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Remarks on variational shape sensitivity analysis based on local coordinates

F.-J. Barthold

Numerical Methods and Information Processing, Technische Universität Dortmund, August-Schmidt-Strasse 8, D-44221 Dortmund, Germany

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ABSTRACT

Shape and topological sensitivity analysis are two closely related research fields of both theoretical and computational mechanics with a high impact on any analytical and numerical approach in structural optimisation. There are close connections to configurational mechanics describing cracks and dislocations as well as to biomechanics observing growth and morphogenesis. Different approaches exist to compute the gradients needed by nonlinear programming algorithms. But it is of utmost importance to acknowledge that mainly a rigorous analysis of the sensitivities provides the deep insight into the nature of the mechanical problems needed to model and to solve inverse problems efficiently.

This paper outlines the author's concept of an *intrinsic formulation in local coordinates* of continuum mechanics which extends Noll's *intrinsic concept* to variable material bodies. This viewpoint is derived by a thorough analysis of their manifold properties and yields the separation of the *phenomena in material space* from the *motion in physical space*. The subsequent variational shape sensitivity analysis is formulated and compared to known approaches.

The interactions with computational techniques such as *computer aided geometrical design* (CAGD), the *finite element method* (FEM) and the *boundary element method* (BEM) are highlighted. Furthermore, the implications on the numerical algorithms for the discrete sensitivity analysis are outlined. Finally, the challenges of a *singular value decomposition* (SVD) of the resulting sensitivities are discussed.

1. Introduction

Engineering analysis applied to a broad spectrum of problems from solid mechanics is based on either the finite element method (FEM), or the boundary element method (BEM) or on a combination of both. The following steps can be recognised in modelling and simulation of all mechanical phenomena.

(i) Field theories are used to formulate basics of kinematics, equilibrium and material laws.
(ii) Strong and weak equilibrium conditions are formulated for continuous solutions.
(iii) Approximation schemes yield the algebraic equations characterising discrete solutions.
(iv) Implementations of the numerical algorithms lead to executable programs.
(v) Applications of these numerical schemes solve engineering problems.

The known theoretical and computational approaches to shape sensitivity analysis can be linked to the different stages in the modelling and the simulation process.

1.1. Overview on methods for sensitivity analysis

The research on sensitivity analysis was initiated from the needs of nonlinear programming, i.e. the gradients of objectives and constraints with respect to a finite number of scalar valued design variables must be supplied. Hence, several methods have been developed to generate these numbers for a large spectrum of problems. Roughly, four different approaches to sensitivity analysis are well known, i.e. the *finite difference approach*, the *automatic differentiation approach*, the *discrete analytical approach* and the *continuous variational approach*. All four strategies finally yield the correct sensitivity values up to manageable deviations, e.g. due to the finite difference approximation error. Thus, the quality of the numerical gradient values can be practically ensured. The advantages and disadvantages of the different approaches have been reported in literature in full length and can be summarised as follows.

A finite difference approach is based on step (v). Here, repeated applications of the executable program with perturbed input data generate the desired sensitivity values. This approach requires almost no theoretical knowledge of the underlying problem but has exorbitant demands on the computing power in case of large analysis and design problems.

An automatic differentiation approach refers to step (iv). The implemented discrete equations are manipulated on the source

E-mail address: franz-joseph.barthold@tu-dortmund.de

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code level by techniques such as function overloading to generate the corresponding derivative code, see e.g. [1]. The gradients are efficiently computed for an increasing number of applications. Nevertheless, there is no increase of profound knowledge because all details are hidden to the user.

An analytical approach focuses on the exact derivatives of the discrete formulation with respect to e.g. nodal point coordinates or other scalar design variables and is based on step (iii), see e.g. [2]. The major reservation to this approach is the fact that a high effort is dedicated to differentiate the discrete formulation which must be repeated almost from scratch for any other problem.

A variational approach is based on step (ii) and design variations of the continuous problem formulations are performed, see e.g. [3]. Two approaches are widely known, i.e. the *material derivative approach* (MDA), see e.g. [4], and the *domain parametrisation approach* (DPA), see e.g. [5,6]. In general, the variational approaches are considered as far to complicated especially for practical engineering problems. But theoretical rigour pays off with a superior computational behaviour as it was shown in literature.

The different approaches should be compared by the efforts needed for their theoretical development, the complexity of the corresponding software implementation and their final computational performance. There is no general and unique choice for all inverse engineering problems. More details are also available e.g. in [7–9] and the references therein.

1.2. Improved concept for shape sensitivity analysis

The classical continuum mechanical field theory, see e.g. [10,11], the FEM, see e.g. [12] or the BEM, see e.g. [13–15], have been developed without any interactions to the field of computer aided geometrical design (CAGD), see e.g. [16]. Thus, the foundations of structural optimisation have been derived almost independently from each other.

Phenomena such as cracking, phase transitions and dislocations occurring in configurational mechanics [17], or growth and morphogenesis observed in biomechanics [18,19] should not be modelled using the classical assumptions in continuum mechanics, i.e. a fixed and closed system during a physical deformation. All above-mentioned approaches use the classical presentation although especially shape modifications are non-classical.

