

The First-Order Comprehensive Sensitivity Analysis Methodology (1st-CASAM) for Scalar-Valued Responses: II. Illustrative Application to a Heat Transport Benchmark Model

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Abstract

This work illustrates the application of the 1st-CASAM to a paradigm heat transport model which admits exact closed-form solutions. The closed-form expressions obtained in this work for the sensitivities of the temperature distributions within the model to the model's parameters, internal interfaces and external boundaries can be used to benchmark commercial and production software packages for simulating heat transport. The 1st-CASAM highlights the novel finding that response sensitivities to the imprecisely known domain boundaries and interfaces can arise both from the definition of the system's response as well as from the equations, interfaces and boundary conditions that characterize the model and its imprecisely known domain. By enabling, in premiere, the exact computations of sensitivities to interface and boundary parameters and conditions, the 1st-CASAM enables the quantification of the effects of manufacturing tolerances on the responses of physical and engineering systems.

Keywords

First-Order Comprehensive Adjoint Sensitivity Analysis Methodology (1st-CASAM), Response Sensitivities for Coupled Systems Involving Imprecisely Known Interfaces, Parameters, And Boundaries, Coupled Heat Conduction and Convection

1. Introduction

An accompanying work [1] has presented the mathematical framework of the first-order comprehensive adjoint sensitivity analysis methodology (1st-CASAM) for computing efficiently, exactly and exhaustively, the first-order response sensitivities to imprecisely known parameters that describe the system, the imprecisely known physical interfaces between systems, and the systems' imprecisely known external boundaries for coupled nonlinear physical systems. This work presents an illustrative application of the 1st-CASAM to a benchmark model [2] [3] [4] that models coupled heat conduction and convection in a physical system comprising an electrically heated rod surrounded by a coolant which simulates the geometry of an advanced ("Generation-IV") nuclear reactor [5]. This benchmark model [2] [3] [4] admits exact closed-form solutions for the sensitivities of the temperature distribution in the coupled rod/coolant system which can be used to benchmark thermal-hydraulics production codes. Notably, this model [2] [3] [4] was used to verify the numerical results produced by the FLUENT Adjoint Solver [6], showing, in particular, that the current version of the FLUENT Adjoint Solver cannot compute sensitivities for the temperature distribution within the solid rod.

This work is structured as follows. Section 2 presents the mathematical modeling of the heat conduction process in the electrically heated rod coupled to the convective heat transport in the coolant surrounding the heated rod. This mathematical model admits exact closed-form solutions for the temperature distributions, which can be used to benchmark thermal-hydraulics production codes. Section 3 presents the application of the 1st-CASAM to the heat conduction/convection model to obtain the exact expressions of the sensitivities of the temperature distribution in the coupled rod/coolant system to the imprecisely known model, internal interface and external boundary parameters. The exact closed-form expressions obtained in this work for the respective sensitivities can also be used to benchmark thermal-hydraulics production codes. Section 4 offers concluding remarks. Ongoing research will generalize the methodology presented in this work, aiming at computing exactly and efficiently higher-order response sensitivities for coupled systems involving imprecisely known interfaces, parameters, and boundaries. As is well known [7], the availability of response sensitivities to imprecisely known parameters, interfaces and boundaries is essential for a variety of subsequent uses, including uncertainty quantification, optimization, data assimilation, model calibration and validation, and reduction of uncertainties in predicted model results.

2. Coupled Heat Conduction and Convection Benchmark: Mathematical Modeling

The benchmark model [2] [3] [4] presented in this Section simulates the steady-state heat conduction in an electrically heated rod coupled through convection heat transfer to coolant surrounding the heated rod. This benchmark [2] [3]

[4] system simulates a fuel rod in an operating nuclear reactor and admits exact closed-form solutions for the sensitivities of the temperature distribution in the coupled rod/coolant system which can be used to benchmark thermal-hydraulics production codes. In particular, this benchmark [2] [3] [4] was used to verify the numerical results produced by the FLUENT Adjoint Solver [6] highlighting some strengths and important weaknesses of the “FLUENT Adjoint Solver” software.

The geometrical characteristics of the electrically heated rod are: radius a and length (height) ℓ . The rod is heated by a heat source of the form $q \cos(\pi z/\ell)$, where $q[\text{W} \cdot \text{m}^{-3}]$ denotes a constant volumetric source and z denotes the coordinate along the rod’s axial (customarily, the vertical) direction. This heat source simulates the axial heat distribution in a nuclear reactor. The heated rod transfers heat by convection to the surrounding coolant that flows along the rod’s vertical direction. The rod’s conductivity, $k[\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}]$, is considered to be a temperature-independent constant. The rod’s surface is cooled by forced convection to a surrounding liquid flowing along the rod’s length, from the rod’s lower end, taken to be located at $z = -\ell/2$, towards the rod’s upper end, located at $z = \ell/2$. The heat transfer coefficient, $h[\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}]$, from the rod’s surface to the coolant is considered to be constant. For this benchmark, the rod’s length is typically two orders of magnitude larger than its diameter, so the heat conduction process in the rod’s axial direction can be neglected by comparison to the heat conduction in the rod’s radial direction. Under these conditions, the steady-state temperature distributions, $T(r, z)$ and $T_{fl}(z)$, within the heated rod and coolant (fluid), respectively, are obtained from the following energy conservation balances:

$$\frac{k}{r} \frac{\partial}{\partial r} \left[r \frac{\partial T(r, z)}{\partial r} \right] = -q \cos \frac{\pi z}{\ell}, \quad 0 \leq r < a, \quad -\frac{\ell}{2} \leq z \leq \frac{\ell}{2}, \quad (1)$$

$$\frac{\partial T(r, z)}{\partial r} = 0, \quad \text{at } r = 0, \quad (2)$$

$$-k \frac{\partial T(r, z)}{\partial r} = h [T(r, z) - T_{fl}(z)], \quad \text{at } r = a, \quad (3)$$

$$\frac{dT_{fl}(z)}{dz} = \frac{\pi a^2 q}{W c_p} \cos \frac{\pi z}{\ell}, \quad -\frac{\ell}{2} \leq z \leq \frac{\ell}{2}, \quad (4)$$

$$T_{fl}(z) = T_{inlet}, \quad \text{at } z = -\ell/2, \quad (5)$$

where $W[\text{kg} \cdot \text{s}^{-1}]$ denotes the mass flow rate, $T_{inlet}[\text{K}]$ denotes the inlet temperature, and $c_p[\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}]$ denotes the coolant’s heat capacity.

For this paradigm benchmark problem, Equations (1)-(5) can be solved exactly to obtain the following closed form expressions:

$$T(r, z) = q \left(\frac{a^2 - r^2}{4k} + \frac{a}{2h} \right) \cos \frac{\pi z}{\ell} + T_{fl}(z), \quad 0 \leq r < a, \quad -\frac{\ell}{2} \leq z \leq \frac{\ell}{2}, \quad (6)$$

$$T_{fl}(z) = \frac{a^2 \ell q}{W c_p} \left(\sin \frac{\pi z}{\ell} + 1 \right) + T_{inlet}, \quad -\frac{\ell}{2} \leq z \leq \frac{\ell}{2}. \quad (7)$$

The imprecisely known parameters underlying the paradigm heat transfer benchmark modeled by Equations (1)-(5) are: $q, k, h, W, c_p, T_{inlet}, a, \ell$. A list of these parameters is provided in the Nomenclature Section at the end of this work. The known nominal values of these parameters will be denoted by using the superscript “zero,” *i.e.*, $q^0, k^0, h^0, W^0, c_p^0, T_{inlet}^0, a^0, \ell^0$. The nominal values of the temperature distributions in the rod and coolant, denoted as $T^0(r, z)$ and $T_{fl}^0(z)$, respectively, have the following expressions:

$$T(r, z) = q^0 \left[\frac{(a^0)^2 - r^2}{4k^0} + \frac{a^0}{2h^0} \right] \cos \frac{\pi z}{\ell^0} + T_{fl}^0(z), \quad 0 \leq r < a^0, \quad -\frac{\ell^0}{2} \leq z \leq \frac{\ell^0}{2}, \quad (8)$$

$$T_{fl}^0(z) = \frac{(a^0)^2 \ell^0 q^0}{W^0 c_p^0} \left(\sin \frac{\pi z}{\ell^0} + 1 \right) + T_{inlet}^0, \quad -\frac{\ell^0}{2} \leq z \leq \frac{\ell^0}{2}. \quad (9)$$

3. Application of the 1st-CASAM to the Coupled Heat Conduction and Convection Benchmark Model

The arbitrary variations in the imprecisely known model parameters, around the respective nominal values, will be denoted as follows: $\delta q \triangleq q - q^0$, $\delta k \triangleq k - k^0$, $\delta h \triangleq h - h^0$, $\delta W \triangleq W - W^0$, $\delta c_p \triangleq c_p - c_p^0$, $\delta T_{inlet} \triangleq T_{inlet} - T_{inlet}^0$, $\delta a \triangleq a - a^0$, $\delta \ell \triangleq \ell - \ell^0$. The variations in the rod and coolant temperatures, respectively, caused by the imprecisely known parameters will be denoted as follows: $\delta T(r, z) \triangleq T(r, z) - T^0(r, z)$ and $\delta T_{fl}(z) \triangleq T_{fl}(z) - T_{fl}^0(z)$, respectively.

