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Fifth-Order Comprehensive Adjoint Sensitivity Analysis Methodology for Nonlinear Systems (5th-CASAM-N): II. Paradigm Application to a Bernoulli Model Comprising Uncertain Parameters

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Abstract

This work presents the application of the recently developed "Fifth-Order Comprehensive Adjoint Sensitivity Analysis Methodology for Nonlinear Systems (5th-CASAM-N)" to a simplified Bernoulli model. The 5th-CASAM-N builds upon and incorporates all of the lower-order (*i.e.*, the first-, second-, third-, and fourth-order) adjoint sensitivities analysis methodologies. The Bernoulli model comprises a nonlinear model response, uncertain model parameters, uncertain model domain boundaries and uncertain model boundary conditions, admitting closed-form explicit expressions for the response sensitivities of all orders. Illustrating the specific mechanisms and advantages of applying the 5th-CASAM-N for the computation of the response sensitivities with respect to the uncertain parameters and boundaries reveals that the 5th-CASAM-N provides a fundamental step towards overcoming the curse of dimensionality in sensitivity and uncertainty analysis.

Keywords

Fifth-Order Sensitivity Analysis of Bernoulli Model, Uncertain Model Parameters, Uncertain Model Domain Boundaries, Uncertain Model Boundary Conditions

1. Introduction

This work presents the application of the recently developed [1] "Fifth-Order Comprehensive Adjoint Sensitivity Analysis Methodology for Nonlinear Systems (5^{th}-CASAM-N)" to a simplified Bernoulli model [2] comprising a nonlinear model response, uncertain model parameters, uncertain model domain boundaries and uncertain model boundary conditions. As is well known [2], the Bernoulli nonlinear differential equation admits exact solutions. The demonstration model selected for illustrating the application of the 5^{th}-CASAM-N is a special case of the Bernoulli equation with quadratic nonlinearity, which is also called [2] the logistic differential equation and is used in economics.

This work is structured as follows: the illustrative Bernoulli model, including the paradigm nonlinear model response, is detailed in Section 2, which also presents the application of the 1^{st}-CASAM-N illustrating the exact and efficient computation of the complete set of first-order response sensitivities with respect to the model parameters. These computations also include the illustrative computation of 1^{st}-order sensitivities with respect to imprecisely known domain boundaries.

Section 3 illustrates the application of the 2^{nd}-CASAM-N to obtain the complete set of 2^{nd}-order sensitivities. It is shown that the complexity of the 2^{nd}-Order Adjoint Sensitivity System used for computing efficiently and exactly the 2^{nd}-order sensitivities is determined by the complexity of the 1^{st}-order sensitivity used as the respective response and, hence, as the respective starting point. Thus, the 2^{nd}-LASS that corresponds to 1^{st}-order sensitivities that involve solely the original state function comprises only as many equations as the corresponding 1^{st}-LASS. On the other hand, if the 1^{st}-order sensitivity under consideration involves both the original state function(s) and the 1^{st}-level adjoint sensitivity function(s), then the 2^{nd}-LASS could comprise twice as many equations as the 1^{st}-LASS. The symmetries inherent to the mixed 2^{nd}-order sensitivities make it possible to choose a priori, based on the expressions of the 1^{st}-order sensitivities, the order of priority and the most advantageous path for computing the 2^{nd}-order sensitivities. The primary consideration when computing 2^{nd}-order sensitivities is the priority order indicated by the magnitudes of the relative 1^{st}-order sensitivities: the 2^{nd}-order sensitivities stemming from the largest 1^{st}-order relative sensitivity should be computed first. Once the priorities for computing the 2^{nd}-order sensitivities have been established, it is important to examine the expressions of the 1^{st}-order sensitivities in order to establish the least expensive (computationally) path for computing the mixed 2^{nd}-order sensitivities.

Section 4 illustrates the application of the 3^{rd}-CASAM-N to obtain representative 3^{rd}-order sensitivities. It is shown that 2^{nd}-order sensitivities that depend solely on the original function will require the solution of a 3^{rd}-Level Adjoint Sensitivity System (3^{rd}-LASS) of the same size as the original system or, equivalently, the 1^{st}-LASS. The 2^{nd}-order sensitivities that depend solely on the original state function and the 1^{st}-level adjoint sensitivity system will give rise to a 3^{rd}-LASS of the same size as the corresponding 2^{nd}-LASS. Finally, 2^{nd}-order sensitivities that depend on all of the components of the 2^{nd}-level adjoint function(s) will need the solution of a 3^{rd}-LASS that will have twice the dimensions of the corresponding 2^{nd}-LASS.

Section 5 discusses the important aspects of applying the 4th-CASAM-N to compute the 4th-order sensitivities and the 5th-CASAM-N to compute the fifth-order sensitivities. Concluding remarks are presented in Section 6.

2. 1st-CASAM-N: Computation of First-Order Response Sensitivities

The illustrative model considered in this work comprises a simplified second-order Bernoulli equation subject to an imprecisely known boundary/initial condition u_{in} at the imprecisely known location λ, having the following standard form:

$$\frac{\mathrm{d}u(x)}{\mathrm{d}x} = qu^2(x);\;\; x \in \Omega_x \triangleq (\lambda, \omega); \tag{1}$$

$$u(x) = u_{in},\;\; x = \lambda . \tag{2}$$

The model's response, denoted as $R[u(x);\boldsymbol{\alpha}]$, is considered to be a nonlinear functional of the state function and parameters and is defined as follows:

$$R[u(x);\boldsymbol{\alpha}] \triangleq \int_{\lambda}^{\omega} \frac{r\mathrm{d}x}{u(x)}. \tag{3}$$

The scalar parameters q, u_{in}, λ, ω, and r, which appear in Equations (1)-(3), are considered to be imprecisely known, subject to uncertainties. These parameters are representative of the type of parameters that can appear in the mathematical model of a physical, as follows: 1) the parameter q typifies uncertain model parameters which appear in the equations underlying the model; 2) the parameter u_{in} typifies uncertain boundary or initial conditions; 3) the parameters λ and ω typify uncertain boundaries of the domain of definition of the independent variable(s); 4) the parameter r typifies uncertain quantities which may appear solely in the definition of the model's response.

For notational convenience, these imprecisely known model parameters are considered to be components of a vector of parameters $\boldsymbol{\alpha}$ defined as follows:

$$\boldsymbol{\alpha} \triangleq (\alpha_1, \cdots, \alpha_{TP})^\dagger \triangleq (q, u_{in}, \lambda, \omega, r)^\dagger , \tag{4}$$

where the subscript $TP = 5$ denotes the "total number of model parameters." The dagger superscript "$\dagger$" will be used in this work to denote "transposition." The information customarily available about the model parameters comprises their nominal (expected/mean) values and, possibly, higher-order moments or cumulants (*i.e.*, variance/covariances, skewness, kurtosis), which are usually determined from evaluation processes external to the physical system under consideration. Occasionally, only lower and upper bounds may be known for some model parameters. The nominal parameter values will be denoted as $\boldsymbol{\alpha}^0 \triangleq [\alpha_1^0, \cdots, \alpha_i^0, \cdots, \alpha_{TP}^0]^\dagger$; the superscript "0" will be used throughout this work to denote "nominal values."

The solution of Equations (1) and (2) is obtained by separation of variables and subsequent integration to obtain the following expression:

$$u(x) = \frac{u_{in}}{1 - q u_{in}(x - \lambda)}. \tag{5}$$

Inserting the result obtained in Equation (5) into Equation (3) yields the following expression for the model response:

$$R[u(x);\boldsymbol{\alpha}] = r(\omega - \lambda)\left(\frac{1}{u_{in}} - q\frac{\omega - \lambda}{2}\right). \tag{6}$$

The parameters q, u_{in} and λ occur in the expression of the state function $u(x)$, which is the solution of Equations (1)-(3), but the parameter ω occurs only in the expression of the response, thus illustrating the fact that model parameters may be introduced in the model solely through the definition of the model's response. Although both the model and its response are nonlinear functions of the state variables, the model has been chosen to be sufficiently simple to admit readily differentiable functions of the model parameters, so that the algebraic manipulations would not distract from following the application of the principles underlying the 5th-CASAM-N to obtain the various sensitivities (up to fifth-order) while enabling the analytical verification of the thus expressions obtained.

The nominal (or mean) parameter vales $\boldsymbol{\alpha}^0$ will differ from their true, but unknown, values by quantities denoted as $\delta\boldsymbol{\alpha} \triangleq (\delta\alpha_1, \cdots, \delta\alpha_{TP})$, where $\delta\alpha_i \triangleq \alpha_i - \alpha_i^0$. Since the forward state function $u(x)$ is related to the model and boundary parameters $\boldsymbol{\alpha}$ through Equations (1) and (2), it follows that the variations $\delta\boldsymbol{\alpha}$ in the model and boundary parameters will cause corresponding variations $v^{(1)}(x) \triangleq \delta u(x)$ around the nominal solution $u^0(x)$ in the forward state functions. In turn, the variations $\delta\boldsymbol{\alpha}$ and $v^{(1)}(x)$ will induce variations in the model's response.

The 1st-order sensitivities of a model response $R[u(x);\boldsymbol{\alpha}]$ are obtained by determining the 1st-order Gateaux- (G-) variation $\delta R[u(x);\boldsymbol{\alpha};v^{(1)}(x);\delta\boldsymbol{\alpha}]$ of the response, which is given, by definition, by the following expression:

$$\begin{aligned}
&\delta R\left[u(x);\boldsymbol{\alpha};v^{(1)}(x);\delta\boldsymbol{\alpha}\right] \triangleq \frac{\partial R}{\partial q}\delta q + \frac{\partial R}{\partial u_{in}}\delta u_{in} + \frac{\partial R}{\partial \lambda}\delta\lambda + \frac{\partial R}{\partial \omega}\delta\omega + \frac{\partial R}{\partial r}\delta r \\
&\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon} R\left[u^0(x) + \varepsilon v^{(1)}(x);\boldsymbol{\alpha}^0 + \varepsilon\delta\boldsymbol{\alpha}\right]\right\}_{\varepsilon=0} = \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega} \frac{(r+\varepsilon\delta r)\mathrm{d}x}{u(x)+\varepsilon v^{(1)}(x)}\right\}_{\varepsilon=0} \\
&= \left\{\delta R\left[u(x);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right]\right\}_{dir} + \left\{\delta R\left[u(x);\boldsymbol{\alpha};v^{(1)}(x)\right]\right\}_{ind},
\end{aligned} \tag{7}$$

where

$$\begin{aligned}
&\left\{\delta R\left[u(x);\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right]\right\}_{dir} \triangleq \delta r\left\{\int_\lambda^\omega \frac{\mathrm{d}x}{u(x)}\right\}_{\boldsymbol{\alpha}^0} + \left\{\frac{r\delta\omega}{u(x=\omega)}\right\}_{\boldsymbol{\alpha}^0} - \left\{\frac{r\delta\lambda}{u(x=\lambda)}\right\}_{\boldsymbol{\alpha}^0} \\
&= \delta r\left\{(\omega-\lambda)\left(\frac{1}{u_{in}} - q\frac{\omega-\lambda}{2}\right)\right\}_{\boldsymbol{\alpha}^0} + \left\{r\left[\frac{1}{u_{in}} - q(\omega-\lambda)\right]\delta\omega - r\frac{\delta\lambda}{u_{in}}\right\}_{\boldsymbol{\alpha}^0},
\end{aligned} \tag{8}$$

$$\left\{\delta R\left[u(x);\boldsymbol{\alpha};v^{(1)}(x)\right]\right\}_{ind} \triangleq \left\{-\int_\lambda^\omega \frac{r\mathrm{d}x}{u^2(x)} v^{(1)}(x)\right\}_{\boldsymbol{\alpha}^0}. \tag{9}$$

The direct-effect term can be computed once the nominal values $\left(\boldsymbol{u}^0, \boldsymbol{\alpha}^0\right)$ are available. The notation $\{\ \}_{\alpha^0}$ will be used in this work to indicate that the quantity enclosed within the bracket is to be evaluated at the nominal values of the respective parameters and state functions. On the other hand, the indirect-effect term can be quantified only after having determined the variations $v^{(1)}(x)$ in terms of the variations $\delta\boldsymbol{\alpha}$. The first-order relationship between the vectors $v^{(1)}(x)$ and $\delta\boldsymbol{\alpha}$ is determined by solving the following 1st-Level Variational Sensitivity System (1st-LVSS) obtained by applying the definition of the G-differential to Equations (1) and (2), which yields the following equations:

$$\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x) = (\delta q)u^2(x);\ x \in \Omega_x; \tag{10}$$

$$v^{(1)}(x=\lambda) + \left\{\frac{\mathrm{d}u(x)}{\mathrm{d}x}\right\}_{x=\lambda}(\delta\lambda) = v^{(1)}(\lambda) + (\delta\lambda)qu_{in}^2 = \delta u_{in},\ \text{at } x=\lambda. \tag{11}$$

The alternative to solving repeatedly the 1st-LVSS to obtain the 1st-level variational function $v^{(1)}(x)$, which depends on the various parameter variations, is to express the indirect-effect term defined in Equation (9) in terms of the solution of the 1st-Level Adjoint Sensitivity System (1st-LASS), which is constructed by applying the principles of the 5th-CASAM-N, as follows:

1) Consider that the functions $u(x)$ and $v^{(1)}(x)$ are elements of a Hilbert space denoted as $\mathsf{H}_1(\Omega_x)$ which is endowed with an inner product of two vectors $f_1(x) \in \mathsf{H}_1(\Omega_x)$ and $f_2(x) \in \mathsf{H}_1(\Omega_x)$ denoted as $\langle f_1, f_2 \rangle_1$ and defined as follows:

$$\langle f_1, f_2 \rangle_1 \triangleq \left\{\int_\lambda^\omega f_1(x) f_2(x)\mathrm{d}x\right\}_{\alpha^0}. \tag{12}$$

2) Using the definition of provided in Equation (12), construct the inner product of Equation (10) with a yet undefined function $a^{(1)}(x) \in \mathsf{H}_1(\Omega_x)$ to obtain the following relation:

$$\left\{\int_\lambda^\omega a^{(1)}(x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\alpha^0} = (\delta q)\left\{\int_\lambda^\omega a^{(1)}(x)u^2(x)\mathrm{d}x\right\}_{\alpha^0}. \tag{13}$$

3) Integrate by parts the left-side of Equation (13) to obtain the following relation:

$$\begin{aligned}&\left\{\int_\lambda^\omega a^{(1)}(x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\alpha^0}\\ &= a^{(1)}(\omega)v^{(1)}(\omega) - a^{(1)}(\lambda)v^{(1)}(\lambda)\\ &-\left\{\int_\lambda^\omega v^{(1)}(x)\left[\frac{\mathrm{d}a^{(1)}(x)}{\mathrm{d}x} + 2qu(x)a^{(1)}(x)\right]\mathrm{d}x\right\}_{\alpha^0}.\end{aligned} \tag{14}$$

4) Use in Equation (14) the boundary condition given in Equation (11) to obtain the following relation:

$$
\begin{aligned}
&-\left\{\int_{\lambda}^{\omega} v^{(1)}(x)\left[\frac{\mathrm{d}a^{(1)}(x)}{\mathrm{d}x}+2qu(x)a^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&=a^{(1)}(\lambda)\left(\delta u_{in}-qu_{in}^2\right)-a^{(1)}(\omega)v^{(1)}(\omega)\\
&+\left\{\int_{\lambda}^{\omega} a^{(1)}(x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x}-2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned}
\tag{15}
$$

5) Require the left-side of Equation (15) to represent the indirect-effect term defined in Equation (9) and eliminate the unknown value $v^{(1)}(\omega)$ in Equation (15) by requiring the function $a^{(1)}(x)\in \mathsf{H}_1(\Omega_x)$ to be the solution of the following 1st-Level Adjoint Sensitivity System (1st-LASS):

$$
\left\{\frac{\mathrm{d}a^{(1)}(x)}{\mathrm{d}x}+2qu(x)a^{(1)}(x)\right\}_{\boldsymbol{\alpha}^0}=\left\{ru^{-2}(x)\right\}_{\boldsymbol{\alpha}^0};\ x\in\Omega_x; \tag{16}
$$

$$
a^{(1)}(x)=0,\ \text{at } x=\omega. \tag{17}
$$

6) Use Equations (15)-(17) together with Equation (13) in Equation (9) to obtain the following alternative expression for the indirect-effect term:

$$
\begin{aligned}
&\left\{\delta R\left[u(x);\boldsymbol{\alpha};v^{(1)}(x)\right]\right\}_{ind}\\
&=a^{(1)}(\lambda)\left[(\delta u_{in})-qu_{in}^2(\delta\lambda)\right]+(\delta q)\left\{\int_{\lambda}^{\omega} a^{(1)}(x)u^2(x)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0},
\end{aligned}
\tag{18}
$$

7) Adding the expressions for the indirect-effect and direct-effect terms obtained in Equations (18) and (8), respectively, and identifying the expressions that multiply the respective parameter variations, as indicated in Equation (7), yields the following expressions for the first-order response sensitivities with respect to the model parameters:

$$
\frac{\partial R}{\partial q}=\int_{\lambda}^{\omega} a^{(1)}(x)u^2(x)\mathrm{d}x, \tag{19}
$$

$$
\frac{\partial R}{\partial u_{in}}=a^{(1)}(\lambda), \tag{20}
$$

$$
\frac{\partial R}{\partial \lambda}=-\frac{r}{u(x=\lambda)}-qu_{in}^2a^{(1)}(\lambda), \tag{21}
$$

$$
\frac{\partial R}{\partial \omega}=\frac{r}{u(x=\omega)}=r\left[\frac{1}{u_{in}}-q(\omega-\lambda)\right], \tag{22}
$$

$$
\frac{\partial R}{\partial r}=\int_{\lambda}^{\omega}\frac{\mathrm{d}x}{u(x)}=(\omega-\lambda)\left(\frac{1}{u_{in}}-q\frac{\omega-\lambda}{2}\right). \tag{23}
$$

The expressions of the sensitivities provided in Equations (19)-(23) are to be evaluated at the nominal values of the respective parameters and state functions but the respective indication $\{\ \}_{\boldsymbol{\alpha}^0}$ has been omitted, for simplicity. The expressions of the sensitivities stemming from the indirect-effect term can be evaluated after solving the 1st-LASS to obtain the 1st-level adjoint sensitivity function

$a^{(1)}(x)$. The 1st-LASS is linear in $a^{(1)}(x)$ and is independent of parameter variations, so it only needs to be solved once. The expression of $a^{(1)}(x)$ obtained by solving the 1st-LASS by the standard integrating-factor method is as follows:

$$a^{(1)}(x)=r(x-\omega)\left[q(x-\lambda)-\frac{1}{u_{in}}\right]^2=\frac{r(x-\omega)}{u^2(x)}. \tag{24}$$

Inserting the result obtained in Equation (24) into in Equations (19)-(21) and evaluating the respective expressions yields the following closed-form results for the respective sensitivities:

$$\frac{\partial R}{\partial q}=-r\frac{(\omega-\lambda)^2}{2}, \tag{25}$$

$$\frac{\partial R}{\partial u_{in}}=\frac{r(\lambda-\omega)}{u_{in}^2}, \tag{26}$$

$$\frac{\partial R}{\partial \lambda}=-\frac{r}{u_{in}}+rq(\omega-\lambda). \tag{27}$$

The closed-form expressions provided in Equations (22), (23), (25)-(27) have been derived for verification purposes, as they can be compared directly with the respective results which would be obtained by differentiating the closed-form expression of model response provided in Equation (6). In practice, however, the model' equations and the 1st-LASS must be solved numerically. Consequently, the sensitivities expressed by Equations (19)-(23) must be evaluated numerically; closed-from expressions for these sensitivities are not available in practice.

