Development of a new algorithm for the time integration of rate-independent crystal plasticity models

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Keywords: *Rate-independent crystal plasticity. Finite strain. Integration algorithm. Schmid's law.*

1 Abstract

The aim of this paper is to develop a new efficient integration scheme, able to integrate the constitutive equations for rate-independent theory of crystal plasticity at finite strain. This algorithm proposes an efficient method to determine the set of active slip systems and the corresponding slip rates. This method is based on the use of a smooth formulation of the Schmid law. The issue of non-uniqueness in the determination of slip rates can be overcome by using two different numerical techniques.

2 Introduction

Due to its ability to relate the inelastic behavior of crystalline materials to their microstructure, the modeling of the mechanical response of single crystals has remained an active research topic. The numerical integration of single crystal constitutive equations is still subject to debate and remains an active research topic, especially with the development of very elaborate scale-transition schemes and computational codes used to predict the mechanical behavior of metallic parts [1,2]. For this reason, it is still of substantial scientific and technical interest to develop robust, efficient and accurate numerical schemes and algorithms to integrate the constitutive equations for rate-independent theory of crystal plasticity. The aim of the present paper is to propose such a scheme. This scheme is reliable because it allows the determination of both the set of active slip systems and the corresponding slip rates at the same iteration level. The issue of non-uniqueness in slip rates is overcome by using two numerical methods: the pseudo-inversion technique [1] and the perturbation approach [2].

3 Mechanical modeling and algorithmic aspects

We consider single crystals obeying Schmid's law. These single crystals are submitted to an Eulerian velocity gradient $\mathbf{g}$. Following Mandel's theory [3], we assume the existence of an elastically relaxed configuration, the arbitrary rotation $\mathbf{r}$ of which being chosen in such a way that the orientations $\bar{\mathbf{M}}^{\alpha}$ of the oriented slip systems remain constant with respect to time. We will denote with a superposed bar all tensors written in an orthonormal basis fixed with respect to these material orientations. Tensor $\mathbf{d}$ (resp. $\mathbf{w}$) denotes the symmetric (resp. skew) part of $\mathbf{g}$. Under small elastic strain assumption, the constitutive equations are written as

$$\begin{gathered}
\bar{\mathbf{d}} = \bar{\mathbf{d}}^{e} + \bar{\mathbf{d}}^{p} \quad ; \quad \bar{\mathbf{w}} = \bar{\mathbf{w}}^{e} + \bar{\mathbf{w}}^{p} \quad ; \quad \bar{\mathbf{d}}^{p} + \bar{\mathbf{w}}^{p} = \sum_{\alpha=1}^{N_s} \dot{\gamma}^{\alpha}\, \bar{\mathbf{M}}^{\alpha} \\
\bar{\mathbf{w}}^{e} = \mathbf{r}^{T}.\dot{\mathbf{r}} \quad ; \quad \dot{\bar{\boldsymbol{\sigma}}} = \mathbf{C}^{e} : \bar{\mathbf{d}}^{e} \\
\forall \alpha = 1,\dots,N_s : \ \tau_c^{\alpha+N_s} = \tau_c^{\alpha} = \tau_{c0}^{\alpha} + \int_0^t \left(h_0 \operatorname{sech}^2\left(\frac{h_0 A}{\tau_{sat} - \tau_0} \right) \dot{A} \right) dt \quad ; \quad \dot{A} = \sum_{\alpha=1}^{N_s} \dot{\gamma}^{\alpha} \\
\forall \alpha = 1,\dots,2N_s : \quad \bar{\mathbf{M}}^{\alpha} : \bar{\boldsymbol{\sigma}} \le \tau_c^{\alpha} \quad ; \quad \dot{\gamma}^{\alpha} > 0 \Rightarrow \bar{\mathbf{M}}^{\alpha} : \bar{\boldsymbol{\sigma}} = \tau_c^{\alpha}
\end{gathered} \tag{1}$$

The constitutive equations (1) are solved by using an incremental algorithm. By analyzing these equations, it is clear that the determination of the slip rates $\dot{\gamma}^{\alpha}$ allows the computation of the evolution of the other mechanical variables over the current time increment $[t_0, t_0 + \Delta t]$. To compute $\dot{\gamma}^{\alpha}$, let us introduce the set of potentially active slip systems P at t_0

$$P = \{\alpha = 1,\dots,2N_s \quad ; \quad \bar{\mathbf{M}}^{\alpha} : \bar{\boldsymbol{\sigma}}(t_0) = \tau_c^{\alpha}(t_0)\}. \tag{2}$$

By using this definition of P, the Schmid law in Eq. $(1)_8$ can be rewritten as follows:

$$\forall \alpha \in P: \quad \phi^{\alpha} = \tau_c^{\alpha} - \bar{\mathbf{M}}^{\alpha} : \bar{\boldsymbol{\sigma}} \ge 0 \quad ; \quad \dot{\gamma}^{\alpha} \ge 0 \quad ; \quad \phi^{\alpha}\dot{\gamma}^{\alpha} = 0. \tag{3}$$

Equation (3) represents a nonlinear complementarity problem and can be equivalently expressed by using a smooth formulation

$$\forall \alpha \in \mathrm{P}: \quad \Gamma^{\alpha} = \sqrt{(\phi^{\alpha})^2 + (\dot{\gamma}^{\alpha})^2} - (\phi^{\alpha} + \dot{\gamma}^{\alpha}) = 0, \tag{4}$$

which can be solved efficiently by using the iterative Newton–Raphson method. The other mechanical variables are updated by Euler's backward integration. The use of the smooth formulation (4) instead of the initial formulation (3) allows combining the two tasks, namely the identification of the set of active slip systems and the calculation of the corresponding slip rates. This combination allows significantly increasing the efficiency of the developed numerical scheme. Further details about this scheme and its comparison with alternative integration schemes will be given in the full paper.

When the Jacobian matrix corresponding to the Newton–Raphson method is singular, two different alternatives are used in the simulations: the pseudo-inversion technique [1] and the perturbation approach [2]. Several numerical results will be given in the full paper in order to investigate the effect of these methods on the numerical predictions at the single crystal and the polycrystal scales (evolution of the stress components and the prediction of plastic localization occurrence).

4 Conclusions

The development of a new numerical integration scheme for constitutive equations of rate-independent theory of crystal plasticity at finite strain is briefly discussed in this paper. This scheme reveals to be more efficient than the earlier schemes available in the literature. Further details about the development of this scheme and the associated numerical predictions will be given in the full paper.

References

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