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An efficient approach for numerical treatment of some inequalities in solid mechanics on examples of Kuhn–Tucker and Signorini–Fichera conditions

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ABSTRACT

A computationally efficient solution scheme is presented for the mechanical problems whose formulations include the Kuhn–Tucker or Signorini–Fichera conditions. It is proposed to reformulate these problems replacing inequalities in these conditions by equations with respect to new unknowns. The solutions of the modified problems have simple physical meanings and determine uniquely the unknowns of the original problems. The approach avoids application of multi-valued operators (inclusions or inequalities) in formulation of the problems. Hence, the modified formulations are suitable for numerical analysis using established powerful mathematical methods and corresponding solvers developed for solving systems of non-linear equations.

To demonstrate the advantages of the proposed approach, it is applied for solving problems in two different areas: constitutive modeling of single-crystal plasticity and mixed boundary value problems of elastic contact mechanics with free boundaries. The original formulations of these problems contain respectively the Kuhn–Tucker and Signorini–Fichera conditions. A problem of the former area is integrated using an implicit integration scheme based on the return-mapping algorithm. The derived integration scheme is free of any update procedure for identification of active slip systems. A problem of the latter area is reduced to solution of non-linear integral boundary equations (NBIEs). Numerical examples demonstrate stability and efficiency of the solution procedures and reflect the mathematical similarities between the both non-linear problems.

1. Introduction

The constitutive relations for modeling of plasticity include a set of equalities and inequalities known as the Kuhn–Tucker conditions (Simo and Hughes, 1998). They appeared originally as the conditions for a solution in non-linear programming to be optimal. In application to single-crystal plasticity, these conditions are equivalent to the following two alternative conditions: on the flow surface the plastic consistency parameter is non-negative; within the region bounded by the flow surface the plastic consistency parameter is zero. However, what a particular condition holds is unknown, because the active constraints, i.e. the set of active slip systems, *a priori* are unknown. Therefore, the traditional approaches to the

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single-crystal plasticity based on the direct mathematical solution of the Kuhn–Tucker conditions lead to application of the slip update procedures. They update the active slip systems until the corresponding solution of the constitutive equations fulfills the inequalities from the Kuhn–Tucker conditions. Iterative determination of active slip systems by means of a slip update procedure is rather time consuming (Anand and Kothari, 1996; Kindrachuk and Fedelich, 2011; Knockaert et al., 2000; Miehe and Schröder, 2001; Schröder and Miehe, 1997; Simo and Hughes, 1998; Zhang et al., 2011). Moreover, usually derivation of a proper slip update procedure is not an easy task because the procedure must ensure the robust numerical algorithm. In addition, some constitutive models, like the multi-mechanisms crystallographic models, need very sophisticated slip update rules to take into account all possible states of a slip system (Kindrachuk and Fedelich, 2011). Therefore, presentation of a mathematical approach that avoids application of the slip update procedures would provide a more robust integration scheme and reduce the numerical costs of integration algorithms to the extent comparable to those of similar isotropic constitutive models.

The Signorini–Fichera conditions (Fichera, 1972) are the functional analogue of the Kuhn–Tucker conditions (Panagiotopoulos, 1985, 1987). Similar to the Kuhn–Tucker conditions, the Signorini–Fichera conditions arise in numerous problems of solid mechanics and may also result in numerical difficulties (Panagiotopoulos, 1985, 1987). For example, many problems of contact mechanics when the contact region is not known in advance, include inequalities with respect to the contact pressure and the gap between the contacting bodies: the gap is positive and the contact pressure is zero outside the contact region; while the contact pressure is positive and the gap is zero within the region. The both relations are known as the Signorini–Fichera conditions. The relations are alternative, similar to the above mentioned example from the single-crystal plasticity. Hence, what particular relation holds at a particular point of the surface can be specified only after solving the contact problem.

Further examples of mechanical problems whose formulations include inequalities can be found in Baiocchi and Capelo (1984) and Glowinski et al. (1981). The common approaches to these problems are based on the employment of the theory of variational inequalities and reduce the original problems to finding minima of some functionals. A serious drawback of the common techniques is that they involve optimization algorithms (Panagiotopoulos, 1987) that in turn makes difficult applications of traditional software packages and requires the development of individual methods, algorithms and programs or involves very serious modifications of the existing general finite element programs. Therefore, it is believed that formulations of the problems that avoid inequalities are more efficient for numerical implementations.

The mathematical theory for replacement of inequalities by equations refers to the algebra of logics (Rvachev, 1974). The origin of such replacement techniques can be traced back to papers by Rvachev dated from the early sixties (Rvachev, 1974, 1982; Shapiro, 2007). He extended Cartesian geometry and derived a general technique for analytical representation of geometrical objects. More specifically, he introduced a special class of functions, also known as R-functions, which provide the connection between set operations on geometrical objects (i.e. logic operations) and analytical expressions. Nowadays, R-functions are used for construction of meshfree methods for solution of boundary value problems (Rvachev and Sheiko, 1995; Tsukanov et al., 2003), geometric modeling and other numerical applications (Shapiro, 2007). R-functions can also be used for replacement of the Kuhn–Tucker or Signorini–Fichera conditions by equations providing more efficient solution schemes for the above mentioned problems. This replacement is not unique since using different R-functions leads to different equations. The choice of proper R-functions is important in order to get equations convenient for their mathematical investigation and numerical solution. There are, however, just few papers dealing with the topic. Replacement of inequalities by equations can be found in the early papers by Galanov (1984, 1985, 1986) devoted to the Hertz type problems of elastic contact. Later Schmidt-Baldassari (2003) proposed to use replacement of inequalities by equations in single-crystal plasticity.

The objective of the present paper is to derive a physical motivated, numerically efficient and generally applicable approach for solving problems with the Kuhn–Tucker or Signorini–Fichera conditions. To develop such an approach, we use the notion of R-functions, and reformulate the problems with respect to new unknowns. They are uniquely related with the unknowns of the original problems. In contrast to the original formulation, the new formulations omit inequalities (constraints).

The paper is organized as follows. In Section 2 we give preliminary information related to the original formulations of multi-surface plasticity and the mixed boundary value problem of elastic contact and show that the formulations contain respectively the Kuhn–Tucker and Signorini–Fichera conditions. Fundamentals of the R-functions and examples of their application to both problems are given in Section 3. Here we provide also the modified formulations of the considered mechanical problems. In addition we show that the presented approach reflects the mathematical similarities between both problems. The constitutive model for face-centered cubic (FCC) single-crystals (Kindrachuk and Fedelich, 2011) is discussed in Section 4. This model is an extension of the widely used viscoplastic crystallographic model of Meric et al. (1991) that further is referred to as the Cailletaud model, to rate-independent behavior. The modified formulation of the extended model is presented and an implicit integration is suggested. Integration of this model is of particular interest to validate the approach of modified formulation. This is because application of conventional integration schemes based on the slip update procedures requires complicated update rules distinguishing between the viscoplastically and plastically active slip systems (Kindrachuk and Fedelich, 2011). On the contrary, the derived implicit stress update algorithm based on the new formulation overcomes the search procedure for identification of the active slip systems. Section 5 demonstrates efficiency of the presented approach on two numerical examples. The computational costs of the stress update algorithms related to the original and modified formulations of the extended model are compared in the first one. Solution of the