3. 2nd-CASAM-N: Computation of Second-Order Response Sensitivities

Since there are five 1st-order sensitivities, it follows that there will be twenty five 2nd-order sensitivities, of which 15 will be distinct. The 2nd-order sensitivities could be computed directly by differentiating the expression of the G-differential of the response provided in Equation (7), to obtain the expression of the 2nd-order G-differential, $\delta^2 R\left[u(x);\boldsymbol{\alpha};v^{(1)}(x);\delta\boldsymbol{\alpha};\delta v^{(1)}(x);v^{(1)}(x)\delta\boldsymbol{\alpha};\delta^2\boldsymbol{\alpha}\right]$, which would require the computation of the 2nd-order differential $\delta v^{(1)}(x)\equiv\delta^2 u(x)$. The second-order G-differential $\delta v^{(1)}(x)\equiv\delta^2 u(x)$ would need to be determined by solving the G-differential of the 1st-LVSS, which would involve 2nd-order differential equations, which would depend on first- and second-order parameter variations. Furthermore, this set of 2nd-order differential equations would depend on the solution of the 1st-LVSS and would need to be solved at least 25 times, to account for all combinations of 1st- and 2nd-order variations in the parameters and state function $u(x)$.

Alternatively, the 2nd-order sensitivities can be defined as the "1st-order sensitivities of the 1st-order sensitivities." This definition stems from the inductive definition of the 2nd-order total G-differential of correspondingly differentiable function, which is also defined inductively as "the total 1st-order differential of the 1st-order total differential." As a general principle, the 2nd-order sensitivities should be computed in a priority order that should follow the ranking of the 1st-order sensitivities: the 2nd-order sensitivities that correspond to the largest relative 1st-order sensitivity should be computed first, the 2nd-order sensitivities that correspond to the second largest relative 1st-order sensitivity should be computed next, and so on. Based on a user-selected a-apriori cut-off criterion, 2nd-order sensitivities that stem from very small relative 1st-order sensitivities might be neglected without actually computing them.

Another criterion for prioritizing the computation of the 2nd-order sensitivities may be based on the difficulty involved in computing them. Examining Equations (19)-(23), it becomes apparent that the expressions of $\partial R/\partial r$ and $\partial R/\partial \omega$ involve only the state function $u(x)$. Therefore, the 2nd-level adjoint sensitivity functions which will be used to compute the sensitivities stemming from $\partial R/\partial r$ and $\partial R/\partial \omega$ will comprise a single component, having the general form $a^{(2)}(1; j_1; x)$, $j_1 = 1,2$. Furthermore, the procedure for computing these 2nd-level sensitivities will be the same as the procedure followed for computing the 1st-order sensitivities, as will be shown in subsections 3.1.1 and 3.1.2, respectively.

On the other hand, the expressions of $\partial R/\partial u_{in}$, $\partial R/\partial q$ and $\partial R/\partial \lambda$ involve the adjoint sensitivity function $a^{(1)}(x)$, which means that the 2nd-level adjoint sensitivity functions that will be needed for computing these sensitivities will comprise two-components, having the general form $\mathbf{A}^{(2)}(2; j_1; x) \triangleq \left[a^{(2)}(1; j_1; x), a^{(2)}(2; j_1; x)\right]^{\dagger}$, $j_1 = 3,4,5$. Thus, the computation of the 2nd-order sensitivities stemming from $\partial R/\partial u_{in}$, $\partial R/\partial q$ and/or $\partial R/\partial \lambda$ will require at least twice as many computations as are required for the computation of the 2nd-order sensitivities stemming from $\partial R/\partial r$ and/or $\partial R/\partial \omega$. This is because solving a 2nd-Level Adjoint Sensitivity System to compute a two-component 2nd-level adjoint sensitivity function of the form $\mathbf{A}^{(2)}(2; j_1; x) \triangleq \left[a^{(2)}(1; j_1; x), a^{(2)}(2; j_1; x)\right]^{\dagger}$ will be at least twice as expensive computationally as solving a 2nd-Level Adjoint Sensitivity System that involves a one-component 2nd-level adjoint sensitivity function of the form $a^{(2)}(2; j_1; x)$. The application of the principles underlying the 5th-CASAM-N to compute the 2nd-order sensitivities stemming from $\partial R/\partial u_{in}$, $\partial R/\partial q$ and $\partial R/\partial \lambda$ will be illustrated in the subsections 3.2.1, 3.2.2 and 3.2.3, respectively.

3.1. Second-Order Sensitivities Stemming from 1st-Order Sensitivities Involving Just the Original State Function

Examining Equations (19)-(23), it becomes apparent that the expressions of $\partial R/\partial r$ and $\partial R/\partial \omega$ involve only the state function $u(x)$. Therefore, the 2nd-level adjoint sensitivity functions which will be used to compute the sensitivities stemming from $\partial R/\partial r$ and $\partial R/\partial \omega$ will comprise a single component, having the general form $a^{(2)}(1; j_1; x)$, $j_1 = 1,2$. Furthermore, the procedure for computing these 2nd-level sensitivities will be the same as the procedure followed for computing the 1st-order sensitivities, as will be shown in subsections 3.1 and 3.2, respectively.

3.1.1. Second-Order Sensitivities Stemming from $\partial R/\partial r$

The 2nd-order sensitivities which arise from $\partial R/\partial r$ are obtained from the G-differential $\delta[\partial R/\partial r]$ of $\partial R/\partial r$, which is obtained by applying the definition of the G-differential to the expression provided in Equation (23). This yields the following expression:

$$\delta\left\{\frac{\partial R}{\partial r}\right\} \triangleq \frac{\partial^2 R}{\partial q \partial r}\delta q + \frac{\partial^2 R}{\partial u_{in} \partial r}\delta u_{in} + \frac{\partial^2 R}{\partial \lambda \partial r}\delta \lambda + \frac{\partial^2 R}{\partial \omega \partial r}\delta \omega + \frac{\partial^2 R}{\partial r \partial r}\delta r$$
$$\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega}\frac{\mathrm{d}x}{u^0(x)+\varepsilon v^{(1)}(x)}\right\}_{\varepsilon=0} \triangleq \left\{\delta[\partial R/\partial r]\right\}_{dir} + \left\{\delta[\partial R/\partial r]\right\}_{ind}, \tag{28}$$

where:

$$\left\{\delta[\partial R/\partial r]\right\}_{dir} \triangleq (\delta\omega)\left\{\frac{1}{u(\omega)}\right\}_{\boldsymbol{\alpha}^0} - (\delta\lambda)\left\{\frac{1}{u(\lambda)}\right\}_{\boldsymbol{\alpha}^0}, \tag{29}$$

$$\left\{\delta[\partial R/\partial r]\right\}_{ind} \triangleq -\left\{\int_\lambda^\omega \frac{v^{(1)}(x)}{u^2(x)}\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}. \tag{30}$$

The direct-effect term has been evaluated at this stage since the function $u(x)$ is already available. The indirect-effect term, however, can be evaluated only after having determined the variational function $v^{(1)}(x)$, which is the solution of the 1st-LVSS. Solving the 1st-LVSS, which depends on parameter variations, can be avoided by expressing the indirect-effect term defined in Equation (30) in terms of the solution of a 2nd-Level Adjoint Sensitivity System (2nd-LASS), which is constructed by applying the same principles as outlined in Section 3.1, as follows:

1) Consider that the functions $u(x)$ and $v^{(1)}(x)$ are elements the Hilbert space denoted as $\mathsf{H}_1(\Omega_x)$ which is endowed with the inner defined in Equation (12). Using the definition of provided in Equation (12), construct the inner product of Equation (10) with a yet undefined function $a^{(2)}(1;1;x) \in \mathsf{H}_1(\Omega_x)$ to obtain the following relation:

$$\left\{\int_\lambda^\omega a^{(2)}(1;1;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}$$
$$= (\delta q)\left\{\int_\lambda^\omega a^{(2)}(1;1;x)u^2(x)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}. \tag{31}$$

2) Integrate by parts the left-side of Equation (31) to obtain the following relation:

$$\left\{\int_\lambda^\omega a^{(2)}(1;1;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}$$
$$= a^{(2)}(1;1;\omega)v^{(1)}(\omega) - a^{(2)}(1;1;\lambda)v^{(1)}(\lambda) \tag{32}$$
$$-\left\{\int_\lambda^\omega v^{(1)}(x)\left[\frac{\mathrm{d}a^{(2)}(1;1;x)}{\mathrm{d}x} + 2qu(x)a^{(2)}(1;1;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}.$$

3) Use in Equation (32) the boundary condition given in Equation (11) to obtain the following relation:

$$
\begin{aligned}
&-\left\{\int_{\lambda}^{\omega} v^{(1)}(x)\left[\frac{\mathrm{d}a^{(2)}(1;1;x)}{\mathrm{d}x}+2qu(x)a^{(2)}(1;1;x)\right]\mathrm{d}x\right\}_{\alpha^0} \\
&= a^{(2)}(1;1;\lambda)\left(\delta u_{in}-qu_{in}^2\right)-a^{(2)}(1;1;\omega)v^{(1)}(\omega) \\
&+\left\{\int_{\lambda}^{\omega} a^{(2)}(1;1;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x}-2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\alpha^0} .
\end{aligned}
\tag{33}
$$

4) Require the left-side of Equation (33) to represent the indirect-effect term defined in Equation (30) and eliminate the unknown value $v^{(1)}(\omega)$ in Equation (33) by requiring the function $a^{(2)}(1;1;x)$ to be the solution of the following 2nd-Level Adjoint Sensitivity System (2nd-LASS):

$$
\left\{\frac{\mathrm{d}a^{(2)}(1;1;x)}{\mathrm{d}x}+2qu(x)a^{(2)}(1;1;x)\right\}_{\alpha^0} = \left\{u^{-2}(x)\right\}_{\alpha^0};\ x\in\Omega_x; \tag{34}
$$

$$
a^{(2)}(1;1;x)=0,\ \text{at}\ x=\omega . \tag{35}
$$

5) Use Equations (33)-(35) together with Equation (31) in Equation (30) to obtain the following alternative expression for the indirect-effect term:

$$
\left\{\delta[\partial R/\partial r]\right\}_{ind} = a^{(2)}(1;1;\lambda)\left[(\delta u_{in})-qu_{in}^2(\delta\lambda)\right]+(\delta q)\left\{\int_{\lambda}^{\omega} a^{(2)}(1;1;x)u^2(x)\mathrm{d}x\right\}_{\alpha^0} . \tag{36}
$$

6) Adding the expressions for the indirect-effect and direct-effect terms obtained in Equations (36) and (29), respectively, and identifying the expressions that multiply the respective parameter variations, as indicated in Equation (28), yields the following expressions for the 2nd-order response sensitivities which stem from the first-order sensitivity $\partial R/\partial r$:

$$
\frac{\partial^2 R}{\partial q\partial r}=\int_{\lambda}^{\omega} a^{(2)}(1;1;x)u^2(x)\mathrm{d}x , \tag{37}
$$

$$
\frac{\partial^2 R}{\partial u_{in}\partial r}=a^{(2)}(1;1;\lambda) , \tag{38}
$$

$$
\frac{\partial^2 R}{\partial \lambda\partial r}=-\frac{1}{u(\lambda)}-qu_{in}^2 a^{(2)}(1;1;\lambda) , \tag{39}
$$

$$
\frac{\partial^2 R}{\partial \omega\partial r}=\frac{1}{u(\omega)}=\frac{1}{u_{in}}-q(\omega-\lambda) , \tag{40}
$$

$$
\frac{\partial^2 R}{\partial r\partial r}=0 . \tag{41}
$$

The expressions of the sensitivities provided in Equations (37)-(40) are to be evaluated at the nominal values of the respective parameters and state functions but the respective indication $\{\ \}_{\alpha^0}$ has been omitted, for simplicity. The expressions of the sensitivities stemming from the indirect-effect term can be evaluated after solving the 2nd-LASS using the standard integrating-factor method to obtain the following expression for the 2nd-level adjoint sensitivity function $a^{(2)}(1;1;x)$:

$$a^{(2)}(1;1;x) = (x-\omega)\left[q(x-\lambda) - \frac{1}{u_{in}}\right]^2 = \frac{x-\omega}{u^2(x)}. \quad (42)$$

Inserting the result obtained in Equation (42) into in Equations (37)-(39) and evaluating the respective expressions yields the following closed-form results for the respective sensitivities:

$$\frac{\partial^2 R}{\partial q \partial r} = -\frac{(\omega-\lambda)^2}{2}, \quad (43)$$

$$\frac{\partial^2 R}{\partial u_{in} \partial r} = -\frac{(\lambda-\omega)}{u_{in}^2}, \quad (44)$$

$$\frac{\partial^2 R}{\partial \lambda \partial r} = -\frac{1}{u_{in}} + q(\omega-\lambda). \quad (45)$$

3.1.2. Second-Order Sensitivities Stemming from $\partial R/\partial \omega$

In preparation for determining the 2nd-order sensitivities that correspond to $\partial R/\partial \omega$, the expression provided in Equation (22) is written in the following integral form:

$$\frac{\partial R}{\partial \omega} = r\int_{\lambda}^{\omega} \frac{\delta(x-\omega)}{u(x)} \mathrm{d}x. \quad (46)$$

The 2nd-order sensitivities which arise from $\partial R/\partial \omega$ are obtained by applying the definition of the G-differential to Equation (22), which yields the following expression:

$$\begin{aligned} \delta\left\{\frac{\partial R}{\partial \omega}\right\} &\triangleq \frac{\partial^2 R}{\partial q \partial \omega}\delta q + \frac{\partial^2 R}{\partial u_{in} \partial \omega}\delta u_{in} + \frac{\partial^2 R}{\partial \lambda \partial \omega}\delta \lambda + \frac{\partial^2 R}{\partial \omega \partial \omega}\delta \omega + \frac{\partial^2 R}{\partial r \partial \omega}\delta r \\ &\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\left(r^0 + \varepsilon \delta r\right)\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega} \frac{\delta\left(x-\omega^0-\varepsilon\delta\omega\right)}{u^0(x)+\varepsilon v^{(1)}(x)}\mathrm{d}x\right\}_{\varepsilon=0} \\ &\triangleq \left\{\delta\left[\frac{\partial R}{\partial \omega}\right]\right\}_{dir} + \left\{\delta\left[\frac{\partial R}{\partial \omega}\right]\right\}_{ind}, \end{aligned} \quad (47)$$

where:

$$\left\{\delta\left[\partial R/\partial \omega\right]\right\}_{dir} \triangleq \left\{(\delta r)\int_{\lambda}^{\omega} \frac{\delta(x-\omega)}{u(x)}\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} - (\delta\omega)\left\{r\int_{\lambda}^{\omega} \frac{\delta'(x-\omega)}{u(x)}\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}, \quad (48)$$

$$\left\{\delta\left[\partial R/\partial \omega\right]\right\}_{ind} \triangleq -\left\{r\int_{\lambda}^{\omega} \frac{\delta(x-\omega)v^{(1)}(x)}{u^2(x)}\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}. \quad (49)$$

The direct-effect term can be evaluated at this stage since the function $u(x)$ is already available. The indirect-effect term, however, can be evaluated only after having determined the variational function $v^{(1)}(x)$, which is the solution of the 1st-LVSS. Solving the 1st-LVSS, which depends on parameter variations, can be avoided by expressing the indirect-effect term defined in Equation (49) in terms of the solution of a 2nd-Level Adjoint Sensitivity System (2nd-LASS), which is constructed by applying the same principles as outlined in Section 3.1, as follows:

1) Using the definition of provided in Equation (12), construct the inner product of Equation (10) with a yet undefined function $a^{(2)}(1;2;x) \in \mathsf{H}_1(\Omega_x)$ to obtain the following relation:

$$\begin{aligned}&\left\{\int_\lambda^\omega a^{(2)}(1;2;x)\left[\frac{dv^{(1)}(x)}{dx} - 2qu(x)v^{(1)}(x)\right]dx\right\}_{\alpha^0} \\ &= (\delta q)\left\{\int_\lambda^\omega a^{(2)}(1;2;x)u^2(x)dx\right\}_{\alpha^0}.\end{aligned} \tag{50}$$

2) Integrate by parts the left-side of Equation (50) to obtain the following relation:

$$\begin{aligned}&\left\{\int_\lambda^\omega a^{(2)}(1;2;x)\left[\frac{dv^{(1)}(x)}{dx} - 2qu(x)v^{(1)}(x)\right]dx\right\}_{\alpha^0} \\ &= a^{(2)}(1;2;\omega)v^{(1)}(\omega) - a^{(2)}(1;2;\lambda)v^{(1)}(\lambda) \\ &-\left\{\int_\lambda^\omega v^{(1)}(x)\left[\frac{da^{(2)}(1;2;x)}{dx} + 2qu(x)a^{(2)}(1;2;x)\right]dx\right\}_{\alpha^0}.\end{aligned} \tag{51}$$

3) Use in Equation (51) the boundary condition given in Equation (11) to obtain the following relation:

$$\begin{aligned}&-\left\{\int_\lambda^\omega v^{(1)}(x)\left[\frac{da^{(2)}(1;2;x)}{dx} + 2qu(x)a^{(2)}(1;2;x)\right]dx\right\}_{\alpha^0} \\ &= a^{(2)}(1;2;\lambda)\left(\delta u_{in} - qu_{in}^2\right) - a^{(2)}(1;2;\omega)v^{(1)}(\omega) \\ &+\left\{\int_\lambda^\omega a^{(2)}(1;2;x)\left[\frac{dv^{(1)}(x)}{dx} - 2qu(x)v^{(1)}(x)\right]dx\right\}_{\alpha^0}.\end{aligned} \tag{52}$$

4) Require the left-side of Equation (52) to represent the indirect-effect term defined in Equation (49) and eliminate the unknown value $v^{(1)}(\omega)$ in Equation (52) by requiring the function $a^{(2)}(1;2;x)$ to be the solution of the following 2nd-Level Adjoint Sensitivity System (2nd-LASS):

$$\left\{\frac{da^{(2)}(1;2;x)}{dx} + 2qu(x)a^{(2)}(1;2;x)\right\}_{\alpha^0} = \left\{\frac{r\delta(x-\omega)}{u^2(x)}\right\}_{\alpha^0};\ x \in \Omega_x; \tag{53}$$

$$a^{(2)}(1;2;x) = 0,\ \text{at}\ x = \omega. \tag{54}$$

5) Use Equations (52)-(54) together with Equation (50) in Equation (49) to obtain the following alternative expression for the indirect-effect term:

$$\{\delta[\partial R/\partial\omega]\}_{ind} = a^{(2)}(1;2;\lambda)\left[(\delta u_{in}) - qu_{in}^2(\delta\lambda)\right] + (\delta q)\left\{\int_\lambda^\omega a^{(2)}(1;2;x)u^2(x)dx\right\}_{\alpha^0}. \tag{55}$$

6) Adding the expressions for the indirect-effect and direct-effect terms obtained in Equations (55) and (48), respectively, and identifying the expressions that multiply the respective parameter variations, as indicated in Equation (47), yields the following expressions for the 2nd-order response sensitivities which stem from the first-order sensitivity $\partial R/\partial r$:

$$\frac{\partial^2 R}{\partial q \partial \omega} = \int_{\lambda}^{\omega} a^{(2)}(1;2;x) u^2(x) \mathrm{d}x, \tag{56}$$

$$\frac{\partial^2 R}{\partial u_{in} \partial \omega} = a^{(2)}(1;2;\lambda), \tag{57}$$

$$\frac{\partial^2 R}{\partial \lambda \partial \omega} = -q u_{in}^2 a^{(2)}(1;2;\lambda), \tag{58}$$

$$\frac{\partial^2 R}{\partial \omega \partial \omega} = -r \int_{\lambda}^{\omega} \frac{\delta'(x-\omega)}{u(x)} \mathrm{d}x = -qr, \tag{59}$$

$$\frac{\partial^2 R}{\partial r \partial \omega} = \int_{\lambda}^{\omega} \frac{\delta(x-\omega)}{u(x)} \mathrm{d}x = \frac{1}{u_{in}} - q(\omega - \lambda). \tag{60}$$

The expressions of the sensitivities provided in Equations (37)-(40) are to be evaluated at the nominal values of the respective parameters and state functions but the respective indication $\{\,\}_{\alpha^0}$ has been omitted, for simplicity. The expressions of the sensitivities stemming from the indirect-effect term can be evaluated after solving the 2nd-LASS using the standard integrating-factor method to obtain the following expression for the 2nd-level adjoint sensitivity function $a^{(2)}(1;2;x)$:

$$a^{(2)}(1;2;x) = -\frac{r}{u_{in}^2}\left[q u_{in}(x-\lambda)-1\right]^2\left[1-H(x-\omega)\right] = -\frac{r}{u^2(x)}\left[1-H(x-\omega)\right]. \tag{61}$$

Inserting the result obtained in Equation (61) into in Equations (56)-(58) and evaluating the respective expressions yields the following closed-form results for the respective sensitivities:

$$\frac{\partial^2 R}{\partial q \partial \omega} = -r(\omega - \lambda), \tag{62}$$

$$\frac{\partial^2 R}{\partial u_{in} \partial \omega} = -\frac{r}{u_{in}^2}, \tag{63}$$

$$\frac{\partial^2 R}{\partial \lambda \partial \omega} = qr. \tag{64}$$

Evidently, the identity of the expressions obtained in Equations (60) and (40) confirms the correct determination of the mixed 2nd-order sensitivity $\partial^2 R/\partial \omega \partial r$.

