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A new implementation of the spectral crystal plasticity framework in implicit finite elements

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ABSTRACT

We present a new implementation of a computationally efficient crystal plasticity model in an implicit finite element (FE) framework. In recent publications, we have reported a standalone version of a crystal plasticity model based on fast Fourier transforms (FFTs) and termed it the spectral crystal plasticity (SCP) model. In this approach, iterative solvers for obtaining the mechanical response of a single crystal of any crystallographic orientation subjected to any deformation mode are replaced by a database of FFTs that allows fast retrieval of the solution. The standalone version of the code facilitates simulations of relatively simple monotonic deformation processes under homogeneous boundary conditions. In this paper, we present a new model that enables simulations of complex, non-monotonic deformation process with heterogeneous boundary conditions. For this purpose, we derive a fully analytical Jacobian enabling an efficient coupling of SCP with implicit finite elements. In our implementation, an FE integration point can represent a single crystal or a polycrystalline material point whose meso-scale mechanical response is obtained by the mean-field Taylor-type homogenization scheme. The finite element spectral crystal plasticity (FE-SCP) implementation has been validated for several monotonic loading conditions and successfully applied to rolling and equi-channel angular extrusion deformation processes. Predictions of the FE-SCP simulations compare favorably with experimental measurements. Details of the FE-SCP implementation and predicted results are presented and discussed in this paper.

1. Introduction

As a consequence of the complex thermo-mechanical loading history experienced during their manufacture, polycrystalline metals possess a non-random distribution of grain orientations, referred to as crystallographic texture (Bunge, 1993). Texture is known to have a strong influence on the anisotropy of various material properties (Adams and Olson, 1998; Fuentes-Cobas et al., 2013; Kocks et al., 1998). Modeling the anisotropy of plastic properties requires consideration of the crystal structure and orientation because of their role in the activation of micro-scale deformation mechanisms (Taylor, 1938). Physically-based, crystal plasticity models provide reliable predictions and help in understanding material anisotropy since they take into account microstructure and the directionality of deformation mechanisms acting at a single-crystal level. Unlike phenomenological models based on continuum plasticity, these models can be used to optimize the microstructure and mechanical properties during production processes

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because they are capable of capturing evolution of the underlying microstructure during finite plastic deformation (Knezevic et al., 2012a, 2008b; Shaffer et al., 2010). As such, they are highly desirable for performing accurate simulations of metal forming processes.

A number of crystal plasticity material models linking the grain scale response to the response of a polycrystalline aggregate have been developed including the self-consistent mean-field models (Knezevic et al., 2013a,b, 2014a; Lebensohn and Tomé, 1993; Lebensohn et al., 2007), Taylor type upper bound models (Knezevic et al., 2008a; Taylor, 1938; Van Houtte et al., 2004), finite-element full-field models (FE) (Kalidindi et al., 1992; Knezevic et al., 2010; Mathur et al., 1989; Roters et al., 2010; Sarma and Dawson, 1996), and Green's function fast Fourier transform (FFT) type full-field models (Lebensohn et al., 2012). While each of these homogenization approaches can be versatile in crystal mechanics and hardening laws, only the FE approach is suitable for non-monotonic deformation and treating heterogeneous boundary conditions and spatial strain gradients. Therefore, an FE implementation of crystal plasticity models is highly desirable in order to simulate complex deformation paths while retaining the micromechanical coupling of texture, stress, and strain. Example applications include simple compression and tension tests (Beaudoin et al., 1993), bending (Knezevic et al., 2013d,e), rolling (Segurado et al., 2012), cup-drawing (Balasubramanian, 1996; Raabe and Roters, 2004), sheet hydroforming (Beaudoin et al., 1994), and bulk forming (Knezevic et al., 2014c, 2013c, 2012b; Kumar and Dawson, 1995). However, the integrated crystal plasticity models within implicit FE simulations tools are computationally intensive and have not been adopted broadly by the metal forming and advanced materials development community.