3.1. First-Order Sensitivities of the Coolant’s Temperature

The sensitivities to model and boundary parameters of several typical responses, including the value of the coolant temperature at a point, the average coolant temperature, and the coolant temperature itself, will be determined in this Section by applying the 1st-CASAM presented in Reference 1. The 1st-LFSS corresponding to Equations (4) and (5) is obtained by determining the G-differentials of these equations to obtain:

$$\left\{ \frac{d}{d\varepsilon} \left[\frac{d}{dz} \left[T_{fl}^0(z) + \varepsilon \delta T_{fl}(z) \right] \right] \right\}_{\varepsilon=0} = \pi \left\{ \frac{d}{d\varepsilon} \frac{(a^0 + \varepsilon \delta a)^2 (q^0 + \varepsilon \delta q)}{(W^0 + \varepsilon \delta W)(c_p^0 + \varepsilon \delta c_p)} \cos \frac{\pi z}{\ell^0 + \varepsilon \delta \ell} \right\}_{\varepsilon=0}, \quad (10)$$

$$\left\{ \frac{d}{d\varepsilon} \left[T_{fl}^0 \left(-\frac{\ell^0 + \varepsilon \delta \ell}{2} \right) + \varepsilon \delta T_{fl} \left(-\frac{\ell^0 + \varepsilon \delta \ell}{2} \right) \right] \right\}_{\varepsilon=0} = \left\{ \frac{d}{d\varepsilon} \left(T_{inlet}^0 + \varepsilon \delta T_{inlet} \right) \right\}_{\varepsilon=0}. \quad (11)$$

Carrying out in Equations (10) and (11) the differentiations with respect to ε and setting $\varepsilon = 0$ in the resulting expressions yields the following set of equations:

$$\begin{aligned} \frac{d}{dz} [\delta T_{fl}(z)] &= \pi \left[\frac{2a^0 q^0 (\delta a)}{W^0 c_p^0} + \frac{(a^0)^2 (\delta q)}{W^0 c_p^0} - \frac{(a^0)^2 q^0 (\delta W)}{(W^0)^2 c_p^0} \right. \\ &\quad \left. + (\delta \ell) \pi^2 z \frac{(a^0)^2 q^0}{W^0 c_p^0 (\ell^0)^2} \sin \frac{\pi z}{\ell^0} \right] \cos \frac{\pi z}{\ell^0} \\ &\triangleq Q_{fl}(z), \quad -\frac{\ell^0}{2} \leq z \leq \frac{\ell^0}{2}, \end{aligned} \tag{12}$$

$$\begin{aligned} \delta T_{fl}(z) &= \frac{dT_{fl}^0(z)}{dz} \frac{\delta \ell}{2} + \delta T_{inlet} = \delta T_{inlet}, \\ \text{at } z &= -\ell^0/2, \end{aligned} \tag{13}$$

since $\{dT_{fl}^0(z)/dz\}_{\ell/2} = 0$, as evidenced by evaluating Equation (4) at $z = -\ell/2$. The 1st-LFSS, comprising Equations (12) and (13), evidently depends on the arbitrary variations which affect the imprecisely known model parameters. The 1st-LFSS can be solved in closed form and its solution can be used for the subsequent verification of the expressions to be obtained for the 1st-order response sensitivities using the 1st-level adjoint functions. For subsequent verification purposes, the solution of Equations (12) and (13) is provided below:

$$\begin{aligned} \delta T_{fl}(z) &= \delta T_{inlet} + \ell^0 \left[\frac{2a^0 q^0 (\delta a)}{W^0 c_p^0} + \frac{(a^0)^2 (\delta q)}{W^0 c_p^0} - \frac{(a^0)^2 q^0 (\delta W)}{(W^0)^2 c_p^0} \right. \\ &\quad \left. - \frac{(a^0)^2 q^0 (\delta c_p)}{W^0 (c_p^0)^2} \right] \left(\sin \frac{\pi z}{\ell^0} + 1 \right) \\ &\quad + (\delta \ell) \frac{(a^0)^2 q^0}{W^0 c_p^0} \left[-\frac{\pi z}{\ell^0} \cos \frac{\pi z}{\ell^0} + \left(\sin \frac{\pi z}{\ell^0} + 1 \right) \right] \end{aligned} \tag{14}$$

It is evident that the expression obtained in Equation (14) is the total differential with respect to the model and boundary parameters of the expression of $T_{fl}(z)$ given in Equation (7).

3.1.1. First-Order Sensitivities of the Coolant's Temperature at a Point in Phase-Space

The coolant temperature, $T_{fl}(z_p)$, at some axial point $z = z_p$, $-\ell/2 < z_p < \ell/2$, can be represented in the form

$$T_{fl}(z_p) = \int_{-\ell/2}^{\ell/2} T_{fl}(z) \delta(z - z_p) dz. \tag{15}$$

The imprecisely known model and boundary parameters that characterize the heat transport benchmark modeled by Equations (1) through (5) and including the imprecisely known location z_p , the response defined in Equation (15) are: $q, k, h, W, c_p, T_{inlet}, a, \ell, z_p$. The total sensitivity of the response defined in Equation (15) is given by its total G-differential, which is

$$\delta T_{fl}(z_p) = \left\{ \frac{d}{d\varepsilon} \int_{-(\ell^0 + \varepsilon\delta\ell)/2}^{(\ell^0 + \varepsilon\delta\ell)/2} [T_{fl}^0(z) + \varepsilon\delta T_{fl}(z)] \delta(z - z_p^0 - \varepsilon\delta z_p) dz \right\}_{\varepsilon=0} \quad (16)$$

$$= \{\delta T_{fl}(z_p)\}^{dir} + \{\delta T_{fl}(z_p)\}^{ind},$$

where the direct-effect term $\{\delta T_{fl}(z_p)\}^{dir}$ is defined as follows:

$$\{\delta T_{fl}(z_p)\}^{dir} = -(\delta z_p) \int_{-\ell^0/2}^{\ell^0/2} T_{fl}^0(z) \delta'(z - z_p^0) dz = (\delta z_p) \left\{ \frac{\partial T_{fl}^0(z)}{\partial z} \right\}_{z=z_p}, \quad (17)$$

while the indirect-effect term $\{\delta T_{fl}(z_p)\}^{ind}$ is defined as follows:

$$\{\delta T_{fl}(z_p)\}^{ind} \triangleq \int_{-\ell^0/2}^{\ell^0/2} \delta T_{fl}(z) \delta(z - z_p) dz, \quad (18)$$

The direct-effect term $\{\delta T_{fl}(z_p)\}^{dir}$ can be evaluated immediately. On the other hand, the indirect-effect term $\{\delta T_{fl}(z_p)\}^{ind}$ depends on the unknown variation $\delta T_{fl}(z)$. In practice, the 1st-LFSS comprising Equations (12) and (13) would need to be solved numerically, repeatedly, for every possible parameter variation. As shown in the companion article¹, application of the 1st-CASAM circumvents the need for solving the 1st-LFSS repeatedly by constructing the 1st-LASS corresponding to the 1st-LFSS. Construction of the 1st-LASS requires the existence of an inner product in the phase-space domain of definition of the 1st-LFSS. For the system defined by Equations (4), (5) and (15), the domain of definition is $-\ell/2 \leq z, z_p \leq \ell/2$. The inner-product of two square-integrable functions $u_1(z)$ and $u_2(z)$ defined on $-\ell/2 \leq z, z_p \leq \ell/2$ has the following expression:

$$\langle u_1(z), u_2(z) \rangle_u \triangleq \int_{-\ell^0/2}^{\ell^0/2} u_1(z) u_2(z) dz. \quad (19)$$

Using the definition provided in Equation (19), construct the inner product of Equation (12) with a square-integrable function $\Psi_{fl}(z)$ to obtain the following relation:

$$\int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \frac{d[\delta T_{fl}(z)]}{dz} dz = \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) Q_{fl}(z) dz. \quad (20)$$