3.2. Second-Order Sensitivities Stemming from 1st-Order Sensitivities Involving the 1st-Level Adjoint Sensitivity Function

The expressions of $\partial R/\partial u_{in}$, $\partial R/\partial q$ and $\partial R/\partial \lambda$ involve the adjoint sensitivity function $a^{(1)}(x)$, which means that the 2nd-level adjoint sensitivity functions that will be needed for computing these sensitivities will comprise two-components, having the general form $\boldsymbol{A}^{(2)}(2;j_1;x) \triangleq \left[a^{(2)}(1;j_1;x), a^{(2)}(2;j_1;x)\right]^{\dagger}$, $j_1 = 3,4,5$. Thus, the computation of the 2nd-order sensitivities stemming from $\partial R/\partial u_{in}$, $\partial R/\partial q$ and/or $\partial R/\partial \lambda$ will require at least twice as many computations as are required for the computation of the 2nd-order sensitivities stemming from $\partial R/\partial r$ and/or $\partial R/\partial \omega$. This is because solving a 2nd-Level Adjoint Sensitivity System to compute a two-component 2nd-level adjoint sensitivity function of the form $\boldsymbol{A}^{(2)}(2;j_1;x) \triangleq \left[a^{(2)}(1;j_1;x), a^{(2)}(2;j_1;x)\right]^{\dagger}$.

3.2.1. Second-Order Sensitivities Stemming from $\partial R/\partial u_{in}$

In preparation for determining the 2nd-order sensitivities that correspond to $\partial R/\partial u_{in}$, the expression provided in Equation (20) is written in the following integral form:

$$\frac{\partial R}{\partial u_{in}} = \int_{\lambda}^{\omega} a^{(1)}(x)\,\delta(x-\lambda)\,\mathrm{d}x. \tag{65}$$

By definition, the G-differential $\delta\left[\partial R/\partial u_{in}\right]$ of $\partial R/\partial u_{in}$ is obtained as follows:

$$\begin{aligned}
\delta\left\{\frac{\partial R}{\partial u_{in}}\right\} &\triangleq \frac{\partial^2 R}{\partial q \partial u_{in}}\delta q + \frac{\partial^2 R}{\partial u_{in}\partial u_{in}}\delta u_{in} + \frac{\partial^2 R}{\partial \lambda \partial u_{in}}\delta\lambda + \frac{\partial^2 R}{\partial \omega \partial u_{in}}\delta\omega + \frac{\partial^2 R}{\partial r \partial u_{in}}\delta r \\
&\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega}\left[a^{(1),0}(x)+\varepsilon\delta a^{(1)}(x)\right]\delta(x-\lambda-\varepsilon\delta\lambda)\,\mathrm{d}x\right\}_{\varepsilon=0} \\
&\triangleq \left\{\delta\left[\partial R/\partial u_{in}\right]\right\}_{dir} + \left\{\delta\left[\partial R/\partial u_{in}\right]\right\}_{ind},
\end{aligned} \tag{66}$$

where:

$$\begin{aligned}
\left\{\delta\left[\partial R/\partial u_{in}\right]\right\}_{dir} &\triangleq -(\delta\lambda)\left\{\int_{\lambda}^{\omega} a^{(1)}(x)\,\delta'(x-\lambda)\,\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \\
&= (\delta\lambda)\left\{\frac{\mathrm{d}a^{(1)}(x)}{\mathrm{d}x}\right\}_{x=\lambda} = \frac{(\delta\lambda)}{u_{in}}\left[\frac{r}{u_{in}} - 2rq(\lambda-\omega)\right],
\end{aligned} \tag{67}$$

$$\left\{\delta\left[\partial R/\partial u_{in}\right]\right\}_{ind} \triangleq \left\{\int_{\lambda}^{\omega} \delta a^{(1)}(x)\,\delta(x-\lambda)\,\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}. \tag{68}$$

The direct-effect term has been evaluated at this stage since the function $a^{(1)}(x)$ is already available. The indirect-effect term, however, can be evaluated only after having determined the variational function $\delta a^{(1)}(x)$, which is the solution of the 2nd-Level Variational Sensitivity System (2nd-LVSS) obtained by G-differentiating the 1st-LASS. The G-differentiation of the 1st-LASS represented by Equations (16) and (17) yields the following system:

$$\begin{aligned}
&\left\{\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x) + 2qu(x)\,\delta a^{(1)}(x) + 2qa^{(1)}(x)\,v^{(1)}(x) + 2ru^{-3}(x)\,v^{(1)}(x)\right\}_{\boldsymbol{\alpha}^0} \\
&= \left\{-2(\delta q)\,u(x)\,a^{(1)}(x) + (\delta r)\,u^{-2}(x)\right\}_{\boldsymbol{\alpha}^0};\; x\in\Omega_x;
\end{aligned} \tag{69}$$

$$\delta a^{(1)}(\omega)+\left\{\frac{\mathrm{d}a^{(1)}(x)}{\mathrm{d}x}\right\}_{x=\omega}\delta\omega$$
$$=\delta a^{(1)}(\omega)+r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2\delta\omega=0,\ \text{at}\ x=\omega. \tag{70}$$

Equation (69) also involves the variational function $v^{(1)}(x)$, which is the solution of the 1st-LVSS comprising Equations (10) and (11). Therefore, Equations (69) and (70) are to be concatenated with the 1st-LVSS to obtain the following 2nd-Level Variational Sensitivity System (2nd-LVSS) which is satisfied by the 2nd-level variational function $\boldsymbol{V}^{(2)}(x)\triangleq\left[v^{(1)}(x),\delta a^{(1)}(x)\right]^{\dagger}$:

$$\left\{\boldsymbol{VM}^{(2)}(2\times2)\boldsymbol{V}^{(2)}(2;x)\right\}_{\alpha^0}=\left\{\boldsymbol{Q}_V^{(2)}(2;x)\right\}_{\alpha^0},\ x\in\Omega_x, \tag{71}$$

$$\boldsymbol{B}_V^{(2)}(2;x)\triangleq\begin{pmatrix} v^{(1)}(\lambda)+(\delta\lambda)qu_{in}^2-\delta u_{in} \\ \delta a^{(1)}(\omega)+r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2\delta\omega \end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix}; \tag{72}$$

where

$$\boldsymbol{V}^{(2)}(2;x)\triangleq\begin{pmatrix} v^{(2)}(1;x) \\ v^{(2)}(2;x)\end{pmatrix}\triangleq\begin{pmatrix} v^{(1)}(x) \\ \delta a^{(1)}(x)\end{pmatrix}; \tag{73}$$

$$\boldsymbol{VM}^{(2)}(2\times2)\triangleq\begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}x}-2qu(x) & 0 \\ 2qa^{(1)}(x)+2ru^{-3}(x) & \frac{\mathrm{d}}{\mathrm{d}x}+2qu(x)\end{pmatrix}; \tag{74}$$

$$\boldsymbol{Q}_V^{(2)}(2;x)\triangleq\begin{pmatrix} (\delta q)u^2(x) \\ -2(\delta q)u(x)a^{(1)}(x)+(\delta r)u^{-2}(x)\end{pmatrix}. \tag{75}$$

The need for solving repeatedly the 2nd-LVSS to obtain the 2nd-level variational function $\boldsymbol{V}^{(2)}(x)$ for every parameter variations is circumvented by expressing the indirect-effect term defined in Equation (68) in terms of the solution of a 2nd-Level Adjoint Sensitivity System (2nd-LASS), which is constructed specifically for the indirect-effect term defined in Equation (68), by applying the principles of the 5th-CASAM-N, as follows:

1) Consider that the function $\boldsymbol{V}^{(2)}(x)$ is an element of a Hilbert space denoted as $\mathsf{H}_2(\Omega_x)$. This Hilbert space is considered to be endowed with an inner product of two vectors $\boldsymbol{\Psi}^{(2)}(2;x)\triangleq\left[\psi^{(2)}(1;x),\psi^{(2)}(2;x)\right]^{\dagger}\in\mathsf{H}_2(\Omega_x)$ and $\boldsymbol{\Phi}^{(2)}(2;x)\triangleq\left[\psi^{(2)}(1;x),\psi^{(2)}(2;x)\right]^{\dagger}\in\mathsf{H}_2(\Omega_x)$ defined as follows:

$$\left\langle\boldsymbol{\Psi}^{(2)}(2;x),\boldsymbol{\Phi}^{(2)}(2;x)\right\rangle_2\triangleq\sum_{i=1}^{2}\left\langle\psi^{(2)}(i;x),\varphi^{(2)}(i;x)\right\rangle_1$$
$$\triangleq\left\{\sum_{i=1}^{2}\int_{\lambda}^{\omega}\psi^{(2)}(i;x),\varphi^{(2)}(i;x)\mathrm{d}x\right\}_{\alpha^0}. \tag{76}$$

2) Using the definition of provided in Equation (76), construct the inner product of Equation (71) with a yet undefined function

$\boldsymbol{A}^{(2)}(2;3;x) \triangleq \left[a^{(2)}(1;3;x), a^{(2)}(2;3;x)\right]^{\dagger} \in \mathsf{H}_2(\Omega_x)$ to obtain the following relation:

$$\left\{\left\langle \boldsymbol{A}^{(2)}(2;3;x), \boldsymbol{VM}^{(2)}(2\times 2)\boldsymbol{V}^{(2)}(2;x)\right\rangle_2\right\}_{\boldsymbol{\alpha}^0} = \left\{\left\langle \boldsymbol{A}^{(2)}(2;3;x), \boldsymbol{Q}_V^{(2)}(2;x)\right\rangle_2\right\}_{\boldsymbol{\alpha}^0}, \quad x \in \Omega_x, \tag{77}$$

which in component form reads as follows:

$$\begin{aligned}
&\left\{\int_{\lambda}^{\omega} a^{(2)}(1;3;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_{\lambda}^{\omega} a^{(2)}(2;3;x)\right.\\
&\left.\times\left[\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x) + 2qu(x)\delta a^{(1)}(x) + 2qa^{(1)}(x)v^{(1)}(x) + 2ru^{-3}(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&= (\delta q)\left\{\int_{\lambda}^{\omega} a^{(2)}(1;3;x)u^2(x)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&+\left\{\int_{\lambda}^{\omega} a^{(2)}(2;3;x)\left[-2(\delta q)u(x)a^{(1)}(x) + (\delta r)u^{-2}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned} \tag{78}$$

3) Integrate by parts the left-side of Equation (78) to obtain the following relation:

$$\begin{aligned}
&\left\{\int_{\lambda}^{\omega} a^{(2)}(1;3;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_{\lambda}^{\omega} a^{(2)}(2;3;x)\right.\\
&\left.\times\left[\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x) + 2qu(x)\delta a^{(1)}(x) + 2qa^{(1)}(x)v^{(1)}(x) + 2ru^{-3}(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&= a^{(2)}(1;3;\omega)v^{(1)}(\omega) - a^{(2)}(1;3;\lambda)v^{(1)}(\lambda)\\
&+\left\{\int_{\lambda}^{\omega} v^{(1)}(x)\left[-\frac{\mathrm{d}a^{(2)}(1;3;x)}{\mathrm{d}x} - 2qu(x)a^{(2)}(1;3;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&+a^{(2)}(2;3;\omega)\delta a^{(1)}(\omega) - a^{(2)}(2;3;\lambda)\delta a^{(1)}(\lambda)\\
&+\left\{\int_{\lambda}^{\omega} \delta a^{(1)}(x)\left[-\frac{\mathrm{d}}{\mathrm{d}x}a^{(2)}(2;3;x) + 2qu(x)a^{(2)}(2;3;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&+\left\{2\int_{\lambda}^{\omega} v^{(1)}(x)\left[qa^{(1)}(x)a^{(2)}(2;3;x) + ru^{-3}(x)a^{(2)}(2;3;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}
\end{aligned} \tag{79}$$

4) Use in Equation (79) the boundary condition given in Equations (11) and (70) to obtain the following relation:

$$\begin{aligned}
&\left\{\int_{\lambda}^{\omega} a^{(2)}(1;3;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_{\lambda}^{\omega} a^{(2)}(2;3;x)\right.\\
&\left.\times\left[\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x) + 2qu(x)\delta a^{(1)}(x) + 2qa^{(1)}(x)v^{(1)}(x) + 2ru^{-3}(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&-a^{(2)}(1;3;\omega)v^{(1)}(\omega) + a^{(2)}(1;3;\lambda)\left[\delta u_{in} - qu_{in}^2(\delta\lambda)\right]\\
&+a^{(2)}(2;3;\omega)r\left[q(\omega-\lambda) - \frac{1}{u_{in}}\right]^2\delta\omega + a^{(2)}(2;3;\lambda)\delta a^{(1)}(\lambda)
\end{aligned}$$

$$=\left\{\int_{\lambda}^{\omega} v^{(1)}(x)\left[-\frac{\mathrm{d}a^{(2)}(1;3;x)}{\mathrm{d}x}-2qu(x)a^{(2)}(1;3;x)\right.\right.$$
$$\left.\left.+2qa^{(1)}(x)a^{(2)}(2;3;x)+2ru^{-3}(x)a^{(2)}(2;3;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \tag{80}$$
$$+\left\{\int_{\lambda}^{\omega}\delta a^{(1)}(x)\left[-\frac{\mathrm{d}}{\mathrm{d}x}a^{(2)}(2;3;x)+2qu(x)a^{(2)}(2;3;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}$$

5) Require the right-side of Equation (80) to represent the indirect-effect term defined in Equation (68) and eliminate the unknown values of the components of $\boldsymbol{V}^{(2)}(x)$ in Equation (80) by requiring the function $\boldsymbol{A}^{(2)}(2;3;x)\triangleq\left[a^{(2)}(1;3;x),a^{(2)}(2;3;x)\right]^{\dagger}$ to be the solution of the following 2nd-Level Adjoint Sensitivity System (2nd-LASS):

$$\left\{\frac{\mathrm{d}a^{(2)}(1;3;x)}{\mathrm{d}x}+2qu(x)a^{(2)}(1;3;x)\right\}_{\boldsymbol{\alpha}^0}=\left\{2a^{(2)}(2;3;x)\left[qa^{(1)}(x)+ru^{-3}(x)\right]\right\}_{\boldsymbol{\alpha}^0}; \tag{81}$$

$$\left\{a^{(2)}(1;3;\omega)\right\}_{\boldsymbol{\alpha}^0}=0,\ \text{at}\ x=\omega; \tag{82}$$

$$\left\{-\frac{\mathrm{d}}{\mathrm{d}x}a^{(2)}(2;3;x)+2qu(x)a^{(2)}(2;3;x)\right\}_{\boldsymbol{\alpha}^0}=\left\{\delta(x-\lambda)\right\}_{\boldsymbol{\alpha}^0};\ x\in\Omega_x; \tag{83}$$

$$\left\{a^{(2)}(2;3;\lambda)\right\}_{\boldsymbol{\alpha}^0}=0,\ \text{at}\ x=\lambda. \tag{84}$$

6) Use Equations (80)-(84) together with Equation (78) in Equation (68) to obtain the following alternative expression for the indirect-effect term:

$$\left\{\delta\left[\partial R/\partial u_{in}\right]\right\}_{ind}=(\delta q)\left\{\int_{\lambda}^{\omega}a^{(2)}(1;3;x)u^2(x)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}$$
$$+\left\{\int_{\lambda}^{\omega}a^{(2)}(2;3;x)\left[-2(\delta q)u(x)a^{(1)}(x)+(\delta r)u^{-2}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \tag{85}$$
$$+\left[\delta u_{in}-qu_{in}^2(\delta\lambda)\right]a^{(2)}(1;3;\lambda)+(\delta\omega)r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2a^{(2)}(2;3;\omega).$$

7) Adding the expressions for the indirect-effect and direct-effect terms obtained in Equations (85) and (67), respectively, and identifying the expressions that multiply the respective parameter variations, as indicated in Equation (66), yields the following expressions for the first-order response sensitivities with respect to the model parameters:

$$\frac{\partial^2 R}{\partial q\partial u_{in}}=\int_{\lambda}^{\omega}a^{(2)}(1;3;x)u^2(x)\mathrm{d}x-2\int_{\lambda}^{\omega}a^{(2)}(2;3;x)u(x)a^{(1)}(x)\mathrm{d}x, \tag{86}$$

$$\frac{\partial^2 R}{\partial u_{in}\partial u_{in}}=a^{(2)}(1;3;\lambda), \tag{87}$$

$$\frac{\partial^2 R}{\partial\lambda\partial u_{in}}=-qu_{in}^2a^{(2)}(1;3;\lambda)+\frac{r}{u_{in}^2}-2r(\lambda-\omega)\frac{q}{u_{in}}, \tag{88}$$

$$\frac{\partial^2 R}{\partial \omega \partial u_{in}} = r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2 a^{(2)}(2;3;\omega), \tag{89}$$

$$\frac{\partial^2 R}{\partial r \partial u_{in}} = \int_{\lambda}^{\omega} a^{(2)}(2;3;x)u^{-2}(x)\mathrm{d}x. \tag{90}$$

The expressions of the sensitivities provided in Equations (86)-(90) are to be evaluated at the nominal values of the respective parameters and state functions but the respective indication $\{\}_{\alpha^0}$ has been omitted, for simplicity. The expressions of the sensitivities stemming from the indirect-effect term can be evaluated after solving the 2nd-LASS to obtain the 2nd-level adjoint sensitivity function $\boldsymbol{A}^{(2)}(2;3;x) \triangleq \left[a^{(2)}(1;3;x), a^{(2)}(2;3;x)\right]^{\dagger}$. The 2nd-LASS is linear in $\boldsymbol{A}^{(2)}(2;3;x) \triangleq \left[a^{(2)}(1;3;x), a^{(2)}(2;3;x)\right]^{\dagger}$ and is independent of parameter variations, so it only needs to be solved once. Furthermore, the 2nd-LASS is an upper-triangular system which can be solved in a decoupled manner, by first obtaining the expression of the function $a^{(2)}(2;3;x)$ and subsequently obtaining the expression of the function $a^{(2)}(1;3;x)$. Solving the 2nd-LASS comprising Equations (81)-(84) yields the following expressions:

$$a^{(2)}(1;3;x) = -2\frac{r(x-\omega)}{u(x)}\frac{1}{u_{in}^2} = -\frac{2r}{u_{in}^3}(x-\omega)\left[1-qu_{in}(x-\lambda)\right], \tag{91}$$

$$a^{(2)}(2;3;x) = -\left[qu_{in}(x-\lambda)-1\right]^{-2} H(x-\lambda) = -\left[\frac{u(x)}{u_{in}}\right]^2 H(x-\lambda). \tag{92}$$

Inserting into Equations (86)-(90) the expressions obtained in Equations (91) and (92) yields the following closed form expressions:

$$\frac{\partial^2 R}{\partial q \partial u_{in}} = 0, \tag{93}$$

$$\frac{\partial^2 R}{\partial u_{in} \partial u_{in}} = -\frac{2r}{u_{in}^3}(\lambda-\omega), \tag{94}$$

$$\frac{\partial^2 R}{\partial \lambda \partial u_{in}} = \frac{r}{u_{in}^2}, \tag{95}$$

$$\frac{\partial^2 R}{\partial \omega \partial u_{in}} = -\frac{r}{u_{in}^2}, \tag{96}$$

$$\frac{\partial^2 R}{\partial r \partial u_{in}} = \frac{(\lambda-\omega)}{u_{in}^2}. \tag{97}$$

Since the expression in Equation (90) must be identical to the expression provided in Equation (38), *i.e.*,

$$\frac{\partial^2 R}{\partial r \partial u_{in}} = \int_{\lambda}^{\omega} a^{(2)}(2;3;x)u^{-2}(x)\mathrm{d}x \equiv \frac{\partial^2 R}{\partial u_{in} \partial r} = a^{(2)}(1;1;\lambda), \tag{98}$$

it follows that the above identity provides a stringent test in practice for verifying the accuracy of the numerical computation of the functions $a^{(2)}(2;3;x)$, $u(x)$ and $a^{(2)}(1;1;x)$.

