{25}$$

Identifying the left-side of Equation (25) with the G-differential $\delta E(\tau)$ of the response $E(\tau)$ and eliminating the unknown value $\delta E(\tau)$ from the right-side of Equation (25) by setting $a^{(1)}(\tau) = 0$ yields the following 1st-Level Adjoint Sensitivity System (1st-LASS) for the 1st-level adjoint sensitivity function $a^{(1)}(t)$:

$$\left\{\left[-\frac{\mathrm{d}}{\mathrm{d}t} + \frac{\alpha_T}{l_p c_p}E(t)\right]a^{(1)}(t)\right\}_{\boldsymbol{\alpha}^0} = \delta(t-\tau),\ t > 0, \tag{26}$$

$$a^{(1)}(\tau) = 0, \quad t = \tau . \tag{27}$$

For further reference, solving the above 1st-LASS yields the following closed-form expression for the 1st-level adjoint sensitivity function $a^{(1)}(t)$:

$$a^{(1)}(t) = H(\tau - t)\left\{\frac{\cosh[t\theta(\boldsymbol{\alpha})]}{\cosh[\tau\theta(\boldsymbol{\alpha})]}\right\}^2, \tag{28}$$

where $H(t - t_f)$ denotes the Heaviside functional.

Using the relations provided by the 1st-LVSS and the 1st-LASS in Equation (24), and recalling Equation (18), yields the following alternate expression of $\delta E(\tau)$ in terms of the 1st-Level adjoint sensitivity function $a^{(1)}(t)$:

$$\delta E(\tau)=\left\{-\frac{\delta\alpha_T}{2l_pc_p}+\frac{\alpha_T}{2l_p\left(c_p\right)^2}\delta c_p+\frac{\alpha_T}{2\left(l_p\right)^2c_p}\delta l_p\right\}_{\boldsymbol{\alpha}^0}\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t$$
$$+\left\{\varphi_0\sigma_fN_f\left(\delta\gamma\right)+\varphi_0\gamma N_f\left(\delta\sigma_f\right)+\varphi_0\gamma\sigma_f\left(\delta N_f\right)+\gamma\sigma_fN_f\left(\delta\varphi_0\right)\right\}_{\boldsymbol{\alpha}^0}\int_0^\tau a^{(1)}(t)\mathrm{d}t. \tag{29}$$

It follows from Equation (29) that the first-order sensitivities of the response $E(\tau)$ with respect to the model parameters have the following expressions in terms of the 1st-Level adjoint sensitivity function $a^{(1)}(t)$:

$$\begin{aligned}\frac{\partial E(\tau)}{\partial\alpha_T}&=-\frac{1}{2l_pc_p}\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t\\&=-\frac{K^2(\boldsymbol{\alpha})}{2l_pc_p}\left\{\frac{\tanh\left[\tau\theta(\boldsymbol{\alpha})\right]}{2\theta(\boldsymbol{\alpha})}-\frac{\tau}{2\cosh^2\left[\tau\theta(\boldsymbol{\alpha})\right]}\right\}\\&=\frac{\tau\varphi_0\gamma\sigma_fN_f}{\left(2\alpha_T\right)\cosh^2\left[\tau\theta(\boldsymbol{\alpha})\right]}-\left[\frac{2\varphi_0\gamma\sigma_fN_fl_pc_p}{\alpha_T}\right]^{1/2}\frac{\tanh\left[\tau\theta(\boldsymbol{\alpha})\right]}{2\alpha_T};\end{aligned}\tag{30}$$

$$\begin{aligned}\frac{\partial E(\tau)}{\partial l_p}&=\frac{\alpha_T}{2\left(l_p\right)^2c_p}\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t\\&=\left[\frac{\varphi_0\gamma\sigma_fN_fc_p}{2\alpha_Tl_p}\right]^{1/2}\tanh\left[\tau\theta(\boldsymbol{\alpha})\right]-\frac{\tau\varphi_0\gamma\sigma_fN_f}{\left(2l_p\right)\cosh^2\left[\tau\theta(\boldsymbol{\alpha})\right]};\end{aligned}\tag{31}$$

$$\begin{aligned}\frac{\partial E(\tau)}{\partial c_p}&=\frac{\alpha_T}{2l_p\left(c_p\right)^2}\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t\\&=\left[\frac{\varphi_0\gamma\sigma_fN_fl_p}{2\alpha_Tc_p}\right]^{1/2}\tanh\left[\tau\theta(\boldsymbol{\alpha})\right]-\frac{\tau\varphi_0\gamma\sigma_fN_f}{\left(2c_p\right)\cosh^2\left[\tau\theta(\boldsymbol{\alpha})\right]};\end{aligned}\tag{32}$$

$$\frac{\partial E(\tau)}{\partial\varphi_0}=\gamma\sigma_fN_f\int_0^\tau a^{(1)}(t)\mathrm{d}t=\gamma\sigma_fN_f\left\{\frac{\tanh\left[\tau\theta(\boldsymbol{\alpha})\right]}{2\theta(\boldsymbol{\alpha})}+\frac{\tau}{2\cosh^2\left[\tau\theta(\boldsymbol{\alpha})\right]}\right\}\tag{33}$$

$$\frac{\partial E(\tau)}{\partial\gamma}=\varphi_0\sigma_fN_f\int_0^\tau a^{(1)}(t)\mathrm{d}t=\varphi_0\sigma_fN_f\left\{\frac{\tanh\left[\tau\theta(\boldsymbol{\alpha})\right]}{2\theta(\boldsymbol{\alpha})}+\frac{\tau}{2\cosh^2\left[\tau\theta(\boldsymbol{\alpha})\right]}\right\}\tag{34}$$

$$\frac{\partial E(\tau)}{\partial\sigma_f}=\varphi_0\gamma N_f\int_0^\tau a^{(1)}(t)\mathrm{d}t=N_f\varphi_0\gamma\left\{\frac{\tanh\left[\tau\theta(\boldsymbol{\alpha})\right]}{2\theta(\boldsymbol{\alpha})}+\frac{\tau}{2\cosh^2\left[\tau\theta(\boldsymbol{\alpha})\right]}\right\}\tag{35}$$

$$\frac{\partial E(\tau)}{\partial N_f}=\varphi_0\gamma\sigma_f\int_0^\tau a^{(1)}(t)\mathrm{d}t=\sigma_f\varphi_0\gamma\left\{\frac{\tanh\left[\tau\theta(\boldsymbol{\alpha})\right]}{2\theta(\boldsymbol{\alpha})}+\frac{\tau}{2\cosh^2\left[\tau\theta(\boldsymbol{\alpha})\right]}\right\}\tag{36}$$

The following formulas have been used to obtain the expressions in Equations (30)-(33): $\int\sinh^2(ax)\mathrm{d}x=\sinh(2ax)/4a-x/2$ and $\int\cosh^2(ax)\mathrm{d}x=\sinh(2ax)/4a+x/2$.

### 3.2. Application of the 1st-FASAM-N to Obtain the First-Order Sensitivities of the Response $E(\tau)$ with Respect to the Features and Model Parameters

The form of Equation (10) indicates that the "features" (*i.e.*, functions) of model parameters characterizing this balance equation can be chosen as follows:

$$f_1(\boldsymbol{\alpha}) \triangleq \frac{\alpha_T}{2 l_p c_p};\; f_2(\boldsymbol{\alpha}) \triangleq \varphi_0 \gamma \sigma_f N_f;\; \boldsymbol{f}(\boldsymbol{\alpha}) \triangleq \left[ f_1(\boldsymbol{\alpha}), f_2(\boldsymbol{\alpha}) \right]^{\dagger}. \tag{37}$$

Consequently, Equation (10) can alternatively be written in terms of the "feature function" $\boldsymbol{f}(\boldsymbol{\alpha}) \triangleq \left[ f_1(\boldsymbol{\alpha}), f_2(\boldsymbol{\alpha}) \right]^{\dagger}$ as follows:

$$\frac{\mathrm{d}E(t)}{\mathrm{d}t} = -f_1(\boldsymbol{\alpha}) E^2(t) + f_2(\boldsymbol{\alpha}),\; E(0) = 0. \tag{38}$$

In terms of the feature function $\boldsymbol{f}(\boldsymbol{\alpha}) \triangleq \left[ f_1(\boldsymbol{\alpha}), f_2(\boldsymbol{\alpha}) \right]^{\dagger}$, the solution of Equation (38) has the following form:

$$E(t) = \left[ \frac{f_2(\boldsymbol{\alpha})}{f_1(\boldsymbol{\alpha})} \right]^{1/2} \tanh\left[ t g(\boldsymbol{\alpha}) \right];\; g(\boldsymbol{\alpha}) \triangleq \sqrt{f_1(\boldsymbol{\alpha}) f_2(\boldsymbol{\alpha})}. \tag{39}$$

Taking the G-differential of Equation (38) yields the following 1st-Level Variational Sensitivity System (1st-LVSS) for the variational function $\delta E(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon} \left\{ \frac{\mathrm{d}\left[ E(t) + \varepsilon \delta E(t) \right]}{\mathrm{d}t} + \left[ f_1 + \varepsilon (\delta f)_1 \right] \left[ E(t) + \varepsilon \delta E(t) \right]^2 - \left[ f_2 + \varepsilon (\delta f_2) \right] \right\}_{\varepsilon = 0} = 0 \tag{40}$$

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon} \left\{ \left[ E(t) + \varepsilon \delta E(t) \right]_{t=0} \right\}_{\varepsilon = 0} = 0. \tag{41}$$

Performing the operations indicated in Equations (40) and (41) yields the following expressions for the 1st-LVSS:

$$\left\{ \left[ \frac{\mathrm{d}}{\mathrm{d}t} + 2 f_1 E(t) \right] \delta E(t) \right\}_{\boldsymbol{f}^0} = \left\{ -\delta f_1 E^2(t) + \delta f_2 \right\}_{\boldsymbol{f}^0},\; t > 0, \tag{42}$$

$$\delta E(0) = 0,\; t = 0. \tag{43}$$

In Equation (42), the notation $\{\;\}_{\boldsymbol{f}^0}$ indicates that the quantity enclosed within the braces is to be evaluated at the nominal values $\boldsymbol{f}^0 \triangleq \left( f_1^0, f_2^0 \right)^{\dagger}$, $f_1^0 \triangleq f_1(\boldsymbol{\alpha}^0)$, $f_2^0 \triangleq f_2(\boldsymbol{\alpha}^0)$, of the components of the feature function $\boldsymbol{f}(\boldsymbol{\alpha})$. The 1st-LVSS would need to be solved anew for all variations $\delta f_1$, $\delta f_2$, in the components of the feature function $\boldsymbol{f}(\boldsymbol{\alpha})$. This need for repeatedly solving the 1st-LVSS can be avoided by constructing the corresponding 1st-Level Adjoint Sensitivity System (1st-LASS). Note that the left-side of Equation (42) is the same as the left-side of Equation (21). Therefore, the Hilbert space appropriate for the construction of the 1st-LASS corresponding to Equation (42) is the same as for the application of the 1st-CASAM-N, being endowed with the inner product defined in Equation (23). It is therefore also expected that the left-side of the 1st-LASS to be constructed for Equation (42) will be the same as the left-side of

Equation (26). Thus, forming the inner product of Equation(42) with a yet undefined function $a^{(1)}(t)$ yields the following relation:

$$\begin{aligned}&\left\{\int_0^\tau a^{(1)}(t)\left[\frac{\mathrm{d}}{\mathrm{d}t}+2f_1E(t)\right]\delta E(t)\,\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\&=\left\{-(\delta f_1)\int_0^\tau a^{(1)}(t)E^2(t)\,\mathrm{d}t+(\delta f_2)\int_0^\tau a^{(1)}(t)\,\mathrm{d}t\right\}_{\boldsymbol{f}^0}.\end{aligned} \tag{44}$$

Integrating by parts the left side of Equation (44) yields the following relation:

$$\begin{aligned}&\left\{\int_0^\tau a^{(1)}(t)\left[\frac{\mathrm{d}}{\mathrm{d}t}+2f_1E(t)\right]\delta E(t)\,\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}\\&=a^{(1)}(\tau)\delta E(\tau)-a^{(1)}(0)\delta E(0)+\left\{\int_0^\tau \delta E(t)\left[-\frac{\mathrm{d}a^{(1)}(t)}{\mathrm{d}t}+2f_1E(t)a^{(1)}(t)\right]\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}.\end{aligned} \tag{45}$$

Identifying the left-side of Equation (45) with the G-differential $\delta E(\tau)$ of the response $E(\tau)$ obtained in Equation (18), and eliminating the unknown value $\delta E(\tau)$ from the right-side of Equation (45) by setting $a^{(1)}(\tau)=0$ yields the following 1st-Level Adjoint Sensitivity System (1st-LASS) for the 1st-Level adjoint sensitivity function $a^{(1)}(t)$:

$$\left\{\left[-\frac{\mathrm{d}}{\mathrm{d}t}+2f_1E(t)\right]a^{(1)}(t)\right\}_{\boldsymbol{f}^0}=\delta(t-\tau),\ t>0, \tag{46}$$

$$a^{(1)}(\tau)=0,\quad t=\tau. \tag{47}$$

Note that the above 1st-LASS, comprising Equations (46) and (47), is the same as the 1st-LASS obtained for determining the sensitivities of the response with respect to the model parameters, *i.e.*, Equations (26) and (27). This outcome is expected since the 1st-LASS is independent of any variations in the model parameters and hence, variations in the feature functions. Therefore, the use of the same symbol, $a^{(1)}(t)$, for the 1st-level adjoint sensitivity function, which is the solution of either of these 1st-LASS, is justified. In terms of the feature function $\boldsymbol{f}(\boldsymbol{\alpha})$, the 1st-level adjoint sensitivity function $a^{(1)}(t)$ has the following closed-form expression:

$$a^{(1)}(t)=H(\tau-t)\left\{\frac{\cosh\left[t(f_1f_2)^{1/2}\right]}{\cosh\left[\tau(f_1f_2)^{1/2}\right]}\right\}^2, \tag{48}$$

where $H(t-\tau)$ denotes the Heaviside functional.

Using Equations (45)-(47) in Equation (44) yields the following expression for the first-order total G-differential $\delta E(\tau)$ of the response $E(\tau)$ in terms of the 1st-level adjoint function $a^{(1)}(t)$:

$$\delta E(\tau)=\left\{-(\delta f_1)\int_0^\tau a^{(1)}(t)E^2(t)\,\mathrm{d}t+(\delta f_2)\int_0^\tau a^{(1)}(t)\,\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}. \tag{49}$$

It follows from Equations (49), (48) and (39) that the two sensitivities of the response $E(\tau)$ with respect to the two components of the feature function $\boldsymbol{f} \triangleq (f_1, f_2)^\dagger$ have the following expressions:

$$\begin{aligned}\frac{\partial E(\tau)}{\partial f_1} &= -\int_0^\tau a^{(1)}(t) E^2(t)\,\mathrm{d}t \\ &= \frac{1}{2}\left[\frac{f_2(\boldsymbol{\alpha})}{f_1(\boldsymbol{\alpha})}\right]^{1/2} \left\{\frac{\tau}{\cosh^2\left[\tau g(\boldsymbol{\alpha})\right]} - \frac{\tanh\left[\tau g(\boldsymbol{\alpha})\right]}{g(\boldsymbol{\alpha})}\right\};\end{aligned} \tag{50}$$

$$\frac{\partial E(\tau)}{\partial f_2} = \int_0^\tau a^{(1)}(t)\,\mathrm{d}t = \frac{1}{2g(\boldsymbol{\alpha})}\tanh\left[\tau g(\boldsymbol{\alpha})\right] + \frac{\tau}{2\cosh^2\left[\tau g(\boldsymbol{\alpha})\right]}. \tag{51}$$

The above expressions are to be evaluated at the nominal parameter values but the notation $\{\ \}_{\alpha^0}$ has been omitted, for simplicity. The expressions obtained in Equations (50) and (51) can be verified by differentiating the expression provided in Equation (39), evaluated at a user-chosen time $t = \tau$ within the interval $0 < \tau < \infty$.

The sensitivities of the response $E(\tau)$ with respect to the model parameters are obtained by using the general relationship:

$$\frac{\partial E(\tau; f_1; f_2)}{\partial \alpha_i} = \frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1(\boldsymbol{\alpha})}{\partial \alpha_i} + \frac{\partial E(\tau)}{\partial f_2}\frac{\partial f_2(\boldsymbol{\alpha})}{\partial \alpha_i};\ i = 1,\cdots,7. \tag{52}$$

Using Equations (50) and (51) while recalling the definitions of the feature functions $f_1(\boldsymbol{\alpha})$ and $f_2(\boldsymbol{\alpha})$ defined in Equation (37) yields the explicit formulas for the particular cases of Equation (52), as follows:

$$\frac{\partial E(\tau)}{\partial \alpha_T} = \frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial \alpha_T} + \frac{\partial E(\tau)}{\partial f_2}\frac{\partial f_2}{\partial \alpha_T} = \frac{1}{2 l_p c_p}\frac{\partial E(\tau)}{\partial f_1}; \tag{53}$$

$$\frac{\partial E(\tau)}{\partial l_p} = \frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial l_p} + \frac{\partial E(\tau)}{\partial f_2}\frac{\partial f_2}{\partial l_p} = -\frac{\alpha_T}{2(l_p)^2 c_p}\frac{\partial E(\tau)}{\partial f_1}; \tag{54}$$

$$\frac{\partial E(\tau)}{\partial c_p} = \frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial c_p} + \frac{\partial E(\tau)}{\partial f_2}\frac{\partial f_2}{\partial c_p} = -\frac{\alpha_T}{2(c_p)^2 l_p}\frac{\partial E(\tau)}{\partial f_1}; \tag{55}$$

$$\frac{\partial E(\tau)}{\partial \varphi_0} = \frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_2}{\partial \varphi_0} + \frac{\partial E(\tau)}{\partial f_2}\frac{\partial f_2}{\partial \varphi_0} = \gamma\sigma_f N_f\frac{\partial E(\tau)}{\partial f_2}; \tag{56}$$

$$\frac{\partial E(\tau)}{\partial \gamma} = \frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial \gamma} + \frac{\partial E(\tau)}{\partial f_2}\frac{\partial f_2}{\partial \gamma} = \varphi_0\sigma_f N_f\frac{\partial E(\tau)}{\partial f_2}; \tag{57}$$

$$\frac{\partial E(\tau)}{\partial \sigma_f} = \frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial \sigma_f} + \frac{\partial E(\tau)}{\partial f_2}\frac{\partial f_2}{\partial \sigma_f} = \varphi_0\gamma N_f\frac{\partial E(\tau)}{\partial f_2}; \tag{58}$$

$$\frac{\partial E(\tau)}{\partial N_f} = \frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial N_f} + \frac{\partial E(\tau)}{\partial f_2}\frac{\partial f_2}{\partial N_f} = \varphi_0\gamma\sigma_f\frac{\partial E(\tau)}{\partial f_2}. \tag{59}$$

### 3.3. Comparative Discussion: Applying the 1st-CASAM-N versus the 1st-FASAM-N for Computing the First-Order Response Sensitivities to Model Parameters

Both the 1st-CASAM-N and the 1st-FASAM-N require the solution of the same

$1^{st}$-LASS. Hence, the application of the $1^{st}$-CASAM-N necessitates a single large-scale computation (for solving the $1^{st}$-LASS) to obtain all of the 7 first-order sensitivities for the instant energy response to the model parameters. The application of the $1^{st}$-FASAM-N also necessitates a single large-scale computation (for solving the same $1^{st}$-LASS as for the $1^{st}$-CASAM-N) to obtain the two first-order sensitivities of the model's response to the model's chosen feature functions. This equivalence between the application of the $1^{st}$-FASAM-N and the $1^{st}$-CASAM-N is as expected, since the $1^{st}$-LASS is independent of parameter variations or, equivalently, of variations in the feature functions. After the $1^{st}$-level adjoint function has been computed, the computation of the sensitivities to the model parameters using the $1^{st}$-FASAM-N additionally requires two quadratures to compute $\partial E(\tau)/\partial f_1$ and $\partial E(\tau)/\partial f_2$ using Equations (50) and (51), respectively, followed by simple differentiations of the feature functions with respect to the component parameters, as shown in Equations (53)-(59). Alternatively, computing the response sensitivities to the same model parameters using the $1^{st}$-CASAM-N additionally requires 7 integrations (quadratures), as shown in Equations (30)-(36). Neither these differentiations nor these quadratures require "large-scale" computations, so the differences in the computational resources needed to apply the $1^{st}$-FASAM-N versus applying the $1^{st}$-CASAM-N are minimal, with a slight advantage towards the $1^{st}$-FASAM-N, since the respective differentiations are computationally somewhat less demanding than the integrations/quadratures required by the application of the $1^{st}$-CASAM-N.

## 4. Computation of the Second-Order Response Sensitivities with Respect to Model Parameters: Applying the $2^{nd}$-FASAM-N Versus the $2^{nd}$-CASAM-N

The fundamental principle underlying both the $2^{nd}$-FASAM-N and the $2^{nd}$-CASAM-N methodologies is to determine the second-order sensitivities by employing their definition of being the "first-order sensitivities of the first-order sensitivities." Thus, each first-order sensitivity is treated as a "model response," and the G-differential of each of these "model responses" subsequently provides the partial second-order sensitivities that stem from the respective first-order sensitivity. As will be highlighted in Section 4.1, below, the computation of the 49 second-order sensitivities (of which 28 are distinct) of the response $E(\tau)$ with respect to the 7 model parameters will require just two large-scale computations (the solving the corresponding two $2^{nd}$-Level Adjoint Sensitivity Systems) when using the $2^{nd}$-FASAM-N methodology, since there are only two sensitivities of the response $E(\tau)$ with respect to the "feature functions" $f_1(\boldsymbol{\alpha})$ and $f_2(\boldsymbol{\alpha})$. In contradistinction, as will be highlighted in Section 4.2, applying the conventional $2^{nd}$-CASAM-N methodology requires 7 large-scale computations for solving the seven $2^{nd}$-Level Adjoint Sensitivity Systems (one $2^{nd}$-LASS for each of the 7 first-order sensitivities with respect to the primary model parameters) for obtaining all second-order sensitivities of the response $E(\tau)$ with respect to the model parameters.

## 4.1. Computation of Second-Order Sensitivities Using the $2^{\text{nd}}$-FASAM-N

The determination of the second-order sensitivities that stem from the first-order sensitivities $\partial E(\tau)/\partial f_1$ of the response $E(\tau)$ with respect to the "feature function" $f_1(\boldsymbol{\alpha})$ is presented in Subsection 4.1.1, while the second-order sensitivities that arise from the first-order sensitivities $\partial E(\tau)/\partial f_2$ of the response $E(\tau)$ with respect to the "feature function" $f_2(\boldsymbol{\alpha})$ will be presented in Subsection 4.1.2.