Integrating by parts the term on the left-side of Equation (20) yields the following relation:

$$\begin{aligned} & \int_{-\ell^0/2}^{\ell^0/2} dz \Psi_{fl}(z) \frac{d[\delta T_{fl}(z)]}{dz} \\ &= \int_{-\ell^0/2}^{\ell^0/2} dz [\delta T_{fl}(z)] \left[-\frac{d\Psi_{fl}(z)}{dz} \right] + \Psi_{fl}\left(\frac{\ell^0}{2}\right) \delta T_{fl}\left(\frac{\ell^0}{2}\right) \\ & \quad - \Psi_{fl}\left(-\frac{\ell^0}{2}\right) \delta T_{fl}\left(-\frac{\ell^0}{2}\right), \end{aligned} \quad (21)$$

Identify the first term on the right-side of Equation (21) with the indirect-effect term defined in Equation (18) to obtain the following relations:

$$-\frac{\partial \Psi_{fl}(z)}{\partial z} = \delta(z - z_p^0), \quad -\frac{\ell^0}{2} \leq z \leq \frac{\ell^0}{2}, \tag{22}$$

$$\begin{aligned} \{\delta T_{fl}(z_p)\}^{ind} &= \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) Q_{fl}(z) dz - \Psi_{fl}\left(\frac{\ell^0}{2}\right) \delta T_{fl}\left(\frac{\ell^0}{2}\right) \\ &+ \Psi_{fl}\left(-\frac{\ell^0}{2}\right) \delta T_{fl}\left(-\frac{\ell^0}{2}\right). \end{aligned} \tag{23}$$

The boundary condition given in Equation (13) is used to replace $\delta T_{fl}(z = -\ell^0/2)$ in the last term on the right side of Equation (23). The remaining term in Equation (23), which contains the unknown value $\delta T_{fl}(\ell^0/2)$, is set to zero by imposing the following boundary condition for the function $\Psi_{fl}(z)$:

$$\Psi_{fl}(z) = 0, \quad \text{at } z = \ell^0/2. \tag{24}$$

It follows from in Equations (24) and (13) that Equation (23) becomes

$$\{\delta T_{fl}(z_p)\}^{ind} = \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) Q_{fl}(z) dz + \Psi_{fl}\left(-\frac{\ell^0}{2}\right) \delta T_{inlet}, \tag{25}$$

where the adjoint function $\Psi_{fl}(z)$ is the solution of the 1st-LASS comprising Equations (22) and (24). As expected from the general methodology underlying the 1st-CASAM, the 1st-LASS, comprising Equations (22) and (24), is independent of any parameter variation. Inserting the definition of $Q_{fl}(z)$ provided in Equation (12) into Equation (25) and identifying the expressions that multiply the respective arbitrary parameter variations yields the following expressions for the sensitivities of the response $T_{fl}(z_p)$ in terms of the adjoint function $\Psi_{fl}(z)$:

$$\frac{\partial T_{fl}(z_p)}{\partial a} = \pi \frac{2a^0 q^0}{W^0 c_p^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz, \tag{26}$$

$$\frac{\partial T_{fl}(z_p)}{\partial q} = \pi \frac{(a^0)^2}{W^0 c_p^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz, \tag{27}$$

$$\frac{\partial T_{fl}(z_p)}{\partial W} = -\pi \frac{(a^0)^2 q^0}{(W^0)^2 c_p^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz, \tag{28}$$

$$\frac{\partial T_{fl}(z_p)}{\partial c_p} = -\pi \frac{(a^0)^2 q^0}{W^0 (c_p^0)^2} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz, \tag{29}$$

$$\frac{\partial T_{fl}(z_p)}{\partial \ell} = \pi^2 \frac{(a^0)^2 q^0}{W^0 c_p^0 (\ell^0)^2} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \left(z \sin \frac{\pi z}{\ell^0} \right) dz, \tag{30}$$

It also follows from Equation (25) that

$$\frac{\partial T_{fl}(z_p^0)}{\partial T_{inlet}} = \Psi_{fl} \left(-\frac{\ell^0}{2} \right). \quad (31)$$

Solving the 1st-LASS comprising Equations (22) and (24), which is notably independent of any parameter variation, yields the following expression for the adjoint function $\Psi_{fl}(z)$:

$$\Psi_{fl}(z) = [1 - H(z - z_p^0)] = H(z_p^0 - z), \quad -\frac{\ell^0}{2} \leq z, z_p^0 \leq \frac{\ell^0}{2}. \quad (32)$$

Replacing the expression obtained in Equation (32) in Equations (26)-(31) and carrying out the respective integrations over the spatial variable z yields the following expressions (where the superscript “zero,” which indicates “nominal values,” has been omitted for notational simplicity) for the first-order sensitivities of $T_{fl}(z_p)$ with respect to the model parameters:

$$\frac{\partial T_{fl}(z_p)}{\partial a} = \frac{2aq\ell}{Wc_p} \left(\sin \frac{\pi z_p}{\ell} + 1 \right), \quad (33)$$

$$\frac{\partial T_{fl}(z_p)}{\partial q} = \frac{a^2\ell}{Wc_p} \left(\sin \frac{\pi z_p}{\ell} + 1 \right), \quad (34)$$

$$\frac{\partial T_{fl}(z_p)}{\partial W} = -\frac{qa^2\ell}{W^2c_p} \left(\sin \frac{\pi z_p}{\ell} + 1 \right), \quad (35)$$

$$\frac{\partial T_{fl}(z_p)}{\partial c_p} = -\frac{qa^2\ell}{Wc_p^2} \left(\sin \frac{\pi z_p}{\ell} + 1 \right), \quad (36)$$

$$\frac{\partial T_{fl}(z_p)}{\partial \ell} = \frac{a^2q}{Wc_p} \left[-\frac{\pi z}{\ell} \cos \frac{\pi z}{\ell} + \left(\sin \frac{\pi z}{\ell} + 1 \right) \right], \quad (37)$$

$$\frac{\partial T_{fl}(z_p)}{\partial T_{inlet}} = 1. \quad (38)$$

It becomes apparent by comparing the expressions obtained in Equations (33)-(38) with the expression provided in Equation (14) that using either the 1st-LASS or the 1st-LFSS yields identical expressions for the respective response sensitivities with respect to the model and boundary parameters. Furthermore, the direct-effect term defined in Equation (17) provides the additional sensitivity of the response with respect to its imprecisely known location, which is computed directly from Equation (7), namely:

$$\left\{ \frac{\partial T_{fl}(z)}{\partial z} \right\}_{z=z_p} = \frac{\pi a^2 q}{Wc_p} \cos \frac{\pi z_p}{\ell}. \quad (39)$$

It is evident from the above illustrative example that the 1st-CASAM is the most efficient way to compute exactly the 1st-order response sensitivities to model and boundary parameters, since it requires a *single* large-scale computation to solve the 1st-LASS, namely Equations (22) and (24) for determining the

1st-level adjoint function needed in the subsequent quadrature formulas to compute *all* of the response sensitivities using Equations (26)-(31).

3.1.2. First-Order Sensitivities of the Average Coolant Temperature

The average coolant temperature, denoted as T_{fl}^{ave} , is given by the expression

$$T_{fl}^{ave} = \frac{1}{\ell} \int_{-\ell/2}^{\ell/2} T_{fl}(z) dz = \left(T_{inlet} + \frac{a^2 \ell q}{Wc_p} \right). \tag{40}$$

The total sensitivity of T_{fl}^{ave} is given by its total G-differential, which is obtained, by definition, by evaluating the following expression:

$$\begin{aligned} \delta T_{fl}^{ave} &= \left\{ \frac{d}{d\varepsilon} \left[\frac{1}{\ell^0 + \varepsilon \delta \ell} \int_{-(\ell^0 + \varepsilon \delta \ell)/2}^{(\ell^0 + \varepsilon \delta \ell)/2} [T_{fl}^0(z) + \varepsilon \delta T_{fl}(z)] dz \right] \right\}_{\varepsilon=0} \\ &= \{ \delta T_{fl}^{ave} \}^{dir} + \{ \delta T_{fl}^{ave} \}^{ind}, \end{aligned} \tag{41}$$

where the direct-effect term is defined as follows:

$$\{ \delta T_{fl}^{ave} \}^{dir} = -\frac{\delta \ell}{(\ell^0)^2} \int_{-\ell^0/2}^{\ell^0/2} T_{fl}^0(z) dz + \frac{\delta \ell}{2\ell^0} \left[T_{fl}^0\left(\frac{\ell^0}{2}\right) - T_{fl}^0\left(-\frac{\ell^0}{2}\right) \right] = 0, \tag{42}$$

while the indirect-effect term is defined as follows:

$$\{ \delta T_{fl}^{ave} \}^{ind} \triangleq \frac{1}{\ell^0} \int_{-\ell^0/2}^{\ell^0/2} \delta T_{fl}(z) dz, \tag{43}$$