Similarly, since the expression in Equation (89) must be identical to the expression provided in Equation (57), *i.e.*,

$$\frac{\partial^2 R}{\partial\omega\partial u_{in}} = r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2 a^{(2)}(2;3;\omega) \equiv \frac{\partial^2 R}{\partial u_{in}\partial\omega} = a^{(2)}(1;2;\lambda), \tag{99}$$

it follows that the above identity provides a stringent test in practice for verifying the accuracy of the numerical computation of the functions $a^{(2)}(2;3;x)$ and $a^{(2)}(1;2;x)$.

3.2.2. Second-Order Sensitivities Stemming from $\partial R/\partial\lambda$

In preparation for determining the 2nd-order sensitivities that correspond to $\partial R/\partial\lambda$, the expression provided in Equation (21) is written in the following integral form:

$$\frac{\partial R}{\partial\lambda} = -r\int_\lambda^\omega \frac{\delta(x-\lambda)}{u(x)}\mathrm{d}x - qu_{in}^2\int_\lambda^\omega a^{(1)}(x)\delta(x-\lambda)\mathrm{d}x. \tag{100}$$

By definition, the G-differential $\delta[\partial R/\partial\lambda]$ of $\partial R/\partial\lambda$ is obtained as follows:

$$\begin{aligned}
\delta\left\{\frac{\partial R}{\partial\lambda}\right\} &\triangleq \frac{\partial^2 R}{\partial q\partial\lambda}\delta q + \frac{\partial^2 R}{\partial u_{in}\partial\lambda}\delta u_{in} + \frac{\partial^2 R}{\partial\lambda\partial\lambda}\delta\lambda + \frac{\partial^2 R}{\partial\omega\partial\lambda}\delta\omega + \frac{\partial^2 R}{\partial r\partial\lambda}\delta r \\
&\triangleq -\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega}\left(r^0+\varepsilon\delta r\right)\frac{\delta\left(x-\lambda^0-\varepsilon\delta\lambda\right)}{u^0(x)+\varepsilon\delta u(x)}\mathrm{d}x\right\}_{\varepsilon=0} \\
&-\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega}\left(q^0+\varepsilon\delta q\right)\left(u_{in}^0+\varepsilon\delta u_{in}\right)^2\left[a^{(1),0}(x)+\varepsilon\delta a^{(1)}(x)\right]\delta\left(x-\lambda^0-\varepsilon\delta\lambda\right)\mathrm{d}x\right\}_{\varepsilon=0} \\
&\triangleq \left\{\delta[\partial R/\partial\lambda]\right\}_{dir} + \left\{\delta[\partial R/\partial\lambda]\right\}_{ind},
\end{aligned} \tag{101}$$

where:

$$\begin{aligned}
\left\{\delta[\partial R/\partial\lambda]\right\}_{dir} &\triangleq -(\delta r)\left\{\int_\lambda^\omega \frac{\delta(x-\lambda)}{u(x)}\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} + (\delta\lambda)\left\{r\int_\lambda^\omega \frac{\delta'(x-\lambda)}{u(x)}\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \\
&-\left\{\left[(\delta q)u_{in}^2 + 2qu_{in}(\delta u_{in})\right]\int_\lambda^\omega a^{(1)}(x)\delta(x-\lambda)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \\
&+(\delta\lambda)\left\{qu_{in}^2\int_\lambda^\omega a^{(1)}(x)\delta'(x-\lambda)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \\
&= -(\delta r)\left\{\frac{1}{u_{in}}\right\}_{\boldsymbol{\alpha}^0} + (\delta\lambda)\{rq\}_{\boldsymbol{\alpha}^0} - \left[(\delta q)u_{in}^2 + 2qu_{in}(\delta u_{in})\right]\frac{r(\lambda-\omega)}{u_{in}^2} \\
&-(\delta\lambda)\left\{qr\left[1-2qu_{in}(\lambda-\omega)\right]\right\}_{\boldsymbol{\alpha}^0},
\end{aligned} \tag{102}$$

$$\left\{\delta[\partial R/\partial\lambda]\right\}_{ind} \triangleq \left\{r\int_\lambda^\omega \frac{\delta(x-\lambda)}{u^2(x)}v^{(1)}(x)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} - \left\{qu_{in}^2\int_\lambda^\omega \delta a^{(1)}(x)\delta(x-\lambda)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}. \tag{103}$$

The direct-effect term has been evaluated at this stage since the functions $u(x)$ and $a^{(1)}(x)$ are already available. The indirect-effect term, however, can be evaluated only after having determined the variational vector $\boldsymbol{V}^{(2)}(x) \triangleq \left[v^{(1)}(x), \delta a^{(1)}(x)\right]^\dagger$, which is the solution of the 2nd-LVSS obtained in

Equations (71)-(75). The need for solving repeatedly the 2nd-LVSS to obtain the 2nd-level variational function $\boldsymbol{V}^{(2)}(x)$ for every parameter variations is circumvented by expressing the indirect-effect term defined in Equation (103) in terms of the solution of a 2nd-LASS, which is constructed specifically for this indirect-effect term, by applying the principles of the 5th-CASAM-N, as follows:

1) Using the definition of provided in Equation (76), construct in the Hilbert $\mathsf{H}_2(\Omega_x)$ the inner product of Equation (71) with a yet undefined function $\boldsymbol{A}^{(2)}(2;4;x) \triangleq \left[a^{(2)}(1;4;x), a^{(2)}(2;4;x)\right]^{\dagger} \in \mathsf{H}_2(\Omega_x)$ to obtain the following relation:

$$\left\{\left\langle \boldsymbol{A}^{(2)}(2;4;x), \boldsymbol{VM}^{(2)}\boldsymbol{V}^{(2)}(x)\right\rangle_2\right\}_{\boldsymbol{\alpha}^0} = \left\{\left\langle \boldsymbol{A}^{(2)}(2;4;x), \boldsymbol{Q}_V^{(2)}\right\rangle_2\right\}_{\boldsymbol{\alpha}^0}, \quad x \in \Omega_x, \tag{104}$$

which in component form reads as follows:

$$\begin{aligned}
&\left\{\int_\lambda^\omega a^{(2)}(1;4;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_\lambda^\omega a^{(2)}(2;4;x)\right.\\
&\left.\times\left[\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x) + 2qu(x)\delta a^{(1)}(x) + 2qa^{(1)}(x)v^{(1)}(x) + 2ru^{-3}(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&= (\delta q)\left\{\int_\lambda^\omega a^{(2)}(1;4;x)u^2(x)\,\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&+\left\{\int_\lambda^\omega a^{(2)}(2;4;x)\left[-2(\delta q)u(x)a^{(1)}(x) + (\delta r)u^{-2}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned} \tag{105}$$

2) Integrate by parts the left-side of Equation (105) to obtain the following relation:

$$\begin{aligned}
&\left\{\int_\lambda^\omega a^{(2)}(1;4;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_\lambda^\omega a^{(2)}(2;4;x)\right.\\
&\left.\times\left[\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x) + 2qu(x)\delta a^{(1)}(x) + 2qa^{(1)}(x)v^{(1)}(x) + 2ru^{-3}(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&= a^{(2)}(1;4;\omega)v^{(1)}(\omega) - a^{(2)}(1;4;\lambda)v^{(1)}(\lambda)\\
&+\left\{\int_\lambda^\omega v^{(1)}(x)\left[-\frac{\mathrm{d}a^{(2)}(1;4;x)}{\mathrm{d}x} - 2qu(x)a^{(2)}(1;4;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&+a^{(2)}(2;4;\omega)\delta a^{(1)}(\omega) - a^{(2)}(2;4;\lambda)\delta a^{(1)}(\lambda)\\
&+\left\{\int_\lambda^\omega \delta a^{(1)}(x)\left[-\frac{\mathrm{d}}{\mathrm{d}x}a^{(2)}(2;4;x) + 2qu(x)a^{(2)}(2;4;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\
&+\left\{2\int_\lambda^\omega v^{(1)}(x)\left[qa^{(1)}(x)a^{(2)}(2;4;x) + ru^{-3}(x)a^{(2)}(2;4;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}
\end{aligned} \tag{106}$$

3) Use in Equation (106) the boundary condition given in Equations (11) and (70) to obtain the following relation:

$$\left\{\int_\lambda^\omega a^{(2)}(1;4;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_\lambda^\omega a^{(2)}(2;4;x)\right.$$

$$\times\left[\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x)+2qu(x)\delta a^{(1)}(x)+2qa^{(1)}(x)v^{(1)}(x)+2ru^{-3}(x)v^{(1)}(x)\right]\mathrm{d}x\Bigg\}_{\boldsymbol{\alpha}^0}$$
$$-a^{(2)}(1;4;\omega)v^{(1)}(\omega)+a^{(2)}(1;4;\lambda)\left[\delta u_{in}-qu_{in}^2(\delta\lambda)\right]$$
$$+a^{(2)}(2;4;\omega)r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2(\delta\omega)+a^{(2)}(2;4;\lambda)\delta a^{(1)}(\lambda)$$
$$=\left\{\int_\lambda^\omega v^{(1)}(x)\left[-\frac{\mathrm{d}a^{(2)}(1;4;x)}{\mathrm{d}x}-2qu(x)a^{(2)}(1;4;x)\right.\right.$$
$$\left.\left.+2qa^{(1)}(x)a^{(2)}(2;4;x)+2ru^{-3}(x)a^{(2)}(2;4;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \tag{107}$$
$$+\left\{\int_\lambda^\omega \delta a^{(1)}(x)\left[-\frac{\mathrm{d}}{\mathrm{d}x}a^{(2)}(2;4;x)+2qu(x)a^{(2)}(2;4;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}$$

4) Require the right-side of Equation (107) to represent the indirect-effect term defined in Equation (103) and eliminate the unknown values of the components of $\boldsymbol{V}^{(2)}(x)$ in Equation (107) by requiring the function $\boldsymbol{A}^{(2)}(2;4;x)\triangleq\left[a^{(2)}(1;4;x),a^{(2)}(2;4;x)\right]^\dagger$ to be the solution of the following 2nd-LASS:

$$\frac{\mathrm{d}a^{(2)}(1;4;x)}{\mathrm{d}x}+2qu(x)a^{(2)}(1;4;x)$$
$$=-\frac{r\delta(x-\lambda)}{u_{in}^2}+2a^{(2)}(2;4;x)\left[qa^{(1)}(x)+2ru^{-3}(x)\right]; \tag{108}$$

$$\left\{a^{(2)}(1;4;\omega)\right\}_{\boldsymbol{\alpha}^0}=0,\ \text{at}\ x=\omega; \tag{109}$$

$$\left\{-\frac{\mathrm{d}}{\mathrm{d}x}a^{(2)}(2;4;x)+2qu(x)a^{(2)}(2;4;x)\right\}_{\boldsymbol{\alpha}^0}=-\left\{qu_{in}^2\delta(x-\lambda)\right\}_{\boldsymbol{\alpha}^0};\ x\in\Omega_x; \tag{110}$$

$$\left\{a^{(2)}(2;4;\lambda)\right\}_{\boldsymbol{\alpha}^0}=0,\ \text{at}\ x=\lambda. \tag{111}$$

5) Use Equations (107)-(111) together with Equation (105) in Equation (103) to obtain the following alternative expression for the indirect-effect term:

$$\left\{\delta[\partial R/\partial\lambda]\right\}_{ind}=(\delta q)\left\{\int_\lambda^\omega a^{(2)}(1;4;x)u^2(x)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}$$
$$+\left\{\int_\lambda^\omega a^{(2)}(2;4;x)\left[-2(\delta q)u(x)a^{(1)}(x)+(\delta r)u^{-2}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}. \tag{112}$$
$$+\left[\delta u_{in}-qu_{in}^2(\delta\lambda)\right]a^{(2)}(1;4;\lambda)+(\delta\omega)r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2a^{(2)}(2;4;\omega)$$

6) Adding the expressions for the indirect-effect and direct-effect terms obtained in Equations (112) and (102), respectively, and identifying the expressions that multiply the respective parameter variations, as indicated in Equation (101), yields the following expressions for the first-order response sensitivities with re-

spect to the model parameters:

$$\frac{\partial^2 R}{\partial q \partial \lambda} = \int_{\lambda}^{\omega} a^{(2)}(1;4;x) u^2(x) \mathrm{d}x - 2\int_{\lambda}^{\omega} a^{(2)}(2;4;x) u(x) a^{(1)}(x) \mathrm{d}x + r(\omega - \lambda), \tag{113}$$

$$\frac{\partial^2 R}{\partial u_{in} \partial \lambda} = a^{(2)}(1;4;\lambda) - 2q \frac{r(\lambda - \omega)}{u_{in}}, \tag{114}$$

$$\frac{\partial^2 R}{\partial \lambda \partial \lambda} = -q u_{in}^2 a^{(2)}(1;4;\lambda) + 2rq^2 u_{in}(\lambda - \omega), \tag{115}$$

$$\frac{\partial^2 R}{\partial \omega \partial \lambda} = r\left[q(\omega - \lambda) - \frac{1}{u_{in}}\right]^2 a^{(2)}(2;4;\omega), \tag{116}$$

$$\frac{\partial^2 R}{\partial r \partial \lambda} = \int_{\lambda}^{\omega} a^{(2)}(2;4;x) u^{-2}(x) \mathrm{d}x - \frac{1}{u_{in}}. \tag{117}$$

The expressions of the sensitivities provided in Equations (113)-(117) are to be evaluated at the nominal values of the respective parameters and state functions but the respective indication $\{\}_{\alpha^0}$ has been omitted, for simplicity. The expressions of the sensitivities stemming from the indirect-effect term can be evaluated after solving the 2nd-LASS defined by Equations (108)-(111) to obtain the 2nd-level adjoint sensitivity function $\mathbf{A}^{(2)}(2;4;x) \triangleq \left[a^{(2)}(1;4;x), a^{(2)}(2;4;x)\right]^{\dagger}$. This 2nd-LASS is linear in $\mathbf{A}^{(2)}(2;4;x) \triangleq \left[a^{(2)}(1;4;x), a^{(2)}(2;4;x)\right]^{\dagger}$ and is independent of parameter variations, so it only needs to be solved once. Furthermore, this 2nd-LASS is an upper-triangular system which can be solved in a decoupled manner, by first obtaining the expression of the function $a^{(2)}(2;4;x)$ and subsequently obtaining the expression of the function $a^{(2)}(1;4;x)$. Solving thus the 2nd-LASS comprising Equations (108)-(111) yields the following expressions:

$$a^{(2)}(1;4;x) = \left[q u_{in}(x - \lambda) - 1\right]^2 \left\{ -\frac{r}{u_{in}^2} H(x - \lambda) - \frac{r}{u_{in}^2} + \frac{2r\left[1 + q u_{in}(\lambda - \omega)\right]}{u_{in}^2 \left[1 + q u_{in}(\lambda - x)\right]} \right\}, \tag{118}$$

$$a^{(2)}(2;4;x) = q u_{in}^2 \left[q u_{in}(x - \lambda) - 1\right]^{-2} H(x - \lambda) = q u^2(x) H(x - \lambda). \tag{119}$$

Inserting into Equations (113)-(117) the expressions obtained in Equations (118) and (119) yields the following closed form expressions:

$$\frac{\partial^2 R}{\partial q \partial \lambda} = r(\omega - \lambda), \tag{120}$$

$$\frac{\partial^2 R}{\partial u_{in} \partial \lambda} = \frac{r}{u_{in}^2}, \tag{121}$$

$$\frac{\partial^2 R}{\partial \lambda \partial \lambda} = -rq, \tag{122}$$

$$\frac{\partial^2 R}{\partial \omega \partial \lambda} = rq, \tag{123}$$

$$\frac{\partial^2 R}{\partial r \partial \lambda} = q(\omega - \lambda) - \frac{1}{u_{in}}. \tag{124}$$

Since the expression in Equation (117) must be identical to the expression provided in Equation (39), *i.e.*,

$$\frac{\partial^2 R}{\partial r \partial \lambda} = \int_{\lambda}^{\omega} a^{(2)}(2;4;x) u^{-2}(x) \mathrm{d}x - \frac{1}{u_{in}} \equiv \frac{\partial^2 R}{\partial \lambda \partial r} = -\frac{1}{u(\lambda)} - q u_{in}^2 a^{(2)}(1;1;\lambda), \quad (125)$$

it follows that the above identity provides a stringent test in practice for verifying the accuracy of the numerical computation of the functions $a^{(2)}(2;4;x)$, $u(x)$ and $a^{(2)}(1;1;x)$.

Similarly, since the expression in Equation (116) must be identical to the expression provided in Equation (58), *i.e.*,

$$\frac{\partial^2 R}{\partial \omega \partial \lambda} = r\left[q(\omega-\lambda) - \frac{1}{u_{in}}\right]^2 a^{(2)}(2;4;\omega) \equiv \frac{\partial^2 R}{\partial \lambda \partial \omega} = -q u_{in}^2 a^{(2)}(1;2;\lambda), \quad (126)$$

it follows that the above identity provides a stringent test in practice for verifying the accuracy of the numerical computation of the functions $a^{(2)}(2;4;x)$ and $a^{(2)}(1;2;x)$.