### 4.1.1. Computation of Second-Order Sensitivities Stemming from the First-Order Sensitivity $\partial E(\tau)/\partial f_1$

The $2^{\text{nd}}$-order sensitivities which stem from the $1^{\text{st}}$-order sensitivity $\partial E(\tau)/\partial f_1$ defined in Equation (50) will be obtained by determining the first-order G-differential $\delta\{\partial E(\tau)/\partial f_1\}$ of $\partial E(\tau)/\partial f_1$. By definition, the first-order G-differential of $\partial E(\tau)/\partial f_1$ is obtained as follows:

$$\begin{aligned}\delta\left\{\frac{\partial E(\tau; f_1, f_2)}{\partial f_1}\right\} &= -\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left[\int_0^\tau \left(a^{(1)}+\varepsilon\delta a^{(1)}\right)\left[E(t)+\varepsilon\delta E(t)\right]^2 \mathrm{d}t\right]\right\}_{\varepsilon=0} \\ &= -\int_0^\tau \left[2a^{(1)}(t)E(t)\delta E(t)+\delta a^{(1)}(t)E^2(t)\right]\mathrm{d}t \\ &= \frac{\partial^2 E(\tau; f_1, f_2)}{\partial f_1 \partial f_1}\delta f_1 + \frac{\partial^2 E(\tau; f_1, f_2)}{\partial f_2 \partial f_1}\delta f_2.\end{aligned} \tag{60}$$

The variational function $\delta a^{(1)}(t)$ is the solution of the system of equations obtained by G-differentiating the $1^{\text{st}}$-LASS defined in Equations (46) and (47). Performing the G-differentiation of this $1^{\text{st}}$-LASS yields the following equations:

$$\begin{aligned}&\left\{\left[-\frac{\mathrm{d}}{\mathrm{d}t}+2f_1E(t)\right]\delta a^{(1)}(t)+2f_1a^{(1)}(t)\left[\delta E(t)\right]\right\}_{\boldsymbol{f}^0} \\ &= -2\left\{(\delta f_1)a^{(1)}(t)E(t)\right\}_{\boldsymbol{f}^0},\ 0<t<\tau,\end{aligned} \tag{61}$$

$$\delta a^{(1)}(\tau)=0, \quad t=\tau. \tag{62}$$

Concatenating Equations (61) and (62) with the $1^{\text{st}}$-LVSS for $\delta E(t)$ defined in Equations (42) and (43) yields the following $2^{\text{nd}}$-Level Variational Sensitivity System ($2^{\text{nd}}$-LVSS) for the $2^{\text{nd}}$-Level variational function $\boldsymbol{V}^{(2)}(2;t) \triangleq \left[v^{(2)}(1;t), v^{(2)}(2;t)\right]^\dagger \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^\dagger$:

$$\left\{\boldsymbol{VM}^{(2)}[2\times 2; \boldsymbol{f}]\boldsymbol{V}^{(2)}(2;t)\right\}_{\boldsymbol{f}^0} = \left\{\boldsymbol{Q}_V^{(2)}[2; \boldsymbol{f}; \delta\boldsymbol{f}]\right\}_{\boldsymbol{f}^0},\ 0<t<\tau, \tag{63}$$

$$\left\{\boldsymbol{B}_V^{(2)}\left[2; \boldsymbol{V}^{(2)}(2;t); \boldsymbol{f}; \delta\boldsymbol{f}\right]\right\}_{\boldsymbol{f}^0} = \boldsymbol{0}[2], \quad \boldsymbol{0}[2] \triangleq [0,0]^\dagger, \tag{64}$$

where

$$\boldsymbol{VM}^{(2)}\left[2\times 2;\boldsymbol{f}\right]\triangleq\begin{pmatrix}\dfrac{\mathrm{d}}{\mathrm{d}t}+2f_1E(t) & 0\\ 2f_1a^{(1)}(t) & -\dfrac{\mathrm{d}}{\mathrm{d}t}+2f_1E(t)\end{pmatrix};\tag{65}$$

$$\boldsymbol{Q}_V^{(2)}\left[2;\boldsymbol{f};\delta\boldsymbol{f}\right]\triangleq\begin{bmatrix}-(\delta f_1)E^2(t)+(\delta f_2)\\ -2(\delta f_1)a^{(1)}(t)E(t)\end{bmatrix};\tag{66}$$

$$\boldsymbol{B}_V^{(2)}\left[2;\boldsymbol{V}^{(2)}(2;t);\boldsymbol{f};\delta\boldsymbol{f}\right]\triangleq\begin{pmatrix}\delta E(0)\\ \delta a^{(1)}(t_f)\end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix}.\tag{67}$$

The need for solving the 2nd-LVSS is circumvented by deriving an alternative expression for the first-order G-differential $\delta\left\{\partial E(\tau)/\partial f_1\right\}$ defined in Equation (60), in which the variational function $\boldsymbol{V}^{(2)}(2;t)\triangleq\left[v^{(2)}(1;t),v^{(2)}(2;t)\right]^{\dagger}\triangleq\left[\delta E(t),\delta a^{(1)}(t)\right]^{\dagger}$ is replaced by a 2nd-level adjoint function which will be denoted as $\boldsymbol{A}^{(2)}(2;1;t)\triangleq\left[a^{(2)}(1;1;t),a^{(2)}(2;1;t)\right]^{\dagger}\in\mathsf{H}_2$. The notation for $\boldsymbol{A}^{(2)}(2;1;t)\triangleq\left[a^{(2)}(1;1;t),a^{(2)}(2;1;t)\right]^{\dagger}\in\mathsf{H}_2$ has the following significance: (i) the bold letter "A" indicates a vector-valued "adjoint" function; (ii) the superscript "(2)" indicates "second-level"; (iii) the first argument, denoted as "2", in $\boldsymbol{A}^{(2)}(2;1;t)$ indicates that this vector has 2 components, denoted as $a^{(2)}(i;1;t)$, $i=1,2$, each of which is a scalar-valued function of time; (iv) the second argument of $\boldsymbol{A}^{(2)}(2;1;t)$, denoted as "1", indicates that this 2nd-level adjoint function corresponds to the first-order sensitivity $\partial E(\tau)/\partial f_1$ of the response with respect to the "first feature function", $f_1(\boldsymbol{\alpha})$. In Equation (63) and in the remainder of this work, matrices will be denoted by using two bold capital letters.

The 2nd-level adjoint function $\boldsymbol{A}^{(2)}(2;1;t)$ will be the solution of a 2nd-Level Adjoint Sensitivity System (2nd-LASS) to be constructed by applying the 2nd-FASAM-N methodology. This 2nd-LASS is constructed in a Hilbert space, denoted as $\mathsf{H}_2$, which comprises as elements block-vectors of the same form as $\boldsymbol{V}^{(2)}(2;t)$, and is endowed with the following inner product of two vectors $\boldsymbol{\Psi}^{(2)}(2;t)\triangleq\left[\psi^{(2)}(1;t),\psi^{(2)}(2;t)\right]^{\dagger}\in\mathsf{H}_2$ and $\boldsymbol{\Phi}^{(2)}(t)\triangleq\left[\varphi^{(2)}(1;t),\varphi^{(2)}(2;t)\right]^{\dagger}\in\mathsf{H}_2$:

$$\left\langle\boldsymbol{\Psi}^{(2)}(2;t),\boldsymbol{\Phi}^{(2)}(2;t)\right\rangle_2\triangleq\sum_{i=1}^{2}\int_0^{\tau}\psi^{(2)}(i;t)\varphi^{(2)}(i;t)\mathrm{d}t.\tag{68}$$

The inner product defined in Equation (68) is now used to construct the 2nd-Level Adjoint Sensitivity System (2nd-LASS) for the 2nd-level adjoint function $\boldsymbol{A}^{(2)}(2;t)\triangleq\left[a^{(2)}(1;t),a^{(2)}(2;t)\right]^{\dagger}\in\mathsf{H}_2$, as follows:

i) Using the inner product defined in Equation (68), form the inner product of $\boldsymbol{A}^{(2)}(2;1;t)\triangleq\left[a^{(2)}(1;1;t),a^{(2)}(2;1;t)\right]^{\dagger}\in\mathsf{H}_2$ with Equation (63), and subsequently integrate by parts the left-side of the resulting equation to obtain the following relation:

$$
\begin{aligned}
&\left\{\left\langle \boldsymbol{A}^{(2)}(2;1;t), \boldsymbol{VM}^{(2)}[2\times 2;\boldsymbol{f}]\boldsymbol{V}^{(2)}(2;t)\right\rangle_2\right\}_{\boldsymbol{f}^0} \\
&= \left\{\left\langle \boldsymbol{A}^{(2)}(2;1;t), \boldsymbol{Q}_V^{(2)}(2;\boldsymbol{f};\delta\boldsymbol{f})\right\rangle_2\right\}_{\boldsymbol{f}^0} \\
&= \left\{a^{(2)}(1;1;t)\,\delta E(t) - a^{(2)}(2;1;t)\,\delta a^{(1)}(t)\right\}_{t=0}^{t=\tau} \\
&\quad + \left\{\left\langle \boldsymbol{V}^{(2)}(2;t), \boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{f}]\boldsymbol{A}^{(2)}(2;1;t)\right\rangle_2\right\}_{\boldsymbol{f}^0}.
\end{aligned}
\tag{69}
$$

where the operator $\boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{f}]$ represents the formal adjoint of the operator $\boldsymbol{VM}^{(2)}(2\times 2;\boldsymbol{f})$, *i.e.*, $\boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{f}] \triangleq \left[\boldsymbol{VM}^{(2)}(2\times 2;\boldsymbol{f})\right]^*$, and is defined as follows:

$$
\begin{aligned}
\boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{f}] &\triangleq \left[\boldsymbol{VM}^{(2)}(2\times 2;\boldsymbol{f})\right]^* \\
&\triangleq \begin{pmatrix} -\dfrac{\mathrm{d}}{\mathrm{d}t} + 2f_1(\boldsymbol{\alpha})E(t) & 2f_1(\boldsymbol{\alpha})a^{(1)}(t) \\ 0 & \dfrac{\mathrm{d}}{\mathrm{d}t} + 2f_1(\boldsymbol{\alpha})E(t) \end{pmatrix}.
\end{aligned}
\tag{70}
$$

ii) Eliminate the boundary terms on the right-side of the second equality in Equation (69) and require the last term on the right-side of the second equality in Equation (69) to represent the right-side of Equation (60) by imposing the following relations:

$$
\left\{\boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{f}]\boldsymbol{A}^{(2)}(2;1;t)\right\}_{\boldsymbol{f}^0} = \left\{\begin{pmatrix} -2a^{(1)}(t)E(t) \\ -E^2(t) \end{pmatrix}\right\}_{\boldsymbol{f}^0}, \quad 0 < t < \tau,
\tag{71}
$$

$$
\left\{\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{A}^{(2)}(2;1;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{f}^0} \triangleq \begin{pmatrix} a^{(2)}(1;1;\tau) \\ a^{(2)}(2;1;0) \end{pmatrix}_{\boldsymbol{f}^0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.
\tag{72}
$$

The relations represented by Equations (71) and (72) constitute the 2nd-LASS for the 2nd-Level adjoint function $\boldsymbol{A}^{(2)}(2;1;t)$. Notably, the 2nd-LASS is independent of variations in the feature functions (and/or parameter variations), so it needs to be solved just once to obtain the 2nd-Level adjoint function $\boldsymbol{A}^{(2)}(2;1;t)$. Furthermore, the 2nd-LASS is an upper-triangular system, so the equations need not solved simultaneously, but can be solved sequentially, first for the component $a^{(2)}(2;1;t)$ and subsequently for the component $a^{(2)}(1;1;t)$.

Solving Equations (71) and (72) yields the following closed-form expressions for the components of the 2nd-Level adjoint sensitivity function $\boldsymbol{A}^{(2)}(2;1;t)$:

$$
\begin{aligned}
a^{(2)}(1;1;t) &= \frac{\int_t^\tau \left[2a^{(1)}(x)E(x) - 2f_1 a^{(2)}(2;1;x)\right]\cosh^2\left[xg(\boldsymbol{\alpha})\right]\mathrm{d}x}{\cosh^2\left[tg(\boldsymbol{\alpha})\right]} \\
&= \cosh^{-2}\left[tg(\boldsymbol{\alpha})\right]\left\{\frac{2}{f_1(\boldsymbol{\alpha})}\left[1 - \frac{\cosh\left[tg(\boldsymbol{\alpha})\right]}{\cosh\left[\tau g(\boldsymbol{\alpha})\right]}\right]\right. \\
&\quad \left. - \frac{2}{3f_1(\boldsymbol{\alpha})}\left[\frac{1}{2}\cosh^2\left[\tau g(\boldsymbol{\alpha})\right] - \frac{1}{2}\cosh^2\left[tg(\boldsymbol{\alpha})\right] - \ln\frac{\cosh\left[\tau g(\boldsymbol{\alpha})\right]}{\cosh\left[tg(\boldsymbol{\alpha})\right]}\right]\right\};
\end{aligned}
\tag{73}
$$

$$\begin{aligned} a^{(2)}(2;1;t) &= \cosh^2\left[tg(\boldsymbol{\alpha})\right]\int_0^t E^2(x)\cosh^{-2}\left[xg(\boldsymbol{\alpha})\right]\mathrm{d}x \\ &= \frac{1}{3g(\boldsymbol{\alpha})}\frac{f_2(\boldsymbol{\alpha})}{f_1(\boldsymbol{\alpha})}\tanh\left[tg(\boldsymbol{\alpha})\right]\sinh^2\left[tg(\boldsymbol{\alpha})\right]. \end{aligned} \tag{74}$$

iii) Use the relations provided by the 2nd-LVSS and the 2nd-LASS in Equation (69) to obtain the following expression for the variation $\delta\left\{\partial E(\tau)/\partial f_1\right\}$ in terms of the 2nd-level adjoint function $\boldsymbol{A}^{(2)}(2;1;t)$:

$$\begin{aligned} &\delta\left\{\frac{\partial E(\tau)}{\partial f_1}\right\} = \frac{\partial^2 E(\tau; f_1, f_2)}{\partial f_1 \partial f_1}\delta f_1 + \frac{\partial^2 E(\tau; f_1, f_2)}{\partial f_2 \partial f_1}\delta f_2 \\ &= \left\{\left\langle \boldsymbol{A}^{(2)}(2;1;t), \boldsymbol{Q}_V^{(2)}(2; \boldsymbol{f}; \delta \boldsymbol{f})\right\rangle_2\right\}_{\boldsymbol{f}^0} \\ &= \int_0^\tau \mathrm{d}t\left\{a^{(2)}(1;1;t)\left[-(\delta f_1)E^2(t) + (\delta f_2)\right] - a^{(2)}(2;1;t)2(\delta f_1)a^{(1)}(t)E(t)\right\}. \end{aligned} \tag{75}$$

It follows from Equation (75) that:

$$\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1} = -\int_0^\tau \left[a^{(2)}(1;1;t)E(t) + 2a^{(2)}(2;1;t)a^{(1)}(t)\right]E(t)\mathrm{d}t; \tag{76}$$

$$\frac{\partial^2 E(\tau)}{\partial f_2 \partial f_1} = \int_0^\tau a^{(2)}(1;1;t)\mathrm{d}t\,. \tag{77}$$

#### 4.1.2. Computation of Second-Order Sensitivities Stemming from the First-Order Sensitivity $\partial E(\tau)/\partial f_2$

The 2nd-order sensitivities which stem from the 1st-order sensitivity $\partial E(\tau)/\partial f_2$ defined in Equation (51) will be obtained from the first-order G-differential $\delta\left\{\partial E(\tau)/\partial f_2\right\}$ of $\partial E(\tau)/\partial f_2$. By definition, the first-order G-differential $\delta\left\{\partial E(\tau)/\partial f_2\right\}$ is obtained as follows:

$$\begin{aligned} \delta\left\{\frac{\partial E(\tau; f_1, f_2)}{\partial f_2}\right\} &= \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left[\int_0^\tau \left(a^{(1)} + \varepsilon \delta a^{(1)}\right)\mathrm{d}t\right]\right\}_{\varepsilon=0} = \int_0^\tau \delta a^{(1)}(t)\mathrm{d}t \\ &= \frac{\partial^2 E(\tau; f_1, f_2)}{\partial f_1 \partial f_2}\delta f_1 + \frac{\partial^2 E(\tau; f_1, f_2)}{\partial f_2 \partial f_2}\delta f_2. \end{aligned} \tag{78}$$

The variational function $\delta a^{(1)}(t)$ is the solution of Equations (61) and (62). Notably, the right-side of Equation (78) depends only on the variational function $\delta a^{(1)}(t)$, but does not depend directly on the variational function $\delta E(t)$. Nevertheless, since the variational function $\delta a^{(1)}(t)$ is related to the variational function $\delta E(t)$ through Equations (61) and (62), the 2nd-level adjoint function that will be constructed in order to eliminate the appearance of $\delta a^{(1)}(t)$ on the right-side of Equation (78) will be the solution of a 2nd-LASS which will correspond to the 2nd-LVSS defined by Equations (63) and (64). The construction of the 2nd-LASS that will be used to eliminate the appearance of the variational function $\delta a^{(1)}(t)$ from Equation (78) follows the same steps as in Subsection 4.1, above. The 2nd-level adjoint function that will be defined for this purpose will be denoted as $\boldsymbol{A}^{(2)}(2;2;t) \triangleq \left[a^{(2)}(1;2;t), a^{(2)}(2;2;t)\right]^\dagger \in \mathsf{H}_2$, where the notation has the following significance: (i) the bold letter "A" indicates a vector-valued "adjoint" function within the 2nd-FASAM-N formalism; (ii) the superscript "(2)" indicates "second-level"; (iii) the first argument, *i.e.*, "2", in $\mathbf{A}^{(2)}(2;2;t)$ indicates that this vector has 2 components, denoted as $a^{(2)}(i;2;t)$, $i=1,2$, each of which is a scalar-valued function of time; (iv) the (second) argument of $\mathbf{A}^{(2)}(2;2;t)$, denoted as "2", indicates that this 2nd-level adjoint function corresponds to the first-order sensitivity $\partial E(\tau)/\partial f_2$ of the response with respect to the "second feature function", *i.e.*, $f_2(\boldsymbol{\alpha})$.

The inner product defined in Equation (68) is now used to construct the 2nd-Level Adjoint Sensitivity System (2nd-LASS) for the 2nd-Level adjoint function $\mathbf{A}^{(2)}(2;2;t)$ by following the same sequence of steps as used in Subsection 4.1, above, but using the expression provided in Equation (78) to determine the right-side ("source") for the 2nd-LASS. This procedure leads to the following 2nd-LASS for the 2nd-Level adjoint function $\mathbf{A}^{(2)}(2;2;t)$:

$$\left\{\mathbf{AM}^{(2)}\left[2\times 2;\mathbf{f}\right]\mathbf{A}^{(2)}(2;2;t)\right\}_{\mathbf{f}^0}=\left\{\begin{pmatrix}0\\1\end{pmatrix}\right\}_{\mathbf{f}^0},\quad 0<t<\tau, \tag{79}$$

$$\left\{\mathbf{B}_A^{(2)}\left[2;\mathbf{A}^{(2)}(2;2;t);\boldsymbol{\alpha}\right]\right\}_{\mathbf{f}^0}\triangleq\left\{\begin{pmatrix}a^{(2)}(1;2;\tau)\\a^{(2)}(2;2;0)\end{pmatrix}\right\}_{\mathbf{f}^0}=\begin{pmatrix}0\\0\end{pmatrix}. \tag{80}$$

Solving Equations (79) and (80) yields the following closed-form expressions for the components of the 2nd-Level adjoint sensitivity function $\mathbf{A}^{(2)}(2;2;t)$:

$$a^{(2)}(1;2;t)=\frac{1}{2f_2(\boldsymbol{\alpha})}\left\{-\cosh^2\left[tg(\boldsymbol{\alpha})\right]+\frac{\cosh^4\left[\tau g(\boldsymbol{\alpha})\right]}{\cosh^2\left[tg(\boldsymbol{\alpha})\right]}\right\}; \tag{81}$$

$$a^{(2)}(2;2;t)=-\frac{1}{2g(\boldsymbol{\alpha})}\sinh\left[2tg(\boldsymbol{\alpha})\right]. \tag{82}$$

The expressions in Equations (81) and (82) are to be evaluated at the nominal values of the feature functions (and, implicitly, at the nominal parameter values) but the notation $\{\ \}_{\mathbf{f}^0}$ has been omitted for simplicity.

Using the relations provided by the 2nd-LVSS and the 2nd-LASS provided in Equations (79) and (80) for the of the 2nd-Level adjoint function $\mathbf{A}^{(2)}(2;2;t)$ leads to the following expression for the variation $\delta\left\{\partial E(\tau)/\partial f_2\right\}$ in terms of the 2nd-Level adjoint function $\mathbf{A}^{(2)}(2;2;t)$:

$$\begin{aligned}\delta\left\{\frac{\partial E(\tau)}{\partial f_2}\right\}&=\frac{\partial^2 E(\tau;f_1,f_2)}{\partial f_1\partial f_2}\delta f_1+\frac{\partial^2 E(\tau;f_1,f_2)}{\partial f_2\partial f_2}\delta f_2\\&=\left\{\left\langle\mathbf{A}^{(2)}(2;2;t),\mathbf{Q}_V^{(2)}(2;\mathbf{f};\delta\mathbf{f})\right\rangle_2\right\}_{\mathbf{f}^0}\\&=\int_0^\tau \mathrm{d}t\left\{a^{(2)}(1;2;t)\left[-(\delta f_1)E^2(t)+(\delta f_2)\right]-a^{(2)}(2;2;t)2(\delta f_1)a^{(1)}(t)E(t)\right\}.\end{aligned} \tag{83}$$

It follows from Equation (83) that:

$$\frac{\partial^2 E(\tau)}{\partial f_1\partial f_2}=-\int_0^\tau\left[a^{(2)}(1;2;t)E(t)+2a^{(2)}(2;2;t)a^{(1)}(t)\right]E(t)\mathrm{d}t; \tag{84}$$

$$\frac{\partial^2 E(\tau)}{\partial f_2 \partial f_2} = \int_0^\tau a^{(2)}(1;2;t)\,\mathrm{d}t \,. \tag{85}$$

It is important to note that the mixed second-order partial derivative $\partial^2 E(\tau)/\partial f_1 \partial f_2$ can be obtained by using either Equation (84) or Equation (77). The equivalence between the two respective expressions provides a stringent verification of the accuracy of solving the two 2nd-LASS, one for $\boldsymbol{A}^{(2)}(2;1;t)$ comprising Equations (71) and (72), and the other 2nd-LASS, comprising Equations (79) and (80) for $\boldsymbol{A}^{(2)}(2;2;t)$.