The indirect-effect term $\{ \delta T_{fl}^{ave} \}^{ind}$ defined in Equation (43) will be expressed in terms of a square-integrable adjoint function, denoted as $\Psi_{fl}^{ave}(z)$, by following the same procedure as used in Section 3.1.1 to obtain the following relation [which corresponds to Equation (25)]:

$$\{ \delta T_{fl}^{ave} \}^{ind} = \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}^{ave}(z) Q_{fl}(z) dz + \Psi_{fl}^{ave}\left(-\frac{\ell^0}{2}\right) \delta T_{inlet}, \tag{44}$$

where the adjoint function $\Psi_{fl}^{ave}(z)$ is the solution of the following 1st-LASS

$$-\frac{\partial \Psi_{fl}^{ave}(z)}{\partial z} = \frac{1}{\ell^0}, \quad -\frac{\ell^0}{2} \leq z \leq \frac{\ell^0}{2}, \tag{45}$$

$$\Psi_{fl}^{ave}(z) = 0, \quad \text{at } z = \ell^0/2. \tag{46}$$

Comparing Equations (44) to Equation (25) indicates that the sensitivities stemming from $\{ \delta T_{fl}^{ave} \}^{ind}$ have the same formal expressions as those given in Equations (26)-(31) but with the adjoint function $\Psi_{fl}^{ave}(z)$ replacing the adjoint $\Psi_{fl}(z)$, namely:

$$\frac{\partial T_{fl}^{ave}}{\partial a} = \pi \frac{2a^0 q^0}{W^0 c_p^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}^{ave}(z) \cos \frac{\pi z}{\ell^0} dz, \tag{47}$$

$$\frac{\partial T_{fl}^{ave}}{\partial q} = \pi \frac{(a^0)^2}{W^0 c_p^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}^{ave}(z) \cos \frac{\pi z}{\ell^0} dz, \tag{48}$$

$$\frac{\partial T_{fl}^{ave}}{\partial W} = -\pi \frac{(a^0)^2 q^0}{(W^0)^2 c_p^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}^{ave}(z) \cos \frac{\pi z}{\ell^0} dz, \quad (49)$$

$$\frac{\partial T_{fl}^{ave}}{\partial c_p} = -\pi \frac{(a^0)^2 q^0}{W^0 (c_p^0)^2} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}^{ave}(z) \cos \frac{\pi z}{\ell^0} dz, \quad (50)$$

$$\frac{\partial T_{fl}^{ave}}{\partial \ell} = \pi^2 \frac{(a^0)^2 q^0}{W^0 c_p^0 (\ell^0)^2} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}^{ave}(z) \left(z \sin \frac{\pi z}{\ell^0} \right) dz, \quad (51)$$

$$\frac{\partial T_{fl}^{ave}}{\partial T_{inlet}} = \Psi_{fl}^{ave} \left(-\frac{\ell}{2} \right). \quad (52)$$

Solving the 1st-LASS comprising Equations (45) and (46) yields the following expression for the adjoint function $\Psi_{fl}^{ave}(z)$:

$$\Psi_{fl}^{ave}(z) = -\frac{z}{\ell^0} + \frac{1}{2}, \quad (53)$$

Replacing the expression obtained in Equation (53) in Equations (47)-(52) and carrying out the respective integrations over the spatial variable z yields the following expressions (where the superscript “zero”, which indicates “nominal values”, has been omitted for notational simplicity) for the first-order sensitivities of $T_{fl}(z_p)$ with respect to the model parameters:

$$\frac{\partial T_{fl}^{ave}}{\partial a} = \frac{2aq\ell}{Wc_p}, \quad (54)$$

$$\frac{\partial T_{fl}^{ave}}{\partial q} = \frac{a^2\ell}{Wc_p}, \quad (55)$$

$$\frac{\partial T_{fl}^{ave}}{\partial W} = -\frac{qa^2\ell}{W^2c_p}, \quad (56)$$

$$\frac{\partial T_{fl}^{ave}}{\partial c_p} = -\frac{qa^2\ell}{Wc_p^2}, \quad (57)$$

$$\frac{\partial T_{fl}^{ave}}{\partial \ell} = \frac{a^2q}{Wc_p}, \quad (58)$$

$$\frac{\partial T_{fl}^{ave}}{\partial T_{inlet}} = 1. \quad (59)$$

For validation purposes, it is noted that the expressions obtained in Equations (54)-(59) are identical to the corresponding expressions that would be obtained by determining the partial sensitivities (1st-order derivatives) of the closed-form expression provided in Equation (40). In practice, the closed-form expression of the response is not available, so that such validation/comparisons are performed approximately by computing the sensitivities of the response numerically, using re-computations with perturbed parameter values in conjunction with finite dif-

ference schemes. The 1st-CASAM is the most efficient way to compute exactly the 1st-order response sensitivities to model and boundary parameters, since it requires a *single* large-scale computation to solve the 1st-LASS, namely Equations (45) and (46) for determining the 1st-level adjoint function needed in the subsequent quadrature formulas to compute *all* of the response sensitivities using Equations (47)-(52).

3.2. First-Order Sensitivities of the Rod's Temperature

The value of the heated rod temperature, $T(r, z)$, at some location (r_p, z_p) , can be represented in the form

$$T(r_p, z_p) = \int_0^a r dr \int_{-\ell/2}^{\ell/2} dz T(r, z) \frac{\delta(r - r_p)}{r} \delta(z - z_p). \tag{60}$$

As indicated in Equations (1)-(5), the imprecisely known parameters that characterize the benchmark heat transfer system are $q, k, h, W, c_p, T_{inlet}, a, \ell$. The known nominal values of these parameters will be denoted by using the superscript “zero,” *i.e.*, $q^0, k^0, h^0, W^0, c_p^0, T_{inlet}^0, a^0, \ell^0$. The arbitrary variations in the model parameters, around the respective nominal values, will be denoted as follows: $\delta q, \delta k, \delta h, \delta W, \delta c_p, \delta T_{inlet}, \delta a, \delta \ell$. For greater generality, it will be assumed that the location (r_p, z_p) is also imprecisely known, being affected by variation (uncertainties) denoted as δr_p and δz_p around the known nominal values denoted as (r_p^0, z_p^0) . The variations in the rod and coolant temperatures, respectively, caused by the imprecisely known model and boundary parameters will be denoted as $\delta T(r, z)$ and $\delta T_\ell(z)$, respectively.

The first-order sensitivities of $T(r_p, z_p)$ to the imprecisely known model and boundary parameters is provided by the G-differential of Equation (60), which is defined as follows:

$$\begin{aligned} \delta T(r_p, z_p) &= \left\{ \frac{d}{d\varepsilon} \int_0^{a^0 + \varepsilon \delta a} r dr \int_{-(\ell^0 + \varepsilon \delta \ell)/2}^{(\ell^0 + \varepsilon \delta \ell)/2} [T(r_p, z_p) + \varepsilon \delta T(r_p, z_p)] \right. \\ &\quad \left. \times \frac{\delta(r - r_p^0 - \varepsilon \delta r_p)}{r} \delta(z - z_p^0 - \varepsilon \delta z_p) dz \right\}_{\varepsilon=0} \tag{61} \\ &= \left\{ \delta T(r_p, z_p) \right\}^{dir} + \left\{ \delta T(r_p, z_p) \right\}^{ind}, \end{aligned}$$

where the direct-effect term $\left\{ \delta T(r_p, z_p) \right\}^{direct}$ is defined as follows:

$$\left\{ \delta T(r_p, z_p) \right\}^{dir} = (\delta z_p) \left\{ \frac{\partial T(r, z)}{\partial z} \right\}_{(z=z_p, r=r_p)} + (\delta r_p) \left\{ \frac{\partial T(r, z)}{\partial r} \right\}_{(z=z_p, r=r_p)}, \tag{62}$$

while the indirect-effect term $\left\{ \delta T(r_p, z_p) \right\}^{ind}$ is defined as follows:

$$\left\{ \delta T(r_p, z_p) \right\}^{ind} \triangleq \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} \delta T(r, z) \frac{\delta(r - r_p^0)}{r} \delta(z - z_p^0) dz. \tag{63}$$