Furthermore, since the expression in Equation (114) must be identical to the expression provided in Equation (88), *i.e.*,

$$\begin{aligned} \frac{\partial^2 R}{\partial u_{in} \partial \lambda} &= a^{(2)}(1;4;\lambda) - 2q\frac{r(\lambda-\omega)}{u_{in}} \\ &\equiv \frac{\partial^2 R}{\partial \lambda \partial u_{in}} = -q u_{in}^2 a^{(2)}(1;3;\lambda) + \frac{r}{u_{in}^2} - 2r(\lambda-\omega)\frac{q}{u_{in}}, \end{aligned} \quad (127)$$

it follows that the above identity provides a stringent test in practice for verifying the accuracy of the numerical computation of the functions $a^{(2)}(1;4;x)$ and $a^{(2)}(1;3;x)$.

3.2.3. Second-Order Sensitivities Stemming from $\partial R/\partial q$

The 2nd-order sensitivities stemming from the 1st-order sensitivity $\partial R/\partial q$ are obtained, by definition, from by determining the G-differential, $\delta[\partial R/\partial q]$, of the expression provided in Equation (19) for $\partial R/\partial q$, which yields:

$$\begin{aligned} \delta\left\{\frac{\partial R}{\partial q}\right\} &\triangleq \frac{\partial^2 R}{\partial q \partial q}\delta q + \frac{\partial^2 R}{\partial u_{in} \partial q}\delta u_{in} + \frac{\partial^2 R}{\partial \lambda \partial q}\delta \lambda + \frac{\partial^2 R}{\partial \omega \partial q}\delta \omega + \frac{\partial^2 R}{\partial r \partial q}\delta r \\ &\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega}\left[a^{(1),0}(x) + \varepsilon \delta a^{(1)}(x)\right]\left[u^0(x) + \varepsilon v^{(1)}(x)\right]^2 \mathrm{d}x\right\}_{\varepsilon=0} \\ &\triangleq \{\delta[\partial R/\partial q]\}_{dir} + \{\delta[\partial R/\partial q]\}_{ind}, \end{aligned} \quad (128)$$

where:

$$\{\delta[\partial R/\partial q]\}_{dir} \triangleq -\left\{a^{(1)}(\lambda) u^2(\lambda)(\delta\lambda)\right\}_{\alpha^0} = (\delta\lambda)\{r(\omega-\lambda)\}_{\alpha^0}, \quad (129)$$

$$\{\delta[\partial R/\partial q]\}_{ind} \triangleq \left\{\int_{\lambda}^{\omega} \delta a^{(1)}(x) u^2(x) \mathrm{d}x\right\}_{\alpha^0} + \left\{2\int_{\lambda}^{\omega} a^{(1)}(x) u(x) v^{(1)}(x) \mathrm{d}x\right\}_{\alpha^0}. \quad (130)$$

The direct-effect term can be evaluated at this stage since the values of the functions $a^{(1)}(x)$ and $u(x)$ are already available. The indirect-effect term, however, can be evaluated only after having determined the vector-valued variational function $\boldsymbol{V}^{(2)}(x) \triangleq \left[v^{(1)}(x), \delta a^{(1)}(x)\right]^{\dagger}$, which is the solution of the 2nd-LVSS obtained in Equations (71)-(75). The need for solving repeatedly the 2nd-LVSS to obtain the 2nd-level variational function $\boldsymbol{V}^{(2)}(x)$ for every parameter variations is circumvented by expressing the indirect-effect term defined in Equation (130) in terms of the solution of a 2nd-LASS, which is constructed specifically for this indirect-effect term, by applying the principles of the 5th-CASAM-N, as follows:

1) Using the definition of provided in Equation (76), construct in the Hilbert $\mathsf{H}_2(\Omega_x)$ the inner product of Equation (71) with a yet undefined function $\boldsymbol{A}^{(2)}(2;5;x) \triangleq \left[a^{(2)}(1;5;x), a^{(2)}(2;5;x)\right]^{\dagger} \in \mathsf{H}_2(\Omega_x)$ to obtain the following relation:

$$\left\{\left\langle \boldsymbol{A}^{(2)}(2;5;x), \boldsymbol{VM}^{(2)}\boldsymbol{V}^{(2)}(x)\right\rangle_2\right\}_{\boldsymbol{\alpha}^0} = \left\{\left\langle \boldsymbol{A}^{(2)}(2;5;x), \boldsymbol{Q}_V^{(2)}\right\rangle_2\right\}_{\boldsymbol{\alpha}^0}, \quad x \in \Omega_x, \tag{131}$$

which in component form reads as follows:

$$\begin{aligned}&\left\{\int_{\lambda}^{\omega} a^{(2)}(1;5;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_{\lambda}^{\omega} a^{(2)}(2;5;x)\right.\\ &\left.\times\left[\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x) + 2qu(x)\delta a^{(1)}(x) + 2qa^{(1)}(x)v^{(1)}(x) + 2ru^{-3}(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\ &= (\delta q)\left\{\int_{\lambda}^{\omega} a^{(2)}(1;5;x)u^2(x)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\ &+\left\{\int_{\lambda}^{\omega} a^{(2)}(2;5;x)\left[-2(\delta q)u(x)a^{(1)}(x) + (\delta r)u^{-2}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}.\end{aligned} \tag{132}$$

2) Integrate by parts the left-side of Equation (132) to obtain the following relation:

$$\begin{aligned}&\left\{\int_{\lambda}^{\omega} a^{(2)}(1;5;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} + \left\{\int_{\lambda}^{\omega} a^{(2)}(2;5;x)\right.\\ &\left.\times\left[\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x) + 2qu(x)\delta a^{(1)}(x) + 2qa^{(1)}(x)v^{(1)}(x) + 2ru^{-3}(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\ &= a^{(2)}(1;5;\omega)v^{(1)}(\omega) - a^{(2)}(1;5;\lambda)v^{(1)}(\lambda)\\ &+\left\{\int_{\lambda}^{\omega} v^{(1)}(x)\left[-\frac{\mathrm{d}a^{(2)}(1;5;x)}{\mathrm{d}x} - 2qu(x)a^{(2)}(1;5;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\ &+a^{(2)}(2;5;\omega)\delta a^{(1)}(\omega) - a^{(2)}(2;5;\lambda)\delta a^{(1)}(\lambda)\\ &+\left\{\int_{\lambda}^{\omega} \delta a^{(1)}(x)\left[-\frac{\mathrm{d}}{\mathrm{d}x}a^{(2)}(2;5;x) + 2qu(x)a^{(2)}(2;5;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\\ &+\left\{2\int_{\lambda}^{\omega} v^{(1)}(x)\left[qa^{(1)}(x)a^{(2)}(2;5;x) + ru^{-3}(x)a^{(2)}(2;5;x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}\end{aligned} \tag{133}$$

3) Use in Equation (133) the boundary condition given in Equations (11) and (70) to obtain the following relation:

$$
\begin{aligned}
&\left\{\int_{\lambda}^{\omega} a^{(2)}(1;5;x)\left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x}-2qu(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\alpha^0}+\left\{\int_{\lambda}^{\omega} a^{(2)}(2;5;x)\right.\\
&\left.\times\left[\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(1)}(x)+2qu(x)\delta a^{(1)}(x)+2qa^{(1)}(x)v^{(1)}(x)+2ru^{-3}(x)v^{(1)}(x)\right]\mathrm{d}x\right\}_{\alpha^0}\\
&-a^{(2)}(1;5;\omega)v^{(1)}(\omega)+a^{(2)}(1;5;\lambda)\left[\delta u_{in}-qu_{in}^{2}(\delta\lambda)\right]\\
&+a^{(2)}(2;5;\omega)r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^{2}(\delta\omega)+a^{(2)}(2;5;\lambda)\delta a^{(1)}(\lambda)\\
&=\left\{\int_{\lambda}^{\omega} v^{(1)}(x)\left[-\frac{\mathrm{d}a^{(2)}(1;5;x)}{\mathrm{d}x}-2qu(x)a^{(2)}(1;1;x)\right.\right.\\
&\left.\left.+2qa^{(1)}(x)a^{(2)}(2;5;x)+2ru^{-3}(x)a^{(2)}(2;5;x)\right]\mathrm{d}x\right\}_{\alpha^0}\\
&+\left\{\int_{\lambda}^{\omega}\delta a^{(1)}(x)\left[-\frac{\mathrm{d}}{\mathrm{d}x}a^{(2)}(2;5;x)+2qu(x)a^{(2)}(2;5;x)\right]\mathrm{d}x\right\}_{\alpha^0}
\end{aligned}
\tag{134}
$$

4) Require the right-side of Equation (134) to represent the indirect-effect term defined in Equation (130) and eliminate the unknown values of the components of $\boldsymbol{V}^{(2)}(x)$ in Equation (134) by requiring the function $\boldsymbol{A}^{(2)}(2;5;x)\triangleq\left[a^{(2)}(1;5;x),a^{(2)}(2;5;x)\right]^{\dagger}$ to be the solution of the following 2nd-Level Adjoint Sensitivity System (2nd-LASS):

$$
\begin{aligned}
&\left\{\frac{\mathrm{d}a^{(2)}(1;5;\omega)}{\mathrm{d}x}+2qu(x)a^{(2)}(1;5;\omega)\right\}_{\alpha^0}\\
&=\left\{-2a^{(1)}(x)u(x)+2a^{(2)}(2;5;x)\left[qa^{(1)}(x)+ru^{-3}(x)\right]\right\}_{\alpha^0};\ x\in\Omega_x;
\end{aligned}
\tag{135}
$$

$$
\left\{a^{(2)}(1;5;\omega)\right\}_{\alpha^0}=0,\ \text{at}\ x=\omega;
\tag{136}
$$

$$
\left\{\frac{\mathrm{d}}{\mathrm{d}x}a^{(2)}(2;5;x)-2qu(x)a^{(2)}(2;5;x)\right\}_{\alpha^0}=-\left\{u^{2}(x)\right\}_{\alpha^0};\ x\in\Omega_x;
\tag{137}
$$

$$
\left\{a^{(2)}(2;5;\lambda)\right\}_{\alpha^0}=0,\ \text{at}\ x=\lambda\ .
\tag{138}
$$

5) Use Equations (134)-(138) together with Equation (132) in Equation (130) to obtain the following alternative expression for the indirect-effect term:

$$
\begin{aligned}
&\left\{\delta\left[\partial R/\partial q\right]\right\}_{ind}=(\delta q)\left\{\int_{\lambda}^{\omega} a^{(2)}(1;5;x)u^{2}(x)\mathrm{d}x\right\}_{\alpha^0}\\
&+\left\{\int_{\lambda}^{\omega} a^{(2)}(2;5;x)\left[-2(\delta q)u(x)a^{(1)}(x)+(\delta r)u^{-2}(x)\right]\mathrm{d}x\right\}_{\alpha^0}\\
&+a^{(2)}(1;5;\lambda)\left[\delta u_{in}-qu_{in}^{2}(\delta\lambda)\right]+a^{(2)}(2;5;\omega)r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^{2}(\delta\omega).
\end{aligned}
\tag{139}
$$

6) Adding the expressions for the indirect-effect and direct-effect terms obtained in Equations (139) and (129), respectively, and identifying the expressions that multiply the respective parameter variations, as indicated in Equation (7),

yields the following expressions for the first-order response sensitivities with respect to the model parameters:

$$\frac{\partial^2 R}{\partial q \partial q} = \int_{\lambda}^{\omega} a^{(2)}(1;5;x) u^2(x) \mathrm{d}x - 2\int_{\lambda}^{\omega} a^{(2)}(2;5;x) u(x) a^{(1)}(x) \mathrm{d}x , \tag{140}$$

$$\frac{\partial^2 R}{\partial u_{in} \partial q} = a^{(2)}(1;5;\lambda), \tag{141}$$

$$\frac{\partial^2 R}{\partial \lambda \partial q} = -q u_{in}^2 a^{(2)}(1;5;\lambda) + r(\omega - \lambda), \tag{142}$$

$$\frac{\partial^2 R}{\partial \omega \partial q} = a^{(2)}(2;5;\omega) r \left[q(\omega - \lambda) - \frac{1}{u_{in}} \right]^2 , \tag{143}$$

$$\frac{\partial^2 R}{\partial r \partial q} = \int_{\lambda}^{\omega} a^{(2)}(2;5;x) u^{-2}(x) \mathrm{d}x . \tag{144}$$

The expressions of the sensitivities provided in Equations (140)-(144) are to be evaluated at the nominal values of the respective parameters and state functions but the respective indication $\{\ \}_{\alpha^0}$ has been omitted, for simplicity. The expressions of the sensitivities stemming from the indirect-effect term can be evaluated after solving the 2nd-LASS to obtain the 2nd-level adjoint sensitivity function $\boldsymbol{A}^{(2)}(2;5;x) \triangleq \left[a^{(2)}(1;5;x), a^{(2)}(2;5;x) \right]^{\dagger}$, which yields:

$$a^{(2)}(1;5;x) = 2r \frac{(\lambda - x)(x - \omega)}{u(x)} , \tag{145}$$

$$a^{(2)}(2;5;x) = (\lambda - x) \left[q(x - \lambda) - \frac{1}{u_{in}} \right]^{-2} = (\lambda - x) u^2(x) . \tag{146}$$

Inserting the results obtained in Equations (145) and (146) into in Equations (140)-(144) and evaluating the respective expressions yields the following closed-form results for the respective sensitivities:

$$\frac{\partial^2 R}{\partial q \partial q} = 0 , \tag{147}$$

$$\frac{\partial^2 R}{\partial u_{in} \partial q} = 0 , \tag{148}$$

$$\frac{\partial^2 R}{\partial \lambda \partial q} = r(\omega - \lambda), \tag{149}$$

$$\frac{\partial^2 R}{\partial \omega \partial q} = r(\lambda - \omega), \tag{150}$$

$$\frac{\partial^2 R}{\partial r \partial q} = -\frac{(\omega - \lambda)^2}{2} . \tag{151}$$

Since the expression in Equation (144) must be identical to the expression provided in Equation (37), *i.e.*,

$$\frac{\partial^2 R}{\partial r \partial q} = \int_\lambda^\omega a^{(2)}(2;5;x) u^{-2}(x) \mathrm{d}x \equiv \frac{\partial^2 R}{\partial q \partial r} = \int_\lambda^\omega a^{(2)}(1;1;x) u^2(x) \mathrm{d}x, \tag{152}$$

it follows that the above identity provides a stringent test in practice for verifying the accuracy of the numerical computation of the functions $a^{(2)}(2;5;x)$, $u(x)$ and $a^{(2)}(1;1;x)$.

Similarly, since the expression in Equation (143) must be identical to the expression provided in Equation (56), *i.e.*,

$$\frac{\partial^2 R}{\partial \omega \partial q} = a^{(2)}(2;5;\omega) r \left[q(\omega - \lambda) - \frac{1}{u_{in}} \right]^2 \equiv \frac{\partial^2 R}{\partial q \partial \omega} = \int_\lambda^\omega a^{(2)}(1;2;x) u^2(x) \mathrm{d}x, \tag{153}$$

it follows that the above identity provides a stringent test in practice for verifying the accuracy of the numerical computation of the functions $a^{(2)}(2;5;x)$, $a^{(2)}(1;2;x)$ and $u(x)$. Furthermore, since the expression in Equation (142) must be identical to the expression provided in Equation (113), *i.e.*,

$$\begin{aligned} \frac{\partial^2 R}{\partial \lambda \partial q} &= -q u_{in}^2 a^{(2)}(1;5;\lambda) + r(\omega - \lambda) \equiv \frac{\partial^2 R}{\partial q \partial \lambda} \\ &= \int_\lambda^\omega a^{(2)}(1;4;x) u^2(x) \mathrm{d}x - 2\int_\lambda^\omega a^{(2)}(2;4;x) u(x) a^{(1)}(x) \mathrm{d}x + r(\omega - \lambda), \end{aligned} \tag{154}$$

it follows that the above identity provides a stringent test in practice for verifying the accuracy of the numerical computation of the functions $a^{(2)}(1;5;x)$, $a^{(2)}(1;4;x)$, $a^{(2)}(2;4;x)$, $a^{(1)}(x)$ and $u(x)$.

Finally, since the expression in Equation (141) must be identical to the expression provided in Equation (86), *i.e.*,

$$\begin{aligned} \frac{\partial^2 R}{\partial u_{in} \partial q} &= a^{(2)}(1;5;\lambda) \equiv \frac{\partial^2 R}{\partial q \partial u_{in}} \\ &= \int_\lambda^\omega a^{(2)}(1;3;x) u^2(x) \mathrm{d}x - 2\int_\lambda^\omega a^{(2)}(2;3;x) u(x) a^{(1)}(x) \mathrm{d}x, \end{aligned} \tag{155}$$

it follows that the above identity provides a stringent test in practice for verifying the accuracy of the numerical computation of the functions $a^{(2)}(1;5;x)$, $a^{(2)}(1;3;x)$, $a^{(2)}(2;3;x)$, $a^{(1)}(x)$, $u(x)$.

3.3. Remarks on the Computation of Second-Order Sensitivities

Each of the 1st-order sensitivities give rise to as many 2nd-order sensitivities as there are model parameters: $TP = 5$ denotes the "total number of model parameters." Each of the 1st-order sensitivity is considered to be a model response for constructing a 2nd-LASS which is independent of parameter variations and therefore needs to be solved just once in order to obtain all (*i.e.*, TP) of the 2nd-order sensitivities that stem from the specific 1st-order sensitivity considered as a model response. The 2nd-LASS may comprise just as many equations as the 1st-LASS, in which case the computational effort required for solving the 2nd-LASS is comparable to that for solving the 1st-LASS. This was the case for determining the 2nd-order sensitivities stemming from the 1st-order sensitivities

$\partial R/\partial r$ and $\partial R/\partial \omega$. On the other hand, the 2nd-LASS could comprise twice as many equations as the 1st-LASS, as was the case for determining the 2nd-order sensitivities stemming from the 1st-order sensitivities $\partial R/\partial u_{in}$, $\partial R/\partial q$ and $\partial R/\partial \lambda$. In such cases, solving the 2nd-LASS would be twice as expensive computationally as solving the 1st-LASS, and requires the prior availability of the state function $u(x)$, which is obtained by solving the original system of nonlinear equations that underly the model under consideration, and the prior availability of the 1st-level adjoint sensitivity function $a^{(1)}(x)$, which is obtained by solving the 1st-LASS. The primary consideration when computing 2nd-order sensitivities is the priority order indicated by the magnitudes of the relative 1st-order sensitivities: the 2nd-order sensitivities stemming from the largest 1st-order relative sensitivity should be computed first. Once the priorities for computing the 2nd-order sensitivities have been established, it is important to examine the expressions of the 1st-order sensitivities in order to establish the least expensive (computationally) path for computing the mixed 2nd-order sensitivities. For example, it is more advantageous computationally to compute most advantageous it is more advantageous to compute those stemming from the 1st-order sensitivities as starting points $\partial R/\partial r$ and $\partial R/\partial \omega$. For example, it is computationally more advantageous to compute $\partial^2 R/\partial u_{in}\partial r$ by using Equation (38), which is obtained by using $\partial R/\partial r$ as the starting point, rather than using Equation (90), which is obtained by using $\partial R/\partial u_{in}$ as the starting point.