The second-order sensitivities of the response $E(\tau)$ with respect to the primary model parameters are obtained by using the parameter-dependencies of the functions $f_1(\boldsymbol{\alpha})$ and $f_2(\boldsymbol{\alpha})$, cf. Equation (37), in conjunction with the expressions obtained in Equations (76), (77), (84) and (85) by using the following general formula, which is obtained by taking the total differential of the expression provided in Equation (52):

$$\begin{aligned}\frac{\partial^2 E(\tau; f_1; f_2)}{\partial \alpha_j \partial \alpha_i} &= \left[\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1}\frac{\partial f_1(\boldsymbol{\alpha})}{\partial \alpha_j} + \frac{\partial^2 E(\tau)}{\partial f_2 \partial f_1}\frac{\partial f_2(\boldsymbol{\alpha})}{\partial \alpha_j}\right]\frac{\partial f_1(\boldsymbol{\alpha})}{\partial \alpha_i} + \frac{\partial E(\tau)}{\partial f_1}\frac{\partial^2 f_1(\boldsymbol{\alpha})}{\partial \alpha_j \partial \alpha_i} \\ &+ \left[\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_2}\frac{\partial f_1(\boldsymbol{\alpha})}{\partial \alpha_j} + \frac{\partial^2 E(\tau)}{\partial f_2 \partial f_2}\frac{\partial f_2(\boldsymbol{\alpha})}{\partial \alpha_j}\right]\frac{\partial f_2(\boldsymbol{\alpha})}{\partial \alpha_i} + \frac{\partial E(\tau)}{\partial f_2}\frac{\partial^2 f_2(\boldsymbol{\alpha})}{\partial \alpha_j \partial \alpha_i};\end{aligned} \tag{86}$$

$i, j = 1, \cdots, 7.$

For example, the second-order sensitivities of the response $E(\tau)$ with respect to the parameter $\alpha_T$ are obtained as follows:

$$\frac{\partial^2 E(\tau)}{\partial \alpha_T \partial \alpha_T} = \frac{\partial}{\partial \alpha_T}\left(\frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial \alpha_T}\right) = \frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1}\left(\frac{\partial f_1}{\partial \alpha_T}\right)^2 = \left(\frac{1}{2 l_p c_p}\right)^2 \frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1}; \tag{87}$$

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial c_p \partial \alpha_T} &= \frac{\partial}{\partial c_p}\left(\frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial \alpha_T}\right) = \frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1}\frac{\partial f_1}{\partial c_p}\frac{\partial f_1}{\partial \alpha_T} + \frac{\partial E(\tau)}{\partial f_1}\frac{\partial^2 f_1}{\partial c_p \partial \alpha_T} \\ &= -\frac{\alpha_T}{4(l_p)^2 (c_p)^3}\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1} - \frac{1}{2 l_p (c_p)^2}\frac{\partial E(\tau)}{\partial f_1}.\end{aligned} \tag{88}$$

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial l_p \partial \alpha_T} &= \frac{\partial}{\partial l_p}\left(\frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial \alpha_T}\right) = \frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1}\frac{\partial f_1}{\partial l_p}\frac{\partial f_1}{\partial \alpha_T} + \frac{\partial E(\tau)}{\partial f_1}\frac{\partial^2 f_1}{\partial l_p \partial \alpha_T} \\ &= -\frac{\alpha_T}{4(c_p)^2 (l_p)^3}\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1} - \frac{1}{2 c_p (l_p)^2}\frac{\partial E(\tau)}{\partial f_1}.\end{aligned} \tag{89}$$

$$\frac{\partial^2 E(\tau)}{\partial \varphi_0 \partial \alpha_T} = \frac{\partial}{\partial \varphi_0}\left(\frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial \alpha_T}\right) = \frac{1}{2 l_p c_p}\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_2}\frac{\partial f_2}{\partial \varphi_0} = \frac{\gamma \sigma_f N_f}{2 l_p c_p}\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_2}; \tag{90}$$

$$\frac{\partial^2 E(t_f)}{\partial \gamma \partial \alpha_T} = \frac{\partial}{\partial \gamma}\left(\frac{\partial E(t_f)}{\partial f_1}\frac{\partial f_1}{\partial \alpha_T}\right) = \frac{1}{2 l_p c_p}\frac{\partial^2 E(t_f)}{\partial f_1 \partial f_2}\frac{\partial f_2}{\partial \gamma} = \frac{\varphi_0 \sigma_f N_f}{2 l_p c_p}\frac{\partial^2 E(t_f)}{\partial f_1 \partial f_2}; \tag{91}$$

$$\frac{\partial^2 E(\tau)}{\partial\sigma_f \partial\alpha_T} = \frac{\partial}{\partial\sigma_f}\left(\frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial\alpha_T}\right) = \frac{1}{2l_p c_p}\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_2}\frac{\partial f_2}{\partial\sigma_f} = \frac{\gamma\varphi_0 N_f}{2l_p c_p}\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_2}; \tag{92}$$

$$\frac{\partial^2 E(\tau)}{\partial N_f \partial\alpha_T} = \frac{\partial}{\partial N_f}\left(\frac{\partial E(\tau)}{\partial f_1}\frac{\partial f_1}{\partial\alpha_T}\right) = \frac{1}{2l_p c_p}\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_2}\frac{\partial f_2}{\partial N_f} = \frac{\gamma\varphi_0 \sigma_f}{2l_p c_p}\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_2}. \tag{93}$$

Because of symmetry, the mixed second-order sensitivities $\partial^2 E(\tau)/\partial f_1 \partial f_2$ or $\partial^2 E(\tau)/\partial f_2 \partial f_1$ can be obtained by using distinct but equivalent expressions in terms of the 2nd-Level adjoint functions $\boldsymbol{A}^{(2)}(2;1;t)$ and $\boldsymbol{A}^{(2)}(2;2;t)$, since the expressions obtained in Equations (77) and (84) represent the same quantity, because $\partial^2 E(\tau)/\partial f_1 \partial f_2 = \partial^2 E(\tau)/\partial f_2 \partial f_1$ by definition. Notably, only two "large-scale computations" are necessary for solving the two distinct 2nd-LASS for obtaining the 2nd-Level adjoint functions $\boldsymbol{A}^{(2)}(2;1;t)$ and $\boldsymbol{A}^{(2)}(2;2;t)$ involved in the computation of the three distinct second-order response sensitivities *i.e.*, $\partial^2 E(\tau)/\partial f_1 \partial f_1$, $\partial^2 E(\tau)/\partial f_1 \partial f_2$ and $\partial^2 E(\tau)/\partial f_2 \partial f_2$, with respect to the two feature functions $f_1$ and $f_2$. The subsequent use of Equation (86) to obtain the 49 second-order sensitivities $\partial^2 E(\tau)/\partial\alpha_i \partial\alpha_j$ of the response with respect to the primary model parameters involves only inexpensive differentiations that are performed exactly, analytically, since the exact dependence of the feature functions on the model parameters is explicitly known. For verification purposes, all of the mixed second-order sensitivities $\partial^2 E(\tau)/\partial\alpha_i \partial\alpha_j$, $i, j = 1,\cdots,7$, with respect to the model parameters can be computed twice, using distinct expressions in terms of the 2nd-Level adjoint functions $\boldsymbol{A}^{(2)}(2;1;t)$ and $\boldsymbol{A}^{(2)}(2;2;t)$.

### 4.2. Computation of Second-Order Sensitivities Using the 2nd-CASAM-N

The conventional 2nd-CASAM-N methodology applies the same fundamental principle (namely that the second-order sensitivities are the "first-order sensitivities of the first-order sensitivities") as the 2nd-FASAM. However, this principle is applied within the 2nd-CASAM-N methodology directly to the first-order sensitivities with respect to the primary model parameters, as opposed to applying this principle to the first-order response sensitivities with respect to the feature functions, as implemented within the application of the 2nd-FASAM-N methodology. This Section illustrates the application of the conventional 2nd-CASAM-N methodology to obtain the second-order response sensitivities from the seven first-order sensitivities with respect to the underlying model parameters (as obtained in Subsection 3.1). It will be shown in this Section that the application of the *2nd-CASAM-N* methodology will require solving *seven* distinct 2nd-Level Adjoint Sensitivity Systems (2nd-LASS), each system comprising a distinct source term which corresponds to one of the seven distinct first-order sensitivities, in order to obtain all of the second-order sensitivities. In contradistinction, the application of the *2nd-FASAM-N* requires solving only *two* 2nd-LASS, as will be shown in Section 6, in the sequel.

#### 4.2.1. Computation of Second-Order Sensitivities Stemming from the First-Order Sensitivity $\partial E(\tau)/\partial \alpha_T$

The second-order sensitivities which stem from the first-order sensitivity $\partial E(\tau)/\partial \alpha_T$ are the components of the first-order G-differential of Equation (30). By definition, the first-order G-differential of Equation (30) is obtained as follows:

$$\delta\left\{\partial E(\tau)/\partial \alpha_T\right\}_{\boldsymbol{\alpha}^0} \triangleq \left\{\delta\left[\partial E(\tau)/\partial \alpha_T\right]\right\}_{dir} + \left\{\delta\left[\partial E(\tau)/\partial \alpha_T\right]\right\}_{ind}$$
$$\triangleq \left\{-\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\left[\frac{1}{2\left(l_p+\varepsilon\delta l_p\right)\left(c_p+\varepsilon\delta c_p\right)}\int_0^\tau\left(a^{(1)}+\varepsilon\delta a^{(1)}\right)\left[E(t)+\varepsilon\delta E(t)\right]^2\mathrm{d}t\right]_{\boldsymbol{\alpha}^0}\right\}\right\}_{\varepsilon=0}, \tag{94}$$

where the "direct-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \alpha_T\right]\right\}_{dir}$ can be determined immediately and is defined as follows:

$$\left\{\delta\left[\partial E(\tau)/\partial \alpha_T\right]\right\}_{dir} \triangleq \left\{\left[\frac{\delta l_p}{2\left(l_p\right)^2 c_p}+\frac{\delta c_p}{2l_p\left(c_p\right)^2}\right]\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0} \tag{95}$$

and where the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \alpha_T\right]\right\}_{ind}$ is defined as follows:

$$\left\{\delta\left[\partial E(\tau)/\partial \alpha_T\right]\right\}_{ind} \triangleq -\left\{\frac{1}{2l_pc_p}\int_0^\tau\left[\delta a^{(1)}(t)E^2(t)+2a^{(1)}(t)E(t)\delta E(t)\right]\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}. \tag{96}$$

The variational function $\delta E(t)$ in Equation (96) is the solution of the 1st-LVSS provided in Equations (21) and (22). The variational function $\delta a^{(1)}(t)$ in Equation (96) is the solution of Equations (61) and (62), but written in terms of the primary model parameters and variations thereof, as follows:

$$\left\{\left[-\frac{\mathrm{d}}{\mathrm{d}t}+\frac{\alpha_T}{l_pc_p}E(t)\right]\delta a^{(1)}(t)+\frac{\alpha_T}{l_pc_p}\left[\delta E(t)\right]\right\}_{\boldsymbol{\alpha}^0}$$
$$=\left\{\left[\frac{\delta\alpha_T}{l_pc_p}-\frac{\alpha_T}{l_p\left(c_p\right)^2}\delta c_p-\frac{\alpha_T}{\left(l_p\right)^2c_p}\delta l_p\right]a^{(1)}(t)E(t)\right\}_{\boldsymbol{\alpha}^0},\ 0<t<\tau, \tag{97}$$

$$\delta a^{(1)}(\tau)=0,\quad t=\tau. \tag{98}$$

Concatenating Equations (97) and (98) with the 1st-LVSS for $\delta E(t)$ represented by Equations (21) and (22) yields the following 2nd-LVSS for the 2nd-level variational function $\boldsymbol{V}^{(2)}(2;t)\triangleq\left[v^{(2)}(1;t),v^{(2)}(2;t)\right]^\dagger\triangleq\left[\delta E(t),\delta a^{(1)}(t)\right]^\dagger$:

$$\left\{\boldsymbol{VM}^{(2)}\left[2\times 2;\boldsymbol{\alpha}\right]\boldsymbol{V}^{(2)}(2;t)\right\}_{\boldsymbol{\alpha}^0}=\left\{\boldsymbol{S}_V^{(2)}\left[2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0},\ 0<t<\tau, \tag{99}$$

$$\left\{\boldsymbol{B}_V^{(2)}\left[2;\boldsymbol{V}^{(2)}(2;t);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0}=\boldsymbol{0}[2],\quad \boldsymbol{0}[2]\triangleq[0,0]^\dagger, \tag{100}$$

where

$$\boldsymbol{VM}^{(2)}[2\times 2;\boldsymbol{\alpha}] \triangleq \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}t} + \frac{\alpha_T}{l_p c_p} E(t) & 0 \\ \frac{\alpha_T}{l_p c_p} & -\frac{\mathrm{d}}{\mathrm{d}t} + {\frac{\alpha_T}{l_p c_p}}_{1} E(t) \end{pmatrix}; \tag{101}$$

$$\boldsymbol{S}_V^{(2)}[2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}] \triangleq \begin{bmatrix} s_V^{(2)}(1;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}) \\ s_V^{(2)}(2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}) \end{bmatrix}; \tag{102}$$

$$\begin{gathered} s_V^{(2)}(1;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}) \triangleq \left\{ -\frac{\delta\alpha_T}{2l_p c_p} + \frac{\alpha_T}{2(l_p)^2 c_p}\delta l_p + \frac{\alpha_T}{2l_p (c_p)^2}\delta c_p \right\}_{\boldsymbol{\alpha}^0} E^2(t) \\ + \left\{ \gamma\sigma_f N_f(\delta\varphi_0) + \varphi_0\sigma_f N_f(\delta\gamma) + \varphi_0\gamma N_f(\delta\sigma_f) + \varphi_0\gamma\sigma_f(\delta N_f) \right\}_{\boldsymbol{\alpha}^0}; \end{gathered} \tag{103}$$

$$s_V^{(2)}(2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}) \triangleq \left\{ -\frac{\delta\alpha_T}{l_p c_p} + \frac{\alpha_T}{(l_p)^2 c_p}\delta l_p + \frac{\alpha_T}{l_p (c_p)^2}\delta c_p \right\}_{\boldsymbol{\alpha}^0} a^{(1)}(t) E(t); \tag{104}$$

$$\boldsymbol{B}_V^{(2)}\left[2;\boldsymbol{V}^{(2)}(2;t);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right] \triangleq \begin{pmatrix} \delta E(0) \\ \delta a^{(1)}(\tau) \end{pmatrix}. \tag{105}$$

Except for the distinct notation, the 2nd-LVSS defined by Equations (99) and (100) is identical with the 2nd-LVSS defined by Equations (63) and (64), which is the reason for having used for both systems of equations the same notation for the respective 2nd-Level variational function, namely $\boldsymbol{V}^{(2)}(2;t) \triangleq \left[v^{(2)}(1;t), v^{(2)}(2;t)\right]^\dagger \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^\dagger$, which is the solution of this 2nd-LVSS. However, the dependence on the components of the vector of parameters, $\boldsymbol{\alpha} \triangleq (\gamma, \sigma_f, N_f, \varphi_0, l_p, \alpha_T, c_p)^\dagger$, is emphasized in Equations (99) and (100), because this explicit dependence is necessary to distinguish the developments of the 2nd-Level Adjoint Sensitivity Systems to follow, which will be distinct from each other depending on the specific expression of each of the seven first-order sensitivities of the response with respect to the primary model parameters.

As discussed in Subsection 4.1, the computationally expensive path of solving the 2nd-LVSS repeatedly for every possible parameter variation will be avoided by replacing the variational function $\boldsymbol{V}^{(2)}(2;t)$ in the expression of the "indirect-effect" term defined in Equation (96) by a corresponding 2nd-level adjoint function, which will be denoted as $\boldsymbol{C}^{(2)}(2;1;t) \triangleq \left[c^{(2)}(1;1;t), c^{(2)}(2;1;t)\right]^\dagger \in \mathsf{H}_2$. This vector-valued function will be the solution of a 2nd-Level Adjoint Sensitivity System (2nd-LASS) to be constructed by applying the 2nd-CASAM-N. The notation used for $\boldsymbol{C}^{(2)}(2;1;t) \triangleq \left[c^{(2)}(1;1;t), c^{(2)}(2;1;t)\right]^\dagger \in \mathsf{H}_2$ has the following significance: (i) the bold letter "C" indicates a vector-valued "adjoint" function within the 2nd-CASAM-N formalism; (ii) the superscript "(2)" indicates "second-level"; (iii) the first argument, namely "2", in $\boldsymbol{C}^{(2)}(2;1;t)$ indicates that this vector has 2 components, denoted as $c^{(2)}(i;2;t)$, $i = 1,2$, each of which is a scalar-valued function of time; (iv) the second argument of $\boldsymbol{C}^{(2)}(2;1;t)$ is denoted as "1" and indicates that this 2nd-level adjoint function corresponds to the first-order sensitivity $\partial E(\tau)/\partial \alpha_T$ of the response with respect to the *first* component of the vector of model parameters $\boldsymbol{\alpha} \triangleq (\alpha_1, \cdots, \alpha_7)^\dagger \triangleq (\alpha_T, l_p, c_p, \varphi_0, \gamma, \sigma_f, N_f)^\dagger$, namely $\alpha_T$.

The 2nd-LASS for the function $\boldsymbol{C}^{(2)}(2;1;t) \triangleq \left[c^{(2)}(1;1;t), c^{(2)}(2;1;t)\right]^\dagger \in \mathsf{H}_2$ is constructed in the same Hilbert space which was denoted as $\mathsf{H}_2$ in the previous Subsection, and which is endowed with the inner product defined in Equation (68). This inner product is used to construct the 2nd-Level Adjoint Sensitivity System (2nd-LASS) for the 2nd-level adjoint function $\boldsymbol{C}^{(2)}(2;1;t) \triangleq \left[c^{(2)}(1;1;t), c^{(2)}(2;1;t)\right]^\dagger \in \mathsf{H}_2$, as follows:

i) Using Equation (68), form the inner product of $\boldsymbol{C}^{(2)}(2;1;t)$ with Equation (99) to obtain the following relation which has the same form as shown in Equation (69), namely:

$$\begin{aligned}
&\left\{\left\langle \boldsymbol{C}^{(2)}(2;1;t), \boldsymbol{VM}^{(2)}[2\times 2;\boldsymbol{\alpha}]\boldsymbol{V}^{(2)}(2;t)\right\rangle_2\right\}_{\boldsymbol{\alpha}^0} \\
&= \left\{\left\langle \boldsymbol{C}^{(2)}(2;1;t), \boldsymbol{S}_V^{(2)}(2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha})\right\rangle_2\right\}_{\boldsymbol{\alpha}^0} \\
&= \left\{c^{(2)}(1;1;t)\,\delta E(t) - c^{(2)}(2;1;t)\,\delta a^{(1)}(t)\right\}_{t=0}^{t=\tau} \\
&\quad + \left\{\left\langle \boldsymbol{V}^{(2)}(2;t), \boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{\alpha}]\boldsymbol{C}^{(2)}(2;1;t)\right\rangle_2\right\}_{\boldsymbol{\alpha}^0},
\end{aligned} \tag{106}$$

where the adjoint operator $\boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{\alpha}]$ is the same as defined in Equation (70).

ii) Eliminate the boundary terms on the right side of Equation (106) and require the term on the right-side of the second equality in Equation (106) to represent the "indirect-effect" term defined in Equation (96) by imposing the following relations:

$$\left\{\boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{\alpha}]\boldsymbol{C}^{(2)}(2;1;t)\right\}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} -\dfrac{a^{(1)}(t)E(t)}{l_p c_p} \\ -\dfrac{E^2(t)}{2 l_p c_p} \end{pmatrix}, \; 0 < t < \tau, \tag{107}$$

$$\left\{\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{C}^{(2)}(2;1;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0} \triangleq \begin{pmatrix} c^{(2)}(1;1;\tau) \\ c^{(2)}(2;1;0) \end{pmatrix}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{108}$$

The relations represented by Equations (107) and (108) constitute the 2nd-LASS for the 2nd-level adjoint function $\boldsymbol{C}^{(2)}(2;1;t) \triangleq \left[c^{(2)}(1;1;t), c^{(2)}(2;1;t)\right]^\dagger \in \mathsf{H}_2$.

Inserting the equations underlying the 2nd-LVSS, *i.e.* Equations (99) and (100), together with those underlying the 2nd-LASS, *i.e.*, Equations (107) and (108), into Equation (106) and recalling Equation (96) yields the following expression for the "indirect-effect" term as a function of $\boldsymbol{C}^{(2)}(2;1;t)$:

$$\left\{\delta\left[\partial E(\tau)/\partial \alpha_T\right]\right\}_{ind} = \left\{\left\langle \boldsymbol{C}^{(2)}(2;1;t), \boldsymbol{S}_V^{(2)}(2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha})\right\rangle_2\right\}_{\boldsymbol{\alpha}^0}. \tag{109}$$

Inserting the result for the indirect-effect term obtained in Equation (109) together with the expression for the direct-effect term shown in Equation (95) into Equation (94) yields the following expression for the first-order G-differential $\delta\left\{\partial E(\tau)/\partial\alpha_T\right\}_{\boldsymbol{\alpha}^0}$:

$$\begin{aligned}\delta\left\{\partial E(\tau)/\partial\alpha_T\right\}_{\boldsymbol{\alpha}^0} &= \left\{\left[\frac{\delta l_p}{2\left(l_p\right)^2 c_p}+\frac{\delta c_p}{2 l_p\left(c_p\right)^2}\right]\int_0^\tau a^{(1)}(t)E^2(t)\,\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}\\ &\quad+\left\{\left\langle \boldsymbol{C}^{(2)}(2;1;t),\boldsymbol{S}_V^{(2)}(2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha})\right\rangle_2\right\}_{\boldsymbol{\alpha}^0}\\ &=\left\{\sum_{i=1}^{7}\left[\partial^2 E(\tau)/\partial\alpha_i\partial\alpha_T\right]\delta\alpha_i\right\}_{\boldsymbol{\alpha}^0}.\end{aligned}\tag{110}$$

Inserting into Equation (110) the expressions provided in Equation (103) and (104) for the respective components of the source $\boldsymbol{S}_V^{(2)}(2;\boldsymbol{\alpha};\delta\boldsymbol{\alpha})$ and collecting the terms that multiply the respective parameter variations yields the following expressions for the second-order partial sensitivities that stem from $\delta\left\{\partial E(\tau)/\partial\alpha_T\right\}_{\boldsymbol{\alpha}^0}$:

$$\frac{\partial^2 E(\tau)}{\partial\alpha_T\partial\alpha_T}=-\frac{1}{2l_p c_p}\int_0^\tau\left[c^{(2)}(1;1;t)E^2(t)+2c^{(2)}(2;1;t)a^{(1)}(t)E(t)\right]\mathrm{d}t\,;\tag{111}$$

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial l_p\partial\alpha_T}&=\frac{1}{2\left(l_p\right)^2 c_p}\int_0^\tau a^{(1)}(t)E^2(t)\,\mathrm{d}t\\ &\quad+\frac{\alpha_T}{2\left(l_p\right)^2 c_p}\int_0^\tau\left[c^{(2)}(1;1;t)E^2(t)+2c^{(2)}(2;1;t)a^{(1)}(t)E(t)\right]\mathrm{d}t;\end{aligned}\tag{112}$$

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial c_p\partial\alpha_T}&=\frac{1}{2\left(c_p\right)^2 l_p}\int_0^\tau a^{(1)}(t)E^2(t)\,\mathrm{d}t\\ &\quad+\frac{\alpha_T}{2\left(c_p\right)^2 l_p}\int_0^\tau\left[c^{(2)}(1;1;t)E^2(t)+2c^{(2)}(2;1;t)a^{(1)}(t)E(t)\right]\mathrm{d}t;\end{aligned}\tag{113}$$

$$\frac{\partial^2 E(\tau)}{\partial\varphi_0\partial\alpha_T}=\gamma\sigma_f N_f\int_0^\tau c^{(2)}(1;1;t)\,\mathrm{d}t\,;\tag{114}$$

$$\frac{\partial^2 E(\tau)}{\partial\gamma\partial\alpha_T}=\varphi_0\sigma_f N_f\int_0^\tau c^{(2)}(1;1;t)\,\mathrm{d}t\,;\tag{115}$$

$$\frac{\partial^2 E(\tau)}{\partial\sigma_f\partial\alpha_T}=\varphi_0\gamma N_f\int_0^\tau c^{(2)}(1;1;t)\,\mathrm{d}t\,;\tag{116}$$

$$\frac{\partial^2 E(\tau)}{\partial N_f\partial\alpha_T}=\varphi_0\gamma\sigma_f\int_0^\tau c^{(2)}(1;1;t)\,\mathrm{d}t\,.\tag{117}$$

### 4.2.2. Computation of Second-Order Sensitivities Stemming from the First-Order Sensitivity $\partial E(\tau)/\partial l_p$

The second-order sensitivities which stem from the first-order sensitivity $\partial E(\tau)/\partial l_p$ are the components of the first-order G-differential of Equation (31). By definition, the first-order G-differential of Equation (31) is obtained as follows:

$$\delta\left\{\partial E(\tau)/\partial l_p\right\}_{\alpha^0} \triangleq \left\{\delta\left[\partial E(\tau)/\partial l_p\right]\right\}_{dir} + \left\{\delta\left[\partial E(\tau)/\partial l_p\right]\right\}_{ind}$$

$$\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\left[\frac{\alpha_T + \varepsilon\delta\alpha_T}{2\left(l_p + \varepsilon\delta l_p\right)^2\left(c_p + \varepsilon\delta c_p\right)}\int_0^\tau\left(a^{(1)} + \varepsilon\delta a^{(1)}\right)\left[E(t) + \varepsilon\delta E(t)\right]^2 \mathrm{d}t\right]_{\alpha^0}\right\}\right\}_{\varepsilon=0}, \tag{118}$$

where the "direct-effect" term $\left\{\delta\left[\partial E(\tau)/\partial l_p\right]\right\}_{dir}$ can be determined immediately and is defined as follows:

$$\left\{\delta\left[\partial E(\tau)/\partial l_p\right]\right\}_{dir}$$

$$\triangleq \left\{\left[\frac{\delta\alpha_T}{2\left(l_p\right)^2 c_p} - \frac{\alpha_T\delta l_p}{\left(l_p\right)^3 c_p} - \frac{\alpha_T\delta c_p}{2\left(l_p c_p\right)^2}\right]\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t\right\}_{\alpha^0} \tag{119}$$

and where the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial l_p\right]\right\}_{ind}$ is defined as follows:

$$\left\{\delta\left[\partial E(\tau)/\partial l_p\right]\right\}_{ind}$$

$$\triangleq \left\{\frac{\alpha_T}{2\left(l_p\right)^2 c_p}\int_0^\tau\left[\delta a^{(1)}(t)E^2(t) + 2a^{(1)}(t)E(t)\delta E(t)\right]\mathrm{d}t\right\}_{\alpha^0}. \tag{120}$$

Just as in Subsection 4.2.1, the 2nd-Level variational function $\boldsymbol{V}^{(2)}(2;t) \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^\dagger$, which is needed to evaluate the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial l_p\right]\right\}_{ind}$, is the solution of the 2nd-LVSS defined by Equations (99) and (100). The computationally expensive path of solving the 2nd-LVSS repeatedly for every possible parameter variation is avoided by replacing the dependence of the "indirect-effect" term defined in Equation (120) on the variational function $\boldsymbol{V}^{(2)}(2;t)$ by a dependence on a corresponding 2nd-Level adjoint function, which will be denoted as $\boldsymbol{C}^{(2)}(2;2;t) \triangleq \left[c^{(2)}(1;2;t), c^{(2)}(2;2;t)\right]^\dagger \in \mathsf{H}_2$, where the notation has the following significance: (i) the bold letter "C" indicates a vector-valued "adjoint" function within the 2nd-CASAM-N formalism; (ii) the superscript "(2)" indicates "second-level"; (iii) the first argument, namely "2", in $\boldsymbol{C}^{(2)}(2;2;t)$ indicates that this vector has 2 components, denoted as $c^{(2)}(i;2;t)$, $i = 1, 2$, each of which is a scalar-valued function of time; (iv) the second argument of $\boldsymbol{C}^{(2)}(2;2;t)$ is denoted as "2" and indicates that this 2nd-Level adjoint function corresponds to the first-order sensitivity $\partial E(\tau)/\partial l_p$ of the response with respect to the *second* component of the vector of model parameters $\boldsymbol{\alpha} \triangleq (\alpha_1, \cdots, \alpha_7)^\dagger \triangleq \left(\alpha_T, l_p, c_p, \varphi_0, \gamma, \sigma_f, N_f\right)^\dagger$, namely $l_p$.