This 1st-LFSS is obtained by determining the G-differentials of Equations (1)-(5), which are as follows:

$$\left\{ \frac{d}{d\varepsilon} \frac{k^0 + \varepsilon\delta k}{r} \frac{\partial}{\partial r} \left[r \frac{\partial (T^0 + \varepsilon\delta T)}{\partial r} \right] \right\}_{\varepsilon=0} = - \left\{ \frac{d}{d\varepsilon} (q^0 + \varepsilon\delta q) \cos \frac{\pi z}{\ell^0 + \varepsilon\delta\ell} \right\}_{\varepsilon=0}, \quad (64)$$

$$\left\{ \frac{d}{d\varepsilon} \frac{\partial (T^0 + \varepsilon\delta T)}{\partial r} \right\}_{\varepsilon=0} = 0, \quad \text{at } r = 0, \quad (65)$$

$$\begin{aligned} & - \left\{ \frac{d}{d\varepsilon} (k^0 + \varepsilon\delta k) \frac{\partial [T^0(a^0 + \varepsilon\delta a, z) + \varepsilon\delta T(a^0 + \varepsilon\delta a, z)]}{\partial (a^0 + \varepsilon\delta a)} \right\}_{\varepsilon=0} \\ & = \left\{ \frac{d}{d\varepsilon} (h^0 + \varepsilon\delta h) [T^0(a^0 + \varepsilon\delta a, z) + \varepsilon\delta T(a^0 + \varepsilon\delta a, z) \right. \\ & \quad \left. - T_{fl}^0(z) - \varepsilon\delta T_{fl}(z)] \right\}_{\varepsilon=0}, \quad \text{at } r = a^0, \end{aligned} \quad (66)$$

$$\begin{aligned} & \left\{ \frac{d}{d\varepsilon} \frac{d [T_{fl}^0(z) + \varepsilon\delta T_{fl}(z)]}{dz} \right\}_{\varepsilon=0} \\ & = \pi \left\{ \frac{d}{d\varepsilon} \frac{(a^0 + \varepsilon\delta a)^2 (q^0 + \varepsilon\delta q)}{(W^0 + \varepsilon\delta W)(c_p^0 + \varepsilon\delta c_p)} \cos \frac{\pi z}{\ell^0 + \varepsilon\delta\ell} \right\}_{\varepsilon=0}, \end{aligned} \quad (67)$$

$$\begin{aligned} & \left\{ \frac{d}{d\varepsilon} \left[T_{fl}^0 \left(-\frac{\ell^0 + \varepsilon\delta\ell}{2} \right) + \varepsilon\delta T_{fl} \left(-\frac{\ell^0 + \varepsilon\delta\ell}{2} \right) \right] \right\}_{\varepsilon=0} \\ & = \left\{ \frac{d}{d\varepsilon} (T_{inlet}^0 + \varepsilon\delta T_{inlet}) \right\}_{\varepsilon=0}. \end{aligned} \quad (68)$$

Carrying out in Equations (64)-(68) the differentiations with respect to ε and setting $\varepsilon = 0$ in the resulting expressions yields the following set of equations comprising 1st-LFSS:

$$\begin{aligned} & \frac{k^0}{r} \frac{\partial}{\partial r} \left\{ r \frac{\partial}{\partial r} [\delta T(r, z)] \right\} \\ & = - \frac{(\delta k)}{r} \frac{\partial}{\partial r} \left[r \frac{\partial T^0(r, z)}{\partial r} \right] - (\delta q) \cos \frac{\pi z}{\ell^0} + (\delta\ell) \frac{q^0 \pi z}{(\ell^0)^2} \sin \frac{\pi z}{\ell^0}, \end{aligned} \quad (69)$$

$$\frac{\partial}{\partial r} [\delta T(r, z)] = 0, \quad \text{at } r = 0, \quad (70)$$

$$\begin{aligned} & -(\delta k) \left\{ \frac{\partial T^0(r, z)}{\partial r} \right\}_{r=a^0} - k^0 (\delta a) \left\{ \frac{\partial^2 T^0(r, z)}{\partial r^2} \right\}_{r=a^0} - k^0 \left\{ \frac{\partial}{\partial r} [\delta T(r, z)] \right\}_{r=a^0} \\ & = (\delta h) \left\{ [T^0(r, z) - T_{fl}^0(z)] \right\}_{r=a^0} + h^0 [\delta T(r) - \delta T_{fl}(z)] \\ & \quad + (\delta a) h^0 \left\{ \frac{\partial T^0(r, z)}{\partial r} \right\}_{r=a^0}, \end{aligned} \quad (71)$$

$$\begin{aligned} \frac{d}{dz} [\delta T_{fl}(z)] &= \pi \cos \frac{\pi z}{\ell^0} \left[\frac{2a^0 q^0 (\delta a)}{W^0 c_p^0} + \frac{(a^0)^2 (\delta q)}{W^0 c_p^0} - \frac{(a^0)^2 q^0 (\delta W)}{(W^0)^2 c_p^0} \right. \\ &\quad \left. - \frac{(a^0)^2 q^0 (\delta c_p)}{W^0 (c_p^0)^2} \right] + (\delta \ell) \pi^2 z \frac{(a^0)^2 q^0}{W^0 c_p^0 (\ell^0)^2} \sin \frac{\pi z}{\ell^0} \quad (72) \\ &\triangleq Q_{fl}(z), \quad -\frac{\ell^0}{2} \leq z \leq \frac{\ell^0}{2}, \\ \delta T_{fl}(z) &= \frac{dT_{fl}^0(z)}{dz} \frac{\delta \ell}{2} + \delta T_{inlet} = \delta T_{inlet}, \quad (73) \\ &\text{at } z = -\ell^0/2. \end{aligned}$$

The first term on the right-side of Equation (69) can be simplified by using Equation (1) to obtain the following equation:

$$\begin{aligned} &\frac{k^0}{r} \frac{\partial}{\partial r} \left\{ r \frac{\partial}{\partial r} [\delta T(r, z)] \right\} \\ &= \left[(\delta k) \frac{q^0}{k^0} - (\delta q) \right] \cos \frac{\pi z}{\ell^0} + (\delta \ell) \frac{q^0 \pi z}{(\ell^0)^2} \sin \frac{\pi z}{\ell^0} \triangleq Q(z). \quad (74) \end{aligned}$$

The terms containing derivatives of $T(r, z)$ in Equation (71) can also be simplified using Equations (1) and (3) to obtain the following equation:

$$\begin{aligned} &\left\{ -k^0 \frac{\partial}{\partial r} [\delta T(r, z)] - h^0 [\delta T(r, z) - \delta T_{fl}(z)] \right\}_{r=a^0} \\ &= (\delta h) \frac{a^0 q^0}{2h^0} \cos \frac{\pi z}{\ell^0} - (\delta k) \frac{a^0 q^0}{2k^0} \cos \frac{\pi z}{\ell^0} - (\delta a) \frac{q^0}{2} \left(\frac{h^0 a^0}{k^0} + 1 \right) \cos \frac{\pi z}{\ell^0}. \quad (75) \end{aligned}$$

The 1st-LFSS comprises Equations (70), (72)-(74), and (75). As has been already discussed throughout this work, it is computationally expensive to solve repeatedly the 1st-LFSS for all possible parameter variations, and this computationally expensive endeavor can be circumvented by expressing the indirect-effect term defined in Equation (63) in terms of the solution of the 1st-LASS, which will be constructed next by applying the 1st-CASAM outlined in the accompanying work [1].

