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Shape sensitivity analysis for dimensionally-heterogeneous models

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1. Abstract
A natural question that arises when working with the so-called kinematically incompatible models is about the positioning of the internal artificial boundary that splits the domain of analysis into the sub-domains for which the different, incompatible, models are established. Although the experience in modeling might provide an *ad hoc* solution to such matter it may also draw misleading conclusions. Here, the sensitivity analysis furnishes a systematic and reliable framework to study the impact of the positioning of the artificial boundary over the solution of the problem. In this sense, the present work is concerned with the sensitivity analysis of the variational formulation corresponding to the kinematically incompatible models when the boundary over which the incompatibility between the models takes place is changed. Assuming the presence of a discontinuity in the fields over a given interface between two incompatible models, this analysis allows to measure the sensitivity of a given cost functional when the location of such interface is changed. The application for which this analysis is envisaged is to assess the correctness, or incorrectness, in the definition of the positioning of such coupling interface between dimensionally-heterogeneous domains. Also, some numerical results are provided to give numerical evidence of the usefulness of the present tool.

2. Keywords: Sensitivity analysis, Kinematically-incompatible models, Shape change.

3. Introduction
From its birth thirty years ago, the sensitivity analysis has proven to be a valuable tool to evaluate how sensible a cost functional associated to a given problem is in front of perturbations in the definition of such problem [4, 11]. This kind of analysis can be encountered under different names according to the nature of the perturbation. Thus, when the parameters that define the problem are perturbed it is referred to as parameter sensitivity analysis [8]. If the perturbations are performed along the boundary of the domain of analysis then it is referred to as shape sensitivity analysis [4, 10]. Finally, when the perturbations are singular such as modifications in the topology of the domain of analysis or discontinuous perturbations in the parameters that define the problem, then it is referred to as topological sensitivity analysis [5, 9].

Kinematically incompatible models are a class of mathematical models that allow the fields in the problem to be discontinuous over a given internal boundary. The role of this internal boundary is to establish a division in the nature of the model when thinking in terms of its kinematics. In the simplest case, a kinematically incompatible model consists of a partition of the domain of analysis into two sub-regions. Over each sub-domain a given kinematics is defined, giving rise to two different sub-models that share a common internal boundary but that are ruled by different kinematics. A theoretical account including the extended variational principles for such models was introduced in [1, 2] for fluid and solid mechanics, respectively.

A natural question that arises when working with incompatible models, when looking to the simple example involving two sub-domains, is about the positioning of the artificial boundary that splits the domain of analysis into the two sub-domains for which the different, incompatible, models will be established. Clearly, a wrong placement of such artificial boundary would produce incorrect solutions because the problem is not appropriately represented by the kinematical incompatible model. Since such internal boundary is artificial, it is not desirable that its position affects significantly the solution of the problem. Although the experience in modeling might provide an *ad hoc* solution to such matter it may also draw misleading conclusions. Hence, the need for a systematic and reliable framework is compulsory, and the sensitivity analysis furnishes such a framework in order to study the impact that a change like the one mentioned before produces over the solution of the problem. The sensitivity analysis to the change in the position of the internal boundary can be understood in two ways: (i) as the sensitivity to the shape change of both domains taking care that they move in an attached fashion, that is at the same time, or

(ii) as the sensitivity to the displacement of the discontinuity that is consequence of the incompatibility. In this work we make use of the concept of sensitivity analysis in a problem involving kinematically incompatible models so as to assess the correctness, or not, in the partitioning of a domain of analysis into two sub-domains for which different models will be used.

This work is organized as follows. In Section 4 we present the bases for the extended variational principle for kinematically incompatible models through its application to the heat transfer problem. Section 5 takes this variational formulation and carries through the sensitivity analysis to the change in the positioning of the discontinuity product of the incompatibility. Section 6 provides some numerical evidences of the usefulness of the analysis performed here. Finally, Section 7 closes the work with some final remarks and conclusions.

4. Kinematically Incompatible Models

This section gives a brief account of kinematically incompatible models in the particular case of the problem of coupling a 3D model with a 1D model for the heat transfer problem. Also, the role of the sensitivity analysis is commented in order to motivate the developments of the forthcoming sections.

4.1. Extended Variational Principle

Consider the heat transfer problem in a domain $\Omega \in \mathbb{R}^3$. A partition of Ω given by an internal boundary Γ_a, is also considered, being $\Omega = (\overline{\Omega_1 \cup \Omega_2})^\circ$. The classical variational principle poses the problem of finding a scalar field $\theta \in \mathcal{U}$ such that it satisfies a variational equation, where $\mathcal{U}$ is the space $H^1(\Omega)$ plus essential boundary conditions. A kinematical incompatibility in a model arises when a kinematical hypothesis is taken over a partition of Ω, while the kinematics for the complementary partition remains invariant (in the simple case of a partition of two sub-domains). In this situation, the field θ is now a pair (θ_1, θ_2), where both fields have their own characteristics. In the problem presented here, due to the particular form of Ω_1 (see Figure 1), over that sub-domain it is possible to make the assumption of a constant scalar field over each transversal section of the domain. Naming z the axial coordinate, the field θ_1 is just a function of that coordinate and the problem can be reduced to a 1D problem over Ω_1 that now ranges in the interval (z_a, z_b). Over Ω_2 the field θ_2 is considered to have a three dimensional description.

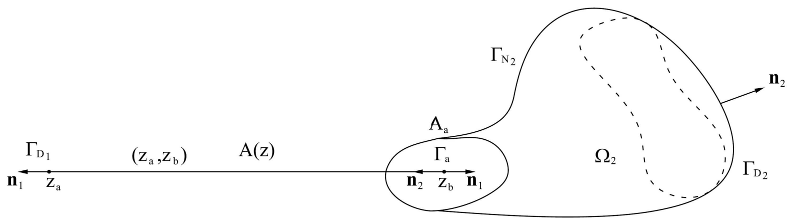

Figure 1: Schematic situation for the kinematically incompatible 3D–1D model.