The 2nd-LASS for the function $\boldsymbol{C}^{(2)}(2;2;t) \triangleq \left[c^{(2)}(1;2;t), c^{(2)}(2;2;t)\right]^\dagger \in \mathsf{H}_2$ is constructed by following the same procedure as in Subsection 4.1.1, except for the source term (*i.e.*, right-side) of the 2nd-LASS; this source-term now corresponds to the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial l_p\right]\right\}_{ind}$ defined in Equation (120). This procedure leads to the following 2nd-LASS for $\boldsymbol{C}^{(2)}(2;2;t)$:

$$\left\{\boldsymbol{AM}^{(2)}\left[2\times 2;\boldsymbol{\alpha}\right]\boldsymbol{C}^{(2)}(2;2;t)\right\}_{\boldsymbol{\alpha}^0}=\begin{pmatrix}\dfrac{\alpha_T}{(l_p)^2 c_p}a^{(1)}(t)E(t)\\[2ex]\dfrac{\alpha_T}{2(l_p)^2 c_p}E^2(t)\end{pmatrix},\ 0<t<\tau, \tag{121}$$

$$\left\{\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{C}^{(2)}(2;2;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0}\triangleq\begin{pmatrix}c^{(2)}(1;2;\tau)\\c^{(2)}(2;2;0)\end{pmatrix}_{\boldsymbol{\alpha}^0}=\begin{pmatrix}0\\0\end{pmatrix}. \tag{122}$$

Furthermore, the 2nd-order partial sensitivities that are obtained in terms of the components of $\boldsymbol{C}^{(2)}(2;2;t)$ have expressions that are formally similar to those obtained in Subsection 4.1.1, above, except for the contributions stemming from the direct effect term defined in Equation (119). Omitting these repetitive derivations, the final expressions for the 2nd-order partial sensitivities that stem from $\partial E(\tau)/\partial l_p$ are as follows:

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial\alpha_T\partial l_p}&=\frac{1}{2(l_p)^2 c_p}\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t\\&-\frac{1}{2l_p c_p}\int_0^\tau\left[c^{(2)}(1;2;t)E^2(t)+2c^{(2)}(2;2;t)a^{(1)}(t)E(t)\right]\mathrm{d}t;\end{aligned} \tag{123}$$

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial l_p\partial l_p}&=-\frac{\alpha_T}{(l_p)^3 c_p}\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t\\&+\frac{\alpha_T}{2(l_p)^2 c_p}\int_0^\tau\left[c^{(2)}(1;2;t)E^2(t)+2c^{(2)}(2;2;t)a^{(1)}(t)E(t)\right]\mathrm{d}t;\end{aligned} \tag{124}$$

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial c_p\partial l_p}&=-\frac{\alpha_T}{2(l_p c_p)^2}\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t\\&+\frac{\alpha_T}{2(c_p)^2 l_p}\int_0^\tau\left[c^{(2)}(1;2;t)E^2(t)+2c^{(2)}(2;2;t)a^{(1)}(t)E(t)\right]\mathrm{d}t;\end{aligned} \tag{125}$$

$$\frac{\partial^2 E(\tau)}{\partial\varphi_0\partial l_p}=\gamma\sigma_f N_f\int_0^\tau c^{(2)}(1;2;t)\mathrm{d}t\,; \tag{126}$$

$$\frac{\partial^2 E(\tau)}{\partial\gamma\partial l_p}=\varphi_0\sigma_f N_f\int_0^\tau c^{(2)}(1;2;t)\mathrm{d}t\,; \tag{127}$$

$$\frac{\partial^2 E(\tau)}{\partial\sigma_f\partial l_p}=\varphi_0\gamma N_f\int_0^\tau c^{(2)}(1;2;t)\mathrm{d}t\,; \tag{128}$$

$$\frac{\partial^2 E(\tau)}{\partial N_f\partial l_p}=\varphi_0\gamma\sigma_f\int_0^\tau c^{(2)}(1;2;t)\mathrm{d}t\,. \tag{129}$$

#### 4.2.3. Computation of Second-Order Sensitivities Stemming from the First-Order Sensitivity $\partial E(\tau)/\partial c_p$

The second-order sensitivities which stem from the first-order sensitivity $\partial E(\tau)/\partial c_p$ are the components of the first-order G-differential of Equation

(32), which has by definition the following expression:

$$\delta\left\{\partial E(\tau)/\partial c_p\right\}_{\alpha^0} \triangleq \left\{\delta\left[\partial E(\tau)/\partial c_p\right]\right\}_{dir} + \left\{\delta\left[\partial E(\tau)/\partial c_p\right]\right\}_{ind}$$

$$\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\left[\frac{\alpha_T + \varepsilon\delta\alpha_T}{2\left(l_p + \varepsilon\delta l_p\right)\left(c_p + \varepsilon\delta c_p\right)^2}\int_0^\tau \left(a^{(1)} + \varepsilon\delta a^{(1)}\right)\left[E(t) + \varepsilon\delta E(t)\right]^2 \mathrm{d}t\right]_{\alpha^0}\right\}\right\}_{\varepsilon=0}, \tag{130}$$

where the "direct-effect" term $\left\{\delta\left[\partial E(\tau)/\partial c_p\right]\right\}_{dir}$ can be determined immediately and is defined as follows:

$$\left\{\delta\left[\partial E(\tau)/\partial c_p\right]\right\}_{dir} \triangleq \left\{\left[\frac{\delta\alpha_T}{2l_p\left(c_p\right)^2} - \frac{\alpha_T\delta l_p}{2\left(l_p c_p\right)^2} - \frac{\alpha_T\delta c_p}{l_p\left(c_p\right)^3}\right]\int_0^\tau a^{(1)}(t)E^2(t)\mathrm{d}t\right\}_{\alpha^0}, \tag{131}$$

and where the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial c_p\right]\right\}_{ind}$ is defined as follows:

$$\left\{\delta\left[\partial E(\tau)/\partial c_p\right]\right\}_{ind} \triangleq \left\{\frac{\alpha_T}{2l_p\left(c_p\right)^2}\int_0^\tau \left[\delta a^{(1)}(t)E^2(t) + 2a^{(1)}(t)E(t)\delta E(t)\right]\mathrm{d}t\right\}_{\alpha^0}. \tag{132}$$

Just as in the previous Subsections of Section 4.2, the 2nd-Level variational function $\boldsymbol{V}^{(2)}(2;t) \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^\dagger$, which is needed to evaluate the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial c_p\right]\right\}_{ind}$, is the solution of the 2nd-LVSS defined by Equations (99) and (100). The computationally expensive path of solving the 2nd-LVSS repeatedly for every possible parameter variation is avoided by replacing the dependence of the "indirect-effect" term defined in Equation (132) on the variational function $\boldsymbol{V}^{(2)}(2;t)$ by a dependence on a corresponding 2nd-Level adjoint function, which will be denoted as $\boldsymbol{C}^{(2)}(2;3;t) \triangleq \left[c^{(2)}(1;3;t), c^{(2)}(2;3;t)\right]^\dagger \in \mathsf{H}_2$, where the notation is as in the previous Subsections, except that the second argument of $\boldsymbol{C}^{(2)}(2;3;t)$ is denoted as "3" and indicates that this 2nd-level adjoint function corresponds to the first-order sensitivity $\partial E(\tau)/\partial c_p$ of the response with respect to the *third* component of the vector of model parameters $\boldsymbol{\alpha} \triangleq (\alpha_1, \cdots, \alpha_7)^\dagger \triangleq \left(\alpha_T, l_p, c_p, \varphi_0, \gamma, \sigma_f, N_f\right)^\dagger$, namely $c_p$.

The 2nd-LASS for the function $\boldsymbol{C}^{(2)}(2;3;t) \triangleq \left[c^{(2)}(1;3;t), c^{(2)}(2;3;t)\right]^\dagger \in \mathsf{H}_2$ is constructed by following the same procedure as in the previous Subsections, except for the source term (*i.e.*, right-side) of the 2nd-LASS which corresponds to the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial c_p\right]\right\}_{ind}$ defined in Equation (132). This procedure leads to the following 2nd-LASS for $\boldsymbol{C}^{(2)}(2;3;t)$:

$$\left\{\boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{\alpha}]\boldsymbol{C}^{(2)}(2;3;t)\right\}_{\boldsymbol{\alpha}^0}=\begin{pmatrix}\dfrac{\alpha_T}{l_p\left(c_p\right)^2}a^{(1)}(t)E(t)\\[2ex]\dfrac{\alpha_T}{2l_p\left(c_p\right)^2}E^2(t)\end{pmatrix},\quad 0<t<\tau, \tag{133}$$

$$\left\{\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{C}^{(2)}(2;3;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0}\triangleq\begin{pmatrix}c^{(2)}(1;3;\tau)\\c^{(2)}(2;3;0)\end{pmatrix}_{\boldsymbol{\alpha}^0}=\begin{pmatrix}0\\0\end{pmatrix}. \tag{134}$$

The 2nd-order partial sensitivities are obtained in terms of the components of $\boldsymbol{C}^{(2)}(2;3;t)$ by applying the same procedure as in Subsections 4.2.1 and 4.2.2, and will have expressions that are formally similar to those obtained in the previous Subsections except for the contributions stemming from the direct effect term defined in Equation (131). The final expressions for the 2nd-order partial sensitivities that stem from $\partial E(\tau)/\partial c_p$ are as follows:

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial\alpha_T\partial c_p}&=\frac{1}{2l_p\left(c_p\right)^2}\int_0^\tau a^{(1)}(t)E^2(t)\,\mathrm{d}t\\&\quad-\frac{1}{2l_pc_p}\int_0^\tau\left[c^{(2)}(1;3;t)E^2(t)+2c^{(2)}(2;3;t)a^{(1)}(t)E(t)\right]\mathrm{d}t;\end{aligned} \tag{135}$$

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial l_p\partial c_p}&=-\frac{\alpha_T}{2\left(l_pc_p\right)^2}\int_0^\tau a^{(1)}(t)E^2(t)\,\mathrm{d}t\\&\quad+\frac{\alpha_T}{2\left(l_p\right)^2c_p}\int_0^\tau\left[c^{(2)}(1;3;t)E^2(t)+2c^{(2)}(2;3;t)a^{(1)}(t)E(t)\right]\mathrm{d}t;\end{aligned} \tag{136}$$

$$\begin{aligned}\frac{\partial^2 E(\tau)}{\partial c_p\partial c_p}&=-\frac{\alpha_T}{l_p\left(c_p\right)^3}\int_0^\tau a^{(1)}(t)E^2(t)\,\mathrm{d}t\\&\quad+\frac{\alpha_T}{2\left(c_p\right)^2l_p}\int_0^\tau\left[c^{(2)}(1;3;t)E^2(t)+2c^{(2)}(2;3;t)a^{(1)}(t)E(t)\right]\mathrm{d}t;\end{aligned} \tag{137}$$

$$\frac{\partial^2 E(\tau)}{\partial\varphi_0\partial c_p}=\gamma\sigma_fN_f\int_0^\tau c^{(2)}(1;3;t)\,\mathrm{d}t\,; \tag{138}$$

$$\frac{\partial^2 E(\tau)}{\partial\gamma\partial c_p}=\varphi_0\sigma_fN_f\int_0^\tau c^{(2)}(1;3;t)\,\mathrm{d}t\,; \tag{139}$$

$$\frac{\partial^2 E(\tau)}{\partial\sigma_f\partial c_p}=\varphi_0\gamma N_f\int_0^\tau c^{(2)}(1;3;t)\,\mathrm{d}t\,; \tag{140}$$

$$\frac{\partial^2 E(\tau)}{\partial N_f\partial c_p}=\varphi_0\gamma\sigma_f\int_0^\tau c^{(2)}(1;3;t)\,\mathrm{d}t\,. \tag{141}$$

#### 4.2.4. Computation of Second-Order Sensitivities Stemming from the First-Order Sensitivity $\partial E(\tau)/\partial\varphi_0$

The second-order sensitivities which stem from the first-order sensitivity

$\partial E(\tau)/\partial \varphi_0$ are the components of the first-order G-differential of Equation (33), which has by definition the following expression:

$$\begin{aligned}&\delta\left\{\partial E(\tau)/\partial \varphi_0\right\}_{\boldsymbol{\alpha}^0} \triangleq \left\{\delta\left[\partial E(\tau)/\partial \varphi_0\right]\right\}_{dir} + \left\{\delta\left[\partial E(\tau)/\partial \varphi_0\right]\right\}_{ind} \\ &\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\left[(\gamma+\varepsilon\delta\gamma)\left(\sigma_f+\varepsilon\delta\sigma_f\right)\left(N_f+\varepsilon\delta N_f\right)\int_0^\tau\left(a^{(1)}+\varepsilon\delta a^{(1)}\right)\mathrm{d}t\right]_{\boldsymbol{\alpha}^0}\right\}\right\}_{\varepsilon=0},\end{aligned} \tag{142}$$

where the "direct-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \varphi_0\right]\right\}_{dir}$ can be determined immediately and is defined as follows:

$$\begin{aligned}&\left\{\delta\left[\partial E(\tau)/\partial \varphi_0\right]\right\}_{dir} \\ &\triangleq \left\{\left[(\delta\gamma)\sigma_f N_f + \left(\delta\sigma_f\right)\gamma N_f + \left(\delta N_f\right)\gamma\sigma_f\right]\int_0^\tau a^{(1)}(t)\,\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0},\end{aligned} \tag{143}$$

and where the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \varphi_0\right]\right\}_{ind}$ is defined as follows:

$$\left\{\delta\left[\partial E(\tau)/\partial \varphi_0\right]\right\}_{ind} \triangleq \left\{\gamma\sigma_f N_f \int_0^\tau \delta a^{(1)}(t)\,\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}. \tag{144}$$

Just as in the previous Subsections of Section 4.2, the 2nd-Level variational function $\boldsymbol{V}^{(2)}(2;t) \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^\dagger$, which is needed to evaluate the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \varphi_0\right]\right\}_{ind}$, is the solution of the 2nd-LVSS defined by Equations (99) and (100). The computationally expensive path of solving the 2nd-LVSS repeatedly for every possible parameter variation is avoided by replacing the dependence of the "indirect-effect" term defined in Equation (144) on the variational function $\boldsymbol{V}^{(2)}(2;t)$ by a dependence on a corresponding 2nd-Level adjoint function, which will be denoted as $\boldsymbol{C}^{(2)}(2;4;t) \triangleq \left[c^{(2)}(1;4;t), c^{(2)}(2;4;t)\right]^\dagger \in \mathsf{H}_2$, where the notation is as in the previous Subsections, except that the second argument of $\boldsymbol{C}^{(2)}(2;4;t)$ is denoted as "4" and indicates that this 2nd-level adjoint function corresponds to the first-order sensitivity $\partial E(\tau)/\partial \varphi_0$ of the response with respect to the *fourth* component of the vector of model parameters $\boldsymbol{\alpha} \triangleq (\alpha_1, \cdots, \alpha_7)^\dagger \triangleq \left(\alpha_T, l_p, c_p, \varphi_0, \gamma, \sigma_f, N_f\right)^\dagger$, namely $\varphi_0$.

The 2nd-LASS for the function $\boldsymbol{C}^{(2)}(2;4;t) \triangleq \left[c^{(2)}(1;4;t), c^{(2)}(2;4;t)\right]^\dagger \in \mathsf{H}_2$ is constructed by following the same procedure as in the previous Subsections, except for the source term (*i.e.*, right-side) of the 2nd-LASS which corresponds to the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \varphi_0\right]\right\}_{ind}$ defined in Equation (144). This procedure leads to the following 2nd-LASS for $\boldsymbol{C}^{(2)}(2;4;t)$:

$$\left\{\boldsymbol{AM}^{(2)}\left[2\times 2;\boldsymbol{\alpha}\right]\boldsymbol{C}^{(2)}(2;4;t)\right\}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ \gamma\sigma_f N_f \end{pmatrix},\ 0<t<\tau,; \tag{145}$$

$$\left\{\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{C}^{(2)}(2;4;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0} \triangleq \begin{pmatrix} c^{(2)}(1;4;\tau) \\ c^{(2)}(2;4;0) \end{pmatrix}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{146}$$

The 2nd-order partial sensitivities are obtained in terms of the components of

$\boldsymbol{C}^{(2)}(2;4;t)$ by applying the same procedure as in Subsections 4.2.1 and 4.2.2, and will have expressions that are formally similar to those obtained in the previous Subsections except for the contributions stemming from the direct-effect term defined in Equation (143). The final expressions for the 2nd-order partial sensitivities that stem from $\partial E(\tau)/\partial \varphi_0$ are as follows:

$$\frac{\partial^2 E(\tau)}{\partial \alpha_T \partial \varphi_0} = -\frac{1}{2 l_p c_p} \int_0^\tau \left[ c^{(2)}(1;4;t) E^2(t) + 2 c^{(2)}(2;4;t) a^{(1)}(t) E(t) \right] \mathrm{d}t; \tag{147}$$

$$\frac{\partial^2 E(\tau)}{\partial l_p \partial \varphi_0} = \frac{\alpha_T}{2 (l_p)^2 c_p} \int_0^\tau \left[ c^{(2)}(1;4;t) E^2(t) + 2 c^{(2)}(2;4;t) a^{(1)}(t) E(t) \right] \mathrm{d}t; \tag{148}$$

$$\frac{\partial^2 E(\tau)}{\partial c_p \partial \varphi_0} = \frac{\alpha_T}{2 (c_p)^2 l_p} \int_0^\tau \left[ c^{(2)}(1;4;t) E^2(t) + 2 c^{(2)}(2;4;t) a^{(1)}(t) E(t) \right] \mathrm{d}t; \tag{149}$$

$$\frac{\partial^2 E(\tau)}{\partial \varphi_0 \partial \varphi_0} = \gamma \sigma_f N_f \int_0^\tau c^{(2)}(1;4;t) \mathrm{d}t\,; \tag{150}$$

$$\frac{\partial^2 E(\tau)}{\partial \gamma \partial \varphi_0} = \sigma_f N_f \int_0^\tau a^{(1)}(t) \mathrm{d}t + \varphi_0 \sigma_f N_f \int_0^\tau c^{(2)}(1;4;t) \mathrm{d}t\,; \tag{151}$$

$$\frac{\partial^2 E(\tau)}{\partial \sigma_f \partial \varphi_0} = \gamma N_f \int_0^\tau a^{(1)}(t) \mathrm{d}t + \varphi_0 \gamma N_f \int_0^\tau c^{(2)}(1;4;t) \mathrm{d}t\,; \tag{152}$$

$$\frac{\partial^2 E(\tau)}{\partial N_f \partial \varphi_0} = \gamma \sigma_f \int_0^\tau a^{(1)}(t) \mathrm{d}t + \varphi_0 \gamma \sigma_f \int_0^\tau c^{(2)}(1;4;t) \mathrm{d}t\,. \tag{153}$$

### 4.2.5. Computation of Second-Order Sensitivities Stemming from the First-Order Sensitivity $\partial E(\tau)/\partial \gamma$

The second-order sensitivities which stem from the first-order sensitivity $\partial E(\tau)/\partial \gamma$ are the components of the first-order G-differential of Equation (34), which has by definition the following expression:

$$\begin{aligned} \delta\left\{\partial E(\tau)/\partial \gamma\right\}_{\alpha^0} &\triangleq \left\{\delta\left[\partial E(\tau)/\partial \gamma\right]\right\}_{dir} + \left\{\delta\left[\partial E(\tau)/\partial \gamma\right]\right\}_{ind} \\ &\triangleq \left\{ \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \left\{ \left[ (\varphi_0 + \varepsilon \delta \varphi_0)(\sigma_f + \varepsilon \delta \sigma_f)(N_f + \varepsilon \delta N_f) \int_0^\tau \left(a^{(1)} + \varepsilon \delta a^{(1)}\right) \mathrm{d}t \right]_{\alpha^0} \right\} \right\}_{\varepsilon=0}, \end{aligned} \tag{154}$$

where the "direct-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \gamma\right]\right\}_{dir}$ can be determined immediately and is defined as follows:

$$\begin{aligned} &\left\{\delta\left[\partial E(\tau)/\partial \gamma\right]\right\}_{dir} \\ &\triangleq \left\{ \left[ (\delta \varphi_0) \sigma_f N_f + (\delta \sigma_f) \varphi_0 N_f + (\delta N_f) \varphi_0 \sigma_f \right] \int_0^\tau a^{(1)}(t) \mathrm{d}t \right\}_{\alpha^0}, \end{aligned} \tag{155}$$

and where the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \gamma\right]\right\}_{ind}$ is defined as follows:

$$\left\{\delta\left[\partial E(\tau)/\partial \gamma\right]\right\}_{ind} \triangleq \left\{ \varphi_0 \sigma_f N_f \int_0^\tau \delta a^{(1)}(t) \mathrm{d}t \right\}_{\alpha^0}. \tag{156}$$

Just as in the previous Subsections of Section 4.2, the 2nd-level variational function $\boldsymbol{V}^{(2)}(2;t)\triangleq\left[\delta E(t),\delta a^{(1)}(t)\right]^{\dagger}$, which is needed to evaluate the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial\gamma\right]\right\}_{ind}$, is the solution of the 2nd-LVSS defined by Equations (99) and (100). The computationally expensive path of solving the 2nd-LVSS repeatedly for every possible parameter variation is avoided by replacing the dependence of the "indirect-effect" term defined in Equation (144) on the variational function $\boldsymbol{V}^{(2)}(2;t)$ by a dependence on a corresponding 2nd-Level adjoint function, which will be denoted as $\boldsymbol{C}^{(2)}(2;5;t)\triangleq\left[c^{(2)}(1;5;t),c^{(2)}(2;5;t)\right]^{\dagger}\in\mathsf{H}_2$, where the notation is as in the previous Subsections, except that the second argument of $\boldsymbol{C}^{(2)}(2;5;t)$ is denoted as "5" and indicates that this 2nd-level adjoint function corresponds to the first-order sensitivity $\partial E(\tau)/\partial\gamma$ of the response with respect to the *fifth* component of the vector of model parameters $\boldsymbol{\alpha}\triangleq(\alpha_1,\cdots,\alpha_7)^{\dagger}\triangleq\left(\alpha_T,l_p,c_p,\varphi_0,\gamma,\sigma_f,N_f\right)^{\dagger}$, namely $\gamma$.

