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A highly accurate 1st- and 2nd-order differentiation scheme for hyperelastic material models based on hyper-dual numbers

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Abstract

In this paper we propose a numerical scheme for the calculation of stresses and corresponding consistent tangent moduli for hyperelastic material models, which are derived in terms of the first and second derivatives of a strain energy function. This numerical scheme provides a compact model-independent framework, which means that once the framework is implemented, any other hyperelastic material model can be incorporated by solely modifying the energy function. The method is based on the numerical calculation of strain energy derivatives using hyper-dual numbers and thus referred to as hyper-dual step derivative (HDSD). The HDSD does neither suffer from roundoff errors nor from truncation errors and is thereby a highly accurate method with high stability being insensitive to perturbation values. Furthermore, it enables the calculation of derivatives of arbitrary order. This is a great advantage compared to other numerical approaches as, e.g., the finite difference approximation which is highly sensitive with respect to the perturbation value and which thus only yields accurate approximations for a small regime of perturbation values. Another alternative, the complex-step derivative approximation enables highly accurate derivatives for a wide range of small perturbation values, but it only provides first derivatives and is thus not able to calculate stresses and moduli at once. In this paper, representative numerical examples using an anisotropic model are provided showing the performance of the proposed method. In detail, an introductory example shows the insensitivity with respect to the perturbation values and the higher accuracy compared to the finite difference scheme. Furthermore, examples demonstrate the robustness and simple implementation of the HDSD scheme in finite element software. It turns out that the higher accuracy compared with other approaches can still be achieved in reasonable computing time.

Keywords: Nonlinear finite element method; Finite deformations; Numerical derivative; Strain energy function; Hyper-dual numbers

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1. Introduction

The numerical simulation of the nonlinear isotropic and anisotropic behavior of materials such as reinforced engineering rubbers, polymers and soft biological tissues, remains an important and challenging topic in computational mechanics. In a wide range of applications, such materials are often described by hyperelastic strain energy functions. For their finite element implementation, the stresses and consistent tangent moduli are derived from an explicitly given strain energy function. The accuracy of the stress calculation determines the accuracy of the physical results of the numerical simulation. Accuracy of the consistent algorithmic tangent moduli influences the convergence behavior in the Newton–Raphson iteration scheme applied in nonlinear finite element problems. Furthermore, it strongly affects the results of an accompanying localization analysis performed for the detection of material instabilities, cf. e.g., [1,2]. However, for some material models their analytic derivatives may be elaborate to be deduced or implemented due to their mathematical complexity, in particular for anisotropic media. In those cases approaches using numerical differentiations may be a useful alternative reducing the implementation time in particular for scientific development purposes. Such numerical approaches have been developed, e.g., by [3–7,2], see also [8], where different numerical differentiation schemes from the literature are recapitulated. However, all of them make use of only first order numerical derivatives. To the best of our knowledge, a numerical scheme for the first and second derivatives in order to derive at once the stresses and consistent tangent moduli directly from the strain energy function has not been reported in the literature. Given the function $f(x)$, most methods are based on the Taylor series expansion

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \cdots . \tag{1}$$

The often-used classical finite difference (FD) schemes consider a real-valued perturbation h and neglect the higher order terms $\mathcal{O}(h^2)$ and thus end up in the approximation

$$f'_{\mathrm{FD}}(x) \approx \frac{f(x+h) - f(x)}{h}, \tag{2}$$

wherein, $\mathcal{O}(h^2)$ denotes Landau's symbol to describe the asymptotic behavior of the higher-order terms. This approach however is highly sensitive with respect to perturbation values and only accurate for a small range of values. For small h the explicit calculation of $f(x+h)$ leads to roundoff errors and for large h the neglection of higher order terms in (1) is not acceptable. To overcome this difficulty of the FD schemes, Lyness [9] devised the complex-step derivative approximation (CSDA) scheme. In order to avoid the direct addition of perturbations along the same (real) axis leading to the roundoff errors in the FD scheme, the CSDA method uses perturbations along the imaginary axis of complex numbers by replacing h by ih in (1), i.e.

$$f(x+ih) = f(x) + ihf'(x) - \frac{h^2}{2!}f''(x) - i\frac{h^3}{3!}f'''(x) + \cdots . \tag{3}$$

Again, the higher order terms $\mathcal{O}(h^3)$ are neglected and thereby small values of h are required in order to obtain a reasonable accuracy. By taking the imaginary part on both sides of (3) one obtains the approximation

$$f'_{\mathrm{CSDA}}(x) \approx \frac{\Im[f(x+ih)]}{h}, \tag{4}$$

wherein, $\Im$ denotes the operation of taking the imaginary part of complex functions. This expression provides a high accuracy for very small values of h being remarkably close to the analytic ones. This is due to the fact that then no roundoff errors occur and technically perturbation values of up to $h = 10^{-99}$ are enabled. The main drawback of this approach is that higher-order derivatives cannot be directly computed and combinations of FD and CSDA have to be considered, see [10]. This however still suffers from the problems of the FD method. Automatic differentiation (AD) techniques, which are typically derived based on repeated application of the chain rule of differentiation, see e.g. [8], are alternatives to compute highly accurate derivatives. However, these schemes are difficult to be derived or implemented, in particular for tensorial derivatives. An equivalent, but more practicable approach can be accomplished by using dual numbers, which have been originally introduced by [11]. These dual numbers represent a modification of complex numbers with a different definition for the imaginary unit ε which has the property $\varepsilon^2 = 0$. Inserting ε into