The extended governing variational principle for this problem, in the steady state case, reads as follows (see [3]): for some $\gamma \in [0, 1]$ find $((\theta_1, \theta_2), t_1, t_2) \in \mathcal{U}_1 \times \mathcal{U}_2 \times \mathbb{R} \times H^{-1/2}(\Gamma_a)$ such that

$$\begin{aligned}\int_{z_a}^{z_b} \left[Ak \frac{\mathrm{d}\theta_1}{\mathrm{d}z} \frac{\mathrm{d}\eta_1}{\mathrm{d}z} - Af\eta_1 \right] \mathrm{d}z &+ \int_{\Omega_2} [k\nabla\theta_2 \cdot \nabla\eta_2 - f\eta_2] \, \mathrm{d}\mathbf{x} \\ &+ \gamma t_1 \left(\eta_1 - \frac{1}{A_a} \int_{\Gamma_a} \eta_2 \, \mathrm{d}\Gamma_a \right)\Big|_{z_b} + (1-\gamma) \int_{\Gamma_a} t_2(\eta_1 - \eta_2) \, \mathrm{d}\Gamma_a \\ &+ \gamma s_1 \left(\theta_1 - \frac{1}{A_a} \int_{\Gamma_a} \theta_2 \, \mathrm{d}\Gamma_a \right)\Big|_{z_b} + (1-\gamma) \int_{\Gamma_a} s_2(\theta_1 - \theta_2) \, \mathrm{d}\Gamma_a = 0 \\ &\qquad \forall((\eta_1, \eta_2), s_1, s_2) \in \mathcal{V}_1 \times \mathcal{V}_2 \times \mathbb{R} \times H^{-1/2}(\Gamma_a), \quad (1)\end{aligned}$$

where $A = A(z)$ is the cross-sectional area in Ω_1, k is the conductivity, f is a volume source, A_a is the measure of boundary Γ_a, and was assumed that the material has an isotropic constitutive behavior such that follows the Fourier law in both domains. Over Ω_1 the both k and f have been assumed constants across the transversal area. Also it is

$$\mathcal{U}_1 = \{\theta_1 \in H^1(]z_a, z_b[);\ \theta_{1|z_a} = \bar{\theta}_1\} \qquad \mathcal{U}_2 = \{\theta_2 \in H^1(\Omega_2);\ \theta_{2|\Gamma_{D_2}} = \bar{\theta}_2\}, \qquad (2)$$

while $\mathcal{V}_1$ and $\mathcal{V}_2$ are the spaces obtained from differences between elements in $\mathcal{U}_1$ and $\mathcal{U}_2$, respectively. The set of Euler–Lagrange equations can be straightforwardly obtained, and are not presented for the sake of brevity.

Remark. The role of the real parameter γ is to provide the sense in which the continuity of the quantities is satisfied (see [3]). Its choice is a decision that should be related to the physical characteristics of the problem that is being dealt with. Indeed, for $\gamma = 1$ the field θ is discontinuous in a pointwise sense while for $\gamma = [0, 1)$ the heat flux is discontinuous in the same strong sense.

The variational problem (1) can be expressed in compact form as follows: for some $\gamma \in [0, 1]$ find $((\theta_1, \theta_2), t_1, t_2) \in \mathcal{U}_1 \times \mathcal{U}_2 \times \mathbb{R} \times H^{-1/2}(\Gamma_a)$ such that

$$\begin{aligned} &a_{\Omega_1}(\theta_1, \eta_1) - f_{\Omega_1}(\eta_1) + a_{\Omega_2}(\theta_2, \eta_2) - f_{\Omega_2}(\eta_2) \\ &\quad + b_1(t_1, \eta_1 - \tfrac{1}{A_a}\textstyle\int_{\Gamma_a} \eta_2 \, d\Gamma_a) + b_2(t_2, \eta_1 - \eta_2) + b_1(s_1, \theta_1 - \tfrac{1}{A_a}\textstyle\int_{\Gamma_a} \theta_2 \, d\Gamma_a) + b_2(s_2, \theta_1 - \theta_2) = 0 \\ &\qquad \forall((\eta_1, \eta_2), s_1, s_2) \in \mathcal{V}_1 \times \mathcal{V}_2 \times \mathbb{R} \times H^{-1/2}(\Gamma_a). \quad (3) \end{aligned}$$

In formulating this problem, as in problem (1), it has been assumed that homogeneous boundary conditions are given over the Neumann boundaries Γ_{N1} and Γ_{N2}.

4.2. The Role of the Sensitivity Analysis

Besides the question that arises about the value of the parameter γ in formulation (1), another decision that comes before is connected with the definition of the partition of Ω, that is with the definition of Ω_1 and Ω_2. The use of the concept of sensitivity analysis comes to the scene to provide the needed tool to answer the question stated above. The study of the sensitivity with respect to the position of the boundary Γ_a (see Figures 1) can be understood in two different ways:

i. the sensitivity of the solution in front of shape changes in both domains Ω_1 and Ω_2, taking into account that they are moved together in an attached way;

ii. the sensitivity of the solution in front of the movement of the discontinuity that there exists in the field θ, that is, the sensitivity to the position of the kinematical incompatibility between the models.

Evidently, the definition of the partition of Ω is, in some sense, correct when the sensitivity of the solution is small.

5. Sensitivity Analysis

In this section we present the main theoretical contribution of the work. After laying a preliminary groundwork we present the calculation of the sensitivity of the variational equation (1) to the change in the position of the artificial boundary Γ_a for a general cost functional. Then, the generalized Eshelby tensor is identified together with the associated balance of configurational forces in our particular application (see [7]). Finally, some specific cost functionals of interest are explored.

5.1. Preliminaries

For the sake of simplicity in the calculation of the sensitivity the following considerations are taken:

i. when moving the boundary Γ_a the lateral boundary from the 3D domain is maintained completely unchanged, then no modification is allowed for the Neumann boundary Γ_{N_2} nor for the Dirichlet boundaries Γ_{D_2} and Γ_{D_1};

ii. the Neumann conditions over the lateral boundaries Γ_{N_1} and Γ_{N_2} are homogeneous as stated by (1);

iii. the conductivity k and the volume source f are constants in both domains.

The methodology employed in the calculation of the sensitivity is the Lagrangian method where the shape change of the given domain Ω is characterized by a vector field $\mathbf{v}$. According to the kinematical hypothesis introduced in deriving the coupled model (1) the velocity shape change $\mathbf{v}$ is characterized by the pair $(v_1, \mathbf{v}_2)$, where v_1 is a scalar field defined in (z_a, z_b) and $\mathbf{v}_2$ is a vector field defined in Ω_2. The shape change velocity must satisfy

$$\begin{aligned} \mathbf{v}_2 \cdot \mathbf{n}_2 &= 0 && \text{on } \Gamma_{N_2}, \\ \mathbf{v}_2 &= 0 && \text{on } \Gamma_{D_2}, \\ v_1 &= 0 && \text{at } \{z_a\}, \end{aligned} \quad (4)$$

and also

$$v_{1|z_b} = (\mathbf{v}_2 \cdot \mathbf{n}_2)|_{\Gamma_a}. \tag{5}$$

The introduction of the vector field $\mathbf{v}$ allows us to establish an analogy between this shape change velocity and the velocity field in the continuum mechanics context [6]. Using this analogy, the shape sensitivity of any expression defined in Ω can be associated to the *material time derivative of spatial fields* (see [6]). Also, the shape change velocity has to meet the following requirement

$$\frac{D}{D\tau}(A_a) = \int_{\Gamma_a} \nabla \mathbf{v}_2 \cdot (\mathbf{I} - \mathbf{n}_2 \otimes \mathbf{n}_2)\, \mathrm{d}\Gamma_a = \int_{\Gamma_a} \mathrm{div}_{\Gamma_a} \mathbf{v}_2 \, \mathrm{d}\Gamma_a, \tag{6}$$

where the operator div_{Γ_a} means the divergence with respect to the coordinates defined over Γ_a. Therefore, the last relation the shape change velocity has to satisfy is the following

$$\left(\frac{\mathrm{d}A}{\mathrm{d}z} v_1\right)\bigg|_{z_b} = \int_{\partial\Gamma_a} \mathbf{v}_2 \cdot \mathbf{m}_2 \, \mathrm{d}\partial\Gamma_a. \tag{7}$$