The 2nd-LASS for the function $\boldsymbol{C}^{(2)}(2;5;t)\triangleq\left[c^{(2)}(1;5;t),c^{(2)}(2;5;t)\right]^{\dagger}\in\mathsf{H}_2$ is constructed by following the same procedure as in the previous Subsections, except for the source term (*i.e.*, right-side) of the 2nd-LASS, which now corresponds to the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial\gamma\right]\right\}_{ind}$ defined in Equation (156). This procedure leads to the following 2nd-LASS for $\boldsymbol{C}^{(2)}(2;5;t)$:

$$\left\{\boldsymbol{AM}^{(2)}\left[2\times 2;\boldsymbol{\alpha}\right]\boldsymbol{C}^{(2)}(2;5;t)\right\}_{\boldsymbol{\alpha}^0}=\begin{pmatrix}0\\ \varphi_0\sigma_f N_f\end{pmatrix},\ 0<t<\tau, \tag{157}$$

$$\left\{\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{C}^{(2)}(2;5;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0}\triangleq\begin{pmatrix}c^{(2)}(1;5;\tau)\\ c^{(2)}(2;5;0)\end{pmatrix}_{\boldsymbol{\alpha}^0}=\begin{pmatrix}0\\ 0\end{pmatrix}. \tag{158}$$

The 2nd-order partial sensitivities are obtained in terms of the components of $\boldsymbol{C}^{(2)}(2;5;t)$ by applying the same procedure as in Subsections 4.2.1-4.2.4, and will have expressions that are formally similar to those obtained in the previous Subsections except for the contributions stemming from the direct-effect term defined in Equation (155). The final expressions for the 2nd-order partial sensitivities that stem from $\partial E(\tau)/\partial\gamma$ are as follows:

$$\frac{\partial^2 E(\tau)}{\partial\alpha_T\partial\gamma}=-\frac{1}{2l_p c_p}\int_0^{\tau}\left[c^{(2)}(1;5;t)E^2(t)+2c^{(2)}(2;5;t)a^{(1)}(t)E(t)\right]\mathrm{d}t; \tag{159}$$

$$\frac{\partial^2 E(\tau)}{\partial l_p\partial\gamma}=\frac{\alpha_T}{2\left(l_p\right)^2 c_p}\int_0^{\tau}\left[c^{(2)}(1;5;t)E^2(t)+2c^{(2)}(2;5;t)a^{(1)}(t)E(t)\right]\mathrm{d}t; \tag{160}$$

$$\frac{\partial^2 E(\tau)}{\partial c_p\partial\gamma}=\frac{\alpha_T}{2\left(c_p\right)^2 l_p}\int_0^{\tau}\left[c^{(2)}(1;5;t)E^2(t)+2c^{(2)}(2;5;t)a^{(1)}(t)E(t)\right]\mathrm{d}t; \tag{161}$$

$$\frac{\partial^2 E(\tau)}{\partial\varphi_0\partial\gamma}=\sigma_f N_f\int_0^{\tau}a^{(1)}(t)\,\mathrm{d}t+\gamma\sigma_f N_f\int_0^{\tau}c^{(2)}(1;5;t)\,\mathrm{d}t\,; \tag{162}$$

$$\frac{\partial^2 E(\tau)}{\partial \gamma \partial \gamma} = \varphi_0 \sigma_f N_f \int_0^\tau c^{(2)}(1;5;t)\,\mathrm{d}t\,; \tag{163}$$

$$\frac{\partial^2 E(\tau)}{\partial \sigma_f \partial \gamma} = \varphi_0 N_f \int_0^\tau a^{(1)}(t)\,\mathrm{d}t + \varphi_0 \gamma N_f \int_0^\tau c^{(2)}(1;5;t)\,\mathrm{d}t\,; \tag{164}$$

$$\frac{\partial^2 E(\tau)}{\partial N_f \partial \gamma} = \varphi_0 \sigma_f \int_0^\tau a^{(1)}(t)\,\mathrm{d}t + \varphi_0 \gamma \sigma_f \int_0^\tau c^{(2)}(1;5;t)\,\mathrm{d}t\,. \tag{165}$$

#### 4.2.6. Computation of Second-Order Sensitivities Stemming from the First-Order Sensitivity $\partial E(\tau)/\partial \sigma_f$

The second-order sensitivities which stem from the first-order sensitivity $\partial E(\tau)/\partial \sigma_f$ are the components of the first-order G-differential of Equation (35), which has by definition the following expression:

$$\begin{aligned}\delta\left\{\partial E(\tau)/\partial \sigma_f\right\}_{\boldsymbol{\alpha}^0} &\triangleq \left\{\delta\left[\partial E(\tau)/\partial \sigma_f\right]\right\}_{dir} + \left\{\delta\left[\partial E(\tau)/\partial \sigma_f\right]\right\}_{ind} \\ &\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\left[\left(\varphi_0 + \varepsilon\delta\varphi_0\right)\left(\gamma + \varepsilon\delta\gamma\right)\left(N_f + \varepsilon\delta N_f\right)\int_0^\tau \left(a^{(1)} + \varepsilon\delta a^{(1)}\right)\mathrm{d}t\right]_{\boldsymbol{\alpha}^0}\right\}\right\}_{\varepsilon=0},\end{aligned} \tag{166}$$

where the "direct-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \sigma_f\right]\right\}_{dir}$ can be determined immediately and is defined as follows:

$$\begin{aligned}&\left\{\delta\left[\partial E(\tau)/\partial \sigma_f\right]\right\}_{dir} \\ &\triangleq \left\{\left[\left(\delta\varphi_0\right)\gamma N_f + \left(\delta\gamma\right)\varphi_0 N_f + \left(\delta N_f\right)\varphi_0\gamma\right]\int_0^\tau a^{(1)}(t)\,\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0},\end{aligned} \tag{167}$$

and where the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial \sigma_f\right]\right\}_{ind}$ is defined as follows:

$$\left\{\delta\left[\partial E(\tau)/\partial \sigma_f\right]\right\}_{ind} \triangleq \left\{\varphi_0 \gamma N_f \int_0^\tau \delta a^{(1)}(t)\,\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}. \tag{168}$$

Just as in the previous Subsections of Section 4.2, the dependence of the "indirect-effect" term defined in Equation (168) on the variational function $\boldsymbol{V}^{(2)}(2;t)$ is replaced by a dependence on a corresponding 2nd-Level adjoint function, which will be denoted as $\boldsymbol{C}^{(2)}(2;6;t) \triangleq \left[c^{(2)}(1;6;t), c^{(2)}(2;6;t)\right]^\dagger \in \mathsf{H}_2$, where the notation is as in the previous Subsections, except that the second argument of $\boldsymbol{C}^{(2)}(2;6;t)$ is denoted as "6" and indicates that this 2nd-Level adjoint function corresponds to the first-order sensitivity $\partial E(\tau)/\partial \sigma_f$ of the response with respect to the *sixth* component of the vector of model parameters $\boldsymbol{\alpha} \triangleq (\alpha_1, \cdots, \alpha_7)^\dagger \triangleq \left(\alpha_T, l_p, c_p, \varphi_0, \gamma, \sigma_f, N_f\right)^\dagger$, namely $\sigma_f$.

The 2nd-LASS for the function $\boldsymbol{C}^{(2)}(2;6;t) \triangleq \left[c^{(2)}(1;6;t), c^{(2)}(2;6;t)\right]^\dagger \in \mathsf{H}_2$ is constructed by following the same procedure as in the previous Subsections, except for the source term (*i.e.*, right-side) of the 2nd-LASS which corresponds to the "indirect-effect" term $\left\{\delta\,\partial E(\tau)/\partial \sigma_f\right\}_{ind}$ defined in Equation (168). This procedure leads to the following 2nd-LASS for $\boldsymbol{C}^{(2)}(2;6;t)$:

$$\left\{\boldsymbol{AM}^{(2)}\left[2\times 2;\boldsymbol{\alpha}\right]\boldsymbol{C}^{(2)}(2;6;t)\right\}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ \varphi_0 \gamma N_f \end{pmatrix},\quad 0 < t < \tau, \tag{169}$$

$$\left\{\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{C}^{(2)}(2;6;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0} \triangleq \begin{pmatrix} c^{(2)}(1;6;\tau) \\ c^{(2)}(2;6;0) \end{pmatrix}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{170}$$

The 2nd-order partial sensitivities are obtained in terms of the components of $\boldsymbol{C}^{(2)}(2;6;t)$ by applying the same procedure as in Subsections 4.2.1-4.2.5, and will have expressions that are formally similar to those obtained in the previous Subsections except for the contributions stemming from the direct-effect term defined in Equation (167). The final expressions for the 2nd-order partial sensitivities that stem from $\partial E(\tau)/\partial\sigma_f$ are as follows:

$$\frac{\partial^2 E(\tau)}{\partial\alpha_T\partial\sigma_f} = -\frac{1}{2l_p c_p}\int_0^\tau\left[c^{(2)}(1;6;t)E^2(t) + 2c^{(2)}(2;6;t)a^{(1)}(t)E(t)\right]\mathrm{d}t; \tag{171}$$

$$\frac{\partial^2 E(\tau)}{\partial l_p\partial\sigma_f} = \frac{\alpha_T}{2(l_p)^2 c_p}\int_0^\tau\left[c^{(2)}(1;6;t)E^2(t) + 2c^{(2)}(2;6;t)a^{(1)}(t)E(t)\right]\mathrm{d}t; \tag{172}$$

$$\frac{\partial^2 E(\tau)}{\partial c_p\partial\sigma_f} = \frac{\alpha_T}{2(c_p)^2 l_p}\int_0^\tau\left[c^{(2)}(1;6;t)E^2(t) + 2c^{(2)}(2;6;t)a^{(1)}(t)E(t)\right]\mathrm{d}t; \tag{173}$$

$$\frac{\partial^2 E(\tau)}{\partial\varphi_0\partial\sigma_f} = \gamma N_f\int_0^\tau a^{(1)}(t)\mathrm{d}t + \gamma\sigma_f N_f\int_0^\tau c^{(2)}(1;6;t)\mathrm{d}t; \tag{174}$$

$$\frac{\partial^2 E(\tau)}{\partial\gamma\partial\sigma_f} = \varphi_0 N_f\int_0^\tau a^{(1)}(t)\mathrm{d}t + \varphi_0\sigma_f N_f\int_0^\tau c^{(2)}(1;6;t)\mathrm{d}t; \tag{175}$$

$$\frac{\partial^2 E(\tau)}{\partial\sigma_f\partial\sigma_f} = \varphi_0\gamma N_f\int_0^\tau c^{(2)}(1;6;t)\mathrm{d}t; \tag{176}$$

$$\frac{\partial^2 E(\tau)}{\partial N_f\partial\sigma_f} = \varphi_0\gamma\int_0^\tau a^{(1)}(t)\mathrm{d}t + \varphi_0\gamma\sigma_f\int_0^\tau c^{(2)}(1;6;t)\mathrm{d}t. \tag{177}$$

### 4.2.7. Computation of Second-Order Sensitivities Stemming from the First-Order Sensitivity $\partial E(\tau)/\partial N_f$

The second-order sensitivities which stem from the first-order sensitivity $\partial E(\tau)/\partial N_f$ are the components of the first-order G-differential of Equation (36), which has by definition the following expression:

$$\begin{aligned} &\delta\left\{\partial E(\tau)/\partial N_f\right\}_{\boldsymbol{\alpha}^0} \triangleq \left\{\delta\left[\partial E(\tau)/\partial N_f\right]\right\}_{dir} + \left\{\delta\left[\partial E(\tau)/\partial N_f\right]\right\}_{ind} \\ &\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\left[(\varphi_0+\varepsilon\delta\varphi_0)(\gamma+\varepsilon\delta\gamma)(\sigma_f+\varepsilon\delta\sigma_f)\int_0^\tau\left(a^{(1)}+\varepsilon\delta a^{(1)}\right)\mathrm{d}t\right]_{\boldsymbol{\alpha}^0}\right\}_{\varepsilon=0}, \end{aligned} \tag{178}$$

where the "direct-effect" term $\left\{\delta\left[\partial E(\tau)/\partial N_f\right]\right\}_{dir}$ can be determined immediately and is defined as follows:

$$\begin{aligned} &\left\{\delta\left[\partial E(\tau)/\partial N_f\right]\right\}_{dir} \\ &\triangleq \left\{\left[(\delta\varphi_0)\gamma\sigma_f + (\delta\gamma)\varphi_0\sigma_f + (\delta\sigma_f)\varphi_0\gamma\right]\int_0^\tau a^{(1)}(t)\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}, \end{aligned} \tag{179}$$

and where the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial N_f\right]\right\}_{ind}$ is defined as follows:

$$\left\{\delta\,\partial E(\tau)/\partial N_f\right\}_{ind} \triangleq \left\{\varphi_0\gamma\sigma_f\int_0^\tau \delta a^{(1)}(t)\,\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}. \tag{180}$$

Just as in the previous Subsections of Section 4.2, the dependence of the "indirect-effect" term defined in Equation (180) on the variational function $\boldsymbol{V}^{(2)}(2;t)$ is replaced by a dependence on a corresponding 2nd-level adjoint function, which will be denoted as $\boldsymbol{C}^{(2)}(2;7;t) \triangleq \left[c^{(2)}(1;7;t), c^{(2)}(2;7;t)\right]^\dagger \in \mathsf{H}_2$, where the notation is as in the previous Subsections, except that the second argument of $\boldsymbol{C}^{(2)}(2;7;t)$ is denoted as "7" and indicates that this 2nd-level adjoint function corresponds to the first-order sensitivity $\partial E(\tau)/\partial N_f$ of the response with respect to the *seventh* component of the vector of model parameters $\boldsymbol{\alpha} \triangleq (\alpha_1,\cdots,\alpha_7)^\dagger \triangleq \left(\alpha_T, l_p, c_p, \varphi_0, \gamma, \sigma_f, N_f\right)^\dagger$, namely $N_f$.

The 2nd-LASS for the function $\boldsymbol{C}^{(2)}(2;7;t) \triangleq \left[c^{(2)}(1;7;t), c^{(2)}(2;7;t)\right]^\dagger \in \mathsf{H}_2$ is constructed by following the same procedure as in the previous Subsections, except for the source term (*i.e.*, right-side) of the 2nd-LASS, which now corresponds to the "indirect-effect" term $\left\{\delta\left[\partial E(\tau)/\partial N_f\right]\right\}_{ind}$ defined in Equation (180). This procedure leads to the following 2nd-LASS for $\boldsymbol{C}^{(2)}(2;7;t)$:

$$\left\{\boldsymbol{AM}^{(2)}\left[2\times 2;\boldsymbol{\alpha}\right]\boldsymbol{C}^{(2)}(2;7;t)\right\}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ \varphi_0\gamma\sigma_f \end{pmatrix},\ 0<t<\tau, \tag{181}$$

$$\left\{\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{C}^{(2)}(2;7;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0} \triangleq \begin{pmatrix} c^{(2)}(1;7;\tau) \\ c^{(2)}(2;7;0) \end{pmatrix}_{\boldsymbol{\alpha}^0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{182}$$

The 2nd-order partial sensitivities are obtained in terms of the components of $\boldsymbol{C}^{(2)}(2;6;t)$ by applying the same procedure as in Subsections 4.2.1-4.2.5, and will have expressions that are formally similar to those obtained in the previous Subsections except for the contributions stemming from the direct-effect term defined in Equation (167). The final expressions for the 2nd-order partial sensitivities that stem from $\partial E(\tau)/\partial\sigma_f$ are as follows:

$$\frac{\partial^2 E(\tau)}{\partial\alpha_T\partial N_f} = -\frac{1}{2l_p c_p}\int_0^\tau\left[c^{(2)}(1;7;t)E^2(t) + 2c^{(2)}(2;7;t)a^{(1)}(t)E(t)\right]\mathrm{d}t; \tag{183}$$

$$\frac{\partial^2 E(\tau)}{\partial l_p\partial N_f} = \frac{\alpha_T}{2\left(l_p\right)^2 c_p}\int_0^\tau\left[c^{(2)}(1;7;t)E^2(t) + 2c^{(2)}(2;7;t)a^{(1)}(t)E(t)\right]\mathrm{d}t; \tag{184}$$

$$\frac{\partial^2 E(\tau)}{\partial c_p\partial N_f} = \frac{\alpha_T}{2\left(c_p\right)^2 l_p}\int_0^\tau\left[c^{(2)}(1;7;t)E^2(t) + 2c^{(2)}(2;7;t)a^{(1)}(t)E(t)\right]\mathrm{d}t; \tag{185}$$

$$\frac{\partial^2 E(\tau)}{\partial\varphi_0\partial N_f} = \gamma\sigma_f\int_0^\tau a^{(1)}(t)\,\mathrm{d}t + \gamma\sigma_f N_f\int_0^\tau c^{(2)}(1;7;t)\,\mathrm{d}t; \tag{186}$$

$$\frac{\partial^2 E(\tau)}{\partial\gamma\partial N_f} = \varphi_0\sigma_f\int_0^\tau a^{(1)}(t)\,\mathrm{d}t + \varphi_0\sigma_f N_f\int_0^\tau c^{(2)}(1;7;t)\,\mathrm{d}t; \tag{187}$$

$$\frac{\partial^2 E(\tau)}{\partial \sigma_f \partial N_f} = \varphi_0 \gamma \int_0^\tau a^{(1)}(t)\,\mathrm{d}t + \varphi_0 \gamma N_f \int_0^\tau c^{(2)}(1;7;t)\,\mathrm{d}t\,; \tag{188}$$

$$\frac{\partial^2 E(\tau)}{\partial N_f \partial N_f} = \varphi_0 \gamma \sigma_f \int_0^\tau c^{(2)}(1;7;t)\,\mathrm{d}t\,. \tag{189}$$

### 4.3. Computational Advantages of Using the 2nd-FASAM-N Versus the 2nd-CASAM-N

"Large-scale" computations are those needed to solve systems of equations (algebraic, differential, integral) such as those underlying the original model and the adjoint sensitivity systems of various levels (1st-LASS, 2nd-LASS, etc.). By comparison, the computational effort involved in evaluating integrals by means of quadrature formulas are "small-scale" computations. The conventional (e.g., "statistical" or "finite-difference") methods for computing response sensitivities with respect to model parameters require at least as many large-scale computations –for solving the original model with altered parameter values– as there are model parameters. If no "feature" functions of parameters can be identified in the model, then the formalisms of 1st-CASAM-N and the 1st-FASAM become identical to one another, requiring a single large-scale computation, which is needed for solving the 1st-LASS to obtain the 1st-level adjoint sensitivity function. Subsequently, the 1st-order sensitivities of the model's response with respect to the underlying model parameters are computed inexpensively using quadrature formulas to evaluate numerically the respective integrals involving the 1st-level adjoint sensitivity function. On the other hand, if "feature" functions of parameters can be identified in the model, then the 1st-FASAM methodology is marginally more efficient than the 1st-CASAM-N: both methodologies require a single large-scale computation, but the 1st-FASAM-N requires fewer numerical quadratures (only as many as there are feature-functions) than the 1st-CASAM (which requires as many quadratures as there are parameters), because the sensitivities with respect to the parameters are obtained from the sensitivities with respect to the feature-functions by analytical differentiations. In both cases, the 1st-LASS to be solved involves the same operators to be inverted (on the left-side of the 1st-LASS); only the source terms on the right-side of the 1st-LASS within the 1st-FASAM-N differ from the source terms on the right-side of the 1st-LASS within the 1st-CASAM-N.

The conventional (e.g., "statistical" or "finite-difference") methods are impractical for computing response sensitivities higher than first-order. Both the 2nd-FASAM-N and the 2nd-CASAM-N methodologies are constructed by using the fundamental definition that "the second-order differential is the first-order differential of the first-order differential." Thus, each of the first-order sensitivities becomes the "model response" for the application of either the 2nd-FASAM-N or the 2nd-CASAM-N. Consequently, there would be as many large-scale computations for solving the 2nd-LASS as there are first-order sensitivities. Consequently, since the number of feature functions is always smaller than the number of model parameters, there would be fewer large-scale computations (to solve the $2^{nd}$-LASS) to be performed within the $2^{nd}$-FASAM-N methodology than there would be within the $2^{nd}$-CASAM-N methodology. In particular, for the Nordheim-Fuchs model analyzed in this work, it was shown that the $2^{nd}$*-FASAM-N* methodology requires $TF = 2$ large-scale computations (as there are two feature-functions) whereas the $2^{nd}$*-CASAM-N* methodology requires $TP = 7$ large-scale computations (*i.e.*, as many computations as there are primary model parameters) for obtaining all of the $TP^2 = 49$ second-order sensitivities to the model parameters; $TP(TP+1)/2 = 28$ (out of the 49) of these $2^{nd}$-order sensitivities are distinct from each other. It is also important to note that the mixed second-order sensitivities are computed twice, using distinct adjoint functions, within either the $2^{nd}$-FASAM-N or the $2^{nd}$-CASAM-N methodology. This characteristic of the $2^{nd}$-FASAM-N and $2^{nd}$-CASAM-N methodologies provide an intrinsic mechanism for verifying the accuracy of the respective first- and second-level adjoint functions. Furthermore, the user can select which of the alternative—but equivalent—expressions of the $2^{nd}$-order mixed sensitivity under consideration is computationally more advantageous to use.

## 5. Computation of the Third-Order Response Sensitivities with Respect to Model Parameters: Applying the $3^{rd}$-FASAM-N Versus the $3^{rd}$-CASAM-N

The fundamental principle underlying both the 3rd-FASAM-N and the 3rd-CASAM-N methodologies is to determine the third-order sensitivities by employing their definition of being the "first-order sensitivities of the second-order sensitivities." Thus, each second-order sensitivity is treated as a "model response," and the G-differential of each of these "model responses" subsequently provides the partial third-order sensitivities that stem from the respective first-order sensitivity. As will be highlighted in Section 5.1, below, the computation of the 343 second-order sensitivities (of which 84 are distinct) of the response $E(\tau)$ with respect to the 7 model parameters will require just three large-scale computations for solving the corresponding three 3rd-Level Adjoint Sensitivity Systems that correspond to the three distinct sensitivities of the response $E(\tau)$ with respect to the "feature functions" $f_1(\boldsymbol{\alpha})$ and $f_2(\boldsymbol{\alpha})$ In contradistinction, as will be highlighted in Section 5.2, applying the conventional 3rd-CASAM-N methodology requires 28 large-scale computations for solving the twenty-eight 3rd-Level Adjoint Sensitivity Systems that correspond to the distinct second-order sensitivities of the response $E(\tau)$ with respect to the model parameters.

### 5.1. Computation of Third-Order Sensitivities Using the $3^{rd}$-FASAM-N

As will be shown in Subsection 5.1.1, the second-order sensitivity $\partial^2 E(\tau)/\partial f_1 \partial f_1$

will give rise to two third-order sensitivities, $\partial^3 E(\tau)/\partial f_1 \partial f_1 \partial f_1$ and $\partial^3 E(\tau)/\partial f_2 \partial f_1 \partial f_1$, which will be determined by solving a corresponding 3rd-Level Adjoint Sensitivity System (3rd-LASS). For bookkeeping purposes, the quantity $\partial^2 E(\tau)/\partial f_1 \partial f_1$ will the labeled "the *first* 2nd-order sensitivity" and the solution of the 3rd-LASS that corresponds to it will be labeled "the *first* 3rd-Level adjoint function.

