DIRECT SIMULATION OF POLYCRYSTALS

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Mesoscale simulations of polycrystalline microstructures are used to understand the role of the material microstructure on material response in both qualitative and quantitative ways. Carrying out the simulations to large strains is frequently challenging because local deformations may have significantly higher strains than the mean strain for the representative volume element being modelled. Indeed, studying localization in the form of shearbands, has been a motivating factor behind performing these simulations. Lagrangian finite element formatulations are attractive for this type of analysis because of their efficiency and accuracy. When the microstructures localize, however, the time step size is reduced for explicit calculations and implicit calculations often fail to converge. Eulerian and arbitrary Lagrangian-Eulerian (ALE) formatulations address these problems by projecting the solution from a deformed to an undeformed mesh. The cost of the calculation increases, and there are issues associated with the projection/transport of the history variables. This talk focuses on the practical difficulties and their solution for applying Eulerian and ALE methods to mesoscale calculations. Results from the two-dimensional Eulerian code Raven, and the three-dimensional ALE code ALE3D, are presented.