5.2. Shape Sensitivity Analysis for a Generic Cost Functional

The assessment of the sensitivity depends upon the definition of a given criterion which is translated in terms of a cost functional. First, let us assume a general cost function given by contributions coming from both models as follows

$$j(\Omega_1, \Omega_2) = \mathcal{J}(\Omega_1, \Omega_2, \theta_1, \tfrac{\mathrm{d}\theta_1}{\mathrm{d}z}, \theta_2, \nabla\theta_2) = \mathcal{J}_1(\Omega_1, \theta_1, \tfrac{\mathrm{d}\theta_1}{\mathrm{d}z}) + \mathcal{J}_2(\Omega_2, \theta_2, \nabla\theta_2), \tag{8}$$

where the sub-indexes denote the correspondence with models over domains Ω_1 and Ω_2. The shape sensitivity analysis of the general cost functional (8) consists in the calculation of the following total (material) derivative

$$\dot{\mathcal{J}}(\Omega_1, \Omega_2, \theta_1, \tfrac{\mathrm{d}\theta_1}{\mathrm{d}z}, \theta_2, \nabla\theta_2) = \frac{D}{D\tau} j(\Omega_1, \Omega_2) \tag{9}$$

Moreover, it is important to remark that in the above expression the variables θ_1, θ_2 and its derivatives are implicit functions of τ (the parameter that controls the shape change) since they are solution of the variational problem (3) defined in the configuration Ω_i, $i = 1, 2$.

As already said the Lagrangian method is used to calculate (9). In order to do so we relax the fact that the fields satisfy the variational problem (3), and introduce such variational equation as a restriction to be satisfied by the fields. Thus, the Lagrangian functional is defined for $((\theta_1, \theta_2), t_1, t_2) \in \mathcal{U}_1 \times \mathcal{U}_2 \times \mathbb{R} \times H^{-1/2}(\Gamma_a)$ and $((\eta_1, \eta_2), s_1, s_2) \in \mathcal{V}_1 \times \mathcal{V}_2 \times \mathbb{R} \times H^{-1/2}(\Gamma_a)$ as follows

$$\begin{aligned}
&\mathcal{L}(\Omega_1, \Omega_2, \theta_1, \theta_2, \eta_1, \eta_2, t_1, t_2, s_1, s_2) = \\
&\qquad \mathcal{J}_1(\Omega_1, \theta_1, \tfrac{\mathrm{d}\theta_1}{\mathrm{d}z}) + \mathcal{J}_2(\Omega_2, \theta_2, \nabla\theta_2) + a_{\Omega_1}(\theta_1, \eta_1) - f_{\Omega_1}(\eta_1) + a_{\Omega_2}(\theta_2, \eta_2) - f_{\Omega_2}(\eta_2) \\
&\qquad + b_1(t_1, \eta_1 - \tfrac{1}{A_a}\textstyle\int_{\Gamma_a} \eta_2 \, \mathrm{d}\Gamma_a) + b_2(t_2, \eta_1 - \eta_2) + b_1(s_1, \theta_1 - \tfrac{1}{A_a}\textstyle\int_{\Gamma_a} \theta_2 \, \mathrm{d}\Gamma_a) + b_2(s_2, \theta_1 - \theta_2).
\end{aligned} \tag{10}$$

Now, the set of variables $((\theta_1, \theta_2), t_1, t_2)$ and its derivatives are *independent* functions of τ since now the variational problem (3) was included as a relaxed constraint. While there is no ambiguity, we get rid of the functional dependence to make the notation shorter. With this consideration, it follows that

$$\begin{aligned}
\frac{D\mathcal{L}}{D\tau} = \left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{x}}, \mathbf{v} \right\rangle + \left\langle \frac{\partial \mathcal{L}}{\partial \theta_1}, \hat{\theta}_1 \right\rangle + \left\langle \frac{\partial \mathcal{L}}{\partial \theta_2}, \hat{\theta}_2 \right\rangle + \left\langle \frac{\partial \mathcal{L}}{\partial \eta_1}, \hat{\eta}_1 \right\rangle + \left\langle \frac{\partial \mathcal{L}}{\partial \eta_2}, \hat{\eta}_2 \right\rangle \\
+ \left\langle \frac{\partial \mathcal{L}}{\partial t_1}, \hat{t}_1 \right\rangle + \left\langle \frac{\partial \mathcal{L}}{\partial t_2}, \hat{t}_2 \right\rangle + \left\langle \frac{\partial \mathcal{L}}{\partial s_1}, \hat{s}_1 \right\rangle + \left\langle \frac{\partial \mathcal{L}}{\partial s_2}, \hat{s}_2 \right\rangle.
\end{aligned} \tag{11}$$

In addition, observe that it has been used the fact that $\dot{\mathbf{x}} = \mathbf{v}$ and $\dot{Z} = \hat{Z}$, for $Z = \theta_1, \theta_2, \eta_1, \eta_2, t_1, t_2, s_1, s_2$. Recall that also it is $((\hat{\eta}_1, \hat{\eta}_2), \hat{s}_1, \hat{s}_2) \in \mathcal{V}_1 \times \mathcal{V}_2 \times \mathbb{R} \times H^{-1/2}(\Gamma_a)$. Now, note that when $((\theta_1, \theta_2), t_1, t_2) = ((\theta_1^s, \theta_2^s), t_1^s, t_2^s)$ is the solution of the original variational problem we have

$$\begin{aligned}
&a_{\Omega_1}(\theta_1^s, \hat{\eta}_1) - f_{\Omega_1}(\hat{\eta}_1) + a_{\Omega_2}(\theta_2^s, \hat{\eta}_2) - f_{\Omega_2}(\hat{\eta}_2) + b_1(t_1^s, \hat{\eta}_1 - \tfrac{1}{A_a}\textstyle\int_{\Gamma_a} \hat{\eta}_2 \, \mathrm{d}\Gamma_a) + b_2(t_2^s, \hat{\eta}_1 - \hat{\eta}_2) \\
&+ b_1(\hat{s}_1, \theta_1^s - \tfrac{1}{A_a}\textstyle\int_{\Gamma_a} \theta_2^s \, \mathrm{d}\Gamma_a) + b_2(\hat{s}_2, \theta_1^s - \theta_2^s) = 0 \qquad \forall ((\hat{\eta}_1, \hat{\eta}_2), \hat{s}_1, \hat{s}_2) \in \mathcal{V}_1 \times \mathcal{V}_2 \times \mathbb{R} \times H^{-1/2}(\Gamma_a).
\end{aligned} \tag{12}$$