Similarly, the second-order sensitivity $\partial^2 E(\tau)/\partial f_2 \partial f_2$ will give rise to two third-order sensitivities, $\partial^3 E(\tau)/\partial f_1 \partial f_2 \partial f_2$ and $\partial^3 E(\tau)/\partial f_2 \partial f_2 \partial f_2$, which will be determined in Subsection 5.1.2 by solving a corresponding 3rd-Level Adjoint Sensitivity System (3rd-LASS). For bookkeeping purposes, the quantity $\partial^2 E(\tau)/\partial f_2 \partial f_2$ will the labeled "the *second* 2nd-order sensitivity" and the solution of the 3rd-LASS that corresponds to it will be labeled "the *second* 3rd-level adjoint function.

Finally, the second-order sensitivity $\partial^2 E(\tau)/\partial f_2 \partial f_1$ or, equivalently, the second-order sensitivity $\partial^2 E(\tau)/\partial f_1 \partial f_2$, will give rise to two third-order sensitivities, $\partial^3 E(\tau)/\partial f_1 \partial f_1 \partial f_2$ and $\partial^3 E(\tau)/\partial f_2 \partial f_1 \partial f_2$, which provide alternative but equivalent expressions for the respective mixed third-order sensitivities obtained as mentioned above. These alternative computations will be discussed in Subsection 5.1.3.

### 5.1.1. Computation of Third-Order Sensitivities Stemming from the Second-Order Sensitivity $\partial^2 E(\tau)/\partial f_1 \partial f_1$

The 3rd-order sensitivities which stem from $\partial^2 E(\tau)/\partial f_1 \partial f_1$ are obtained by applying the definition of the first-order G-differential to Equation (76), which yields the following expression:

$$\begin{aligned}
&\delta\left\{\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1}\right\} \triangleq \frac{\partial^3 E(\tau)}{\partial f_1 \partial f_1 \partial f_1}\delta f_1 + \frac{\partial^3 E(\tau)}{\partial f_2 \partial f_1 \partial f_1}\delta f_2 \\
&\triangleq -\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\int_0^\tau \left[a^{(2)}(1;1;t) + \varepsilon \delta a^{(2)}(1;1;t)\right]\left[E(t) + \varepsilon \delta E(t)\right]^2 \mathrm{d}t\right\}_{f^0}\right\}_{\varepsilon=0}; \\
&\quad -2\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\int_0^\tau \left[a^{(2)}(2;1;t) + \varepsilon \delta a^{(2)}(2;1;t)\right]\left(a^{(1)} + \varepsilon \delta a^{(1)}\right)\left(E + \varepsilon \delta E\right)\mathrm{d}t\right\}_{f^0}\right\}_{\varepsilon=0} \\
&= -\left\{\int_0^\tau \delta a^{(2)}(1;1;t) E^2(t)\mathrm{d}t\right\}_{f^0} - 2\left\{\int_0^\tau \left[a^{(2)}(1;1;t)E(t) + a^{(2)}(2;1;t)a^{(1)}(t)\right]\delta E(t)\mathrm{d}t\right\}_{f^0} \\
&\quad -2\left\{\int_0^\tau \delta a^{(2)}(2;1;t)a^{(1)}(t)E(t)\mathrm{d}t\right\}_{f^0} - 2\left\{\int_0^\tau \delta a^{(1)}(t)a^{(2)}(2;1;t)E(t)\mathrm{d}t\right\}_{f^0}.
\end{aligned} \tag{190}$$

The expression obtained in Equation (190) comprises no direct-effect term, and it can be evaluated after having determined the vector-valued variational functions $\mathbf{V}^{(2)}(2;t) \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^\dagger$ and $\delta \mathbf{A}^{(2)}(2;1;t) \triangleq \left[\delta a^{(2)}(1;1;t), \delta a^{(2)}(2;1;t)\right]^\dagger$. The vector-valued variational function $\mathbf{V}^{(2)}(2;t) \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^\dagger$ is the solution of the 2nd-Level Variational Sensitivity System (2nd-LVSS) defined by Equations (63) and (64). On the other hand, the vector-valued variational function $\delta \boldsymbol{A}^{(2)}(2;1;t) \triangleq \left[\delta a^{(2)}(1;1;t), \delta a^{(2)}(2;1;t)\right]^{\dagger}$ is the solution of the G-differentiated 2nd-LASS defined by Equations (71) and (72), evaluated at the nominal values of the feature functions and state functions (*i.e.*, dependent variables). Using the superscript "zero" to denote the respective nominal values of the various quantities and applying the definition of the G-differential to Equations (71) and (72) yields the following system of equations:

$$\begin{aligned} &\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left[-\frac{\mathrm{d}}{\mathrm{d}t}+2\left(f_1^0+\varepsilon\delta f_1\right)\left(E^0+\varepsilon\delta E\right)\right]\left[a^{(2,0)}(1;1;t)+\varepsilon\delta a^{(2)}(1;1;t)\right]\right\}_{\varepsilon=0} \\ &+2\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(f_1^0+\varepsilon\delta f_1\right)\left(a^{(1,0)}+\varepsilon\delta a^{(1)}\right)\left[a^{(2,0)}(2;1;t)+\varepsilon\delta a^{(2)}(2;1;t)\right]\right\}_{\varepsilon=0} \\ &=-2\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left[\left(a^{(1,0)}+\varepsilon\delta a^{(1)}\right)\left(E^0+\varepsilon\delta E\right)\right]\right\}_{\varepsilon=0}, \end{aligned} \tag{191}$$

$$\begin{aligned} &\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left[\frac{\mathrm{d}}{\mathrm{d}t}+2\left(f_1^0+\varepsilon\delta f_1\right)\left(E^0+\varepsilon\delta E\right)\right]\left[a^{(2,0)}(2;1;t)+\varepsilon\delta a^{(2)}(2;1;t)\right]\right\}_{\varepsilon=0} \\ &=-\left\{\left(E^0+\varepsilon\delta E\right)^2\right\}_{\varepsilon=0} \end{aligned} \tag{192}$$

$$\left\{\delta \boldsymbol{B}_A^{(2)}\left[2;\delta\boldsymbol{A}^{(2)}(2;1;t);\boldsymbol{f}\right]\right\}_{\boldsymbol{f}^0} \triangleq \left\{\begin{pmatrix}\delta a^{(2)}(1;1;\tau) \\ \delta a^{(2)}(2;1;0)\end{pmatrix}\right\}_{\boldsymbol{f}^0} = \begin{pmatrix}0\\0\end{pmatrix}. \tag{193}$$

Carrying out the operations with respect to $\varepsilon$ indicated in Equations (191)-(193) yields the following system of equations:

$$\begin{aligned} &\left[2f_1^0a^{(2,0)}(1;1;t)+2a^{(1,0)}(t)\right]\delta E(t)+\left[2f_1^0a^{(2,0)}(2;1;t)+2E^0\right]\delta a^{(1)}(t) \\ &+\left[-\frac{\mathrm{d}}{\mathrm{d}t}+2f_1^0E^0(t)\right]\delta a^{(2)}(1;1;t)+2f_1^0a^{(1,0)}(t)\delta a^{(2)}(2;1;t) \\ &=-2\left(\delta f_1\right)\left[E^0(t)a^{(2,0)}(1;1;t)+a^{(1,0)}(t)a^{(2,0)}(2;1;t)\right], \end{aligned} \tag{194}$$

$$\begin{aligned} &\left[f_1^0a^{(2,0)}(2;1;t)+2E^0(t)\right]\delta E(t)+\left[\frac{\mathrm{d}}{\mathrm{d}t}+2f_1^0E^0(t)\right]\delta a^{(2)}(2;1;t) \\ &=-2E^0(t)a^{(2,0)}(2;1;t)\left(\delta f_1\right) \end{aligned} \tag{195}$$

Concatenating Equations (194) and (195) with the equations underlying the 2nd-LVSS provided in Equations (63) and (64) yields the following 3rd-Level Variational Sensitivity System (3rd-LVSS) for the 3rd-level vector-valued variational function $\boldsymbol{V}^{(3)}(4;1;t) \triangleq \left[\boldsymbol{V}^{(2)}(2;t), \delta\boldsymbol{A}^{(2)}(2;1;t)\right]^{\dagger}$:

$$\left\{\boldsymbol{VM}^{(3)}\left[4\times 4;1;\boldsymbol{f}\right]\boldsymbol{V}^{(3)}(4;1;t)\right\}_{\boldsymbol{f}^0} = \left\{\boldsymbol{Q}_V^{(3)}\left[4;1;\boldsymbol{f};\delta\boldsymbol{f}\right]\right\}_{\boldsymbol{f}^0}, \quad 0<t<\tau, \tag{196}$$

together with the following boundary conditions:

$$\left[\delta E(0), \delta a^{(1)}(\tau), \delta a^{(2)}(1;1;\tau), \delta a^{(2)}(2;1;0)\right]^{\dagger} = \left[0,0,0,0\right]^{\dagger}. \tag{197}$$

The quantities which appear in Equation (196) are defined as follows:

$$\boldsymbol{VM}^{(3)}\left[4\times 4;1;\,\boldsymbol{f}\,\right]\triangleq\begin{pmatrix}\boldsymbol{VM}^{(2)}\left[2\times 2;\,\boldsymbol{f}\,\right] & \mathbf{0}\left[2\times 2\right]\\ \boldsymbol{VM}_{21}^{(3)}\left[2\times 2;1;\,\boldsymbol{f}\,\right] & \boldsymbol{VM}_{22}^{(3)}\left[2\times 2;1;\,\boldsymbol{f}\,\right]\end{pmatrix};\tag{198}$$

$$\begin{gathered}\boldsymbol{VM}_{21}^{(3)}\left[2\times 2;1;\,\boldsymbol{f}\,\right]\triangleq\begin{pmatrix}2f_1^{0}a^{(2,0)}(1;1;t)+2a^{(1,0)}(t) & 2f_1^{0}a^{(2,0)}(2;1;t)+2E^{0}\\ 2f_1(\boldsymbol{\alpha})a^{(2)}(2;1;t)+2E(t) & 0\end{pmatrix};\\ \mathbf{0}\left[2\times 2\right]\triangleq\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix};\end{gathered}\tag{199}$$

$$\begin{aligned}\boldsymbol{VM}_{22}^{(3)}\left[2\times 2;1;\,\boldsymbol{f}\,\right]&\triangleq\boldsymbol{AM}^{(2)}\left[2\times 2;\,\boldsymbol{f}\,\right]\\ &\triangleq\begin{pmatrix}-\dfrac{\mathrm{d}}{\mathrm{d}t}+2f_1(\boldsymbol{\alpha})E(t) & 2f_1(\boldsymbol{\alpha})a^{(1)}(t)\\ 0 & \dfrac{\mathrm{d}}{\mathrm{d}t}+2f_1(\boldsymbol{\alpha})E(t)\end{pmatrix};\end{aligned}\tag{200}$$

$$\begin{gathered}\boldsymbol{Q}_V^{(3)}\left[4;1;\,\boldsymbol{f};\delta\boldsymbol{f}\,\right]\triangleq\begin{pmatrix}\boldsymbol{Q}_V^{(2)}\left[2;\,\boldsymbol{f};\delta\boldsymbol{f}\,\right]\\ \boldsymbol{Q}_2^{(3)}\left[2;1;\,\boldsymbol{f};\delta\boldsymbol{f}\,\right]\end{pmatrix};\\ \boldsymbol{Q}_2^{(3)}\left[2;1;\,\boldsymbol{f};\delta\boldsymbol{f}\,\right]\triangleq\begin{pmatrix}-2(\delta f_1)\left[E(t)a^{(2)}(1;1;t)+a^{(1)}(t)a^{(2)}(2;1;t)\right]\\ -2(\delta f_1)E(t)a^{(2)}(2;1;t)\end{pmatrix}.\end{gathered}\tag{201}$$

The notation used for the above quantities is as follows: (i) the argument "4 × 4"of the block-matrix $\boldsymbol{VM}^{(3)}\left[4\times 4;1;\,\boldsymbol{f}\,\right]$ indicates the dimensions of this matrix; (ii) the second argument, namely "1", of the block-matrix $\boldsymbol{VM}^{(3)}\left[4\times 4;1;\,\boldsymbol{f}\,\right]$ indicates that this matrix corresponds to the quantity $\partial^2 E(\tau)/\partial f_1\partial f_1$, which was labeled (by convention) the "*first* 2nd-order sensitivity"; (iii) the first argument (*i.e.*, "4") of the 3rd-level variational vector $\boldsymbol{V}^{(3)}(4;1;t)$ indicates that this vector has 4 components; (iv) the second argument of $\boldsymbol{V}^{(3)}(4;1;t)$, namely "1", indicates that this vector corresponds to $\partial^2 E(\tau)/\partial f_1\partial f_1$, which was labeled (by convention) the "*first* $2nd$-order sensitivity." The notation for the arguments of the vector-function $\boldsymbol{Q}_V^{(3)}\left[4;1;\,\boldsymbol{f};\delta\boldsymbol{f}\,\right]$ is similar to the notation used for the block-vector $\boldsymbol{V}^{(3)}(4;1;t)$.

The need for repeatedly solving the 3rd-LVSS represented by Equations (196) and (197) for all parameter variations of interest is circumvented by applying the 3rd-FASAM-N to eliminate the appearance of the variational function $\boldsymbol{V}^{(3)}(4;1;t)$ in Equation (190) by expressing this indirect-effect term in terms of a 3rd-level adjoint sensitivity function which will have the same number of components as $\boldsymbol{V}^{(3)}(4;1;t)$ but would be independent of parameter variations. This 3rd-level adjoint function will be denoted as $\boldsymbol{A}^{(3)}(4;1;t)\triangleq\left[a^{(3)}(1;1;t),a^{(3)}(2;1;t),a^{(3)}(3;1;t),a^{(3)}(4;1;t)\right]^{\dagger}$, where: (i) the first argument of $\boldsymbol{A}^{(3)}(4;1;t)$, namely "4", indicates that this vector-valued function has 4-components; (ii) the second argument of $\boldsymbol{A}^{(3)}(4;1;t)$, namely "1", indicates that this vector-valued function corresponds to $\partial^2 E(\tau)/\partial f_1\partial f_1$, which was labeled (by convention) the "*first* 2nd-order sensitivity." The 3rd-level adjoint function $\boldsymbol{A}^{(3)}(4;1;t)$ will be obtained as the solution of a 3rd-Level Adjoint Sensitivity System (3rd-LASS) which will be constructed in a Hilbert space denoted as $\mathsf{H}_3$, and which comprises as elements block-vectors of the same form as $\boldsymbol{V}^{(3)}(4;1;t)$. The inner product, denoted as $\left\langle \boldsymbol{\Psi}^{(3)}(4;t), \boldsymbol{\Phi}^{(3)}(4;t) \right\rangle_3$, of two generic vectors $\boldsymbol{\Psi}^{(3)}(4;t) \triangleq \left[\psi^{(3)}(1;t), \cdots, \psi^{(3)}(4;t)\right]^\dagger \in \mathsf{H}_3$ and $\boldsymbol{\Phi}^{(3)}(4;t) \triangleq \left[\varphi^{(3)}(1;t), \cdots, \varphi^{(3)}(4;t)\right]^\dagger \in \mathsf{H}_3$ in the Hilbert space $\mathsf{H}_3$ is defined as follows:

$$\left\langle \boldsymbol{\Psi}^{(3)}(4;t), \boldsymbol{\Phi}^{(3)}(4;t) \right\rangle_3 \triangleq \sum_{i=1}^{4} \int_0^\tau \psi^{(3)}(i;t)\varphi^{(3)}(i;t)\,\mathrm{d}t. \tag{202}$$

The 3rd-Level Adjoint Sensitivity System (3rd-LASS) for the 3rd-level adjoint function $\boldsymbol{A}^{(3)}(4;1;t) \triangleq \left[a^{(3)}(1;1;t), a^{(3)}(2;1;t), a^{(3)}(3;1;t), a^{(3)}(4;1;t)\right]^\dagger \in \mathsf{H}_3$, is constructed as follows:

i) Using Equation (202), form the inner product of the vector $\boldsymbol{A}^{(3)}(4;1;t)$ with Equation (196) to obtain the following relation:

$$\begin{aligned} &\left\{ \left\langle \boldsymbol{A}^{(3)}(4;1;t), \boldsymbol{VM}^{(3)}[4\times 4;1]\boldsymbol{V}^{(3)}(4;1;t) \right\rangle_3 \right\}_{\boldsymbol{f}^0} \\ &= \Big\{ a^{(3)}(1;1;t)\delta E(t) - a^{(3)}(2;1;t)\delta a^{(1)}(t) - a^{(3)}(3;1;t)\delta a^{(2)}(1;1;t) \\ &\quad + a^{(3)}(4;1;t)\delta a^{(2)}(2;1;t) \Big\}_{t=0}^{t=\tau} + \left\{ \left\langle \boldsymbol{V}^{(3)}(4;1;t), \boldsymbol{AM}^{(3)}[4\times 4;1]\boldsymbol{A}^{(3)}(4;1;t) \right\rangle_3 \right\}_{\boldsymbol{f}^0} \\ &= \left\{ \left\langle \boldsymbol{A}^{(3)}(4;1;t), \boldsymbol{Q}_V^{(3)}[4;1;\boldsymbol{f};\delta\boldsymbol{f}] \right\rangle_3 \right\}_{\boldsymbol{f}^0}. \end{aligned} \tag{203}$$

ii) Eliminate the boundary terms on the right side of Equation (203) and require the second term on the right-side of the first equality in Equation (203) to represent the G-differential defined in Equation (190) by imposing the following relations:

$$\left\{ \boldsymbol{AM}^{(3)}[4\times 4;1]\boldsymbol{A}^{(3)}(4;1;t) \right\}_{\boldsymbol{f}^0} = \left\{ \boldsymbol{Q}_A^{(3)}[4;1;\boldsymbol{f}] \right\}_{\boldsymbol{f}^0}, \quad 0 < t < \tau, \tag{204}$$

$$\left\{ \boldsymbol{B}_A^{(3)}\left[4;\boldsymbol{A}^{(3)}(4;1;t);\boldsymbol{f}\right] \right\}_{\boldsymbol{f}^0} \triangleq \begin{pmatrix} a^{(3)}(1;1;\tau) \\ a^{(3)}(2;1;0) \\ a^{(3)}(3;1;0) \\ a^{(3)}(4;1;\tau) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}; \tag{205}$$

where the block-matrix $\boldsymbol{AM}^{(3)}[4\times 4;1] \triangleq \left[\boldsymbol{VM}^{(3)}[4\times 4;1]\right]^*$ is the formal adjoint of the block-matrix $\boldsymbol{VM}^{(3)}[4\times 4;1]$, obtained by transposing the adjoints of the elements of $\boldsymbol{VM}^{(3)}[4\times 4;1]$, namely:

$$\boldsymbol{AM}^{(3)}[4\times 4;1] \triangleq \left[\boldsymbol{VM}^{(3)}[4\times 4;1]\right]^* = \begin{pmatrix} \left\{\left[\boldsymbol{VM}^{(2)}\right]^*\right\}^\dagger & \left\{\left[\boldsymbol{VM}_{21}^{(3)}\right]^*\right\}^\dagger \\ \boldsymbol{0}[2\times 2] & \left\{\left[\boldsymbol{VM}_{22}^{(3)}\right]^*\right\}^\dagger \end{pmatrix}; \tag{206}$$

and where the following definitions were used:

$$\boldsymbol{Q}_A^{(3)}[4;1;\boldsymbol{f}] \triangleq \left[\boldsymbol{q}_A^{(3)}(1;1;\boldsymbol{f}),\cdots,\boldsymbol{q}_A^{(3)}(4;1;\boldsymbol{f})\right]^\dagger; \tag{207}$$

$$\boldsymbol{q}_A^{(3)}(1;1;\boldsymbol{f}) \triangleq -2\left[a^{(2)}(1;1;t)E(t)+a^{(2)}(2;1;t)a^{(1)}(t)\right]; \tag{208}$$

$$\boldsymbol{q}_A^{(3)}(2;1;\boldsymbol{f}) \triangleq -2a^{(2)}(2;1;t)E(t); \tag{209}$$

$$\boldsymbol{q}_A^{(3)}(3;1;\boldsymbol{f}) \triangleq -E^2(t); \tag{210}$$

$$\boldsymbol{q}_A^{(3)}(4;1;\boldsymbol{f}) \triangleq -2a^{(1)}(t)E(t). \tag{211}$$

Replacing Equations (196), (197), and (190) into Equation (203) reduces the latter to the following expression:

$$\begin{aligned}
&\frac{\partial^3 E(\tau)}{\partial f_1 \partial f_1 \partial f_1}\delta f_1+\frac{\partial^3 E(\tau)}{\partial f_2 \partial f_1 \partial f_1}\delta f_2=\left\{\left\langle \boldsymbol{A}^{(3)}(4;1;t),\boldsymbol{Q}_V^{(3)}[4;1;\boldsymbol{f};\delta\boldsymbol{f}]\right\rangle_3\right\}_{\boldsymbol{f}^0}\\
&=\left\{\int_0^\tau a^{(3)}(1;1;t)\left[-(\delta f_1)E^2(t)+(\delta f_2)\right]\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&\quad+\left\{\int_0^\tau a^{(3)}(2;1;t)\left[-2(\delta f_1)a^{(1)}(t)E(t)\right]\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&\quad-2(\delta f_1)\left\{\int_0^\tau a^{(3)}(3;1;t)\left[E(t)a^{(2)}(1;1;t)+a^{(1)}(t)a^{(2)}(2;1;t)\right]\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&\quad-2(\delta f_1)\left\{\int_0^\tau a^{(3)}(4;1;t)E(t)a^{(2)}(2;1;t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}.
\end{aligned} \tag{212}$$

It follows from Equation (212) that:

$$\begin{aligned}
\frac{\partial^3 E(\tau)}{\partial f_1 \partial f_1 \partial f_1}=&-\left\{\int_0^\tau a^{(3)}(1;1;t)E^2(t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}-2\left\{\int_0^\tau a^{(3)}(2;1;t)a^{(1)}(t)E(t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&-2\left\{\int_0^\tau a^{(3)}(3;1;t)\left[E(t)a^{(2)}(1;1;t)+a^{(1)}(t)a^{(2)}(2;1;t)\right]\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&-2\left\{\int_0^\tau a^{(3)}(4;1;t)E(t)a^{(2)}(2;1;t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}.
\end{aligned} \tag{213}$$

$$\frac{\partial^3 E(\tau)}{\partial f_2 \partial f_1 \partial f_1}=\left\{\int_0^\tau a^{(3)}(1;1;t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}; \tag{214}$$

### 5.1.2. Computation of Third-Order Sensitivities Stemming from the Second-Order Sensitivity $\partial^2 E(\tau)/\partial f_2 \partial f_2$

The 3rd-order sensitivities that stem from $\partial^2 E(\tau)/\partial f_2 \partial f_2$ are obtained by applying the definition of the first-order G-differential to Equation (85), which yields the following expression:

$$\begin{aligned}
\delta\left\{\frac{\partial^2 E(\tau)}{\partial f_2 \partial f_2}\right\} &\triangleq \frac{\partial^3 E(\tau)}{\partial f_1 \partial f_2 \partial f_2}\delta f_1+\frac{\partial^3 E(\tau)}{\partial f_2 \partial f_2 \partial f_2}\delta f_2\\
&\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left\{\int_0^\tau\left[a^{(2)}(1;2;t)+\varepsilon\delta a^{(2)}(1;2;t)\right]\mathrm{d}t\right\}_{\boldsymbol{f}^0}\right\}_{\varepsilon=0}\\
&=\left\{\int_0^\tau \delta a^{(2)}(1;2;t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}.
\end{aligned} \tag{215}$$

Evidently, the second-order sensitivity $\partial^2 E(\tau)/\partial f_2 \partial f_2$ gives rise to two third-order sensitivities, $\partial^3 E(\tau)/\partial f_1 \partial f_2 \partial f_2$ and $\partial^3 E(\tau)/\partial f_2 \partial f_2 \partial f_2$, which will be determined in this Subsection by solving a corresponding 3rd-Level Adjoint Sensitivity System (3rd-LASS). For bookkeeping purposes, the quantity $\partial^2 E(\tau)/\partial f_2 \partial f_2$ will the labeled "the *second* 2nd-order sensitivity" and the solution of the 3rd-LASS that corresponds to it will be labeled "the *second* 3rd-level adjoint function."