4. 3rd-CASAM-N: Computation of Third-Order Response Sensitivities

Each of the 2nd-order sensitivities would give rise to five 3rd-order sensitivities, for a total of 125 third-order sensitivities. The 3rd-order sensitivities could be computed directly by differentiating the expression of the 2nd-order G-differential, $\delta^2 R\left[u(x);\boldsymbol{\alpha};v^{(1)}(x);\delta\boldsymbol{\alpha};\delta v^{(1)}(x);v^{(1)}(x)\delta\boldsymbol{\alpha};\delta^2\boldsymbol{\alpha}\right]$, of the response, to obtain the 3rd-order G-differential which would require the computation of the G-differentials $\delta^n u(x)$, $n=1,2,3$. In this case, the G-differentials $\delta^n u(x)$, $n=1,2,3$ would need to be determined by solving nth-LVSS, the differentials $\delta^n u(x)$, $n=1,2,3$, which would involve 3rd-order differential equations, which would depend on 1st-, 2nd- and 3rd-order parameter variations. Furthermore, this set of 3rd-order differential equations would need to be solved at least 125 times, to account for all combinations of 1st- and 2nd-order variations in the parameters and state function $u(x)$. Alternatively, the 3rd-order sensitivities can be defined as the "1st-order sensitivities of the 2nd-order sensitivities," which enables the 3rd-order sensitivities to be computed by using 3rd-level adjoint sensitivity functions determined as will be illustrated in the remainder of this Section.

4.1. Third-Order Sensitivities Stemming from 2nd-Order Sensitivities Involving One-Component of the State Functions

Examining the expressions of the 2nd-order sensitivities reveals that the sensitivities $\partial^2 R/\partial\omega\partial r$ and $\partial^2 R/\partial\omega\partial\omega$ depend solely on the original function $u(x)$. Therefore, the 3rd-order sensitivities stemming from these 2nd-order sensitivities will involve a one-component 3rd-level adjoint sensitivity function, as will be illustrated on this Section by determining the 3rd-order sensitivities arising from $\partial^2 R/\partial\omega\partial r = \partial^2 R/\partial r\,\partial\omega$. The expression of $\partial^2 R/\partial\omega\partial r$ is provided by Equation (40), which is identical to Equation (60). The 3rd-order sensitivities stemming from $\partial^2 R/\partial\omega\partial r$ are obtained from by G-differentiating Equation (60), which by definition yields the following expression:

$$\begin{aligned}\delta\left\{\frac{\partial^2 R}{\partial r\partial\omega}\right\} &\triangleq \frac{\partial^3 R}{\partial q\partial r\partial\omega}\delta q + \frac{\partial^3 R}{\partial u_{in}\partial r\partial\omega}\delta u_{in} \\ &+ \frac{\partial^3 R}{\partial\lambda\partial r\partial\omega}\delta\lambda + \frac{\partial^3 R}{\partial\omega\partial r\partial\omega}\delta\omega + \frac{\partial^3 R}{\partial r\partial r\partial\omega}\delta r \\ &\triangleq \left\{\frac{d}{d\varepsilon}\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega}\frac{\delta\left(x-\omega^0-\varepsilon\delta\omega\right)}{u^0(x)+\varepsilon v^{(1)}(x)}dx\right\}_{\varepsilon=0} \\ &\triangleq \left\{\delta\left[\partial^2 R/\partial r\partial\omega\right]\right\}_{dir} + \left\{\delta\left[\partial^2 R/\partial r\partial\omega\right]\right\}_{ind},\end{aligned} \tag{156}$$

where:

$$\left\{\delta\left[\partial^2 R/\partial r\partial\omega\right]\right\}_{dir} \triangleq (\delta\omega)\left\{-\int_{\lambda}^{\omega}\frac{\delta'(x-\omega)}{u(x)}dx\right\}_{\alpha^0}, \tag{157}$$

$$\left\{\delta\left[\partial^2 R/\partial r\partial\lambda\right]\right\}_{ind} \triangleq \left\{-\int_{\lambda}^{\omega}\delta(x-\omega)u^{-2}(x)v^{(1)}(x)dx\right\}_{\alpha^0}. \tag{158}$$

The direct-effect term defined in Equation (157) has been evaluated at this stage by using the already available value expression of $u(x)$ from Equation (5). On the other hand, the indirect-effect term defined in Equation (158) can be evaluated only after having determined the variational function $v^{(1)}(x)$, which is the solution of the 1st-LVSS provided in Equations (10) and (11), which is computationally expensive to solve in practice for systems comprising many parameter variations. The alternative to solving repeatedly the 1st-LVSS to obtain the 1st-level variational function $v^{(1)}(x)$, which depends on the various parameter variations, is to express the indirect-effect term defined in Equation (158) in terms of the solution of a 3rd-Level Adjoint Sensitivity System (3rd-LASS), which is constructed by following the same steps as outlined in subsection 3.1.1. Thus, the definition of provided in Equation (12) is used to construct the inner product of Equation (10) with a yet undefined function $a^{(3)}(x) \in \mathsf{H}_1(\Omega_x)$ to obtain the following relation:

$$\left\{\int_{\lambda}^{\omega}a^{(3)}(x)\left[\frac{dv^{(1)}(x)}{dx} - 2qu(x)v^{(1)}(x)\right]dx\right\}_{\alpha^0} = (\delta q)\left\{\int_{\lambda}^{\omega}a^{(3)}(x)u^2(x)dx\right\}_{\alpha^0}. \tag{159}$$

Integrating by parts the left-side of Equation (159) yields the following relation:

$$\begin{aligned}&\left\{\int_\lambda^\omega a^{(3)}(x)\left[\frac{dv^{(1)}(x)}{dx}-2qu(x)v^{(1)}(x)\right]dx\right\}_{\alpha^0}\\&=a^{(3)}(\omega)v^{(3)}(\omega)-a^{(3)}(\lambda)v^{(3)}(\lambda)\\&-\left\{\int_\lambda^\omega v^{(1)}(x)\left[\frac{da^{(3)}(x)}{dx}+2qu(x)a^{(3)}(x)\right]dx\right\}_{\alpha^0}.\end{aligned} \tag{160}$$

Using in Equation (160) the boundary condition given in Equation (11) yields the following relation:

$$\begin{aligned}&-\left\{\int_\lambda^\omega v^{(1)}(x)\left[\frac{da^{(3)}(x)}{dx}+2qu(x)a^{(3)}(x)\right]dx\right\}_{\alpha^0}\\&=a^{(3)}(\lambda)\left(\delta u_{in}-qu_{in}^2\right)-a^{(3)}(\omega)v^{(1)}(\omega)\\&+\left\{\int_\lambda^\omega a^{(3)}(x)\left[\frac{dv^{(1)}(x)}{dx}-2qu(x)v^{(1)}(x)\right]dx\right\}_{\alpha^0}.\end{aligned} \tag{161}$$

The left-side of Equation (161) is required to represent the indirect-effect term defined in Equation (158) and the unknown value $v^{(1)}(\omega)$ in Equation (160) is eliminated by requiring the function $a^{(3)}(x)\in \mathsf{H}_1(\Omega_x)$ to be the solution of the following 3rd-Level Adjoint Sensitivity System (3rd-LASS):

$$\left\{\frac{da^{(3)}(x)}{dx}+2qu(x)a^{(3)}(x)\right\}_{\alpha^0}=-\left\{\delta(x-\omega)u^{-2}(x)\right\}_{\alpha^0};\ x\in\Omega_x; \tag{162}$$

$$a^{(3)}(x)=0,\ \text{at}\ x=\omega. \tag{163}$$

Using Equations (162), (163), (161), and (159) in Equation (158) yields the following alternative expression for the indirect-effect term:

$$\left\{\delta\left[\partial^2 R/\partial r\partial\lambda\right]\right\}_{ind}=a^{(3)}(\lambda)\left[(\delta u_{in})-qu_{in}^2(\delta\lambda)\right]+(\delta q)\left\{\int_\lambda^\omega a^{(3)}(x)u^2(x)dx\right\}_{\alpha^0}, \tag{164}$$

Adding the expressions for the indirect-effect and direct-effect terms obtained in Equations (164) and (157), respectively, and identifying the expressions that multiply the respective parameter variations, as indicated in Equation (156), yields the following expressions for the third-order response sensitivities which stem from $\partial^2 R/\partial r\partial\omega$:

$$\frac{\partial^3 R}{\partial q\partial r\partial\omega}=\int_\lambda^\omega a^{(3)}(x)u^2(x)dx, \tag{165}$$

$$\frac{\partial^3 R}{\partial u_{in}\partial r\partial\omega}=a^{(3)}(\lambda), \tag{166}$$

$$\frac{\partial^3 R}{\partial\lambda\partial r\partial\omega}=-qu_{in}^2a^{(3)}(\lambda), \tag{167}$$

$$\frac{\partial^3 R}{\partial\omega\partial r\partial\omega}=-q, \tag{168}$$

$$\frac{\partial^3 R}{\partial r \partial r \partial \omega} = 0 . \tag{169}$$

The expressions of the sensitivities provided in Equations (165)-(168) are to be evaluated at the nominal values of the respective parameters and state functions but the respective indication $\{\ \}_{\boldsymbol{\alpha}^0}$ has been omitted, for simplicity. These expressions can be evaluated after solving the 3rd-LASS to obtain the 3rd-level adjoint sensitivity function $a^{(3)}(x)$.

Solving 3rd-LASS by the standard integrating-factor method yields the following expression for the 3rd-level adjoint sensitivity function $a^{(3)}(x)$:

$$a^{(3)}(x) = -u^{-2}(x) H(x-\omega) . \tag{170}$$

Inserting the result obtained in Equation (170) into in Equations (165)-(167) and evaluating the respective expressions yields the following closed-form results for the respective sensitivities:

$$\frac{\partial^3 R}{\partial q \partial r \partial \omega} = \lambda - \omega , \tag{171}$$

$$\frac{\partial^3 R}{\partial u_{in} \partial r \partial \omega} = -u_{in}^{-2} , \tag{172}$$

$$\frac{\partial^3 R}{\partial \lambda \partial r \partial \omega} = q . \tag{173}$$

4.2. Third-Order Sensitivities Stemming from 2nd-Order Sensitivities Involving Two Components of the State Functions

The 2nd-order sensitivities $\partial^2 R / \partial q \partial r$ and $\partial^2 R / \partial u_{in} \partial r$ depend only on the functions $a^{(2)}(1;1;x)$ and $u(x)$. Similarly, the 2nd-order sensitivities $\partial^2 R / \partial \omega \partial u_{in}$ and $\partial^2 R / \partial r \partial u_{in}$ depend only on the functions $a^{(2)}(2;3;x)$ and $u(x)$. Furthermore, the 2nd-order sensitivities $\partial^2 R / \partial \omega \partial \lambda$ and $\partial^2 R / \partial r \partial \lambda$ depend only on the functions $a^{(2)}(2;4;x)$ and $u(x)$. Finally, the 2nd-order sensitivities $\partial^2 R / \partial \omega \partial q$ and $\partial^2 R / \partial r \partial q$ depend only on the functions $a^{(2)}(2;5;x)$ and $u(x)$. Consequently, the 3rd-order sensitivities that stem from these 2nd-order sensitivities can be expressed in terms of a 3rd-level adjoint sensitivity function which will comprise only two components, as will be illustrated by determining the 3rd-order sensitivities that stem from $\partial^2 R / \partial r \partial \lambda$. These 3rd-order sensitivities are obtained from the G-differential of Equation (117), which has, by definition, the following expression:

$$\begin{aligned} \delta \left\{ \frac{\partial^2 R}{\partial r \partial \lambda} \right\} &\triangleq \frac{\partial^3 R}{\partial q \partial r \partial \lambda} \delta q + \frac{\partial^3 R}{\partial u_{in} \partial r \partial \lambda} \delta u_{in} \\ &+ \frac{\partial^3 R}{\partial \lambda \partial r \partial \lambda} \delta \lambda + \frac{\partial^3 R}{\partial \omega \partial r \partial \lambda} \delta \omega + \frac{\partial^3 R}{\partial r \partial r \partial \lambda} \delta r \\ &\triangleq -\left\{ \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \left[\frac{1}{u_{in}^0 + \varepsilon \delta u_{in}} \right] \right\}_{\varepsilon = 0} \end{aligned}$$

$$+\left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega}\left[a^{(2),0}(2;4;x)+\varepsilon\delta a^{(2)}(2;4;x)\right]\left[u^0(x)+\varepsilon v^{(1)}(x)\right]^{-2}\mathrm{d}x\right\}_{\varepsilon=0} \triangleq \left\{\delta\left[\partial^2 R/\partial r\partial\lambda\right]\right\}_{dir}+\left\{\delta\left[\partial^2 R/\partial r\partial\lambda\right]\right\}_{ind}, \tag{174}$$

where:

$$\begin{aligned}&\left\{\delta\left[\partial^2 R/\partial r\partial\lambda\right]\right\}_{dir}\\ &\triangleq(\delta u_{in})\left\{(u_{in})^{-2}\right\}_{\boldsymbol{\alpha}^0}+(\delta\omega)\left\{\left[a^{(2)}(2;4;\omega)u^{-2}(\omega)\right]\right\}_{\boldsymbol{\alpha}^0}\\ &-(\delta\lambda)\left\{\left[a^{(2)}(2;4;\lambda)u^{-2}(\lambda)\right]\right\}_{\boldsymbol{\alpha}^0}\\ &=(\delta u_{in})\left\{(u_{in})^{-2}\right\}_{\boldsymbol{\alpha}^0}+(\delta\omega)q-(\delta\lambda)q,\end{aligned} \tag{175}$$

$$\begin{aligned}&\left\{\delta\left[\partial^2 R/\partial r\partial\lambda\right]\right\}_{ind}\\ &\triangleq\left\{\int_\lambda^\omega \delta a^{(2)}(2;4;x)u^{-2}(x)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}-2\left\{\int_\lambda^\omega a^{(2)}(2;4;x)u^{-3}(x)v^{(1)}(x)\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}.\end{aligned} \tag{176}$$

The direct-effect term defined in Equation (175) has been evaluated at this stage by using the already available values of the 2nd-level adjoint sensitivity function $a^{(2)}(2;4;x)$, cf. Equation (119), and $u(x)$, cf. Equation (5). On the other hand, the indirect-effect term defined in Equation (176) can be evaluated only after having determined the variational function $\delta a^{(2)}(2;4;x)$, which is the solution of the G-differentiated system of Equations (110) and (111), which has the following form:

$$\begin{aligned}&\left\{-\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(2)}(2;4;x)+2qu(x)\delta a^{(2)}(2;4;x)+2qa^{(2)}(2;4;x)v^{(1)}(x)\right\}_{\boldsymbol{\alpha}^0}\\ &=-\left\{2(\delta q)u(x)a^{(2)}(2;4;x)+(\delta q)u_{in}^2\delta(x-\lambda)+2(\delta u_{in})qu_{in}\delta(x-\lambda)\right\}_{\boldsymbol{\alpha}^0};\end{aligned} \tag{177}$$

$$\begin{aligned}&\delta a^{(2)}(2;4;\lambda)+\left\{\frac{\mathrm{d}a^{(2)}(2;4;x)}{\mathrm{d}x}\right\}_{x=\lambda}(\delta\lambda)\\ &=\delta a^{(2)}(2;4;\lambda)+(\delta\lambda)\left\{2q^2u_{in}^3\right\}_{\boldsymbol{\alpha}^0}=0,\ \text{at } x=\lambda.\end{aligned} \tag{178}$$

Equation (177) also involves the variational function $v^{(1)}(x)$, which is the solution of the 1st-LVSS comprising Equations (10) and (11). Therefore, Equations (177) and (178) are to be concatenated with the 1st-LVSS to obtain a 3rd-Level Variational Sensitivity System (3rd-LVSS) which is satisfied by a two-component 3rd-level variational function of the form $\boldsymbol{V}^{(3)}(2;x)\triangleq\left[v^{(1)}(x),\delta a^{(2)}(2;4;x)\right]^\dagger$. This 3rd-LVSS will therefore have a structure similar to the 2nd-LVSS derived in Sections 3.3-3.5, namely:

$$\left\{\boldsymbol{VM}^{(3)}(2\times 2)\boldsymbol{V}^{(3)}(2;x)\right\}_{\boldsymbol{\alpha}^0}=\left\{\boldsymbol{Q}_V^{(3)}(2;x)\right\}_{\boldsymbol{\alpha}^0},\ x\in\Omega_x, \tag{179}$$

$$\boldsymbol{B}_V^{(3)}(2;x)\triangleq\begin{pmatrix}v^{(1)}(\lambda)+(\delta\lambda)qu_{in}^2-\delta u_{in}\\ \delta a^{(2)}(2;4;\lambda)+2(\delta\lambda)q^2u_{in}^3\end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix}; \tag{180}$$

where

$$\boldsymbol{V}^{(3)}(2;x) \triangleq \begin{pmatrix} v^{(3)}(1;x) \\ v^{(3)}(2;x) \end{pmatrix} \triangleq \begin{pmatrix} v^{(1)}(x) \\ \delta a^{(2)}(2;4;x) \end{pmatrix}; \tag{181}$$

$$\boldsymbol{VM}^{(3)}(2\times 2) \triangleq \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}x} - 2qu(x) & 0 \\ 2qa^{(2)}(2;4;x) & -\frac{\mathrm{d}}{\mathrm{d}x} + 2qu(x) \end{pmatrix}; \tag{182}$$

$$\begin{gathered} \boldsymbol{Q}_V^{(3)}(2;x) \triangleq \begin{pmatrix} \boldsymbol{q}_V^{(3)}(1;x) \\ \boldsymbol{q}_V^{(3)}(2;x) \end{pmatrix}; \ \boldsymbol{q}_V^{(3)}(1;x) \triangleq (\delta q) u^2(x); \\ \boldsymbol{q}_V^{(3)}(2;x) \triangleq -2(\delta q) u(x) a^{(2)}(2;4;x) - (\delta q) u_{in}^2 \delta(x-\lambda) - 2(\delta u_{in}) q u_{in} \delta(x-\lambda); \end{gathered} \tag{183}$$

The need for solving repeatedly the 3rd-LVSS to obtain the 3rd-level variational function $\boldsymbol{V}^{(3)}(2;x)$ for every parameter variations is circumvented by expressing the indirect-effect term defined in Equation (176) in terms of the solution of a 3rd-Level Adjoint Sensitivity System (3rd-LASS), which is constructed specifically for the indirect-effect term defined in Equation (176), by applying the principles of the 5th-CASAM-N, as follows:

1) Using the definition of provided in Equation (76), construct the inner product of Equation (179) with a yet undefined function $\boldsymbol{F}^{(3)}(2;x) \triangleq \left[f^{(3)}(1;x), f^{(3)}(2;x) \right]^{\dagger} \in \mathsf{H}_2(\Omega_x)$ to obtain the following relation:

$$\begin{aligned} &\left\{ \left\langle \boldsymbol{F}^{(3)}(2;x), \boldsymbol{VM}^{(3)}(2\times 2) \boldsymbol{V}^{(3)}(2;x) \right\rangle_2 \right\}_{\boldsymbol{\alpha}^0} \\ &= \left\{ \left\langle \boldsymbol{F}^{(3)}(2;x), \boldsymbol{Q}_V^{(3)}(2;x) \right\rangle_2 \right\}_{\boldsymbol{\alpha}^0}, \ x \in \Omega_x, \end{aligned} \tag{184}$$

which in component form reads as follows:

$$\begin{aligned} &\left\{ \int_\lambda^\omega f^{(3)}(1;x) \left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x) v^{(1)}(x) \right] \mathrm{d}x \right\}_{\boldsymbol{\alpha}^0} + \left\{ \int_\lambda^\omega f^{(3)}(2;x) \right. \\ &\left. \times \left[-\frac{\mathrm{d}}{\mathrm{d}x} \delta a^{(2)}(2;4;x) + 2qu(x) \delta a^{(2)}(2;4;x) + 2qa^{(2)}(2;4;x) v^{(1)}(x) \right] \mathrm{d}x \right\}_{\boldsymbol{\alpha}^0} \\ &= (\delta q) \left\{ \int_\lambda^\omega f^{(3)}(1;x) u^2(x) \mathrm{d}x \right\}_{\boldsymbol{\alpha}^0} - \left\{ \int_\lambda^\omega f^{(3)}(2;x) \left[2(\delta q) u(x) a^{(2)}(2;4;x) \right. \right. \\ &\left. \left. + (\delta q) u_{in}^2 \delta(x-\lambda) + 2(\delta u_{in}) q u_{in} \delta(x-\lambda) \right] \mathrm{d}x \right\}_{\boldsymbol{\alpha}^0}; \end{aligned} \tag{185}$$