Several strategies have been explored for speeding up crystal plasticity calculations. An approach relying on the adaptive sampling algorithm has been reported in Barton et al. (2011, 2008). In this approach, each calculated response of a polycrystalline material point is recorded in a database on the fly as a function of input parameters. These solutions become subdomains from which subsequent model solutions can be interpolated for material points close to the already computed points instead of requiring a new call to the crystal plasticity model. Therefore, the number of direct interrogations of the intensive crystal plasticity model can be dramatically reduced. Using this approach, wall-clock speedup factors exceeding an order of magnitude relative to direct crystal plasticity calculations were demonstrated. Other attempts to improve efficiency of the crystal plasticity codes rely on a process plane concept based on proper orthogonal decomposition in Rodrigues–Frank space (Sundararaghavan and Zabaras, 2007). It has also been shown that solving crystal plasticity using the Jacobian-Free Newton–Krylov (JFNK) technique in place of the Newton–Raphson method can yield some computational benefits (Chockalingam et al., 2013).

In recent work, we have developed a computationally efficient crystal plasticity model in the spectral representation termed spectral crystal plasticity (SCP) (Knezevic et al., 2009). In the SCP framework, the crystal plasticity solutions are organized into a set of functions that describe the dependence of the stresses, the lattice spin, and the total slip rates in single crystals on their lattice orientation and the strain rate imposed on them. The domain of these functions is the product space of all possible crystal orientations and all possible isochoric strain rates. These functions were evaluated using a conventional crystal plasticity code (Kalidindi et al., 1992) and represented using Fourier bases to obtain databases of spectral coefficients. The viability of this framework was initially demonstrated using generalized spherical harmonics (GSH) bases (Fast et al., 2008; Kalidindi et al., 2006; Knezevic and Kalidindi, 2007). Subsequently, in place of the GSH bases we have explored the use of Discrete Fourier Transforms (DFTs) to generate the spectral databases (Kalidindi et al., 2009; Knezevic et al., 2009, 2008a). The major advantage of using DFTs is that the DFTs can be computed using highly efficient fast Fourier transforms (FFTs) algorithms (Briggs and Henson, 1995; Brigham, 1988; Cooley and Tukey, 1965; Duhamel and Vetterli, 1990; Press et al., 2002). The most remarkable discovery in this framework is only as few as several hundred dominant Fourier transforms are sufficient to recover the functions of interest on their respective domains. We reported speed up factors of about two orders of magnitude relative to conventional iterative solvers.

Building on these prior advances in efficient numerical schemes, we successfully developed a high performance computational application of SCP that runs on specialized hardware incorporating graphic processing units (GPUs) (Mihaila et al., 2014), and an improved version that takes advantage of an efficient GPU8 algorithm for matrix–matrix multiplication (Knezevic and Savage, 2014). The latter implementation resulted in remarkable improvements in computational speed, exceeding three orders of magnitude over the conventional numerical schemes. We have also presented a work distribution scheme on a hybrid computer architecture consisting of a cluster of Linux nodes that individually integrates multi-core processors (CPUs) and Graphics Processing Units (GPUs) intended for performing future tractable multi-scale process simulations (Knezevic and Savage, 2014). This combined framework, consisting of the computationally efficient SCP and specialized hybrid CPU–GPU hardware, has only been presented in the form of a standalone code.

The current paper is focused on a new implementation of the computationally efficient SCP framework (Al-Harbi et al., 2010; Knezevic et al., 2009, 2008a) within the implicit solver of the FE package ABAQUS through a user material subroutine (UMAT). We produce a new finite element spectral crystal plasticity (FE-SCP) model. In an implicit nonlinear FE formulation, the material constitutive model provides the stress and the tangent stiffness matrix (Jacobian). We derive and present a fully analytical Jacobian matrix ensuring fast convergence towards global stress equilibrium. The new implementation follows the main aspects of the constructive coupling presented in Knezevic et al. (2013d) and Segurado et al. (2012)) and therefore differs from the first implementation presented in Al-Harbi and Kalidindi (2015). Moreover, the new implementation includes the hardening term in the Jacobian matrix, which we found improves the convergence. Simple