The expression obtained in Equation (215) comprises no direct-effect term and can be evaluated after having determined the function $\delta a^{(2)}(1;2;t)$, which can be obtained as (part of) the solution of the G-differentiated 2nd-LASS defined by Equations (79) and (80), evaluated at the nominal values of the feature functions and state functions (*i.e.*, dependent variables). Using the superscript "zero" to denote the respective nominal values of the various quantities and applying the definition of the G-differential to Equations (79) and (80) yields the following system of equations for the vector-valued variational function $\delta \boldsymbol{A}^{(2)}(2;2;t) \triangleq \left[\delta a^{(2)}(1;2;t),\, \delta a^{(2)}(2;2;t)\right]^{\dagger}$:

$$\begin{aligned}&\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left[-\frac{\mathrm{d}}{\mathrm{d}t}+2\left(f_1^0+\varepsilon\delta f_1\right)\left(E^0+\varepsilon\delta E\right)\right]\left[a^{(2,0)}(1;2;t)+\varepsilon\delta a^{(2)}(1;2;t)\right]\right\}_{\varepsilon=0}\\&+2\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(f_1^0+\varepsilon\delta f_1\right)\left(a^{(1,0)}+\varepsilon\delta a^{(1)}\right)\left[a^{(2,0)}(2;2;t)+\varepsilon\delta a^{(2)}(2;2;t)\right]\right\}_{\varepsilon=0}=0,\end{aligned} \tag{216}$$

$$\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left[\frac{\mathrm{d}}{\mathrm{d}t}+2\left(f_1^0+\varepsilon\delta f_1\right)\left(E^0+\varepsilon\delta E\right)\right]\left[a^{(2,0)}(2;2;t)+\varepsilon\delta a^{(2)}(2;2;t)\right]\right\}_{\varepsilon=0}=0. \tag{217}$$

$$\left\{\delta \boldsymbol{B}_A^{(2)}\left[2;\delta\boldsymbol{A}^{(2)}(2;2;t);\boldsymbol{f}\right]\right\}_{\boldsymbol{f}^0} \triangleq \left\{\begin{pmatrix}\delta a^{(2)}(1;2;\tau)\\ \delta a^{(2)}(2;2;0)\end{pmatrix}\right\}_{\boldsymbol{f}^0}=\begin{pmatrix}0\\0\end{pmatrix}. \tag{218}$$

Carrying out the operations with respect to $\varepsilon$ indicated in Equations (216)-(218) yields the following system of equations:

$$\begin{aligned}&\left(2f_1^0\right)\delta E(t)+\left(2f_1^0\right)\delta a^{(1)}+\left[-\frac{\mathrm{d}}{\mathrm{d}t}+2f_1^0E^0(t)\right]\delta a^{(2)}(1;2;t)\\&+\left(2f_1^0a^{(1)}\right)\delta a^{(2)}(2;2;t)=-\left[E^0(t)a^{(2,0)}(1;2;t)+2a^{(1,0)}a^{(2,0)}(2;2;t)\right]\delta f_1;\end{aligned} \tag{219}$$

$$\begin{aligned}&2f_1^0a^{(2,0)}(2;2;t)\delta E+\left[\frac{\mathrm{d}}{\mathrm{d}t}+2f_1^0E^0(t_1)\right]\delta a^{(2)}(2;2;t)\\&=-2E^0(t)a^{(2,0)}(2;2;t)\delta f_1.\end{aligned} \tag{220}$$

Concatenating Equations (219) and (220) with the equations underlying the 2nd-LVSS provided in Equations (63) and (64) for the 2nd-Level vector-valued variational function $\boldsymbol{V}^{(2)}(2;t) \triangleq \left[\delta E(t), \delta a^{(1)}(t)\right]^{\dagger}$ yields the following 3rd-Level Variational Sensitivity System (3rd-LVSS) for the 3rd-Level vector-valued variational function $\boldsymbol{V}^{(3)}(4;2;t) \triangleq \left[\boldsymbol{V}^{(2)}(2;t), \delta\boldsymbol{A}^{(2)}(2;2;t)\right]^{\dagger}$:

$$\left\{\boldsymbol{VM}^{(3)}\left[4\times 4;2;\boldsymbol{f}\right]\boldsymbol{V}^{(3)}(4;2;t)\right\}_{\boldsymbol{f}^0}=\left\{\boldsymbol{Q}_V^{(3)}\left[4;2;\boldsymbol{f};\delta\boldsymbol{f}\right]\right\}_{\boldsymbol{f}^0},\ 0<t<\tau, \tag{221}$$

together with the following boundary conditions:

$$\left[\delta E(0),\delta a^{(1)}(\tau),\delta a^{(2)}(1;2;\tau),\delta a^{(2)}(2;2;0)\right]^{\dagger}=[0,0,0,0]^{\dagger}. \tag{222}$$

The quantities which appear in Equation (221) are defined as follows:

$$\boldsymbol{VM}^{(3)}[4\times 4;2;\boldsymbol{f}]\triangleq\begin{pmatrix}\boldsymbol{VM}^{(2)}[2\times 2;\boldsymbol{f}] & \mathbf{0}[2\times 2]\\ \boldsymbol{VM}_{21}^{(3)}[2\times 2;2;\boldsymbol{f}] & \boldsymbol{VM}_{22}^{(3)}[2\times 2;2;\boldsymbol{f}]\end{pmatrix}; \tag{223}$$

$$\boldsymbol{VM}_{21}^{(3)}[2\times 2;2;\boldsymbol{f}]\triangleq\begin{pmatrix}2f_1(\boldsymbol{\alpha}) & 2f_1(\boldsymbol{\alpha})\\ 2f_1(\boldsymbol{\alpha})a^{(2)}(2;2;t) & 0\end{pmatrix}; \tag{224}$$

$$\boldsymbol{VM}_{22}^{(3)}[2\times 2;1;\boldsymbol{f}]\triangleq\boldsymbol{AM}^{(2)}[2\times 2;\boldsymbol{f}]$$
$$\triangleq\begin{pmatrix}-\dfrac{\mathrm{d}}{\mathrm{d}t}+2f_1(\boldsymbol{\alpha})E(t) & 2f_1(\boldsymbol{\alpha})a^{(1)}(t)\\ 0 & \dfrac{\mathrm{d}}{\mathrm{d}t}+2f_1(\boldsymbol{\alpha})E(t)\end{pmatrix}; \tag{225}$$

$$\boldsymbol{Q}_V^{(3)}[4;2;\boldsymbol{f};\delta\boldsymbol{f}]\triangleq\begin{pmatrix}\boldsymbol{Q}_V^{(2)}[2;\boldsymbol{f};\delta\boldsymbol{f}]\\ \boldsymbol{Q}_2^{(3)}[2;2;\boldsymbol{f};\delta\boldsymbol{f}]\end{pmatrix};$$
$$\boldsymbol{Q}_2^{(3)}[2;2;\boldsymbol{f};\delta\boldsymbol{f}]\triangleq\begin{pmatrix}-(\delta f_1)\left[E(t)a^{(2)}(1;2;t)+2a^{(1)}(t)a^{(2)}(2;2;t)\right]\\ -2(\delta f_1)E(t)a^{(2)}(2;2;t)\end{pmatrix}. \tag{226}$$

The notation used for the above quantities is similar to that used in Subsection 5.1.1, above, except for the replacement of the argument ”1” with the argument “2” for the quantities that appear in Equation (223), to indicate that all of the respective quantities now correspond to $\partial^2 E(\tau)/\partial f_2\partial f_2$, which was labeled (by convention) the “*second* 2nd-order sensitivity.”

The need for solving the 3rd-LVSS for all parameter variations is circumvented by applying the 3rd-FASAM-N to eliminate the appearance of the variational function $\boldsymbol{V}^{(3)}(4;2;t)$ in Equation (215) by expressing this indirect-effect term in terms of a 3rd-Level adjoint sensitivity function which will be denoted as $\boldsymbol{A}^{(3)}(4;2;t)\triangleq\left[a^{(3)}(1;2;t),a^{(3)}(2;2;t),a^{(3)}(3;2;t),a^{(3)}(4;2;t)\right]^{\dagger}$, where: (i) the first argument of $\boldsymbol{A}^{(3)}(4;2;t)$, namely “4”, indicates that this vector-valued function has 4-components; (ii) the second argument of $\boldsymbol{A}^{(3)}(4;2;t)$, namely “2”, indicates that this vector-valued function corresponds to $\partial^2 E(\tau)/\partial f_2\partial f_2$, which was labeled (by convention) the “*second* 2nd-order sensitivity.” The 3rd-Level adjoint function $\boldsymbol{A}^{(3)}(4;2;t)$ will be obtained as the solution of a 3rd-Level Adjoint Sensitivity System (3rd-LASS) which is constructed in the Hilbert space $\mathsf{H}_3$ (as introduced in Subsection 5.1.1), as follows:

i) Form the inner product of the vector $\boldsymbol{A}^{(3)}(4;2;t)$ with Equation (221) to obtain the following relation:

$$\begin{aligned}
&\left\{\left\langle \boldsymbol{A}^{(3)}(4;2;t),\boldsymbol{VM}^{(3)}[4\times 4;2]\boldsymbol{V}^{(3)}(4;2;t)\right\rangle_3\right\}_{\boldsymbol{f}^0}\\
&=\Big\{a^{(3)}(1;2;t)\delta E(t)-a^{(3)}(2;2;t)\delta a^{(1)}(t)-a^{(3)}(3;2;t)\delta a^{(2)}(1;2;t)\\
&\quad +a^{(3)}(4;2;t)\delta a^{(2)}(2;2;t)\Big\}_{t=0}^{t=\tau}+\left\{\left\langle \boldsymbol{V}^{(3)}(4;2;t),\boldsymbol{AM}^{(3)}[4\times 4;2]\boldsymbol{A}^{(3)}(4;2;t)\right\rangle_3\right\}_{\boldsymbol{f}^0}\\
&=\left\{\left\langle \boldsymbol{A}^{(3)}(4;2;t),\boldsymbol{Q}_V^{(3)}[4;2;\boldsymbol{f};\delta\boldsymbol{f}]\right\rangle_3\right\}_{\boldsymbol{f}^0}.
\end{aligned} \tag{227}$$

ii) Eliminate the boundary terms on the right side of Equation (227) and require the second term on the right-side of the first equality in Equation (227) to represent the G-differential defined in Equation (215) by imposing the following relations:

$$\left\{\boldsymbol{AM}^{(3)}[4\times 4;2]\boldsymbol{A}^{(3)}(4;2;t)\right\}_{\boldsymbol{f}^0}=\left\{\boldsymbol{Q}_A^{(3)}[4;2;\boldsymbol{f}]\right\}_{\boldsymbol{f}^0},\ 0<t<\tau, \tag{228}$$

$$\left\{\boldsymbol{B}_A^{(3)}\left[4;\boldsymbol{A}^{(3)}(4;2;t);\boldsymbol{f}\right]\right\}_{\boldsymbol{f}^0}\triangleq\begin{pmatrix}a^{(3)}(1;2;\tau)\\ a^{(3)}(2;2;0)\\ a^{(3)}(3;2;0)\\ a^{(3)}(4;2;\tau)\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\end{pmatrix}; \tag{229}$$

where the block-matrix $\boldsymbol{AM}^{(3)}[4\times 4;2]\triangleq\left[\boldsymbol{VM}^{(3)}[4\times 4;2]\right]^*$ is the formal adjoint of the block-matrix $\boldsymbol{VM}^{(3)}[4\times 4;2]$.

Replacing Equations (228), (229), and (215) into Equation (227) reduces the latter to the following expression:

$$\begin{aligned}
&\frac{\partial^3 E(\tau)}{\partial f_1\partial f_2\partial f_2}\delta f_1+\frac{\partial^3 E(\tau)}{\partial f_2\partial f_2\partial f_2}\delta f_2=\left\{\left\langle \boldsymbol{A}^{(3)}(4;2;t),\boldsymbol{Q}_V^{(3)}[4;2;\boldsymbol{f};\delta\boldsymbol{f}]\right\rangle_3\right\}_{\boldsymbol{f}^0}\\
&=\left\{\int_0^\tau a^{(3)}(1;2;t)\left[-(\delta f_1)E^2(t)+(\delta f_2)\right]\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&\quad+\left\{\int_0^\tau a^{(3)}(2;2;t)\left[-2(\delta f_1)a^{(1)}(t)E(t)\right]\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&\quad-(\delta f_1)\left\{\int_0^\tau a^{(3)}(3;2;t)\left[E(t)a^{(2)}(1;2;t)+2a^{(1)}(t)a^{(2)}(2;2;t)\right]\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&\quad-2(\delta f_1)\left\{\int_0^\tau a^{(3)}(4;2;t)E(t)a^{(2)}(2;2;t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}.
\end{aligned} \tag{230}$$

It follows from Equation (230) that:

$$\begin{aligned}
\frac{\partial^3 E(\tau)}{\partial f_1\partial f_2\partial f_2}=&-\left\{\int_0^\tau a^{(3)}(1;2;t)E^2(t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}-2\left\{\int_0^\tau a^{(3)}(2;2;t)a^{(1)}(t)E(t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&-\left\{\int_0^\tau a^{(3)}(3;2;t)\left[E(t)a^{(2)}(1;2;t)+2a^{(1)}(t)a^{(2)}(2;2;t)\right]\mathrm{d}t\right\}_{\boldsymbol{f}^0}\\
&-\left\{\int_0^\tau a^{(3)}(4;2;t)E(t)a^{(2)}(2;2;t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}.
\end{aligned} \tag{231}$$

$$\frac{\partial^3 E(\tau)}{\partial f_2\partial f_2\partial f_2}=\left\{\int_0^\tau a^{(3)}(1;2;t)\mathrm{d}t\right\}_{\boldsymbol{f}^0}. \tag{232}$$

### 5.1.3. Using Sensitivities with Respect to the Feature Functions to Compute Most Efficiently Third-Order Response Sensitivities to Primary Model Parameters

The expression of $\partial^2 E(\tau)/\partial f_2 \partial f_1$ is provided in Equation (77) in terms of the 1st-level adjoint function $\boldsymbol{A}^{(2)}(2;1;t) \triangleq \left[a^{(2)}(1;1;t), a^{(2)}(2;1;t)\right]^\dagger$ while the equivalent expression of $\partial^2 E(\tau)/\partial f_1 \partial f_2$ is provided in Equation (84) in terms of the 1st-level adjoint function $\boldsymbol{A}^{(2)}(2;2;t) \triangleq \left[a^{(2)}(1;2;t), a^{(2)}(2;2;t)\right]^\dagger$. Examining these two equivalent expressions indicates that the expression for $\partial^2 E(\tau)/\partial f_2 \partial f_1$ is much simpler and hence, more convenient to use, than the expression for $\partial^2 E(\tau)/\partial f_1 \partial f_2$. The second-order sensitivity $\partial^2 E(\tau)/\partial f_2 \partial f_1$ gives rise to the third-order sensitivities $\partial^3 E(\tau)/\partial f_1 \partial f_2 \partial f_1$ and $\partial^3 E(\tau)/\partial f_2 \partial f_2 \partial f_1$, while the second-order sensitivity $\partial^2 E(\tau)/\partial f_1 \partial f_2$ gives rise to the third-order sensitivities $\partial^3 E(\tau)/\partial f_1 \partial f_1 \partial f_2$ and $\partial^3 E(\tau)/\partial f_2 \partial f_1 \partial f_2$.

In summary, one large-scale computation is needed for solving the 3rd-LASS defined by Equations (204) and (205), which yields the unmixed third-order sensitivity $\partial^3 E(\tau)/\partial f_1 \partial f_1 \partial f_1$. A second large-scale computation is needed for solving the 3rd-LASS defined by Equations (228) and (229), which yields the unmixed third-order sensitivity $\partial^3 E(\tau)/\partial f_2 \partial f_2 \partial f_2$. These two large-scale computations also yield the mixed third-order sensitivities $\partial^3 E(\tau)/\partial f_2 \partial f_1 \partial f_1$ and $\partial^3 E(\tau)/\partial f_1 \partial f_2 \partial f_2$. Thus, *the computation of all third-order sensitivities necessitates just two large-scale computations*. For verification purpose, one may consider performing a third and/or fourth large-scale computation for solving the 3rd-LASS that corresponds to $\partial^2 E(\tau)/\partial f_2 \partial f_1$ and/or $\partial^2 E(\tau)/\partial f_1 \partial f_2$. These additional large-scale computations yield alternative equivalent expressions/results for the mixed third-order sensitivities.

The third-order sensitivities of the response with respect to the primary model parameters are obtained by analytical, exact differentiation of the general expression provided in Equation (86) with respect to an arbitrary primary model parameter $\alpha_k$, *i.e.*,

$$\begin{aligned}\frac{\partial^3 E(\tau; f_1; f_2)}{\partial \alpha_k \partial \alpha_j \partial \alpha_i} &= \frac{\partial}{\partial \alpha_k}\left\{\left[\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_1}\frac{\partial f_1(\boldsymbol{\alpha})}{\partial \alpha_j} + \frac{\partial^2 E(\tau)}{\partial f_2 \partial f_1}\frac{\partial f_2(\boldsymbol{\alpha})}{\partial \alpha_j}\right]\frac{\partial f_1(\boldsymbol{\alpha})}{\partial \alpha_i}\right\} \\ &+ \frac{\partial}{\partial \alpha_k}\left\{\frac{\partial E(\tau)}{\partial f_1}\frac{\partial^2 f_1(\boldsymbol{\alpha})}{\partial \alpha_j \partial \alpha_i}\right\} + \frac{\partial}{\partial \alpha_k}\left\{\frac{\partial E(\tau)}{\partial f_2}\frac{\partial^2 f_2(\boldsymbol{\alpha})}{\partial \alpha_j \partial \alpha_i}\right\} \\ &+ \frac{\partial}{\partial \alpha_k}\left\{\left[\frac{\partial^2 E(\tau)}{\partial f_1 \partial f_2}\frac{\partial f_1(\boldsymbol{\alpha})}{\partial \alpha_j} + \frac{\partial^2 E(\tau)}{\partial f_2 \partial f_2}\frac{\partial f_2(\boldsymbol{\alpha})}{\partial \alpha_j}\right]\frac{\partial f_2(\boldsymbol{\alpha})}{\partial \alpha_i}\right\}; \; i, j, k = 1, \cdots, 7.\end{aligned} \tag{233}$$

The numerical result for any of the third-order sensitivity of the response with respect to a primary model parameter is obtained by performing the actual differentiation in Equation (233) and subsequently replacing in the resulting expression the analytical expression of the sensitivity of the respective feature-functions with respect to the parameter(s) under consideration, together with the (numerical) results for the respective sensitivities of the response with respect to the feature functions. Evidently, no additional large-scale computations are required to obtain the third-order response sensitivities to the primary parameters from the response sensitivities to the feature functions. Altogether, *two large-scale computations (for solving the aforementioned 3rd-LASS) suffice for obtaining all of the 343 third-order sensitivities* (of which 84 are distinct from each other) of the response with respect to the primary model parameters.

### 5.2. Generic Computation of Third-Order Sensitivities Using the 3rd-CASAM-N

Just like the 3rd-FASAM-N, the 3rd-CASAM-N methodology generically considers that the third-order sensitivities are the "first-order sensitivities of the second-order sensitivities." The application of the 3rd-CASAM-N for determining the third-order sensitivities of the response with respect to the primary model parameters will be generally illustrated in this Subsection by considering the general functional dependence of the second-order sensitivities obtained in Subsection 4.2. As has been shown in Section 4.2, as many large-scale computations as there are primary model parameters (TP = 7) are needed to solve the seven distinct 2nd-Level Adjoint Sensitivity Systems (2nd-LASS) for obtaining all of the $TP^2 = 49$ second-order sensitivities to the model parameters, of which $TP(TP+1)/2 = 28$ are distinct from each other. Examining the expressions obtained in Section 4.2 for the second-order sensitivities of the response with respect to the primary model parameters indicates that they all have the following generic form:

$$\begin{gathered}\frac{\partial^2 E(\tau)}{\partial\alpha_j\partial\alpha_i} = \int_0^\tau F\left[j;i;E(t);a^{(1)}(t);c^{(2)}(1;i;t),c^{(2)}(2;i;t);\boldsymbol{\alpha}\right]\mathrm{d}t, \\ i,j = 1,\cdots,TP = 7.\end{gathered} \tag{234}$$

The third-order sensitivities of the response $E(\tau)$ with respect to the primary model parameters is obtained as the first-order G-differential of the expression considered in Equation (234) which by definition yields the following expression:

$$\begin{aligned}&\delta\left\{\frac{\partial^2 E(\tau)}{\partial\alpha_j\partial\alpha_i}\right\} \triangleq \left\{\left\{\frac{d}{d\varepsilon}\int_0^\tau F\left[j;i;E(t);a^{(1)}(t);c^{(2)}(1;i;t),c^{(2)}(2;i;t);\boldsymbol{\alpha}\right]\mathrm{d}t\right\}_{\varepsilon=0}\right\}_{\boldsymbol{\alpha}^0} \\ &\triangleq \left\{\delta\left[\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_i\right]\right\}_{dir} + \left\{\delta\left[\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_i\right]\right\}_{ind}, \quad j,i = 1,\cdots,7;\end{aligned} \tag{235}$$

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

$$\left\{\delta\left[\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_i\right]\right\}_{dir} \triangleq \sum_{k=1}^{TP=7}\left\{\int_0^\tau\left[\partial F(j;i;\cdots;\boldsymbol{\alpha})/\partial\alpha_k\right]\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}\delta\alpha_k; \tag{236}$$

$$\begin{aligned}&\left\{\delta\left[\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_i\right]\right\}_{ind}\\&\triangleq\left\{\int_0^\tau \frac{\partial F[j;i;\cdots;\boldsymbol{\alpha}]}{\partial E}\delta E(t)\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}+\left\{\int_0^\tau \frac{\partial F[j;i;\cdots;\boldsymbol{\alpha}]}{\partial a^{(1)}}\delta a^{(1)}(t)\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}\\&\quad+\left\{\int_0^\tau \frac{\partial F[j;i;\cdots;\boldsymbol{\alpha}]}{\partial c^{(2)}(1;i;t)}\delta c^{(2)}(1;i;t)\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}+\left\{\int_0^\tau \frac{\partial F[j;i;\cdots;\boldsymbol{\alpha}]}{\partial c^{(2)}(2;i;t)}\delta c^{(2)}(2;i;t)\mathrm{d}t\right\}_{\boldsymbol{\alpha}^0}.\end{aligned}\tag{237}$$

The direct-effect term defined in Equation (236) can be computed already at this stage. The indirect-effect term may, in principle, be computed after having determined the variational functions $\delta E(t)$, $\delta a^{(1)}(t)$, $\delta c^{(2)}(1;i;t)$ and $\delta c^{(2)}(2;i;t)$. The variational functions $\delta E(t)$ and $\delta a^{(1)}(t)$ are the solutions of the 1st-LVSS represented by Equations (99) and (100).

Recall that the functions 2nd-Level adjoint functions $c^{(2)}(1;i;t), c^{(2)}(2;i;t), i=1,\cdots,7$, are the solutions of the corresponding 2nd-LASS, namely:

i) the functions $c^{(2)}(1;1;t), c^{(2)}(2;1;t)$ are the solutions of Equations (107) and (108);

ii) the functions $c^{(2)}(1;2;t), c^{(2)}(2;2;t)$ are the solutions of Equations (121) and (122);

iii) the functions $c^{(2)}(1;3;t), c^{(2)}(2;3;t)$ are the solutions of Equations (133) and (134);

iv) the functions $c^{(2)}(1;4;t), c^{(2)}(2;4;t)$ are the solutions of Equations (145) and (146);

v) the functions $c^{(2)}(1;5;t), c^{(2)}(2;5;t)$ are the solutions of Equations (157) and (158);

vi) the functions $c^{(2)}(1;6;t), c^{(2)}(2;6;t)$ are the solutions of Equations (169) and (170);

vii) the functions $c^{(2)}(1;7;t), c^{(2)}(2;7;t)$ are the solutions of Equations (181) and (182).

