Implement a remeshing scheme into a spectral method based crystal plasticity code

M. Diehl

August 19, 2011

At MPIE, the flexible crystal plasticity framework "Düsseldorf Advanced MAterial Simulation Kit" (DAMASK) is developed. It consists of different constitutive models, homogenization schemes, and tools for post- and preprocessing [1]. It has interfaces to different solvers to the mechanical boundary value problem. To compute the boundary value problem, commercial FEM software like MSC.Marc or Abaqus or a solver based on a so-called spectral method [2, 3]. Spectral methods have advantages concerning accuracy, performance, and memory efficiency compared to the de-facto standard FEM. However, their use is limited to periodic boundary conditions due to the approximation of the solution by plane waves. The spectral method implemented at MPIE uses a finite-strain formulation proposed in [4] that is written in terms of deformation gradient $\boldsymbol{F}$ and Piola–Kirchhoff stress $\boldsymbol{P}$ and can therefore be used to solve the mechanical boundary value problem in the reference configuration. Calculations have shown that for inhomogeneous material convergence cannot be achieved any longer at strains larger than ca. 15–20 %. We presently believe that this is due to the fact that the regular mesh in the reference configuration is locally heavily deformed to an extent where single points cross the path of neighboring points. To reach higher strains, a remeshing scheme should be implemented as follows.

1. Write out the current state
2. Approximate the deformed configuration by a regular (undeformed, new) mesh
3. Translate the old state values to the new mesh

References

[1] F. Roters, P. Eisenlohr, L. Hantcherli, D.D. Tjahjanto, T.R. Bieler, and D. Raabe. Overview of constitutive laws, kinematics, homogenization, and multiscale methods in crystal plasticity finite element modeling: theory, experiments, applications. *Acta Mater.*, 58:1152–1211, 2010. doi: 10.1016/j.actamat.2009.10.058.

[2] H. Moulinec and P. Suquet. A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Computer Methods in Applied Mechanics and Engineering*, 157(1-2):69–94, 1998. doi: 10.1016/S0045-7825(97)00218-1.

[3] R.A. Lebensohn. N-site modeling of a 3D viscoplastic polycrystal using Fast Fourier Transform. *Acta Mater.*, 49(14):2723–2737, 2001. doi: 10.1016/S1359-6454(01)00172-0.

[4] N. Lahellec, J.C. Michel, H. Moulinec, and P. Suquet. Analysis of inhomogeneous materials at large strains using fast Fourier transforms. In C. Miehe, editor, *Proc. IUTAM Symposium*, volume 108 of *Solid Mechanics and its Applications*, pages 247–258, Dordrecht, The Netherlands, 2001. Kluwer Academic Publishers.