The Hilbert space appropriate for the heat transport benchmark under consideration comprises the space of all square-integrable two-component vector functions of the form $\mathbf{u}(\mathbf{x}) \equiv [u_1(r, z), u_2(z)]^\dagger$, endowed with an inner product $\langle \mathbf{u}(\mathbf{x}), \boldsymbol{\psi}(\mathbf{x}) \rangle$ of the form

$$\langle \mathbf{u}(\mathbf{x}), \boldsymbol{\psi}(\mathbf{x}) \rangle \equiv \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz [u_1(r, z) \psi_1(r, z) + u_2(z) \psi_2(z)]. \quad (76)$$

Using the definition provided in Equation (76), construct the inner product of a square integrable vector function $\boldsymbol{\psi}(\mathbf{x}) = [\Psi(r, z), \Psi_{fl}(z)]$, where $\Psi(r, z)$ and $\Psi_{fl}(z)$ denote the adjoint sensitivity functions that correspond to the forward functions $\delta T(r, z)$ and $\delta T_{fl}(z)$, with Equations (74) and (72), re-

spectively, to obtain the following relation:

$$\int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz \left\{ \Psi(r, z) \frac{k^0}{r} \frac{\partial}{\partial r} \left[r \frac{\partial}{\partial r} \delta T(r, z) \right] + \Psi_{\beta}(z) \frac{d[\delta T_{\beta}(z)]}{dz} \right\} = \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz [\Psi(r, z) Q(z) + \Psi_{\beta}(z) Q_{\beta}(z)]. \tag{77}$$

The left-side of Equation (77) is now integrated by parts (twice over the variable r and once over the variable z) to obtain

$$\begin{aligned} & \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz \left\{ \Psi(r, z) \frac{k^0}{r} \frac{\partial}{\partial r} \left[r \frac{\partial}{\partial r} \delta T(r, z) \right] + \Psi_{\beta}(z) \frac{d[\delta T_{\beta}(z)]}{dz} \right\} \\ &= \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz [\delta T_{\beta}(z)] \left[-\frac{d\Psi_{\beta}(z)}{dz} \right] \\ &+ \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz \left\{ [\delta T(r, z)] \frac{k^0}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Psi(r, z)}{\partial r} \right) \right\} \\ &+ \int_0^{a^0} r dr \left[\Psi_{\beta} \left(\frac{\ell^0}{2} \right) \delta T_{\beta} \left(\frac{\ell^0}{2} \right) - \Psi_{\beta} \left(-\frac{\ell^0}{2} \right) \delta T_{\beta} \left(-\frac{\ell^0}{2} \right) \right] \\ &+ \int_{-\ell^0/2}^{\ell^0/2} dz \left[\Psi(r, z) r k^0 \frac{\partial}{\partial r} \delta T(r, z) - \delta T(r, z) r k^0 \frac{\partial \Psi(r, z)}{\partial r} \right]_{r=a^0} \\ &- \int_{-\ell^0/2}^{\ell^0/2} dz \left[\Psi(r, z) r k^0 \frac{\partial}{\partial r} \delta T(r, z) - \delta T(r, z) r k^0 \frac{\partial \Psi(r, z)}{\partial r} \right]_{r=0}. \end{aligned} \tag{78}$$

Using the boundary condition given in Equations (70) and imposing the boundary condition

$$\frac{\partial \Psi(r, z)}{\partial r} = 0, \text{ at } r = 0, \tag{79}$$

eliminates the last term on the right-side of Equation (78), including the unknown function $\left\{ \frac{\partial [\delta T(r, z)]}{\partial r} \right\}_{r=0}$. Imposing the boundary condition

$$\Psi_{\beta}(z) = 0, \text{ at } z = \ell^0/2, \tag{80}$$

eliminates the unknown function $\delta T_{\beta}(z = \ell^0/2)$ on the right-side of Equation (78). Using the boundary condition given in Equation (73) to replace the term $\delta T_{\beta}(z = -\ell/2)$ on the right side of Equation (78) and replacing the left-side of Equation (78) by the right-side of Equation (77) yields the following expression equivalent to Equation (78):

$$\begin{aligned} & \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz [\Psi(r, z) Q(z) + \Psi_{\beta}(z) Q_{\beta}(z)] \\ &= \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz \left\{ [\delta T(r, z)] \frac{k^0}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Psi(r, z)}{\partial r} \right) \right\} \\ &+ [\delta T_{\beta}(z)] \left[-\frac{d\Psi_{\beta}(z)}{dz} \right] \left\{ -\int_0^{a^0} r dr \Psi_{\beta} \left(-\frac{\ell}{2} \right) \delta T_{inlet} \right\} \end{aligned}$$

$$+ \int_{-\ell^0/2}^{\ell^0/2} dz \left[\Psi(r, z) rk^0 \frac{\partial}{\partial r} \delta T(r, z) - \delta T(r, z) rk^0 \frac{\partial \Psi(r, z)}{\partial r} \right]_{r=a^0}. \quad (81)$$

The unknown quantity $\left\{ \partial [\delta T(r, z)] / \partial r \right\}_{r=a^0}$, which appears in the last term on the right-side of Equation (81) is eliminated by using the boundary condition given in Equation (75); this operation transforms Equation (81) into the following form:

$$\begin{aligned} & \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz \left[\Psi(r, z) Q(z) + \Psi_{fl}(z) Q_{fl}(z) \right] \\ &= \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz \left\{ [\delta T(r, z)] \frac{k^0}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Psi(r, z)}{\partial r} \right) + [\delta T_{fl}(z)] \left[-\frac{d\Psi_{fl}(z)}{dz} \right] \right\} \\ & \quad - \int_0^{a^0} r dr \Psi_{fl} \left(-\frac{\ell}{2} \right) (\delta T_{inlet}) - \int_{-\ell^0/2}^{\ell^0/2} dz \left[\delta T(r, z) rk^0 \frac{\partial \Psi(r, z)}{\partial r} \right]_{r=a^0} \\ & \quad - \int_{-\ell^0/2}^{\ell^0/2} dz \left\{ \Psi(a^0, z) h^0 a^0 [\delta T(r, z) - \delta T_{fl}(z)] \right\}_{r=a^0} \\ & \quad - \int_{-\ell^0/2}^{\ell^0/2} dz \Psi(a^0, z) a^0 \left\{ (\delta h) \frac{a^0 q^0}{2h^0} \cos \frac{\pi z}{\ell^0} - (\delta k) \frac{a^0 q^0}{2k^0} \cos \frac{\pi z}{\ell^0} \right. \\ & \quad \left. - (\delta a) \frac{q^0}{2} \left(\frac{h^0 a^0}{k^0} + 1 \right) \cos \frac{\pi z}{\ell^0} \right\}. \end{aligned} \quad (82)$$

The unknown quantity $\delta T(a^0, z)$, which appears in third and fourth terms on the right-side of Equation (82), is eliminated by imposing the following interface condition on the (adjoint) function $\Psi(r, z)$:

$$\begin{aligned} -k^0 \frac{\partial \Psi(r, z)}{\partial r} &= h^0 \Psi(r, z), \\ \text{at } r &= a^0 \end{aligned} \quad (83)$$

Inserting Equation (83) into the right-side of Equation (82) reduces it to the following form:

$$\begin{aligned} & \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz \left[\Psi(r, z) Q(z) + \Psi_{fl}(z) Q_{fl}(z) \right] \\ &= \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz \left\{ [\delta T(r, z)] \frac{k^0}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Psi(r, z)}{\partial r} \right) + [\delta T_{fl}(z)] \left[-\frac{d\Psi_{fl}(z)}{dz} \right] \right\} \\ & \quad - \frac{(a^0)^2}{2} \Psi_{fl} \left(-\frac{\ell}{2} \right) (\delta T_{inlet}) + h^0 a^0 \int_{-\ell^0/2}^{\ell^0/2} dz \Psi(a^0, z) [\delta T_{fl}(z)] \\ & \quad - a^0 \left[(\delta h) \frac{a^0 q^0}{2h^0} - (\delta k) \frac{a^0 q^0}{2k^0} - (\delta a) \frac{q^0}{2} \left(\frac{h^0 a^0}{k^0} + 1 \right) \right] \int_{-\ell^0/2}^{\ell^0/2} dz \Psi(a^0, z) \cos \frac{\pi z}{\ell^0}. \end{aligned} \quad (84)$$

The two terms that contain the unknown function $\delta T_{fl}(z)$ are grouped together, transforming Equation (84) into the following form:

$$\begin{aligned}
 & \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz [\Psi(r, z)Q(z) + \Psi_{fl}(z)Q_{fl}(z)] \\
 &= -\frac{(a^0)^2}{2} \Psi_{fl}\left(-\frac{\ell}{2}\right) (\delta T_{inlet}) + \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz \left\{ [\delta T(r, z)] \frac{k^0}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Psi(r, z)}{\partial r} \right) \right. \\
 & \quad \left. + [\delta T_{fl}(z)] \left[-\frac{d\Psi_{fl}(z)}{dz} + \frac{2h^0}{a^0} \Psi(a^0, z) \right] \right\} \\
 & \quad - a^0 \left[(\delta h) \frac{a^0 q^0}{2h^0} - (\delta k) \frac{a^0 q^0}{2k^0} - (\delta a) \frac{q^0}{2} \left(\frac{h^0 a^0}{k^0} + 1 \right) \right] \int_{-\ell^0/2}^{\ell^0/2} dz \Psi(a^0, z) \cos \frac{\pi z}{\ell^0}.
 \end{aligned} \tag{85}$$