The 2nd-LASSystems enumerated above can be written in the following generic form $i=1,\cdots,7=TP$, where "TP" denotes the "total number of primary model parameters":

$$\begin{aligned}&\left\{\boldsymbol{AM}^{(2)}\left[2\times 2;E(t),a^{(1)}(t);\boldsymbol{\alpha}\right]\boldsymbol{C}^{(2)}(2;i;t)\right\}_{\boldsymbol{\alpha}^0}\\&=\left\{\boldsymbol{Q}_A^{(2)}\left[2;i;E(t),a^{(1)}(t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0},\ 0<t<\tau;\end{aligned}\tag{238}$$

$$\left\{\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{C}^{(2)}(2;i;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0}\triangleq\begin{pmatrix}c^{(2)}(1;i;\tau)\\c^{(2)}(2;i;0)\end{pmatrix}_{\boldsymbol{\alpha}^0}=\begin{pmatrix}0\\0\end{pmatrix};\tag{239}$$

where:

$$\boldsymbol{Q}_A^{(2)}\left[2;i;E(t),a^{(1)}(t);\boldsymbol{\alpha}\right]\triangleq\begin{pmatrix}q_A^{(2)}\left(1;i;E(t),a^{(1)}(t);\boldsymbol{\alpha}\right)\\q_A^{(2)}\left(2;i;E(t),a^{(1)}(t);\boldsymbol{\alpha}\right)\end{pmatrix}.\tag{240}$$

The variational functions $\delta c^{(2)}(1;i;t)$ and $\delta c^{(2)}(2;i;t)$ are the solutions of the equations that result by G-differentiating Equations (238) and (239), which can be generically represented as follows:

$$\begin{aligned}&\left\{\frac{\partial\left[\boldsymbol{AM}^{(2)}\boldsymbol{C}^{(2)}(2;i;t)-\boldsymbol{Q}_A^{(2)}\right]}{\partial E}\delta E(t)\right\}_{\boldsymbol{\alpha}^0}\\&+\left\{\frac{\partial\left[\boldsymbol{AM}^{(2)}\boldsymbol{C}^{(2)}(2;i;t)-\boldsymbol{Q}_A^{(2)}\right]}{\partial a^{(1)}}\delta a^{(1)}(t)\right\}_{\boldsymbol{\alpha}^0}\\&+\left\{\boldsymbol{AM}^{(2)}\left[\delta\boldsymbol{C}^{(2)}(2;i;t)\right]\right\}_{\boldsymbol{\alpha}^0}=\left\{\frac{\partial\left[\boldsymbol{Q}_A^{(2)}-\boldsymbol{AM}^{(2)}\boldsymbol{C}^{(2)}(2;i;t)\right]}{\partial\boldsymbol{\alpha}}\delta\boldsymbol{\alpha}\right\}_{\boldsymbol{\alpha}^0}.\end{aligned}\tag{241}$$

$$\left\{\delta\boldsymbol{B}_A^{(2)}\left[2;\boldsymbol{C}^{(2)}(2;i;t);\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0}\triangleq\begin{pmatrix}\delta c^{(2)}(1;i;\tau)\\ \delta c^{(2)}(2;i;0)\end{pmatrix}_{\boldsymbol{\alpha}^0}=\begin{pmatrix}0\\0\end{pmatrix};\ i=1,\cdots,7.. \tag{242}$$

As indicated by Equations (241) and (242), the variational functions $\delta c^{(2)}(1;i;t)$ and $\delta c^{(2)}(2;i;t)$ are coupled to the variational functions $\delta E(t)$ and $\delta a^{(1)}(t)$. It follows that these variational functions can be determined as the solution of the system of equations obtained by concatenating Equations (241) and (242) with Equations (63) and (64). The 4×4-dimensional system thus obtain is called the 3rd-Level Variational Sensitivity System (3rd-LVSS) for the 3rd-Level variational vector-valued function $\boldsymbol{U}^{(3)}(4;i;t)\triangleq\left[\boldsymbol{V}^{(2)}(2;t),\delta\boldsymbol{C}^{(2)}(2;i;t)\right]^{\dagger}$, where $\boldsymbol{V}^{(2)}(2;t)\triangleq\left[\delta E(t),\delta a^{(1)}(t)\right]^{\dagger}$ and $\boldsymbol{C}^{(2)}(2;i;t)\triangleq\left[\delta c^{(2)}(1;i;t),\delta c^{(2)}(2;i;t)\right]^{\dagger}$, for $i=1,\cdots,TP=7$. This 3rd-LVSS is linear in $\boldsymbol{U}^{(3)}(4;i;t)$ and can be generically represented in the following form:

$$\left\{\boldsymbol{UM}^{(3)}\left[4\times4;i;\boldsymbol{\alpha}\right]\boldsymbol{U}^{(3)}(4;i;t)\right\}_{\boldsymbol{\alpha}^0}=\left\{\boldsymbol{S}_V^{(3)}\left[4;i;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right]\right\}_{\boldsymbol{\alpha}^0},\ 0<t<\tau, \tag{243}$$

together with the following boundary conditions:

$$\left[\delta E(0),\delta a^{(1)}(\tau),\delta a^{(2)}(1;i;\tau),\delta a^{(2)}(2;i;0)\right]^{\dagger}=\left[0,0,0,0\right]^{\dagger}. \tag{244}$$

The specific expressions of the 4×4-dimensional matrix $\boldsymbol{UM}^{(3)}\left[4\times4;i;\boldsymbol{\alpha}\right]$ and 4-dimensional vector $\boldsymbol{S}_V^{(3)}\left[4;i;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right]$ which appear in Equation (243) differ according to the value of the index $i=1,\cdots,TP=7$, but their specific expressions are not needed for the purpose of presenting the generic characteristics of computing the third-order response sensitivities with respect to the primary model parameters by applying the 3rd-CASAM-N methodology. Following the principles underlying this methodology, the need for determining explicitly the variational vector-valued function $\boldsymbol{U}^{(3)}(4;i;t)$ is avoided by eliminating its appearance in Equation (237) by recasting the indirect-effect term into an equivalent expression involving a corresponding (4-dimensional vector-valued)

3rd-Level adjoint sensitivity function, which will be constructed in the Hilbert space $\mathsf{H}_3$. Correspondingly, the third-level vector-valued adjoint function which will be denoted as $\boldsymbol{C}^{(3)}(4;j;i;t)\triangleq\left[c^{(3)}(1;j;i;t),\cdots,c^{(3)}(4;j;i;t)\right]^{\dagger}\in\mathsf{H}_3$, where the indices "$(j;i)$" indicate that this adjoint function corresponds to the "$(j;i)$ th second-order sensitivity" in Equation (237). The 3rd-LASS for $\boldsymbol{C}^{(3)}(4;j;i;t)$ is constructed by applying the 3rd-CASAM-N, which employs the same principles as the 3rd-FASAM-N, as follows:

1) Using the definition provided by Equation (202), form the inner product in $\mathsf{H}_3$ of the vector $\boldsymbol{C}^{(3)}(4;j;i;t)$ with Equation (243) to obtain the following relation:

$$\begin{aligned}&\left\{\left\langle \boldsymbol{C}^{(3)}(4;j;i;t),\boldsymbol{UM}^{(3)}[4\times4;i;\boldsymbol{\alpha}]\boldsymbol{U}^{(3)}(4;i;t)\right\rangle_3\right\}_{\boldsymbol{\alpha}^0}\\&=\Big\{c^{(3)}(1;j;i;t)\delta E(t)-c^{(3)}(2;j;i;t)\delta a^{(1)}(t)\\&\quad-c^{(3)}(3;j;i;t)\delta c^{(2)}(1;i;t)+c^{(3)}(4;j;i;t)\delta c^{(2)}(2;i;t)\Big\}_{t=0}^{t=t_f}\\&\quad+\left\{\left\langle \boldsymbol{U}^{(3)}(4;i;t),\left[\boldsymbol{UM}^{(3)}(4\times4;i;\boldsymbol{\alpha})\right]^{*}\boldsymbol{C}^{(3)}(4;j;i;t)\right\rangle_3\right\}_{\boldsymbol{\alpha}^0}\\&=\left\{\left\langle \boldsymbol{C}^{(3)}(4;j;i;t),\boldsymbol{S}_V^{(3)}[4;i;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\right\rangle_3\right\}_{\boldsymbol{\alpha}^0},\end{aligned}\tag{245}$$

where $\left[\boldsymbol{UM}^{(3)}(4\times4;i;\boldsymbol{\alpha})\right]^{*}$ denotes the formal adjoint of the operator-valued matrix $\boldsymbol{UM}^{(3)}[4\times4;i;\boldsymbol{\alpha}]$.

2) Eliminate the boundary terms on the right side of Equation (245) and require the term $\left\{\left\langle \boldsymbol{U}^{(3)}(4;i;t),\left[\boldsymbol{UM}^{(3)}(4\times4;i;\boldsymbol{\alpha})\right]^{*}\boldsymbol{C}^{(3)}(4;j;i;t)\right\rangle_3\right\}_{\boldsymbol{\alpha}^0}$ in Equation (245) to represent the indirect-effect term defined in Equation (237) by imposing the following relations:

$$\begin{aligned}&\left\{\left[\boldsymbol{UM}^{(3)}(4\times4;i;\boldsymbol{\alpha})\right]^{*}\boldsymbol{C}^{(3)}(4;j;i;t)\right\}_{\boldsymbol{\alpha}^0}\\&=\left\{\left[\frac{\partial F[j;i;\cdots;\boldsymbol{\alpha}]}{\partial E},\frac{\partial F[j;i;\cdots;\boldsymbol{\alpha}]}{\partial a^{(1)}},\frac{\partial F[j;i;\cdots;\boldsymbol{\alpha}]}{\partial c^{(2)}(1;i;t)},\frac{\partial F[j;i;\cdots;\boldsymbol{\alpha}]}{\partial c^{(2)}(2;i;t)}\right]^{\dagger}\right\}_{\boldsymbol{\alpha}^0}.\end{aligned}\tag{246}$$

$$c^{(3)}(1;j;i;\tau)=c^{(3)}(2;j;i;0)=c^{(3)}(3;j;i;0)=c^{(3)}(4;j;i;\tau)=0\,.\tag{247}$$

The relations represented by Equations (246) and (247) constitute the 3rd-LASS for the 3rd-Level adjoint function $\boldsymbol{C}^{(3)}(4;j;i;t)$.

3) Use the relations provided in Equations (245)-(247) in Equation (237) to obtain the following expression for the indirect-effect term $\left\{\delta\left[\partial^2 E(t_f)/\partial\gamma\partial l_p\right]\right\}_{ind}$:

$$\left\{\delta\left[\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_i\right]\right\}_{ind}\triangleq\left\{\left\langle \boldsymbol{C}^{(3)}(4;j;i;t),\boldsymbol{S}_V^{(3)}[4;i;\boldsymbol{\alpha};\delta\boldsymbol{\alpha}]\right\rangle_3\right\}_{\boldsymbol{\alpha}^0}.\tag{248}$$

4) Finally, the third-order sensitivities, $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_j\partial\alpha_i$, $i,j,k=1,\cdots,7=TP$, of the response with respect to the primary model parame-

ters are obtained by adding the expression for the indirect-effect term obtained in Equation (248) with the expression for the direct-effect term defined by Equation (236) and subsequently identifying the quantities that multiply the parameter variations $\delta\alpha_k$, $k = 1,\cdots,7 = TP$.

Evidently, because of the symmetry of the mixed second-order sensitivities $\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_i = \partial^2 E(\tau)/\partial\alpha_i\partial\alpha_j$, $i, j = 1,\cdots,7 = TP$, only $TP(TP+1)/2 = 28$ of the total of 49 second-order response sensitivities with respect to the primary model parameters need to be considered for providing the source terms for the right-side of the 3rd-LASS defined in Equation (246). This means that at most 28 "responses" would need to be considered for providing the sources on the right-side of the 3rd-LASS defined in Equation (246), which in turn implies that at most 28 "large-scale" computations would be needed to obtain all of the third-order sensitivities, $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_j\partial\alpha_i$, $i, j, k = 1,\cdots,7 = TP$. However, if all of these large-scale computations were performed, many of the mixed third-order sensitivities would be computed twice, and some of them would even be computed thrice.

Note that of the total number of $TP^3 = 343$ third-order sensitivities, only $TP(TP+1)(TP+2)/6 = 84$ of them are distinct. The minimum number of "large-scale" computations needed to obtain all of these 84 distinct third-order sensitivities can be deduced as follows:

a) The second-order sensitivities $\partial^2 E(\tau)/\partial\alpha_i\partial\alpha_i$, $i = 1,\cdots,7 = TP$, are uniquely obtained when solving the 2nd-LASS, so they certainly must serve as "responses" for the "large-scale" computations needed to solve the corresponding 3rd-LASS. Performing these 7 large-scale computations (*i.e.*, solving the 3rd-LASSystems that correspond to $\partial^2 E(\tau)/\partial\alpha_i\partial\alpha_i$) yields 49 third-order sensitivities of the form $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_i\partial\alpha_i$, $i, k = 1,\cdots,7 = TP$. These 7 "large-scale" computations are mandatory since these are the only ones that will produce the unique third-order sensitivities of the form $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_k\partial\alpha_k$, $k = 1,\cdots,7 = TP$, included in the 49 sensitivities of the form $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_i\partial\alpha_i$, $i, k = 1,\cdots,7 = TP$, that are obtained this way.

b) Five "large-scale computations" are performed using the second-order sensitivities of the form $\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_1 = \partial^2 E(\tau)/\partial\alpha_1\partial\alpha_j$, $j = 2,\cdots,6 = TP-1$, as "responses" for the respective 3rd-LASSystems. These 5 "large-scale computations" yield 35 third-order sensitivities of the form $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_j\partial\alpha_1$, $k = 1,\cdots,7 = TP$ of which the following 15 are distinct: (i) $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_2\partial\alpha_1$ for $k = 3,\cdots,7 = TP$; (ii) $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_3\partial\alpha_1$ for $k = 4,5,6,7 = TP$; (iii) $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_4\partial\alpha_1$ for $k = 5,6,7 = TP$; (iv) $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_5\partial\alpha_1$ for $k = 6,7 = TP$; (v) $\partial^3 E(\tau)/\partial\alpha_7\partial\alpha_6\partial\alpha_1$.

c) Four "large-scale computations" are performed using the second-order sensitivities of the form $\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_2 = \partial^2 E(\tau)/\partial\alpha_2\partial\alpha_j$, $j = 3,\cdots,6 = TP-1$, as "responses" for the respective 3rd-LASSystems. These 4 "large-scale computations" yield 28 third-order sensitivities of the form $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_j\partial\alpha_2$, $k = 1,\cdots,7 = TP$, of which the following 10 are distinct: (i)

$\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_3\partial\alpha_2$ for $k=4,5,6,7=TP$; (ii) $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_4\partial\alpha_2$ for $k=5,6,7=TP$; (iii) $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_5\partial\alpha_2$ for $k=6,7=TP$; (iv) $\partial^3 E(\tau)/\partial\alpha_7\partial\alpha_6\partial\alpha_2$.

d) Three "large-scale computations" are performed using the second-order sensitivities of the form $\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_3=\partial^2 E(\tau)/\partial\alpha_3\partial\alpha_j$, $j=4,5,6=TP-1$, as "responses" for the respective 3rd-LASSystems. These 3 "large-scale computations" yield 21 third-order sensitivities of the form $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_j\partial\alpha_2$, $k=1,\cdots,7=TP$, of which the following 6 are distinct: (i) $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_4\partial\alpha_3$ for $k=5,6,7=TP$; (ii) $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_5\partial\alpha_3$ for $k=6,7=TP$; (iii) $\partial^3 E(\tau)/\partial\alpha_7\partial\alpha_6\partial\alpha_3$.

e) Two "large-scale computations" are performed using the second-order sensitivities of the form $\partial^2 E(\tau)/\partial\alpha_j\partial\alpha_4=\partial^2 E(\tau)/\partial\alpha_4\partial\alpha_j$, $j=5,6=TP-1$, as "responses" for the respective 3rd-LASSystems. These 2 "large-scale computations" yield 14 third-order sensitivities of the form $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_j\partial\alpha_4$, $k=1,\cdots,7=TP$, of which the following 3 are distinct: (i) $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_5\partial\alpha_4$ for $k=6,7=TP$; (ii) $\partial^3 E(\tau)/\partial\alpha_7\partial\alpha_6\partial\alpha_4$.

f) One "large-scale computation" is performed using the second-order sensitivity $\partial^2 E(\tau)/\partial\alpha_6\partial\alpha_5=\partial^2 E(\tau)/\partial\alpha_5\partial\alpha_6$ as the "response" for the respective 3rd-LASS. This "large-scale computation" yields 7 third-order sensitivities of the form $\partial^3 E(\tau)/\partial\alpha_k\partial\alpha_6\partial\alpha_5$, $k=1,\cdots,7=TP$, of which the following is distinct: $\partial^3 E(\tau)/\partial\alpha_7\partial\alpha_6\partial\alpha_5$.

In summary, a minimum of 22 "large-scale" computations for solving 22 distinct 3rd-LASSystems are necessary to obtain all of the distinct third-order sensitivities of the response with respect to the 7 primary model parameters. In addition to the distinct third-order sensitivities, these 22 computations will also yield alternative expressions/results for the third-order sensitivities enumerated above. On the other hand, if duplicate computations of all of the mixed third-order sensitivities are desired, then all of 28 distinct second-order sensitivities should be used as "responses" for the corresponding twenty-eight 3rd-LASSystems.

## 6. Concluding Discussion

Computational models of physical systems often comprise not only imprecisely known primary model parameters (e.g., geometrical dimensions, microscopic nuclear cross sections, atomic number densities, etc.) but often comprise "feature" functions of such parameters, such as macroscopic cross sections, Reynolds numbers, Nusselt numbers, etc. When such "feature" functions of model parameters can be identified, the "nth-order Feature Sensitivity Analysis Methodology for Nonlinear Systems" (abbreviated as "nth-FASAM-N") presented in the accompanying "Part 1" by Cacuci [1] provides the ultimate efficiency for deriving and computing the exact explicit expressions of the sensitivities of arbitrarily-high order of model responses with respect to the model's parameters, by first determining the sensitivities of the respective responses with respect to the feature functions and subsequently determining analytically the sensitivities with respect to the model's parameters. The number of large-scale computations for determining the second-and higher-order sensitivities within the n<sup>th</sup>-FASAM-N methodology is proportional to the number of feature-functions (as opposed to the number of primary parameters). For the computation of the first-order sensitivities, both the n<sup>th</sup>-FASAM-N [1] and the n<sup>th</sup>-CASAM-N [2] methodologies require a single "large-scale" "adjoint" computation, regardless of the number of model parameters. On the other hand, the application of the n<sup>th</sup>-FASAM-N methodology for obtaining the higher-order sensitivities requires the least number of large-scale computations, since the number of feature-functions is much smaller than the number of model parameters.

The above characteristics of the n<sup>th</sup>-FASAM-N [1] and the n<sup>th</sup>-CASAM-N [2] methodologies have been comparatively illustrated in this work by using the well-known Nordheim-Fuchs reactor dynamics/safety model [3] [4]. This phenomenological model describes a short-time self-limiting power transient in a nuclear reactor system having a negative temperature coefficient in which a large amount of reactivity is suddenly inserted, either intentionally or by accident. This model is sufficiently complex to demonstrate all of the important features of applying the n<sup>th</sup>-FASAM-N and n<sup>th</sup>-CASAM-N methodologies yet admits exact closed-form solutions for the energy released in the transient (which is the most important system response) and its sensitivities to the model's uncertain parameters. This model comprises 7 uncertain parameters which can be grouped into two "feature" functions of these parameters. The expressions of the first, second, and third-order sensitivities of the released energy to the model's parameters were obtained analytically in closed form, and their respective computations revealed the following characteristics:

1) Computation of all first-order response sensitivities with respect to the model's primary parameters:

a) The 1<sup>st</sup>-FASAM-N and the 1<sup>st</sup>-CASAM-N methodologies are equally efficient; each methodology requires a single large-scale computation for solving the "First-Level Adjoint Sensitivity System" (1<sup>st</sup>-LASS) to obtain all 7 first-order response sensitivities with respect to the 7 parameters involved in the Nordheim-Fuchs model.

b) The simplest conventional first-order finite difference scheme requires at least 2 large-scale computations per parameter, using the original model with "perturbed" parameter values, to produce an approximate value for a first-order sensitivity. For the 7 parameters involved in the Nordheim-Fuchs model, at least 14 large-scale computations would be required to compute the first-order sensitivities within a first-order accuracy in the considered parameter perturbation. Evidently, both the 1<sup>st</sup>-FASAM-N and the 1<sup>st</sup>-CASAM-N are vastly more efficient than finite-difference schemes. Furthermore, the finite difference schemes produce approximate values, while the 1<sup>st</sup>-FASAM-N and the 1<sup>st</sup>-CASAM-N accurately compute exact expressions of the respective sensitivities.

2) Computation of all second-order response sensitivities with respect to the model's primary parameters:

a) The 2nd-CASAM-N methodology requires as many large-scale computations (for solving the 2nd-LASS) as there are first-order sensitivities to model parameters, or, equivalently, as many as there are parameters (*i.e.*, *TP*).

b) The 2nd-FASAM-N methodology requires as many large-scale computations (for solving the 2nd-LASS) as there are first-order sensitivities with respect to the feature functions, which is equivalent to "as many computations as there are feature functions" (*i.e.*, *TF*). Since the number of feature-functions is much smaller than the number of primary parameters, *i.e.*, $TF \ll TP$, the 2nd-FASAM-N methodology is considerably more efficient than the 2nd-CASAM-N methodology. For the illustrative example of the Nordheim-Fuchs model, the 2nd-FASAM-N methodology required 2 large-scale computations to obtain all of the exact expressions of the 28 distinct second-order response sensitivities with respect to the model parameters, while the 2nd-FASAM-N methodology required 7 large-scale computations for obtaining these 28 distinct second-order sensitivities. Both the 2nd-FASAM-N and the 2nd-CASAM-N methodologies yield exact values for the expressions of the second-order sensitivities

3) Computation of all third-order response sensitivities with respect to the model's primary parameters:

a) The 3rd-CASAM-N methodology requires at most $TP(TP+1)/2$ large-scale computations for solving the "3rd-Level Adjoint Sensitivity System" (3rd-LASS). For the illustrative example of the Nordheim-Fuchs model, 22 large-scale computations were needed by applying the 3rd-CASAM-N methodology to obtain the exact expressions of the 84 distinct third-order response sensitivities with respect to the model parameters.

b) The 3rd-FASAM-N methodology requires at most $TF(TF+1)/2$ large-scale computations for solving the "3rd-Level Adjoint Sensitivity System" (3rd-LASS). For the illustrative example of the Nordheim-Fuchs model, 2 large-scale computations within the 3rd-FASAM-N methodology sufficed to obtain all of the exact expressions of the 84 distinct third-order response sensitivities with respect to the model parameters. Evidently, the 3rd-FASAM methodology is significantly more efficient for computing the second-and higher-order sensitivities than the 3rd-CASAM-N methodology. Both the 3rd-FASAM-N and the 3rd-CASAM-N methodologies yield exact values for the expressions of the third-order sensitivities.

In summary, when no feature functions of parameters can be identified, the mathematical frameworks of the nth-FASAM-N and the nth-CASAM-N methodologies coincide. When feature-functions of parameters can be identified within the model, the nth-FASAM-N methodology requires the least number of large-scale computations of any practical methodology for computing exact expressions of second- and higher-order sensitivities. Evidently, both the nth-FASAM-N and the nth-CASAM-N are vastly more efficient than fi-

finite-difference schemes. Furthermore, the finite difference-schemes are approximate, while the $n^{th}$-FASAM-N and the $n^{th}$-CASAM-N accurately compute exact expressions of these sensitivities. Together, the $n^{th}$-FASAM-N and the $n^{th}$-CASAM-N methodologies remain the most practical methodologies for computing response sensitivities comprehensively and accurately, overcoming the curse of dimensionality in sensitivity analysis of nonlinear systems.

## Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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