Due to the arbitrariness in the choice of the element $((\eta_1, \eta_2), s_1, s_2)$ we select the element denoted by $((\eta_1^a, \eta_2^a), s_1^a, s_2^a)$ (the so-called adjoint state) which satisfies the following problem (adjoint problem)

$$\left\langle \frac{\partial \mathcal{J}_1}{\partial \theta_1}, \hat{\theta}_1 \right\rangle \bigg|_{\theta_1=\theta_1^s} + \left\langle \frac{\partial \mathcal{J}_2}{\partial \theta_2}, \hat{\theta}_2 \right\rangle \bigg|_{\theta_2=\theta_2^s} + a_{\Omega_1}(\hat{\theta}_1, \eta_1^a) + a_{\Omega_2}(\hat{\theta}_2, \eta_2^a)$$
$$+ b_1(s_1^a, \hat{\theta}_1 - \tfrac{1}{A_a}\textstyle\int_{\Gamma_a} \hat{\theta}_2 \,\mathrm{d}\Gamma_a) + b_2(s_2^a, \hat{\theta}_1 - \hat{\theta}_2) + b_1(\hat{t}_1, \eta_1^a - \tfrac{1}{A_a}\textstyle\int_{\Gamma_a} \eta_2^a \,\mathrm{d}\Gamma_a) + b_2(\hat{t}_2, \eta_1^a - \eta_2^a) = 0$$
$$\forall ((\hat{\theta}_1, \hat{\theta}_2), \hat{t}_1, \hat{t}_2) \in \mathcal{V}_1 \times \mathcal{V}_2 \times \mathbb{R} \times H^{-1/2}(\Gamma_a). \quad (13)$$

Hereafter it will be denoted directly $\mathcal{S} = ((\theta_1, \theta_2), t_1, t_2)$ and $\mathcal{A} = ((\eta_1, \eta_2), s_1, s_2)$, so we have $\mathcal{S}^s = ((\theta_1^s, \theta_2^s), t_1^s, t_2^s)$ and $\mathcal{A}^a = ((\eta_1^a, \eta_2^a), s_1^a, s_2^a)$. Using the above results in (11) yields

$$\dot{\mathcal{J}} = \frac{Dj}{D\tau} = \frac{D\mathcal{L}}{D\tau}\bigg|_{\substack{\mathcal{S}=\mathcal{S}^s\\ \mathcal{A}=\mathcal{A}^a}} = \left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{x}}, \mathbf{v} \right\rangle \bigg|_{\substack{\mathcal{S}=\mathcal{S}^s\\ \mathcal{A}=\mathcal{A}^a}} = \frac{\partial \mathcal{L}}{\partial \tau}\bigg|_{\substack{\mathcal{S}=\mathcal{S}^s\\ \mathcal{A}=\mathcal{A}^a}}. \quad (14)$$

Then, the sensitivity can be assessed through the calculation of the partial derivative of $\mathcal{L}$ with respect to τ, and then by evaluating such derivative at states $\mathcal{S}^s$ and $\mathcal{A}^a$. To do that it is necessary to make use of the classical expressions of the material derivatives of spatial fields.

5.3. Boundary Integral Form of the Sensitivity and the Eshelby Tensor

Assume now that both cost functionals $\mathcal{J}_1$ and $\mathcal{J}_2$ in (8) have the following more specific forms

$$\mathcal{J}_1(\Omega_1, \theta_1, \tfrac{\mathrm{d}\theta_1}{\mathrm{d}z}) = \int_{z_a}^{z_b} A \mathcal{F}_1(\theta_1, \tfrac{\mathrm{d}\theta_1}{\mathrm{d}z}) \,\mathrm{d}z \qquad \mathcal{J}_2(\Omega_2, \theta_2, \nabla\theta_2) = \int_{\Omega_1} \mathcal{F}_2(\theta_2, \nabla\theta_2) \,\mathrm{d}\mathbf{x}. \quad (15)$$

Proper choices for $\mathcal{F}_1$ and $\mathcal{F}_2$ will lead to energy-based cost functionals as will be seen in next sections. Also, from (14) it is necessary to calculate the following terms

$$\begin{aligned} \frac{\partial \mathcal{J}_1}{\partial \tau}\bigg|_{\mathcal{S}=\mathcal{S}^s} &= \int_{z_a}^{z_b} \left[-A \frac{\partial \mathcal{F}_1}{\partial \frac{\mathrm{d}\theta_1}{\mathrm{d}z}}\bigg|_{\mathcal{S}=\mathcal{S}^s} \frac{\mathrm{d}v_1}{\mathrm{d}z}\frac{\mathrm{d}\theta_1^s}{\mathrm{d}z} + \frac{\mathrm{d}A}{\mathrm{d}z}\mathcal{F}_1\bigg|_{\mathcal{S}=\mathcal{S}^s} v_1 + A\mathcal{F}_1\bigg|_{\mathcal{S}=\mathcal{S}^s} \frac{\mathrm{d}v_1}{\mathrm{d}z} \right] \mathrm{d}z, \\ \frac{\partial \mathcal{J}_2}{\partial \tau}\bigg|_{\mathcal{S}=\mathcal{S}^s} &= \int_{\Omega_2} \left[-\frac{\partial \mathcal{F}_2}{\partial \nabla\theta_2}\bigg|_{\mathcal{S}=\mathcal{S}^s} \cdot (\nabla \mathbf{v}_2)^T \nabla\theta_2^s + \mathcal{F}_2\bigg|_{\mathcal{S}=\mathcal{S}^s} \operatorname{div} \mathbf{v}_2 \right] \mathrm{d}\mathbf{x}. \end{aligned} \quad (16)$$