The question is how to integrate modifications of the material body, its mass and its shape canonically into continuum mechanics with a minimal and optimal enhancement of its theoretical foundation?

This objective is achieved by tracing, highlighting and separating the influences of design dependent (reference) configurations and time dependent deformation processes in continuum mechanics. The corresponding scheme to fulfil this task is closely related to the intrinsic viewpoint proposed by Noll [20]. An integrated approach of variations within direct analysis and variational design sensitivity analysis in line with the considerations made above has been developed over the last decade. Firstly, e.g. [21] and up to about 1998, independently and without any knowledge of the intrinsic ideas of Noll. Since then, and with an increasing interest, understanding and sympathy, in line with the novel presentation [20,22,23]. Several mechanical phenomena have been considered from both theoretical and computational point of view, see [21,24–30].

This paper summarises the basic ideas starting from the kinematical background on the continuum mechanical level and ending with an investigation of the sensitivity information on the discrete level.

1.3. Outline of the paper

The kinematical background of the continuum mechanical field theories, i.e. the concept of a *differentiable manifold*, is discussed in Section 2, and a *local representation* with two mutually independent mappings is highlighted. The functional dependencies of continuum mechanical quantities from design and time are traced in detail in Section 3, and the advocated viewpoint for sensitivity analysis is explained. The following three sections treat the gradients and tangent mappings (Section 4), the strain and stress tensors (Section 5) as well as different equilibrium conditions (Section 6). Here, the local formulation is given and the corresponding variations are derived. Section 7 deals with the sensitivity analysis on the continuous and discrete level. The considerations allow a novel examination of the sensitivity information via a *singular value decomposition* (SVD) (Section 8). The paper ends up with the summary in Section 9.

1.4. Notation

The Kronecker delta δ_{ij} with values $\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for $i \neq j$ as well as the Einstein summation convention over repeated indices are frequently used. Scalars and scalar functions are represented in italic shape, i.e. for Latin letters a, b, A, C or for Greek letters $\alpha, \beta, \Gamma, \Theta$. Vectors are written using boldface letters in upright shape, e.g. $\mathbf{X}, \mathbf{x}, \mathbf{u}$ and with the Einstein summation convention as $\mathbf{x} = \sum_{i=1}^{3} x^i \mathbf{g}_i = x^i \mathbf{g}_i$. The corresponding matrix of vector coefficients or coordinates is denoted by boldface letters in italic shape, i.e. $\boldsymbol{x} = [x^i] = [x^1, x^2, x^3]^{\mathrm{T}}$. Tensors of second order are printed using a boldface sans serif font, e.g. $\mathsf{T} = T^{ij} \mathbf{g}_i \otimes \mathbf{g}_j$. The corresponding matrix of tensor coefficients is again written in bold letters and italic shape, i.e. $\boldsymbol{T} = [T^{ij}]$. Tensors of higher order are printed in a hollowed Roman font, i.e. $\mathbb{C} = C^{ijkl} \mathbf{g}_i \otimes \mathbf{g}_j \otimes \mathbf{g}_k \otimes \mathbf{g}_l$. This font can be distinguished from the blackboard bold font used to denote the real numbers $\mathbb{R}$, the Euclidean point space $\mathbb{E}^3$ and the Euclidean vector spaces $\mathbb{V}^3$ and $\mathbb{Z}^3$. Sets are denoted using the upright Roman font like U and D. Quantities of the material body are expressed using a Fraktur alphabet, i.e. the material point $\mathfrak{x}$, the material body $\mathfrak{B}$, the balls $\mathfrak{U}$ around $\mathfrak{x}$ and the corresponding atlas $\mathfrak{A}$. The gradient and divergence operators on different placements are depicted by $\mathrm{GRAD}_\Theta, \mathrm{DIV}_\Theta$ and $\mathrm{Grad}_\mathrm{X}, \mathrm{Div}_\mathrm{X}$ as well as $\mathrm{grad}_\mathrm{x}, \mathrm{div}_\mathrm{x}$. The variation operator is given by δ yielding virtual vectors $\delta\mathbf{X}, \delta\mathbf{u}$ and corresponding matrices $\delta\boldsymbol{X}, \delta\boldsymbol{U}$.

Additional hints to notation are given at the place of their first usage.

2. Bodies and placements

The particular importance of differentiable manifolds in continuum mechanics is elaborated.

2.1. The concept of a differentiable manifold

The concept of a *differentiable manifold* is outstanding in continuum mechanics, see e.g. [10,11,20,31,32] and further hints to literature therein. A thorough mathematical viewpoint can be found e.g. in [33]. The central properties of manifolds are summarised below.

- A set of points, say $\mathfrak{B}$, is said to be a differentiable manifold if it can be covered by a finite number of *charts*. All charts together build up an *atlas* $\mathfrak{A}$ of the manifold $\mathfrak{B}$.