2) Integrate by parts the left-side of Equation (185) to obtain the following relation:

$$\begin{aligned} &\left\{ \int_\lambda^\omega f^{(3)}(1;x) \left[\frac{\mathrm{d}v^{(1)}(x)}{\mathrm{d}x} - 2qu(x) v^{(1)}(x) \right] \mathrm{d}x \right\}_{\boldsymbol{\alpha}^0} + \left\{ \int_\lambda^\omega f^{(3)}(2;x) \right. \\ &\left. \times \left[-\frac{\mathrm{d}}{\mathrm{d}x} \delta a^{(2)}(2;4;x) + 2qu(x) \delta a^{(2)}(2;4;x) + 2qa^{(2)}(2;4;x) v^{(1)}(x) \right] \mathrm{d}x \right\}_{\boldsymbol{\alpha}^0} \\ &= f^{(3)}(1;\omega) v^{(1)}(\omega) - f^{(3)}(1;\lambda) v^{(1)}(\lambda) \\ &+ \left\{ \int_\lambda^\omega v^{(1)}(x) \left[-\frac{\mathrm{d}f^{(3)}(1;x)}{\mathrm{d}x} - 2qu(x) f^{(3)}(1;x) \right] \mathrm{d}x \right\}_{\boldsymbol{\alpha}^0} \end{aligned}$$

$$
\begin{aligned}
&-f^{(3)}(2;\omega)\delta a^{(2)}(2;4;\omega)+f^{(3)}(2;\lambda)\delta a^{(2)}(2;4;\lambda)\\
&+\left\{\int_{\lambda}^{\omega}\delta a^{(2)}(2;4;x)\left[\frac{d}{dx}f^{(3)}(2;x)+2qu(x)f^{(3)}(2;x)\right]dx\right\}_{\alpha^0}\\
&+\left\{2q\int_{\lambda}^{\omega}v^{(1)}(x)a^{(2)}(2;4;x)f^{(3)}(2;x)dx\right\}_{\alpha^0}.
\end{aligned}
\tag{186}
$$

3) Use in Equation (186) the boundary condition given in Equation (180) to obtain the following relation:

$$
\begin{aligned}
&\left\{\int_{\lambda}^{\omega}f^{(3)}(1;x)\left[\frac{dv^{(1)}(x)}{dx}-2qu(x)v^{(1)}(x)\right]dx\right\}_{\alpha^0}+\left\{\int_{\lambda}^{\omega}f^{(3)}(2;x)\right.\\
&\left.\times\left[-\frac{d}{dx}\delta a^{(2)}(2;4;x)+2qu(x)\delta a^{(2)}(2;4;x)+2qa^{(2)}(2;4;x)v^{(1)}(x)\right]dx\right\}_{\alpha^0}\\
&=f^{(3)}(1;\omega)v^{(1)}(\omega)-f^{(3)}(1;\lambda)\left[\delta u_{in}-(\delta\lambda)qu_{in}^2\right]\\
&+\left\{\int_{\lambda}^{\omega}v^{(1)}(x)\left[-\frac{df^{(3)}(1;x)}{dx}-2qu(x)f^{(3)}(1;x)\right]dx\right\}_{\alpha^0}\\
&-f^{(3)}(2;\omega)\delta a^{(2)}(2;4;\omega)-2(\delta\lambda)q^2u_{in}^3a^{(3)}(2;\lambda)\\
&+\left\{\int_{\lambda}^{\omega}\delta a^{(2)}(2;4;x)\left[\frac{d}{dx}f^{(3)}(2;x)+2qu(x)f^{(3)}(2;x)\right]dx\right\}_{\alpha^0}\\
&+\left\{2q\int_{\lambda}^{\omega}v^{(1)}(x)a^{(2)}(2;4;x)f^{(3)}(2;x)dx\right\}_{\alpha^0}.
\end{aligned}
\tag{187}
$$

4) Require the right-side of Equation (187) to represent the indirect-effect term defined in Equation (176) and eliminate the unknown values of the components of $\boldsymbol{V}^{(3)}(2;x)\triangleq\left[v^{(1)}(x),\delta a^{(2)}(2;4;x)\right]^\dagger$ in Equation (187) by requiring the function $\boldsymbol{F}^{(3)}(2;x)\triangleq\left[f^{(3)}(1;x),f^{(3)}(2;x)\right]^\dagger$ to be the solution of the following 3rd-Level Adjoint Sensitivity System (3rd-LASS):

$$
\begin{aligned}
&\left\{\frac{df^{(3)}(1;x)}{dx}+2qu(x)f^{(3)}(1;x)\right\}_{\alpha^0}\\
&=2\left\{a^{(2)}(2;4;x)\left[u^{-3}(x)+qf^{(3)}(2;x)\right]\right\}_{\alpha^0}=\frac{2q}{u_{in}}\left[1+qu_{in}(\lambda-\omega)\right];
\end{aligned}
\tag{188}
$$

$$
\left\{f^{(3)}(1;\omega)\right\}_{\alpha^0}=0,\ \text{at}\ x=\omega;
\tag{189}
$$

$$
\left\{\frac{d}{dx}f^{(3)}(2;x)+2qu(x)f^{(3)}(2;x)\right\}_{\alpha^0}=\left\{u^{-2}(x)\right\}_{\alpha^0};\ x\in\Omega_x;
\tag{190}
$$

$$
\left\{f^{(3)}(2;\omega)\right\}_{\alpha^0}=0,\ \text{at}\ x=\omega.
\tag{191}
$$

5) Use Equations (188)-(191) together with Equations (187) and (185) in Equation (176) to obtain the following alternative expression for the indirect-effect term:

$$
\left\{\delta\left[\partial^2R/\partial r\partial\lambda\right]\right\}_{ind}=f^{(3)}(1;\lambda)\left[\delta u_{in}-(\delta\lambda)qu_{in}^2\right]+2(\delta\lambda)q^2u_{in}^3f^{(3)}(2;\lambda)
$$

$$+(\delta q)\left\{\int_{\lambda}^{\omega} f^{(3)}(1;x)u^{2}(x)\mathrm{d}x\right\}_{\alpha^0} -\left\{\int_{\lambda}^{\omega} f^{(3)}(2;x)\left[2(\delta q)u(x)a^{(2)}(2;4;x)\right.\right.$$
$$\left.\left.+(\delta q)u_{in}^{2}\delta(x-\lambda)+2(\delta u_{in})qu_{in}\delta(x-\lambda)\right]\mathrm{d}x\right\}_{\alpha^0}. \tag{192}$$

6) Adding the expressions for the indirect-effect and direct-effect terms obtained in Equations (192) and (175), respectively, and identifying the expressions that multiply the respective parameter variations, as indicated in Equation (174), yields the following expressions for the first-order response sensitivities with respect to the model parameters:

$$\frac{\partial^3 R}{\partial q \partial r \partial \lambda}=\int_{\lambda}^{\omega}\left\{f^{(3)}(1;x)u^{2}(x)-f^{(3)}(2;x)\left[2u(x)a^{(2)}(2;4;x)+u_{in}^{2}\delta(x-\lambda)\right]\right\}\mathrm{d}x\,; \tag{193}$$

$$\frac{\partial^3 R}{\partial u_{in} \partial r \partial \lambda}=f^{(3)}(1;\lambda)-2qu_{in}\int_{\lambda}^{\omega} f^{(3)}(2;x)\delta(x-\lambda)\mathrm{d}x+(u_{in})^{-2}\,; \tag{194}$$

$$\frac{\partial^3 R}{\partial \lambda \partial r \partial \lambda}=-qu_{in}^{2}f^{(3)}(1;\lambda)+2q^{2}u_{in}^{3}f^{(3)}(2;\lambda)-q\,; \tag{195}$$

$$\frac{\partial^3 R}{\partial \omega \partial r \partial \lambda}=q\,; \tag{196}$$

$$\frac{\partial^3 R}{\partial r \partial r \partial \lambda}=0\,. \tag{197}$$

The expressions of the sensitivities provided in Equations (193)-(196) are to be evaluated at the nominal values of the respective parameters and state functions. The expressions of the sensitivities stemming from the indirect-effect term can be evaluated after solving the 3rd-LASS comprising Equations (188)-(191) in order to obtain the 3rd-level adjoint sensitivity function $\boldsymbol{F}^{(3)}(2;x)\triangleq\left[f^{(3)}(1;x),f^{(3)}(2;x)\right]^{\dagger}$. The 3rd-LASS is independent of parameter variations, so it only needs to be solved once, to obtain the following expressions:

$$f^{(3)}(1;x)=\frac{2q(x-\omega)}{u(x)}\,, \tag{198}$$

$$f^{(3)}(2;x)=\frac{(x-\omega)}{u^{2}(x)}\,. \tag{199}$$

Inserting into Equations (193)-(195) the expressions obtained in Equations (198) and (199) yields the following closed form expressions:

$$\frac{\partial^3 R}{\partial q \partial r \partial \lambda}=\omega-\lambda\,; \tag{200}$$

$$\frac{\partial^3 R}{\partial u_{in} \partial r \partial \lambda}=(u_{in})^{-2}\,; \tag{201}$$

$$\frac{\partial^3 R}{\partial \lambda \partial r \partial \lambda}=-q\,. \tag{202}$$

4.3. Third-Order Sensitivities Stemming from 2nd-Order Sensitivities Involving Four Components of the State Functions

The 2nd-order sensitivities mentioned in Sections 4.1 and 4.2, above, involve one or two components of the original or adjoint sensitivity functions. The expressions of the remaining 2nd-order sensitivities involve as many as four distinct functions, as follows: 1) the two components of respective 2nd-level adjoint sensitivity functions; 2) the one-component 1st-level adjoint sensitivity function $a^{(1)}(x)$; and 3) the original forward function $u(x)$. Consequently, the 3rd-order sensitivities that stem from such 2nd-order sensitivities will need to be expressed in terms of a 3rd-level adjoint sensitivity function which will comprise four components, as will be illustrated in this Section by determining the 3rd-order sensitivities stemming from of a typical such 2nd-order sensitivity, namely the unmixed 2nd-order sensitivity $\partial^2 R/\partial u_{in}\partial u_{in}$. Notably, there is a single expression for the unmixed 2nd-order sensitivity $\partial^2 R/\partial u_{in}\partial u_{in}$, namely the expression provided in Equation (87), in contradistinction to the expressions for the unmixed 2nd-order sensitivities, for which two alternative expressions are available, as discussed and illustrated in Section 3. This, the expression provided in Equation (87) must be used as the starting point for computing the higher-order unmixed sensitivities of the response $R[u(x);\boldsymbol{\alpha}]$ with respect to the parameter u_{in}.

In preparation for determining the expressions of the 3rd-order sensitivities which stem from $\partial^2 R/\partial u_{in}\partial u_{in}$, Equation (87) is written in the following integral form:

$$\frac{\partial^2 R}{\partial u_{in}\partial u_{in}} = \int_{\lambda}^{\omega} a^{(2)}(1;3;x)\,\delta(x-\lambda)\,\mathrm{d}x. \tag{203}$$

Performing the G-differentiation of the expression provided in Equation (203) yields the following relation:

$$\begin{aligned}
\delta\left\{\frac{\partial^2 R}{\partial u_{in}\partial u_{in}}\right\} &\triangleq \frac{\partial^3 R}{\partial q\partial u_{in}\partial u_{in}}\delta q + \frac{\partial^3 R}{\partial u_{in}\partial u_{in}\partial u_{in}}\delta u_{in} + \frac{\partial^3 R}{\partial \lambda\partial u_{in}\partial u_{in}}\delta\lambda \\
&+ \frac{\partial^3 R}{\partial \omega\partial u_{in}\partial u_{in}}\delta\omega + \frac{\partial^3 R}{\partial r\partial u_{in}\partial u_{in}}\delta r \\
&\triangleq \left\{\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\lambda^0+\varepsilon\delta\lambda}^{\omega^0+\varepsilon\delta\omega}\left[a^{(2),0}(1;3;x)+\varepsilon\delta a^{(2)}(1;3;x)\right]\delta\left(x-\lambda^0-\varepsilon\delta\lambda\right)\mathrm{d}x\right\}_{\varepsilon=0} \\
&\triangleq \left\{\delta\left[\partial^2 R/\partial u_{in}\partial u_{in}\right]\right\}_{dir} + \left\{\delta\left[\partial^2 R/\partial u_{in}\partial u_{in}\right]\right\}_{ind}
\end{aligned} \tag{204}$$

where:

$$\begin{aligned}
&\left\{\delta\left[\partial^2 R/\partial u_{in}\partial u_{in}\right]\right\}_{dir} \\
&\triangleq -(\delta\lambda)\left\{a^{(2)}(1;3;\lambda)\right\}_{\boldsymbol{\alpha}^0} - (\delta\lambda)\int_{\lambda}^{\omega} a^{(2)}(1;3;x)\,\delta'(x-\lambda)\,\mathrm{d}x \\
&= (\delta\lambda)\left\{\frac{2r}{u_{in}^3}(\lambda-\omega)\right\}_{\boldsymbol{\alpha}^0} + (\delta\lambda)\left[-\frac{2r}{u_{in}^3}+\frac{2r}{u_{in}^2}(\lambda-\omega)q\right],
\end{aligned} \tag{205}$$

$$\left\{\delta\left[\partial^2 R/\partial u_{in}\partial u_{in}\right]\right\}_{ind} \triangleq \left\{\int_{\lambda}^{\omega}\delta a^{(2)}(1;3;x)\delta(x-\lambda)\,\mathrm{d}x\right\}_{\alpha^0}. \tag{206}$$

The direct-effect term defined in Equation (205) has been evaluated at this stage since the values of the 2nd-level adjoint sensitivity function $a^{(2)}(1;3;x)$ is already available. However, the indirect-effect term defined in Equation (206) depends on the variational function $\delta a^{(2)}(1;3;x)$, which is the solution of the system of equations obtained by G-differentiating the 2nd-LASS provided in Equations (81)-(84), namely:

$$\begin{aligned}&\left\{\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(2)}(1;3;x)+2qu(x)\delta a^{(2)}(1;3;x)-2\left[qa^{(1)}(x)+ru^{-3}(x)\right]\delta a^{(2)}(2;3;x)\right.\\&\left.+\left[2qa^{(2)}(1;3;x)+6a^{(2)}(2;3;x)ru^{-4}(x)\right]v^{(1)}(x)-2qa^{(2)}(2;3;x)\delta a^{(1)}(x)\right\}_{\alpha^0}\\&=\left\{-2(\delta q)a^{(2)}(1;3;x)u(x)+2a^{(2)}(2;3;x)\left[(\delta q)a^{(1)}(x)+(\delta r)u^{-3}(x)\right]\right\}_{\alpha^0};\end{aligned} \tag{207}$$

$$\delta a^{(2)}(1;3;\omega)+\left\{\frac{\mathrm{d}a^{(2)}(1;3;x)}{\mathrm{d}x}\right\}_{x=\omega}(\delta\omega)=0,\ \text{at}\ x=\omega; \tag{208}$$

$$\begin{aligned}&\left\{-\frac{\mathrm{d}}{\mathrm{d}x}\delta a^{(2)}(2;3;x)+2qu(x)\delta a^{(2)}(2;3;x)+2qa^{(2)}(2;3;x)v^{(1)}(x)\right\}_{\alpha^0}\\&=-\left\{2(\delta q)u(x)a^{(2)}(2;3;x)+(\delta\lambda)\delta'(x-\lambda)\right\}_{\alpha^0};\ x\in\Omega_x;\end{aligned} \tag{209}$$

$$\delta a^{(2)}(2;3;\lambda)+\left\{\frac{\mathrm{d}a^{(2)}(2;3;x)}{\mathrm{d}x}\right\}_{x=\lambda}(\delta\lambda)=0,\ \text{at}\ x=\lambda. \tag{210}$$

Evidently, Equations (207)-(210) involve not only the vector-valued function $\delta\boldsymbol{A}^{(2)}(2;3;x)\triangleq\left[\delta a^{(2)}(1;3;x),\delta a^{(2)}(2;3;x)\right]^{\dagger}$ but also involve the variational vector function $\boldsymbol{V}^{(2)}(x)\triangleq\left[v^{(1)}(x),\delta a^{(1)}(x)\right]^{\dagger}$, which is the solution of the 2nd-LVSS. Therefore, Equations (207)-(210) must be concatenated with the 2nd-LVSS, namely Equations (71) and (72), to obtain the following 3rd-Level Variational Sensitivity System (3rd-LVSS) to be satisfied by the four-component 3rd-level variational function

$$\begin{aligned}&\boldsymbol{V}^{(3)}(4;\boldsymbol{x})\triangleq\left[\boldsymbol{V}^{(2)}(2;x),\delta\boldsymbol{A}^{(2)}(2;3;x)\right]^{\dagger}\\&\equiv\left[v^{(1)}(x),\delta a^{(1)}(x),\delta a^{(2)}(1;3;x),\delta a^{(2)}(2;3;x)\right]^{\dagger}\end{aligned}:$$

$$\left\{\boldsymbol{VM}^{(3)}(4\times4)\boldsymbol{V}^{(3)}(4;x)\right\}_{\alpha^0}=\left\{\boldsymbol{Q}_V^{(3)}\right\}_{\alpha^0},\ x\in\Omega_x, \tag{211}$$

$$\boldsymbol{B}_V^{(3)}=[0,0,0,0]^{\dagger},\ x\in\partial\Omega_x, \tag{212}$$

where:

$$\boldsymbol{VM}^{(3)}(4\times4)\triangleq\begin{pmatrix}\boldsymbol{VM}^{(2)}(2\times2) & \boldsymbol{0}[2\times2]\\ \boldsymbol{VM}_{21}^{(3)}(2\times2) & \boldsymbol{VM}_{22}^{(3)}(2\times2)\end{pmatrix};\ \boldsymbol{0}[2\times2]\triangleq\begin{pmatrix}0&0\\0&0\end{pmatrix}; \tag{213}$$

$$\boldsymbol{VM}_{21}^{(3)}(2\times2)\triangleq\begin{pmatrix}2qa^{(2)}(1;3;x)+6a^{(2)}(2;3;x)ru^{-4}(x) & -2qa^{(2)}(2;3;x)\\ 2qa^{(2)}(2;3;x) & 0\end{pmatrix}; \tag{214}$$

$$\boldsymbol{VM}_{22}^{(3)}(2\times 2)\triangleq\begin{pmatrix}\frac{\mathrm{d}}{\mathrm{d}x}+2qu(x) & -2\left[qa^{(1)}(x)+ru^{-3}(x)\right]\\ 0 & -\frac{\mathrm{d}}{\mathrm{d}x}+2qu(x)\end{pmatrix};\tag{215}$$

$$\boldsymbol{Q}_{V}^{(3)}(4;x)\triangleq\begin{pmatrix}\boldsymbol{Q}_{V}^{(2)}(2;x)\\ \boldsymbol{Q}_{2}^{(3)}(2;x)\end{pmatrix};$$

$$\boldsymbol{Q}_{2}^{(3)}(2;x)\triangleq\begin{pmatrix}-2(\delta q)a^{(2)}(1;3;x)u(x)+2a^{(2)}(2;3;x)\left[(\delta q)a^{(1)}(x)+(\delta r)u^{-3}(x)\right]\\ -2(\delta q)u(x)a^{(2)}(2;3;x)-(\delta\lambda)\delta'(x-\lambda)\end{pmatrix};\tag{216}$$