With such choices, after some calculus and manipulations, it can be shown that for our coupled problem it is

$$\begin{aligned} \dot{\mathcal{J}} = \frac{\partial \mathcal{L}}{\partial \tau}\bigg|_{\substack{\mathcal{S}=\mathcal{S}^s\\ \mathcal{A}=\mathcal{A}^a}} &= \int_{z_a}^{z_b} \left[\frac{\mathrm{d}A}{\mathrm{d}z}\mathcal{F}_1\bigg|_{\mathcal{S}=\mathcal{S}^s} v_1 + A\frac{\mathrm{d}v_1}{\mathrm{d}z}\left(\mathcal{F}_1\bigg|_{\mathcal{S}=\mathcal{S}^s} - \frac{\partial \mathcal{F}_1}{\partial \frac{\mathrm{d}\theta_1}{\mathrm{d}z}}\bigg|_{\mathcal{S}=\mathcal{S}^s} \frac{\mathrm{d}\theta_1^s}{\mathrm{d}z} \right) \right] \mathrm{d}z \\ &+ \int_{\Omega_2} \left[\mathcal{F}_2\bigg|_{\mathcal{S}=\mathcal{S}^s} \mathbf{I} - \nabla\theta_2^s \otimes \frac{\partial \mathcal{F}_2}{\partial \nabla\theta_2}\bigg|_{\mathcal{S}=\mathcal{S}^s} \right] \cdot \nabla \mathbf{v}_2 \,\mathrm{d}\mathbf{x} + \int_{z_a}^{z_b} \left[\frac{\mathrm{d}A}{\mathrm{d}z} k \frac{\mathrm{d}\theta_1^s}{\mathrm{d}z}\frac{\mathrm{d}\eta_1^a}{\mathrm{d}z} v_1 - A\frac{\mathrm{d}v_1}{\mathrm{d}z} k \frac{\mathrm{d}\theta_1^s}{\mathrm{d}z}\frac{\mathrm{d}\eta_1^a}{\mathrm{d}z} \right] \mathrm{d}z \\ &+ \int_{\Omega_2} [k(\nabla\theta_2^s \cdot \nabla\eta_2^a)\mathbf{I} - k(\nabla\theta_2^s \otimes \nabla\eta_2^a + \nabla\eta_2^a \otimes \nabla\theta_2^s)] \cdot \nabla \mathbf{v}_2 \,\mathrm{d}\mathbf{x} \\ &- \int_{z_a}^{z_b} \left[\frac{\mathrm{d}A}{\mathrm{d}z} f\eta_1^a v_1 + A\frac{\mathrm{d}v_1}{\mathrm{d}z} f\eta_1^a \right] \mathrm{d}z - \int_{\Omega_2} f\eta_2^a \mathbf{I} \cdot \nabla \mathbf{v}_2 \,\mathrm{d}\mathbf{x} \\ &+ t_1^s \frac{1}{A_a}\left[\frac{\mathrm{d}A_a}{\mathrm{d}z} v_1 \eta_1^a - \int_{\Gamma_a} \eta_2^a \operatorname{div}_{\Gamma_a} \mathbf{v}_2 \,\mathrm{d}\Gamma_a \right]\bigg|_{z_b} + s_1^a \frac{1}{A_a}\left[\frac{\mathrm{d}A_a}{\mathrm{d}z} v_1 \theta_1^s - \int_{\Gamma_a} \theta_2^s \operatorname{div}_{\Gamma_a} \mathbf{v}_2 \,\mathrm{d}\Gamma_a \right]\bigg|_{z_b}. \end{aligned} \quad (17)$$

In order to recast expression (17) as a boundary integral it is necessary to introduce the so-called generalized Eshelby tensor. Consider the definition of the following quantities

$$\begin{aligned} \Sigma_1 &= A\left[\mathcal{F}_1\bigg|_{\mathcal{S}=\mathcal{S}^s} - \frac{\partial \mathcal{F}_1}{\partial \frac{\mathrm{d}\theta_1}{\mathrm{d}z}}\bigg|_{\mathcal{S}=\mathcal{S}^s} \frac{\mathrm{d}\theta_1^s}{\mathrm{d}z} - k\frac{\mathrm{d}\theta_1^s}{\mathrm{d}z}\frac{\mathrm{d}\eta_1^a}{\mathrm{d}z} - f\eta_1^a \right], \\ \mathbf{\Sigma}_2 &= \mathcal{F}_2\bigg|_{\mathcal{S}=\mathcal{S}^s} \mathbf{I} - \nabla\theta_2^s \otimes \frac{\partial \mathcal{F}_2}{\partial \nabla\theta_2}\bigg|_{\mathcal{S}=\mathcal{S}^s} + k(\nabla\theta_2^s \cdot \nabla\eta_2^a)\mathbf{I} - k(\nabla\theta_2^s \otimes \nabla\eta_2^a + \nabla\eta_2^a \otimes \nabla\theta_2^s) - f\eta_2^a \mathbf{I}. \end{aligned} \quad (18)$$

After some manipulations and the use of the Euler–Lagrange equations corresponding to the direct and adjoint states, it is possible to show the following property of the generalized Eshelby tensor

$$\begin{cases} \dfrac{\mathrm{d}\Sigma_1}{\mathrm{d}z} = \dfrac{\mathrm{d}A}{\mathrm{d}z}\left(\mathcal{F}_1\bigg|_{\mathcal{S}=\mathcal{S}^s} + k\dfrac{\mathrm{d}\theta_1^s}{\mathrm{d}z}\dfrac{\mathrm{d}\eta_1^a}{\mathrm{d}z} - f\eta_1^a \right) & \text{in } (z_a, z_b), \\ \operatorname{div} \mathbf{\Sigma}_2 = 0 & \text{in } \Omega_2. \end{cases} \quad (19)$$

These expressions are recognized as the balances of configurational forces associated to the shape change in both domains Ω_1 and Ω_2 of our problem.

Using the Green's formula in (17) and the balances of configurational forces (19) allows us to find

$$\dot{\mathcal{J}} = \Sigma_1 v_1\Big|_{z_b} + \int_{\Gamma_a} \boldsymbol{\Sigma}_2 \mathbf{n}_2 \cdot \mathbf{v}_2 \, \mathrm{d}\Gamma_a + \int_{\Gamma_{N2}} \boldsymbol{\Sigma}_2 \mathbf{n}_2 \cdot \mathbf{v}_2 \, \mathrm{d}\Gamma$$
$$+ t_1^s \frac{1}{A_a} \left[\frac{\mathrm{d}A_a}{\mathrm{d}z} v_1 \eta_1^a - \int_{\Gamma_a} \eta_2^a \operatorname{div}_{\Gamma_a} \mathbf{v}_2 \, \mathrm{d}\Gamma_a \right]\Bigg|_{z_b} + s_1^a \frac{1}{A_a} \left[\frac{\mathrm{d}A_a}{\mathrm{d}z} v_1 \theta_1^s - \int_{\Gamma_a} \theta_2^s \operatorname{div}_{\Gamma_a} \mathbf{v}_2 \, \mathrm{d}\Gamma_a \right]\Bigg|_{z_b}. \quad (20)$$

Note that the shape sensitivity (20) depends upon the state and adjoint variables evaluated at the configuration Ω_i, $i = 1, 2$. Then, and from the computational point of view the shape sensitivity is easily achieved through a simple post-processing computation.

