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Determination of the tangent stiffness tensor in materials modeling in case of large deformations by calculation of a directed strain perturbation

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Abstract

The Finite Element Method in the field of materials modeling is often relying to the tangent stiffness tensor of the constitutive law. This so called Jacobian matrix is required at each time increment and describes the local material behavior. It assigns a stress increment to a strain increment and is of fundamental importance for the numerical determination of the equilibrium state. For increasingly sophisticated material models the tangent stiffness tensor can be derived analytically only with great effort, if at all. Numerical methods like the forward-difference, the central-difference, and the complex-step derivative approximation approach are widely used for its calculation. For each of these methods it is necessary to generate a specific strain perturbation. However, in large strain formulations it is not possible to perturb the strain directly but one can only modify the deformation gradient.

We present our methods to generate a directed strain perturbation for the Green–Lagrange, Euler–Almansi and logarithmic strain measures as a function of the deformation gradient and compare them with other commonly used methods. An increase in accuracy and rate of convergence can be achieved with the proposed procedures.

Keywords: Jacobian matrix; Tangent stiffness tensor; Numerical calculation; Directed strain perturbation; Materials modeling

1. Introduction

Commercial finite element software as ABAQUS [1] or MARC [2] is widely used in the field of materials research. They allow the user to incorporate a subroutine describing the material behavior. This subroutine is called at each integration point and provides the local stress response $\boldsymbol{\sigma}$ and the tangent stiffness tensor $\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\boldsymbol{\varepsilon}}$, where $\boldsymbol{\varepsilon}$ is the local strain, to the solver of the finite element software. Thereby the tangent stiffness tensor not only affects the rate of convergence to the state of equilibrium, but also specifies the direction in stress–strain space in which it is sought. Hence, the determined state of equilibrium depends significantly on the correctness of $\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\boldsymbol{\varepsilon}}$. The most direct way is to derive the stiffness analytically as conducted in [3–5]. For sophisticated material models, e.g. multiscale [6] or crystal plasticity

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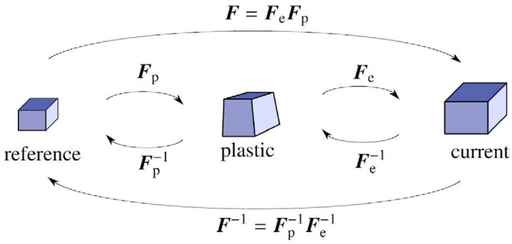

Fig. 1. Multiplicative decomposition of the deformation gradient $\boldsymbol{F}$ into an elastic and a plastic part, and denotation of the different configurations.

models [7], however, it is complex and inflexible to derive an analytical expression. In this context it becomes convenient to conduct the derivation numerically. In order to reduce the computational effort Starman [5] decomposes the tangent stiffness tensor into a part which can be calculated analytically and a part determined numerically. Irrespective of whether you decompose the stiffness tensor or not, you come to the point where you have to perform a numerical approximation. The common approach for the numerical calculation of the tangent stiffness tensor is to conduct a controlled perturbation at the assumed state of equilibrium [8–13]. The general idea for this is outlined in Section 3. In Section 4 of this contribution, we present a survey of both established and novel strategies [10–13]. Since it is not possible to perform a strain perturbation directly in a large strain formulation, one can only modify the deformation gradient. In Section 5 we present a new approach how this deformation gradient can be determined precisely depending on a prescribed strain perturbation. As demonstrated in Section 6 our methods are able to increase the accuracy of the numerical approximation of the tangent stiffness tensor because the approximation works the better the preciser the strain perturbation was determined. Since one key feature which discriminates the different methods is the coordinate system they are based on, we prepend in Section 2 a short recapitulation of the relevant continuum mechanics basics.

2. Configurations and strain measures

In continuum mechanics, we distinguish mainly between the reference configuration, generated by the Lagrangian basis vectors and describing the initial, undeformed state, and the current configuration, generated by the Eulerian basis vectors and describing the current, deformed state [14,15], Fig. 1. The fundamental kinematic variable, the deformation gradient $\boldsymbol{F} := \frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}\boldsymbol{X}}$, transforms an infinitesimal vector $\mathrm{d}\boldsymbol{X}$ within the reference configuration to its new dimension $\mathrm{d}\boldsymbol{x}$ within the current configuration. Since only elastic strains cause stresses, the deformation gradient $\boldsymbol{F}$ is decomposed multiplicatively into the elastic and the plastic deformation gradients $\boldsymbol{F}_\mathrm{e}$ and $\boldsymbol{F}_\mathrm{p}$, so that $\boldsymbol{F} = \boldsymbol{F}_\mathrm{e}\boldsymbol{F}_\mathrm{p}$. Thus we introduced the plastic configuration which describes the state of purely plastic deformation. The elastic Green–Lagrange strain $\boldsymbol{E}^\mathrm{e}$ is defined within the plastic configuration:

$$\boldsymbol{E}^\mathrm{e}(\boldsymbol{F}_\mathrm{e}) := \frac{1}{2}(\boldsymbol{F}_\mathrm{e}^\mathrm{T}\boldsymbol{F}_\mathrm{e} - \boldsymbol{I}), \tag{1}$$

where $\boldsymbol{I}$ is the 3×3 unit tensor. Within the current configuration we denote the elastic strain $\boldsymbol{\varepsilon}^\mathrm{e}$ and distinguish between the logarithmic ($\boldsymbol{\varepsilon}^\mathrm{e}_\mathrm{log}$) and the Euler–Almansi strain measure ($\boldsymbol{\varepsilon}^\mathrm{e}_\mathrm{EA}$):

$$\boldsymbol{\varepsilon}^\mathrm{e}_\mathrm{log}(\boldsymbol{F}_\mathrm{e}) := \frac{1}{2}\ln(\boldsymbol{F}_\mathrm{e}\boldsymbol{F}_\mathrm{e}^\mathrm{T}), \tag{2}$$

$$\boldsymbol{\varepsilon}^\mathrm{e}_\mathrm{EA}(\boldsymbol{F}_\mathrm{e}) := \frac{1}{2}(\boldsymbol{I} - (\boldsymbol{F}_\mathrm{e}\boldsymbol{F}_\mathrm{e}^\mathrm{T})^{-1}). \tag{3}$$

Performing the double contraction with the elastic tangent stiffness tensor $\mathbb{C}^\mathrm{pla}_\mathrm{e}$ (defined within the plastic configuration) or $\mathbb{C}^\mathrm{cur}_\mathrm{e}$ (defined within the current configuration), we obtain the 2nd Piola–Kirchhoff stress $\boldsymbol{S}$ within the plastic configuration and the Cauchy stress $\boldsymbol{\sigma}$ within the current configuration:

$$\boldsymbol{S} := \mathbb{C}^\mathrm{pla}_\mathrm{e} : \boldsymbol{E}^\mathrm{e}, \tag{4}$$

$$\boldsymbol{\sigma} := \mathbb{C}^\mathrm{cur}_\mathrm{e} : \boldsymbol{\varepsilon}^\mathrm{e}. \tag{5}$$

Using the elastic deformation gradient $\boldsymbol{F}_\mathrm{e}$ we can transform any tensor from the plastic to the current configuration and vice versa [16].