The need for solving repeatedly the 3rd-LVSS to obtain the 3rd-level variational function $\boldsymbol{V}^{(3)}(4;x)$ for every parameter variations is circumvented by recasting the indirect-effect term defined in Equation (206) using the solution of a 3rd-Level Adjoint Sensitivity System (3rd-LASS), which will be independent of parameter variations and is constructed specifically for this indirect-effect term. The requisite 3rd-LASS is constructed by applying the principles of the 5th-CASAM-N, as follows:

1) Consider that the function $\boldsymbol{V}^{(3)}(4;x)\in\mathsf{H}_{3}(\Omega_{x})$ is an element in a Hilbert space $\mathsf{H}_{3}(\Omega_{x})$ endowed with an inner product between two elements $\boldsymbol{\Psi}^{(3)}(4;x)\triangleq\left[\psi^{(3)}(1;x),\psi^{(3)}(2;x),\psi^{(3)}(3;x),\psi^{(3)}(4;x)\right]\in\mathsf{H}_{3}(\Omega_{x})$ and $\boldsymbol{\Phi}^{(3)}(4;x)\triangleq\left[\varphi^{(3)}(1;x),\varphi^{(3)}(2;x),\varphi^{(3)}(3;x),\varphi^{(3)}(4;x)\right]\in\mathsf{H}_{3}(\Omega_{x})$ defined as follows:

$$\begin{aligned}&\left\langle\boldsymbol{\Psi}^{(3)}(4;x),\boldsymbol{\Phi}^{(3)}(4;x)\right\rangle_{3}\triangleq\sum_{i=1}^{4}\left\langle\psi^{(3)}(i;x),\varphi^{(3)}(i;x)\right\rangle_{1}\\&\triangleq\left\{\sum_{i=1}^{4}\int_{\lambda}^{\omega}\psi^{(3)}(i;x),\varphi^{(3)}(i;x)\,\mathrm{d}x\right\}_{\boldsymbol{\alpha}^{0}}.\end{aligned}\tag{217}$$

2) Using the definition of provided in Equation (217), construct the inner product of Equation (211) with a yet undefined function $\boldsymbol{A}^{(3)}(4;x)\triangleq\left[a^{(3)}(1;x),a^{(3)}(2;x),a^{(3)}(3;x),a^{(3)}(4;x)\right]\in\mathsf{H}_{3}(\Omega_{x})$ to obtain the following relation:

$$\left\{\left\langle\boldsymbol{A}^{(3)}(4;x),\boldsymbol{VM}^{(3)}(4\times 4)\boldsymbol{V}^{(3)}(4;x)\right\rangle_{2}\right\}_{\boldsymbol{\alpha}^{0}}=\left\{\left\langle\boldsymbol{A}^{(3)}(4;x),\boldsymbol{Q}_{V}^{(3)}\right\rangle_{2}\right\}_{\boldsymbol{\alpha}^{0}},\tag{218}$$

3) Integrate by parts the left-side of Equation (218) to obtain the following relation:

$$\begin{aligned}&\left\{\left\langle\boldsymbol{A}^{(3)}(4;x),\boldsymbol{VM}^{(3)}(4\times 4)\boldsymbol{V}^{(3)}(4;x)\right\rangle_{3}\right\}_{\boldsymbol{\alpha}^{0}}-\left\{\left[P^{(3)}\left(\boldsymbol{A}^{(3)};\boldsymbol{V}^{(3)};\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right)\right]_{\partial\Omega_{x}}\right\}_{\boldsymbol{\alpha}^{0}}\\&=\left\{\left\langle\boldsymbol{V}^{(3)}(4;x),\boldsymbol{AM}^{(3)}(4\times 4)\boldsymbol{A}^{(3)}(4;x)\right\rangle_{3}\right\}_{\boldsymbol{\alpha}^{0}},\end{aligned}\tag{219}$$

where

$$\boldsymbol{AM}^{(3)}(4\times 4)\triangleq\left[\boldsymbol{VM}^{(3)}(4\times 4)\right]^{*}=\begin{pmatrix}\left\{\left[\boldsymbol{VM}^{(2)}(2\times 2)\right]^{*}\right\}^{\dagger} & \left\{\left[\boldsymbol{VM}_{21}^{(3)}(2\times 2)\right]^{*}\right\}^{\dagger}\\ \boldsymbol{0}[2\times 2] & \left\{\left[\boldsymbol{VM}_{22}^{(3)}(2\times 2)\right]^{*}\right\}^{\dagger}\end{pmatrix},\tag{220}$$

$$\left[P^{(3)}\left(\boldsymbol{A}^{(3)};\boldsymbol{V}^{(3)};\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right)\right]_{\partial\Omega_x} \triangleq a^{(3)}(1;\omega)v^{(1)}(\omega)-a^{(3)}(1;\lambda)v^{(1)}(\lambda)$$
$$+a^{(3)}(2;\omega)\delta a^{(1)}(\omega)-a^{(3)}(2;\lambda)\delta a^{(1)}(\lambda)+a^{(3)}(3;\omega)\delta a^{(2)}(1;3;\omega) \quad (221)$$
$$-a^{(3)}(3;\lambda)\delta a^{(2)}(1;3;\lambda)-a^{(3)}(4;\omega)\delta a^{(2)}(2;3;\omega)+a^{(3)}(4;\lambda)\delta a^{(2)}(2;3;\lambda).$$

4) Use in Equation (221) the boundary condition given in Equations (11), (70), (208) and (210) to obtain the following relation:

$$\left[P^{(3)}\left(\boldsymbol{A}^{(3)};\boldsymbol{V}^{(3)};\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right)\right]_{\partial\Omega_x} \triangleq \left[\hat{P}^{(3)}\left(\boldsymbol{A}^{(3)};\boldsymbol{V}^{(3)};\boldsymbol{\alpha};\delta\boldsymbol{\alpha}\right)\right]_{\partial\Omega_x}$$
$$= a^{(3)}(1;\omega)v^{(1)}(\omega)-a^{(3)}(1;\lambda)\left[(\delta u_{in})-(\delta\lambda)qu_{in}^2\right]$$
$$-a^{(3)}(2;\omega)r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2(\delta\omega)-a^{(3)}(2;\lambda)\delta a^{(1)}(\lambda) \quad (222)$$
$$+a^{(3)}(3;\omega)\frac{2r}{u_{in}^3}\left[1-qu_{in}(\omega-\lambda)\right](\delta\omega)-a^{(3)}(3;\lambda)\delta a^{(2)}(1;3;\lambda)$$
$$-a^{(3)}(4;\omega)\delta a^{(2)}(2;3;\omega).$$

5) The right-side of Equation (219) is now required to represent the indirect-effect term defined in Equation (206) and the unknown values of the components of $\boldsymbol{V}^{(3)}(4;x)$ are eliminated in Equation (222) by requiring the function $\boldsymbol{A}^{(3)}(4;x)\triangleq\left[a^{(3)}(1;x),a^{(3)}(2;x),a^{(3)}(3;x),a^{(3)}(4;x)\right]$ to be the solution of the following 3rd-Level Adjoint Sensitivity System (3rd-LASS):

$$\boldsymbol{AM}^{(3)}(4\times4)\boldsymbol{A}^{(3)}(4;x)=\left[0,0,\delta(x-\lambda),0\right]^{\dagger}, \quad (223)$$

$$\left\{a^{(3)}(1;\omega)\right\}_{\boldsymbol{\alpha}^0}=0,\ \text{at } x=\omega; \quad (224)$$

$$\left\{a^{(3)}(2;\lambda)\right\}_{\boldsymbol{\alpha}^0}=0,\ \text{at } x=\lambda; \quad (225)$$

$$\left\{a^{(3)}(3;\lambda)\right\}_{\boldsymbol{\alpha}^0}=0,\ \text{at } x=\lambda; \quad (226)$$

$$\left\{a^{(3)}(4;\omega)\right\}_{\boldsymbol{\alpha}^0}=0,\ \text{at } x=\omega. \quad (227)$$

In component form, Equation (223) comprises the following equations:

$$-\frac{\mathrm{d}a^{(3)}(1;x)}{\mathrm{d}x}-2qu(x)a^{(3)}(1;x)+2a^{(3)}(2;x)\left[qa^{(1)}(x)+ru^{-3}(x)\right]$$
$$+2a^{(3)}(3;x)\left[qa^{(2)}(1;3;\omega)+3a^{(2)}(2;3;x)ru^{-4}(x)\right] \quad (228)$$
$$+2qa^{(2)}(2;3;x)a^{(3)}(4;x)=0;$$

$$-\frac{\mathrm{d}}{\mathrm{d}x}a^{(3)}(2;x)+2qu(x)a^{(3)}(2;x)-2qa^{(2)}(2;3;x)a^{(3)}(3;x)=0; \quad (229)$$

$$-\frac{\mathrm{d}}{\mathrm{d}x}a^{(3)}(3;x)+2qu(x)a^{(3)}(3;x)=\delta(x-\lambda); \quad (230)$$

$$-\frac{\mathrm{d}}{\mathrm{d}x}a^{(3)}(4;x)+2qu(x)a^{(3)}(4;x)-2a^{(3)}(3;x)\left[qa^{(1)}(x)+ru^{-3}(x)\right]=0. \quad (231)$$

6) Using Equations (223)-(227), (219) and (211) in Equation (206) yields the following alternative expression for the indirect-effect term:

$$
\begin{aligned}
&\left\{\delta\left[\partial^2 R/\partial u_{in}\partial u_{in}\right]\right\}_{ind} \\
&= a^{(3)}(1;\lambda)\left[(\delta u_{in})-(\delta\lambda)qu_{in}^2\right]+a^{(3)}(2;\omega)r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2(\delta\omega) \\
&+a^{(3)}(3;\omega)\frac{2r}{u_{in}^3}\left[1-qu_{in}(\omega-\lambda)\right](\delta\omega)+(\delta q)\left\{\int_\lambda^\omega a^{(3)}(1;x)u^2(x)\,\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \\
&+\left\{\int_\lambda^\omega a^{(3)}(2;x)\left[-2(\delta q)u(x)a^{(1)}(x)+(\delta r)u^{-2}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \\
&+2\left\{\int_\lambda^\omega a^{(3)}(3;x)a^{(2)}(2;3;x)\left[(\delta q)a^{(1)}(x)+(\delta r)u^{-3}(x)\right]\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \\
&-2(\delta q)\left\{\int_\lambda^\omega a^{(3)}(3;x)a^{(2)}(1;3;x)u(x)\,\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \\
&-2(\delta q)\left\{\int_\lambda^\omega a^{(3)}(4;x)u(x)a^{(2)}(2;3;x)\,\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0} \\
&-(\delta\lambda)\left\{\int_\lambda^\omega \delta'(x-\lambda)a^{(3)}(4;x)u(x)a^{(2)}(2;3;x)\,\mathrm{d}x\right\}_{\boldsymbol{\alpha}^0}.
\end{aligned}
\tag{232}
$$

7) Adding the expressions for the indirect-effect and direct-effect terms obtained in Equations (232) and (205), respectively, and identifying the expressions that multiply the respective parameter variations, as indicated in Equation (204), yields the following expressions for the first-order response sensitivities with respect to the model parameters:

$$
\begin{aligned}
\frac{\partial^3 R}{\partial q\partial u_{in}\partial u_{in}} &= \int_\lambda^\omega a^{(3)}(1;x)u^2(x)\,\mathrm{d}x-2\int_\lambda^\omega a^{(3)}(2;x)u(x)a^{(1)}(x)\,\mathrm{d}x \\
&+2\int_\lambda^\omega a^{(3)}(3;x)a^{(2)}(2;3;x)a^{(1)}(x)\,\mathrm{d}x-2\int_\lambda^\omega a^{(3)}(3;x)a^{(2)}(1;3;x)u(x)\,\mathrm{d}x \\
&-2\int_\lambda^\omega a^{(3)}(4;x)u(x)a^{(2)}(2;3;x)\,\mathrm{d}x;
\end{aligned}
\tag{233}
$$

$$
\frac{\partial^3 R}{\partial u_{in}\partial u_{in}\partial u_{in}} = a^{(3)}(1;\lambda); \tag{234}
$$

$$
\frac{\partial^3 R}{\partial\lambda\partial u_{in}\partial u_{in}} = -qu_{in}^2 a^{(3)}(1;\lambda)-\int_\lambda^\omega \delta'(x-\lambda)a^{(3)}(4;x)u(x)a^{(2)}(2;3;x)\,\mathrm{d}x; \tag{235}
$$

$$
\frac{\partial^3 R}{\partial\omega\partial u_{in}\partial u_{in}} = -a^{(3)}(2;\omega)r\left[q(\omega-\lambda)-\frac{1}{u_{in}}\right]^2+a^{(3)}(3;\omega)\frac{2r}{u_{in}^3}\left[1-qu_{in}(\omega-\lambda)\right]; \tag{236}
$$

$$
\frac{\partial^3 R}{\partial r\partial u_{in}\partial u_{in}} = \int_\lambda^\omega\left[a^{(3)}(2;x)u^{-2}(x)+2a^{(3)}(3;x)a^{(2)}(2;3;x)u^{-3}(x)\right]\mathrm{d}x \tag{237}
$$

The expressions of the sensitivities provided in Equations (233)-(237) are to be evaluated at the nominal values of the respective parameters and state functions but the respective indication $\{\;\}_{\boldsymbol{\alpha}^0}$ has been omitted, for simplicity. The expressions of the sensitivities stemming from the indirect-effect term can be evaluated after solving the 3rd-LASS comprising Equations (223)-(227) to obtain the 3rd-level adjoint sensitivity function $\boldsymbol{A}^{(3)}(4;x)$, the components of which are determined in the following order: 1) $a^{(3)}(3;x)$; 2) $a^{(3)}(4;x)$; 3) $a^{(3)}(2;x)$; 4) $a^{(3)}(1;x)$. It is evident that determining the components of $\boldsymbol{A}^{(3)}(4;x)$ involves a considerable amount of straightforward, albeit tedious, algebraic operations, which will not be reproduced here because they do not involve any new concepts.

4.4. Remarks on the Application of the 3rd-CASAM-N for Computing Third-Order Sensitivities

The 3rd-order sensitivities are computed by using the 2nd-order sensitivities as "model responses". For each 2nd-order sensitivity, a single computation of the corresponding 3rd-Level Adjoint Sensitivity System (3rd-LASS) enables the efficient computation of all of the 3rd-order sensitivities that stem from the 2nd-order sensitivity considered as the "model response." If the 2nd-order sensitivity involves only the original state function, the corresponding 3rd-LASS needed to compute the corresponding 3rd-order sensitivities will have the same dimensions as the original system or the 1st-LASS. If the starting 2nd-order sensitivity involves only both the original state function and the 1st-level adjoint sensitivity function, the corresponding 3rd-LASS needed to compute the corresponding 3rd-order sensitivities will have twice the dimensions of the original system or the 1st-LASS. When the starting 2nd-order sensitivity involves in its expression the original state function, the 1st-level and 2nd-level adjoint sensitivity functions, the corresponding 3rd-LASS which is solved for computing the 3rd-order sensitivities stemming from such a 2nd-order sensitivity will have four times the dimensions of the original system or the 1st-LASS. These considerations provide guidelines for prioritizing the computation of the 3rd-order sensitivities: 1) the largest 2nd-order relative sensitivities should be given priority consideration, and 2) the simplest expressions of the 2nd-order sensitivities should be used as starting points for computing the mixed 3rd-order sensitivities. Furthermore, the symmetries inherent to the 3rd-order sensitivities provide verification opportunities for assessing the computational numerical accuracy of the various adjoint sensitivity functions.

5. Computation of Fourth- and Fifth-Order Response Sensitivities

The 4th-order sensitivities are obtained by using the 3rd-order sensitivities of interest as "model responses" and computing their G-differentials by applying the 4th-CASAM-N. If the 3rd-order sensitivity under consideration involves only the original state function, the corresponding 4th-LASS needed to compute the corresponding 4th-order sensitivities will have the same dimensions as the 1st-LASS. If the starting 2nd-order sensitivity involves only both the original state function and the 1st-level adjoint sensitivity function, the corresponding 4th-LASS needed to compute the corresponding 4th-order sensitivities will have twice the dimensions of the original system or the 1st-LASS. When the starting 3rd-order sensitivity involves in its expression the original state function, the 1st-level and 2nd-level adjoint sensitivity functions, the corresponding 4th-LASS which is solved for computing the 4th-order sensitivities stemming from such a 3rd-order sensitivity will have four times the dimensions of the 1st-LASS. Finally, the starting 3rd-order sensitivity may depend on the original state function, the 1st-level, 2nd-level and 3rd-level adjoint sensitivity functions. In such a case, the corresponding 4th-LASS (to be solved for computing the 4th-order sensitivities stemming from such a 3rd-order sensitivity) will have eight times the dimensions of the 1st-LASS. These considerations provide guidelines for prioritizing the computation of the 4th-order sensitivities: 1) the largest 3rd-order relative sensitivities should be given priority consideration, and 2) the simplest expressions of the 3rd-order sensitivities should be used as starting points for computing the mixed -order sensitivities. Furthermore, the symmetries inherent to the 4th-order sensitivities provide verification opportunities for assessing the computational numerical accuracy of the various adjoint sensitivity functions.

The 5th-order sensitivities are obtained by using the 4th-order sensitivities of interest as "model responses" and computing their G-differentials by applying the 5th-CASAM-N. The dimensions of the 2nd-LASS, 3rd-LASS, and 4th-LASS which would correspond to a specific 4th-order sensitivity have the same characteristics as mentioned above. In addition, if the 4th-order sensitivity of interest depends on all of the lower-level adjoint sensitivity state functions (*i.e.*, the 4th-order sensitivity under consideration depends on the original function, 1st-, 2nd-, 3rd-, and 4th-level adjoint sensitivity functions) characteristics, then the 5th-LASS to be solved for determining the 5th-order sensitivities will have dimensions that are 16 times larger than the dimensions of the 1st-LASS. As for the computation of lower-order sensitivities, the above considerations provide guidelines for prioritizing the computation of the 5th-order sensitivities: 1) the largest 4th-order relative sensitivities should be given priority consideration, and 2) the simplest expressions of the 4th-order sensitivities should be used as starting points for computing the mixed -order sensitivities. Furthermore, the symmetries inherent to the 5th-order sensitivities provide verification opportunities for assessing the computational numerical accuracy of the various adjoint sensitivity functions.

6. Concluding Remarks

This work has illustrated the application of the recently developed [1] "Fifth-Order Comprehensive Adjoint Sensitivity Analysis Methodology for Nonlinear Systems (5th-CASAM-N)" to a simplified Bernoulli model [2] comprising a nonlinear model response, uncertain model parameters, uncertain model domain boundaries and uncertain model boundary conditions. The demonstration model selected for illustrating the application of the 5th-CASAM-N admits exact, closed form expressions for the various adjoint sensitivity functions, as well as for the model response sensitivities with respect to the uncertain model parameters, uncertain model domain boundaries and uncertain model boundary conditions. While illustrating the fundamental aspects of applying the 5th-CASAM-N, the guidelines for prioritizing the computation of sensitivities of various orders have also been outlined, indicating how the symmetries inherent if the mixed-sensitivities of various orders enable multi-faceted comparisons and mutual verifications of the various adjoint sensitivity functions, aiming at minimizing the number of large-scale computations.

The 5th-CASAM-N provides the foundation for developing a comprehensive adjoint sensitivity analysis methodology for computing efficiently and exactly model response sensitivities of arbitrarily high-order, aimed at overcoming the curse of dimensionality in sensitivity and uncertainty analysis.

Conflicts of Interest

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

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