5.4. Sensitivity of Energy-Based Cost Functionals

Consider now that the contributions of $\mathcal{J}_1$ and $\mathcal{J}_2$ for the cost functional (8) have the following forms

$$\mathcal{J}_1(\Omega_1, \tfrac{\mathrm{d}\theta_1}{\mathrm{d}z}) = \frac{1}{2} \int_{z_a}^{z_b} Ak \left(\frac{\mathrm{d}\theta_1}{\mathrm{d}z} \right)^2 \mathrm{d}z \qquad \mathcal{J}_2(\Omega_2, \nabla\theta_2) = \frac{1}{2} \int_{\Omega_2} k |\nabla\theta_2|^2 \, \mathrm{d}\mathbf{x}, \quad (21)$$

which account for the internal energy of each one of the domains. Then, from (20) we reach

$$\dot{\mathcal{J}} = A\left[-\frac{1}{2} k \left(\frac{\mathrm{d}\theta_1^s}{\mathrm{d}z} \right)^2 - k \frac{\mathrm{d}\theta_1^s}{\mathrm{d}z} \frac{\mathrm{d}\eta_1^a}{\mathrm{d}z} - f\eta_1^a \right] v_1 \Bigg|_{z_b} + \int_{\Gamma_a} \left(\frac{1}{2} k |\nabla\theta_2^s|^2 + k(\nabla\theta_2^s \cdot \nabla\eta_2^a) - f\eta_2^a \right) \mathbf{n}_2 \cdot \mathbf{v}_2 \, \mathrm{d}\Gamma_a$$
$$- \int_{\Gamma_a} k(\nabla\theta_2^s \otimes \nabla\theta_2^s + \nabla\theta_2^s \otimes \nabla\eta_2^a + \nabla\eta_2^a \otimes \nabla\theta_2^s) \mathbf{n}_2 \cdot \mathbf{v}_2 \, \mathrm{d}\Gamma_a$$
$$+ t_1^s \frac{1}{A_a} \left[\frac{\mathrm{d}A_a}{\mathrm{d}z} v_1 \eta_1^a - \int_{\Gamma_a} \eta_2^a \operatorname{div}_{\Gamma_a} \mathbf{v}_2 \, \mathrm{d}\Gamma_a \right]\Bigg|_{z_b} + s_1^a \frac{1}{A_a} \left[\frac{\mathrm{d}A_a}{\mathrm{d}z} v_1 \theta_1^s - \int_{\Gamma_a} \theta_2^s \operatorname{div}_{\Gamma_a} \mathbf{v}_2 \, \mathrm{d}\Gamma_a \right]\Bigg|_{z_b}. \quad (22)$$

This formula provides the sensitivity of the cost functional $\mathcal{J} = \mathcal{J}_1 + \mathcal{J}_2$ as a function of the shape change velocity which is characterized by the pair $(v_1, \mathbf{v}_2)$, more specifically by $(v_{1|z_b}, \mathbf{v}_{2|\Gamma_a})$.

6. Numerical Results

In this section two examples of applications are developed. Firstly, a brief comment on the use of the sensitivity is presented.

6.1. Sensitivity Factors

Our main goal is to employ the value of $\dot{\mathcal{J}}$ to assess the quality of the partitioning of an original problem into coupled dimensionally-heterogeneous models. In order to do so, we define the following shape sensitivity factor

$$\mathsf{f_{ss}} = |\lambda(\ln \mathcal{J})^{\cdot}| = \frac{\lambda|\dot{\mathcal{J}}|}{\mathcal{J}}, \quad (23)$$

which measures an specific change in the value of $\mathcal{J}$ with respect to the energy per unit of length λ, being λ a characteristic length within the model. Because we are dealing with energy-based functionals, the factor $\mathsf{f_{ss}}$ measures the relative alteration in the energy of the system, given by the contributions of the 3D and 1D sub-systems, that is $\mathcal{J} = \mathcal{J}_1 + \mathcal{J}_2$. Nonetheless, since in our examples most of the energy is stored in the 3D model, we change it to

$$\tilde{\mathsf{f}}_{\mathsf{ss}} = \frac{\lambda_1|\dot{\mathcal{J}}|}{\mathcal{J}_1}, \quad (24)$$

where we measure the sensitivity relative to the energy stored in the 1D model per unit of length. Thus, λ_1 is the length of the 1D model, what provides us with a reference value for the energy stored in the 1D model per unit of area, that is $\frac{\mathcal{J}_1}{\lambda_1}$. Certainly, this choice might change according to the application.

In a real problem, we pre-define a degree of correctness based on the value of this factor $\tilde{\mathsf{f}}_{\mathsf{ss}}$, say $\tilde{\mathsf{f}}^{\mathsf{c}}_{\mathsf{ss}}$. Hence, a given 3D–1D model is a *good* model, regarding the partitioning of the original domain into 1D and 3D models, when the sensitivity analysis yields $\tilde{\mathsf{f}}_{\mathsf{ss}} < \tilde{\mathsf{f}}^{\mathsf{c}}_{\mathsf{ss}}$.

6.2. Case 1

This first case shows the simplest situation we could imagine. Figure 2 sketches the problem in a cylindrical domain with radius R and length L (the top part of the figure). Over the leftmost and rightmost boundaries (corresponding to 1D and 3D domains respectively) homogeneous Dirichlet boundary conditions are considered. Also, over te transversal cylinder a non-homogeneous Dirichlet boundary condition is considered. Also in that figure two possible representations are given, cases (i) and (ii), according to the placement of the coupling interface. In this example we pre-define $\tilde{\mathsf{f}}_{\mathsf{ss}}^{\mathsf{c}} = 1.0 \cdot 10^{-2}$ and we look for that model which satisfies $\tilde{\mathsf{f}}_{\mathsf{ss}} < \tilde{\mathsf{f}}_{\mathsf{ss}}^{\mathsf{c}}$.

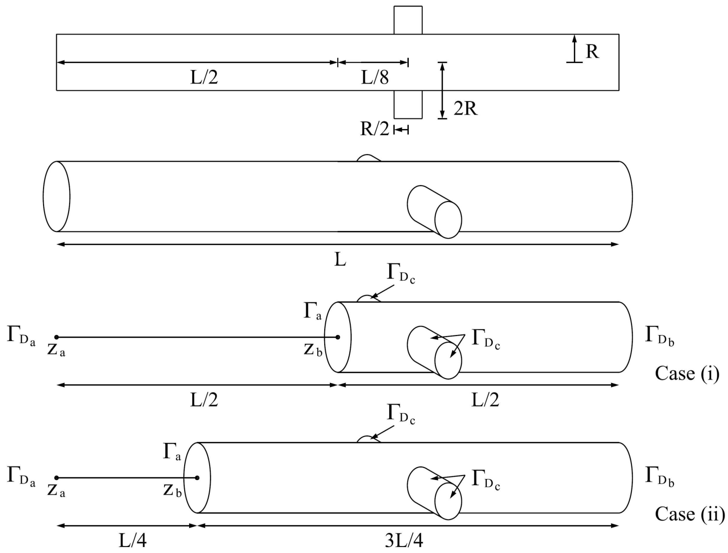

Figure 2: Scheme for case 1. Representation through coupled models.