The second-term on the right-side of Equation (85) will represent the indirect-effect term $\{\delta T(r_p, z_p)\}^{ind}$ defined in Equation (63) by requiring that the following equations be satisfied:

$$k^0 \frac{\partial}{\partial r} \left[r \frac{\partial \Psi(r, z)}{\partial r} \right] = \delta(r - r_p^0) \delta(z - z_p^0), \quad 0 \leq r < a^0, \quad -\frac{\ell^0}{2} \leq z \leq \frac{\ell^0}{2}, \tag{86}$$

$$-\frac{\partial \Psi_{fl}(z)}{\partial z} + \frac{2h^0}{a^0} \Psi(a, z) = 0, \quad -\frac{\ell^0}{2} \leq z \leq \frac{\ell^0}{2}, \tag{87}$$

Inserting the relations provide in Equations (63), (86) and (87) into Equation (85) and re-arranging the resulting equation yields the following expression for the indirect-effect term $\{\delta T(r_p, z_p)\}^{ind}$:

$$\begin{aligned}
 & \{\delta T(r_p, z_p)\}_{indirect} \\
 &= \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} dz [\Psi(r, z)Q(z) + \Psi_{fl}(z)Q_{fl}(z)] \\
 & \quad + a^0 \left[(\delta h) \frac{a^0 q^0}{2h^0} - (\delta k) \frac{a^0 q^0}{2k^0} - (\delta a) \frac{q^0}{2} \left(\frac{h^0 a^0}{k^0} + 1 \right) \right] \int_{-\ell^0/2}^{\ell^0/2} dz \Psi(a^0, z) \cos \frac{\pi z}{\ell^0} \\
 & \quad + \frac{(a^0)^2}{2} \Psi_{fl}\left(-\frac{\ell}{2}\right) (\delta T_{inlet}).
 \end{aligned} \tag{88}$$

Inserting the definitions provided for $Q(z)$ and $Q_{fl}(z)$ in Equations (74) and (72), respectively, into Equation (88) yields the following expression:

$$\begin{aligned}
 & \{\delta T(r_p, z_p)\}_{indirect} \\
 &= \left[(\delta k) \frac{q^0}{k^0} - (\delta q) \right] \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} \Psi(r, z) \cos \frac{\pi z}{\ell^0} dz \\
 & \quad + (\delta \ell) \frac{q^0 \pi}{(\ell^0)^2} \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} \Psi(r, z) z \sin \frac{\pi z}{\ell^0} dz \\
 & \quad + (\delta \ell) \pi^2 \frac{(a^0)^2 q^0}{W^0 c_p^0 (\ell^0)^2} \frac{(a^0)^2}{2} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) z \sin \frac{\pi z}{\ell^0} dz
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{(a^0)^2}{2} \pi \left[\frac{2a^0 q^0 (\delta a)}{W^0 c_p^0} + \frac{(a^0)^2 (\delta q)}{W^0 c_p^0} - \frac{(a^0)^2 q^0 (\delta W)}{(W^0)^2 c_p^0} \right. \\
 & \left. - \frac{(a^0)^2 q^0 (\delta c_p)}{W^0 (c_p^0)^2} \right] \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz + \frac{(a^0)^2}{2} \Psi_{fl} \left(-\frac{\ell}{2} \right) (\delta T_{inlet}) \quad (89) \\
 & + a^0 \left[(\delta h) \frac{a^0 q^0}{2h^0} - (\delta k) \frac{a^0 q^0}{2k^0} - (\delta a) \frac{q^0}{2} \left(\frac{h^0 a^0}{k^0} + 1 \right) \right] \int_{-\ell^0/2}^{\ell^0/2} \Psi(a^0, z) \cos \frac{\pi z}{\ell^0} dz.
 \end{aligned}$$

The 1st-LASS, which comprises Equations (79), (80), (83), (86) and (87), is independent of parameter variations and needs to be solved only once for each response of interest. Therefore, once the adjoint functions have been computed for the specific response, they are used in Equation (89) to obtain very efficiently all of the first-order response sensitivities to all model parameters.

It follows from Equation (89) that the respective partial sensitivities of $T(r_p, z_p)$ have the following expressions:

$$\frac{\partial T(r_p, z_p)}{\partial q} = - \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} \Psi(r, z) \cos \frac{\pi z}{\ell^0} dz + \frac{(a^0)^4}{W^0 c_p^0} \frac{\pi}{2} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz, \quad (90)$$

$$\frac{\partial T(r_p, z_p)}{\partial k} = \frac{q^0}{k^0} \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} \Psi(r, z) \cos \frac{\pi z}{\ell^0} dz - \frac{(a^0)^2 q^0}{2k^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi(a^0, z) \cos \frac{\pi z}{\ell^0} dz, \quad (91)$$

$$\frac{\partial T(r_p, z_p)}{\partial h} = \frac{(a^0)^2 q^0}{2h^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi(a^0, z) \cos \frac{\pi z}{\ell^0} dz, \quad (92)$$

$$\frac{\partial T(r_p, z_p)}{\partial W} = - \frac{\pi q^0 (a^0)^4}{2(W^0)^2 c_p^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz, \quad (93)$$

$$\frac{\partial T(r_p, z_p)}{\partial c_p} = - \frac{\pi (a^0)^4 q^0}{2W^0 (c_p^0)^2} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz, \quad (94)$$

$$\frac{\partial T(r_p, z_p)}{\partial T_{inlet}} = \frac{(a^0)^2}{2} \Psi_{fl} \left(-\frac{\ell}{2} \right) \quad (95)$$

$$\begin{aligned}
 \frac{\partial T(r_p, z_p)}{\partial \ell} &= \frac{q^0 \pi}{(\ell^0)^2} \frac{q^0 \pi}{2} \int_0^{a^0} r dr \int_{-\ell^0/2}^{\ell^0/2} \Psi(r, z) z \sin \frac{\pi z}{\ell^0} dz \\
 &+ \pi^2 \frac{(a^0)^4 q^0}{2W^0 c_p^0 (\ell^0)^2} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) z \sin \frac{\pi z}{\ell^0} dz, \quad (96)
 \end{aligned}$$

$$\begin{aligned}
 \frac{\partial T(r_p, z_p)}{\partial a} &= \pi \frac{(a^0)^3 q^0}{W^0 c_p^0} \int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz \\
 &- \frac{a^0 q^0}{2} \left(\frac{h^0 a^0}{k^0} + 1 \right) \int_{-\ell^0/2}^{\ell^0/2} \Psi(a^0, z) \cos \frac{\pi z}{\ell^0} dz, \quad (97)
 \end{aligned}$$

The following additional sensitivities arise from the direct-effect term $\{\delta T(r_p, z_p)\}^{dir}$ defined in Equation (62):

$$\frac{\partial T(r_p, z_p)}{\partial z_p} = -q^0 \frac{\pi}{\ell^0} \left[\frac{(a^0)^2 - r_p^2}{4k^0} + \frac{a^0}{2h^0} \right] \sin \frac{\pi z_p}{\ell^0} + \pi \frac{(a^0)^2 q^0}{W^0 c_p^0} \cos \frac{\pi z_p}{\ell^0}, \quad (98)$$

$$\frac{\partial T(r_p, z_p)}{\partial r_p} = -\frac{r_p^0 q^0}{2k^0} \cos \frac{\pi z_p}{\ell^0}. \quad (99)$$

Solving the 1st-LASS yields the following expressions for the adjoint functions $\Psi(r, z)$ and $\Psi_{fl}(z)$, respectively:

$$\Psi(r, z) = \delta(z - z_p) \left[-\frac{1}{a^0 h^0} + H(r - r_p) \frac{1}{k^0} \ln \frac{r}{r_p} - \frac{1}{k^0} \ln \frac{a^0}{r_p} \right], \quad (100)$$

$$\text{for } 0 \leq r, r_p \leq a^0, \quad -\frac{\ell^0}{2} \leq z, z_p \leq \frac{\ell^0}{2},$$

$$\Psi_{fl}(z) = \frac{2}{(a^0)^2} [1 - H(z - z_p)] = \frac{2}{(a^0)^2} H(z_p - z), \quad -\frac{\ell^0}{2} \leq z, z_p \leq \frac{\ell^0}{2}. \quad (101)$$

Using the results obtained in Equations (100) and (101) yields the following expressions for the integrals in Equations (90)-(97) involving the adjoint functions $\Psi(r, z)$ and $\Psi_{fl}(z)$:

$$\int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) \cos \frac{\pi z}{\ell^0} dz = \frac{2}{(a^0)^2} \int_{-\ell^0/2}^{z_p} \cos \frac{\pi z}{\ell^0} dz = \frac{2}{(a^0)^2} \frac{\ell^0}{\pi} \left(\sin \frac{\pi z_p}{\ell^0} + 1 \right), \quad (102)$$

$$\int_{-\ell^0/2}^{\ell^0/2} \Psi(a^0, z) \cos \frac{\pi z}{\ell^0} dz = -\frac{1}{a^0 h^0} \cos \frac{\pi z_p}{\ell^0} \quad (103)$$

$$\int_{-\ell^0/2}^{\ell^0/2} \Psi_{fl}(z) z \sin \frac{\pi z}{\ell^0} dz = \frac{2}{(a^0)^2} \left[-\frac{\ell^0 z_p}{\pi} \cos \frac{\pi z_p}{\ell^0} + \left(\frac{\ell^0}{\pi} \right)^2 \left(\sin \frac{\pi z_p}{\ell^0} + 1 \right) \right]. \quad (104)$$

