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Implementation of incremental variational formulations based on the numerical calculation of derivatives using hyper dual numbers

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Abstract

In this paper, novel implementation schemes for the automatic calculation of internal variables, stresses and consistent tangent moduli for incremental variational formulations (IVFs) describing inelastic material behavior are proposed. IVFs recast inelasticity theory as an equivalent optimization problem where the incremental stress potential within a discrete time interval is minimized in order to obtain the values of internal variables. In the so-called Multilevel Newton–Raphson method for the inelasticity theory, this minimization problem is typically solved by using second derivatives with respect to the internal variables. In addition to that, to calculate the stresses and moduli further second derivatives with respect to deformation tensors are required. Compared with classical formulations such as the return mapping method, the IVFs are relatively new and their implementation is much less documented. Furthermore, higher order derivatives are required in the algorithms demanding increased implementation efforts. Therefore, even though IVFs are mathematically and physically elegant, their application is not standard. Here, novel approaches for the implementation of IVFs using HDNs of second and higher order are presented to arrive at a fully automatic and robust scheme with computer accuracy. The proposed formulations are quite general and can be applied to a broad range of different constitutive models, which means that once the proposed schemes are implemented as a framework, any other dissipative material model can be implemented in a straightforward way by solely modifying the constitutive functions. These include the Helmholtz free energy function, the dissipation potential function and additional side constraints such as e.g. the yield function in the case of plasticity. Its uncomplicated implementation for associative finite strain elasto-plasticity and performance is illustrated by some representative numerical examples.

Keywords: Inelasticity; Incremental variational formulations; Finite strains; Higher-order hyper-dual numbers

1. Introduction

Numerical simulation of the nonlinear and in particular inelastic mechanical behavior of materials undergoing finite strains remains an important and challenging topic in computational mechanics. For their implicit finite element

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implementation, the stresses and consistent tangent moduli are required. The precision quality of the stress calculation is important for the verification of the algorithmic implementation of the material models. Furthermore, the accuracy of the algorithmic tangent moduli influences the convergence behavior in an iterative solution scheme as well as the detection of material instabilities in localization analysis, cf. e.g., [1]. For conventional material formulations, evolution equations are defined for the internal variables associated with the dissipative material behavior. For some classical models such as von Mises plasticity, these equations can be obtained by exploiting the principle of maximum dissipation. As an alternative way, a generalized variational approach was proposed by Ortiz and Stainier [2]. The basic idea there is based on a variational principle stating that stationary points of a functional are identical to solutions of the problem. This scheme recasts inelasticity theory as an equivalent optimization problem where the incremental stress potential within time interval $[t_n, t_{n+1}]$ is minimized with respect to the internal variables. The scheme is referred to as incremental variational formulation (IVF). The IVF provides a general numerical framework which is suitable for the implementation of a broad range of constitutive models and their thermodynamical consistency is a priori guaranteed, cf. e.g., [3] and [4]. One of the important advantages of IVFs is their incremental quasi-hyperelastic potential structure which allows to investigate the existence of minimizers by analyzing generalized convexity conditions which were originally designed for finite elasticity theory. In this context particularly polyconvex strain energy functions are important and various formulations are given in the literature for different application fields, e.g. soft biological tissues or fiber-reinforced structures, see e.g. [5–8]. For an overview of convexity conditions and their applications see [9]. As a consequence, a convexification of the IVF can provide a numerical treatment for instabilities which may result from e.g. loss of ellipticity eventually leading to mesh dependency, cf. e.g., [10–15]. In addition to that, an error estimation for adaptive mesh refinements can be obtained by IVFs, cf. e.g., [16–18].

Compared with classical formulations such as the return mapping method, the IVFs are relatively new and their implementation is much less documented. Particularly, in the so-called Multilevel Newton–Raphson method (see e.g. [19,20]) for the inelasticity theory, higher-order derivatives are required in the algorithms not only for the calculation of stresses and tangents (functional matrices). The inner minimization problem, which is usually solved by the Newton method, additionally requires the derivatives of the incremental stress potential with respect to the internal variables. Therefore, numerical approximations of the derivatives may be a useful alternative reducing the implementation time in particular for scientific development purposes, see e.g., [21–27]. However, most of them make use of only first order numerical derivatives, where they compute the approximated tangent moduli from the stresses or tangent stiffness matrices from the residual vectors. Often-used classical finite differences (FD) unfortunately lead to a poorly accurate scheme being sensitive with respect to perturbation values, especially for the second-order derivatives. A robust and accurate alternative based on the complex-step derivative approximation (CSDA), cf. [28], is also problematic since no second derivatives can be computed. Fike [29] developed a method for exact (in the sense of computer accuracy) first- and second-order derivative calculations independent of the choice of perturbation values using hyper dual numbers (HDNs). Tanaka et al. [30] exploited this for a numerical scheme to implement hyperelastic materials. There it is shown that the numerical calculation of stresses and tangent moduli is almost identical to the implementation of the analytic derivatives. Korelc [31] and Rothe and Hartmann [32] utilized symbolic and automatic differentiation tools, respectively, which are alternatives to numerical derivative approximations in terms of HDNs. Regarding the computational cost of each scheme, analytically derived differentiations are least expensive followed by FD, CSDA and HDNs or automatic differentiation in this order, which is reported by Rothe and Hartmann [32] and Tanaka et al. [30]. However, with large numbers of elements, the difference in computational cost of the overall calculation decreases significantly, because then the solution time, not the assembling time becomes dominant.

In this contribution, a novel implementation of IVFs using HDNs of second and higher order is presented to arrive at a fully automatic and robust scheme with computer accuracy. This method can be easily applied to a broad range of different constitutive models since the only things that need to be implemented are the strain energy density, the dissipation potential and further side constraints such as e.g. for elasto-plasticity the yield criterion and the flow rule.

This paper is organized as follows. In Section 2, a recapitulation of HDNs is presented, where the important characteristics regarding the numerical differentiation scheme and its application to tensor fields and continuum mechanics are given. Section 3 recalls the fundamentals of IVFs. In Section 4 the novel implementation schemes for the general case of IVFs are proposed using 2nd- and 4th-order HDNs. Section 5 shows the application of the proposed schemes for a specialization, where associative finite strain elasto-plasticity is considered. In Section 6, representative numerical examples are provided, and Section 7 concludes the paper.