According to Figure 2 and to equation (1) we have $\Gamma_{D1} = \Gamma_{Da} = \{z_a\}$ and $\Gamma_{D2} = \Gamma_{Db} \cup \Gamma_{Dc}$. The geometrical parameters that define this problem are $L = 20$, $R = 1$, and thus $A = \pi R^2 = \pi$, $\theta_{|\Gamma_{Da}} = 0$, $\theta_{|\Gamma_{Db}} = 0$, $\theta_{|\Gamma_{Dc}} = 100$, while the rest of the lateral boundary has an homogeneous Neumann boundary condition. The physical parameters are $k = 1$ and $f = 0$. For this problem we consider that the characteristic length is the length of the 1D model, and therefore $\lambda_1^{(i)} = \frac{L}{2}$ and $\lambda_1^{(ii)} = \frac{L}{4}$.

Figure 3 presents the results of the direct problem. The figures on the left do not convey any conclusive result and here is where we resort to the calculation of the sensitivity. When we look at the coupling interfaces, where we plot the value $\theta^s_{2|\Gamma_a} - \theta^s_{1|z_b}$ (taking out the mean value) it can be observed that the discontinuity is more noticeable in the Case (i).

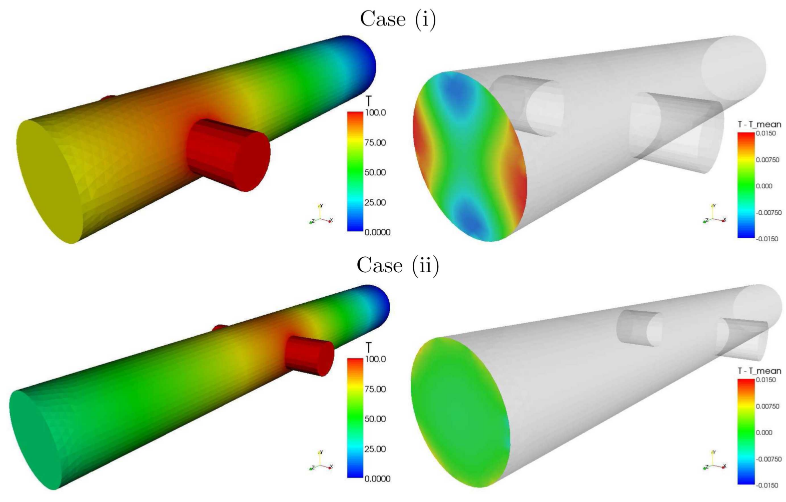

Figure 3: Results of the direct problem and detail of the coupling interface.

In this particular case the adjoint state $((\eta_1^a, \eta_2^a), s_1^a)$ is also null. Thus, taking into account that $f = 0$, k is constant, $\mathbf{v}_2 = -\mathbf{n}_2$ and that $v_1 = 1$ (here we assume a displacement of Γ_a in the direction of the 3D domain) the expression of the sensitivity is simplified to

$$\dot{\mathcal{J}} = \frac{1}{2} k \int_{\Gamma_a} \left(|\nabla \theta_2^s|^2 - \left(\frac{\mathrm{d}\theta_1^s}{\mathrm{d}z} \right)^2 \right) \mathrm{d}\Gamma_a. \tag{25}$$

This expression clearly states that the sensitivity is associated with the flux of energy between the representations given by the 1D model and the 3D model. As a matter of fact, the first term represents the energy lost by the system because the 3D model is becoming shorter, whereas the second term denotes the energy gained by the system because the 1D model is becoming larger.

The calculation of the sensitivity for both cases yielded

$$\text{Case (i)}: \quad \tilde{\mathsf{f}}_{\mathsf{ss}} = 4.624 \cdot 10^{-3} < \tilde{\mathsf{f}}_{\mathsf{ss}}^{\mathsf{c}} \qquad \text{Case (ii)}: \quad \tilde{\mathsf{f}}_{\mathsf{ss}} = 4.536 \cdot 10^{-3} < \tilde{\mathsf{f}}_{\mathsf{ss}}^{\mathsf{c}}. \tag{26}$$

This tells us, through $\tilde{\mathsf{f}}_{\mathsf{ss}}$, that both cases are in fact quite good representations of the original problem according to the value established for $\tilde{\mathsf{f}}_{\mathsf{ss}}^{\mathsf{c}}$. As expected, the Case (ii) is closer from the original problem than the Case (i) which is determined by the lower value of the sensitivity factor.

6.3. Case 2

In this second example we introduce the fact that the area of the 3D model is not constant. Figure 4 is a scheme of the problem. All the geometrical quantities are specified in such figure. Over the leftmost boundary (1D boundary) an homogeneous Dirichlet boundary condition is considered. Over the rightmost boundary and part of the lateral boundary (3D boundaries) Dirichlet conditions are imposed. Two possible representations are given for this problem, namely, cases (i) and (ii) that correspond to different placements of the coupling interface (shown also in Figure 4). As in the previous example we again pre-define $\tilde{\mathsf{f}}_{\mathsf{ss}}^{\mathsf{c}} = 1.0 \cdot 10^{-2}$ as the threshold which determines whether a certain kinematically incompatible model is a good approximation of the original one.