Replacing the results obtained in Equations (100) and (101) yields the following expressions for the partial sensitivities of $T(r_p, z_p)$ with respect to all model and boundary parameters:

$$\frac{\partial T(r_p, z_p)}{\partial q} = \left[\frac{(a^0)^2 - r_p^2}{4k^0} + \frac{a^0}{2h^0} \right] \cos \frac{\pi z_p}{\ell^0} + \frac{(a^0)^2 \ell^0}{W^0 c_p^0} \left(\sin \frac{\pi z_p}{\ell^0} + 1 \right), \quad (105)$$

$$\frac{\partial T(r_p, z_p)}{\partial k} = -q^0 \frac{(a^0)^2 - r_p^2}{4(k^0)^2} \cos \frac{\pi z_p}{\ell^0}, \quad (106)$$

$$\frac{\partial T(r_p, z_p)}{\partial h} = -\frac{a^0 q^0}{2(h^0)^2} \cos \frac{\pi z_p}{\ell^0}, \quad (107)$$

$$\frac{\partial T(r_p, z_p)}{\partial W} = -\frac{q^0 \ell^0}{c_p^0} \left(\frac{a^0}{W^0} \right)^2 \left(\sin \frac{\pi z_p}{\ell^0} + 1 \right), \quad (108)$$

$$\frac{\partial T(r_p, z_p)}{\partial c_p} = -\frac{q^0 \ell^0}{W^0} \left(\frac{a^0}{c_p^0} \right)^2 \left(\sin \frac{\pi z_p}{\ell^0} + 1 \right), \quad (109)$$

$$\frac{\partial T(r_p, z_p)}{\partial T_{inlet}} = 1, \quad (110)$$

$$\begin{aligned} \frac{\partial T(r_p, z_p)}{\partial \ell} = & -\frac{q^0 \pi z}{(\ell^0)^2} \left(\frac{a^2 - r_p^2}{4k^0} + \frac{a^0}{2h^0} \right) \sin \frac{\pi z_p}{\ell^0} \\ & + \frac{(a^0)^2 q^0}{W^0 c_p^0} \left(-\frac{\pi z_p}{\ell^0} \cos \frac{\pi z_p}{\ell^0} + \sin \frac{\pi z_p}{\ell^0} + 1 \right), \end{aligned} \quad (111)$$

$$\frac{\partial T(r_p, z_p)}{\partial a} = \frac{q^0}{2} \left(\frac{a^0}{k^0} + \frac{1}{h^0} \right) \cos \frac{\pi z_p}{\ell^0} + \frac{2a^0 q^0 \ell^0}{W^0 c_p^0} \left(\sin \frac{\pi z_p}{\ell^0} + 1 \right). \quad (112)$$

$$\frac{\partial T(r_p, z_p)}{\partial z_p} = -q^0 \frac{\pi}{\ell^0} \left[\frac{(a^0)^2 - r_p^2}{4k^0} + \frac{a^0}{2h^0} \right] \sin \frac{\pi z_p}{\ell^0} + \pi \frac{(a^0)^2 q^0}{W^0 c_p^0} \cos \frac{\pi z_p}{\ell^0}, \quad (113)$$

$$\frac{\partial T(r_p, z_p)}{\partial r_p} = -\frac{r_p^0 q^0}{2k^0} \cos \frac{\pi z_p}{\ell^0}. \quad (114)$$

For verification and validation purposes, the solution of the 1st-LFSS, comprising Equations (70), (72)-(74), and (75) is presented below:

$$\begin{aligned} \delta T(r, z) = & (\delta q) \left[\frac{(a^0)^2 - r^2}{4k^0} + \frac{a}{2h^0} \right] \cos \frac{\pi z}{\ell^0} - (\delta k) \frac{q^0 \left[(a^0)^2 - r^2 \right]}{4(k^0)^2} \cos \frac{\pi z}{\ell^0} \\ & - (\delta h) \frac{a^0 q^0}{2(h^0)^2} \cos \frac{\pi z}{\ell^0} - (\delta \ell) \frac{q^0 \pi z}{(\ell^0)^2} \left[\frac{(a^0)^2 - r^2}{4k^0} + \frac{a^0}{2h^0} \right] \sin \frac{\pi z}{\ell^0} \\ & + (\delta a) \frac{q^0}{2} \left(\frac{a^0}{k^0} + \frac{1}{h^0} \right) \cos \frac{\pi z}{\ell^0} + \delta T_{fl}^0(z), \end{aligned} \quad (115)$$

where the expression of $\delta T_{fl}^0(z)$ is provided in Equation (14). It is evident that the expression provided in Equation (115) is the total differential with respect to the model and boundary parameters of the expression of $T(r, z)$ given in Equation (6). The additional sensitivities of the response $T(r_p, z_p)$ arise directly from the direct-effect term defined in Equation (62).

Notably, the 1st-LASS is solved in a manner that is “reverse/backwards” by comparison to the way in which solution proceeds for solving the 1st-LFSS as well as the original heat transport model. Thus, while the 1st-LFSS and the original heat transport model are solved by starting with the fluid flow equation (which is solved from the inlet to the outlet of the fluid flow) and subsequently solving the heat conduction equation in the rod, the solution of the 1st-LASS proceeds in the reverse manner, by first solving the heat conduction in the rod, followed by solving the fluid flow equation from the outlet to the inlet.

4. Concluding Remarks

The *first-order comprehensive adjoint sensitivity analysis methodology* (1st-CASAM) has been presented in a previous work¹. The 1st-CASAM enables the most efficient computing of the exact first-order response sensitivities for large-scale coupled nonlinear physical systems characterized by imprecisely known parameters characterizing the systems, the interfaces between systems and the systems' domain boundaries. The larger the number of imprecisely known parameters, the more efficient the 1st-CASAM becomes for computing the sensitivities of a scalar-valued response to the respective parameters.

This work has illustrated the application of the 1st-CASAM to a benchmark problem [2] [3] [4] that models heat conduction and convection in a physical system comprising an electrically heated rod surrounded by a coolant which simulates the geometry of an advanced ("Generation-IV") nuclear reactor [5]. This benchmark has deliberately been chosen for illustrative purposes, because it admits exact closed-form solutions for the sensitivities of the temperature distribution in the coupled rod/coolant system. This work has highlighted the novel finding that response sensitivities to the imprecisely known domain boundaries and interfaces can arise both from the definition of the system's response as well as from the equations, interfaces and boundary conditions that characterize the model and its imprecisely known domain. Furthermore, the novel analytical results obtained for the sensitivities of the temperature distribution in the coupled rod/coolant system to the model's internal interfaces and external boundaries can be used to benchmark thermal-hydraulics production and/or commercially-available codes, such as the FLUENT Adjoint Solver [6].

The 1st-CASAM fundamentally generalizes and extends all previously published theoretical works on this topic, enabling the quantification of the effects of manufacturing tolerances on the responses of physical and engineering systems. Ongoing research will generalize the methodology presented in this work, aiming at computing exactly and efficiently higher-order response sensitivities for coupled systems involving imprecisely known interfaces, parameters, and boundaries. As is well known [7], the availability of response sensitivities to imprecisely known parameters, interfaces and boundaries is essential for a variety of subsequent uses, including uncertainty quantification, optimization, data assimilation, model calibration and validation, and reduction of uncertainties in predicted model results.

Conflicts of Interest

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

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Nomenclature

a [m]: radius of electrically heated rod;

ℓ [m]: length of electrically heated rod and length of coolant channel;

z : coordinate along the rod's axial (customarily, the vertical) direction;

c_p [$\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$]: coolant heat capacity;

h [$\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$]: heat transfer coefficient;

k [$\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$]: rod conductivity;

q [$\text{W} \cdot \text{m}^{-3}$]: volumetric source;

T_{inlet} [K]: inlet temperature;

W [$\text{kg} \cdot \text{s}^{-1}$]: mass flow rate;

$T(r, z)$: steady-state temperature distribution within the heated rod;

$T_f(z)$: steady-state temperature distribution within the coolant (fluid).