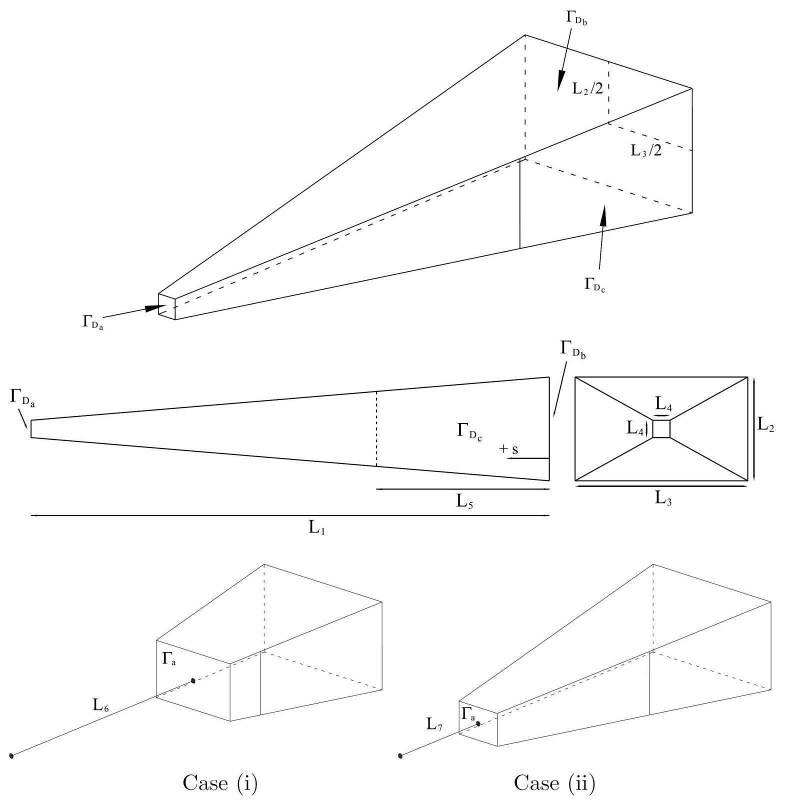

Figure 4: Scheme for case 2. Representation through coupled models.

According to Figure 4 we have $\Gamma_{D1} = \Gamma_{Da} = \{z_a\}$ (the anterior boundary) and $\Gamma_{D2} = \Gamma_{Db} \cup \Gamma_{Dc}$ (the posterior and a portion of the lateral boundary respectively). The problem is completely defined by setting

$L_1 = 60$, $L_2 = 12$, $L_3 = 20$, $L_4 = 2$ and $L_5 = 20$. We take $\theta_{|\Gamma_{D_a}} = 0$, $\theta_{|\Gamma_{D_b}}(x, y) = 100 \cos\left(\frac{\pi x}{L_3}\right) \cos\left(\frac{\pi y}{L_2}\right)$ (x, y are the coordinates in the plane, with the origin located in its center), $\theta_{|\Gamma_{D_c}}(s) = 100 \sin\left(\frac{\pi s}{2L_5}\right)$ (observe the dependence upon the s coordinate, which is aligned with the z coordinate), whilst the rest of lateral boundary has an homogeneous Neumann boundary condition. The physical parameters are, again, $k = 1$ and $f = 0$. The two cases for which the sensitivity is calculated are defined with $L_6 = 35$ and $L_7 = 15$ (see Figure 4). Once again we consider that the characteristic length is the length of the 1D model, i.e. $\lambda_1^{(i)} = L_6$ and $\lambda_1^{(ii)} = L_7$.

The calculation of the sensitivity for both cases leads to

$$\text{Case (i)}: \quad \tilde{\mathsf{f}}_{\mathsf{ss}} = 8.6669 \cdot 10^{-1} > \tilde{\mathsf{f}}^{\mathsf{c}}_{\mathsf{ss}} \qquad\qquad \text{Case (ii)}: \quad \tilde{\mathsf{f}}_{\mathsf{ss}} = 4.3386 \cdot 10^{-3} < \tilde{\mathsf{f}}^{\mathsf{c}}_{\mathsf{ss}}. \tag{27}$$

Hence, we conclude that just the Case (ii) is a good representation of the original problem. Figure 5 shows the results of the direct problem for both cases, supporting the previous statement. For Case (i) the distribution of the field over the coupling interface is far from being constant, which is the main assumption taken when the model is reduced to a 1D representation. On the other hand, for Case (ii) we observe that the distribution over the coupling interface is almost constant, which is in agreement with the characteristic hypothesis of the 1D model.

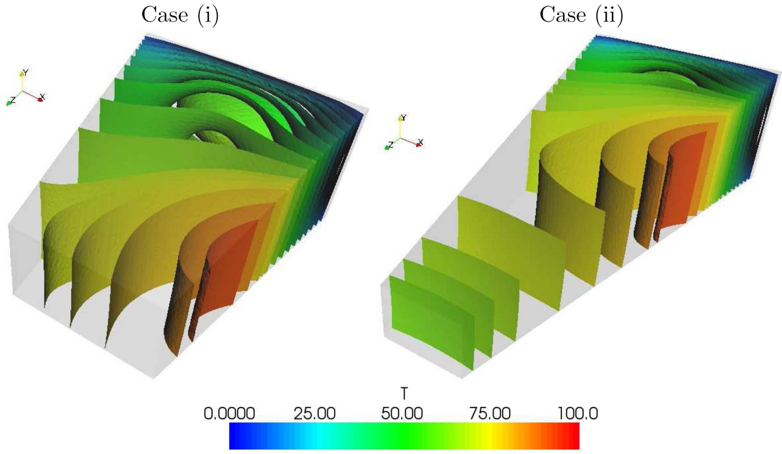

Figure 5: Iso-surfaces of field θ_2^s for both cases.

If we compare both solutions over the 1D domains, see Figure 6, we see that they are almost identical. This comparison tells us that although both representations render similar mean distributions, just one of them is cabale of representing accurately the essential phenomena in the 3D domain.

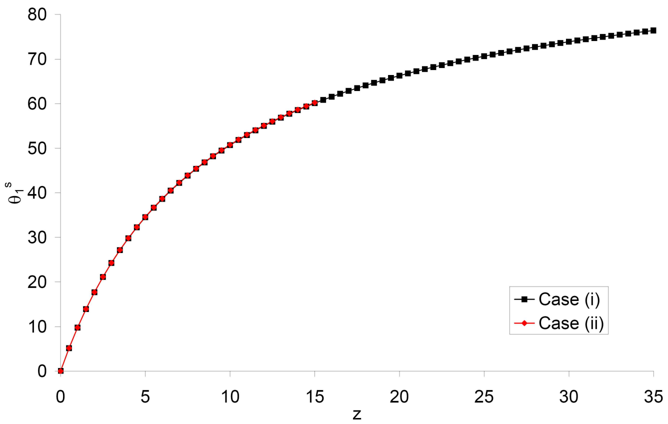

Figure 6: Distribution of θ_1^s in the 1D domains.

7. Conclusions

This work has been concerned with the application of the shape sensitivity analysis to a new kind of problem. Specifically, it has been employed to assess the suitability in the representation of a system via a given partitioning through kinematically incompatible models (dimensionally-heterogeneous models). Thus, the need for introducing concepts borrowed from the continuum mechanics and the variational theory to deal with the presence of a discontinuity has been established and elucidated. In view of the natural question related to the placement of the coupling interface (where the discontinuity is manifested) between dimensionally-heterogeneous models, the present study has proven to be a valuable tool in order to provide a systematic procedure for analysis. This has been shown along the theoretical development and confirmed by the results obtained in the numerical experiments.

8. Acnknowledgements

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