Modelling self-contact in metallic alloys with the Discrete Element Method

Robin Gibaud*, Étienne Guesnet, Pierre Lhuissier, Luc Salvo

Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, F-38000 Grenoble, France
e-mail: robin.gibaud@simap.grenoble-inp.fr

ABSTRACT

Structural metallic alloys often exibhits a meso-scale porosity at early stages of the elaboration process. Such defects of the material, potential failure factors, are eliminated with hot or cold forming, for example rolling. From a numerical point of view, the issues of modelling interactions between initialy free interfaces must be adressed. Using a traditionnal Finite Element Method (FEM) approach, the proper description of these phenomena involves heavy and costly procedures such as interface description, periodic re-meshing and contact detection [1]. The costs in terms of development and computation can be limiting factors for large geometrical domain where contact phenonema become dominant and cannot be considered independant.

Alternative strategies to continuum mechanics can be built based on discrete descriptions of the material, which are innately suited to model arbitrary contacts between sets of discrete objects, and topological changes. In the context of pore closure and large strains, particle based method must rely on an updated Lagrangian description, for the interfaces as well as the neighors. The Discrete Element Method (DEM) has been used in the literature to model elastic continuous materials, in the objective of model for example brittle failure [2] or buckling [3]. To our knowledge, these works rely on initially bonded neighbors and are limited to volumic plastic strain.

In this work, the DEM is used as a numerical tool to phenomenologically describe metallic plasticity in large strain. Custom attractive-repulsive contact laws are implemented in the open-source DEM code liggghts [4], taking advantage on the numerical scalability of the solver. Irreversible strains are modelled by the collective rearrangement of a packing of spherical particles, arbitrarly changing neighbors, with macroscopic volume conservation. The accuracy of the behavior, with respect to continuum mechanics, is evaluated on elementary geometries.

In the large strain context, the initial position of the particles cannot be used to define free interfaces, as in more classical approaches. Our method is based on pseudo-normals, an approximation of the outward normal vectors, computed for each particle using the position of the neighbors. At each time step, depending on the magnitude and orientation of their respective pseudo-normals, particles interactions can be discriminated in two categories: cohesive interaction inside the material; repulsive interaction across interfaces.

The numerical methodology is applied to experimental porosity determined by X-ray tomography. The initial geometry is discretized using the 3D image as a mask on a random packing of spherical particles. This numerically cheap procedure can applied to abritrarly tortuous experimental or realistic microstructure.

Implemented for the DEM, our interfaces description methodology could be used in a variety of particle based methods, providing a fully updated Lagrangian description of topological events in continuum mechanics. Associated with criteria for cohesion and decohesion, this methodology can be used to phenomenologically model physical phenomena such as fragmentation of phases and voids closure and healing, in irreversible large strains or displacement.

REFERENCES

[1] M. Saby, M. Bernacki, E. Roux and P.O. Bouchard. *Computational materials science*, *77*, 194-201, 2013.

[2] D. André, I. Iordanoff, J.-L. Charles and J. Néauport. *Computer Methods in Applied Mechanics and Engineering*, 213-216:113-125, 2012.

[3] R. Kumar, S. Rommel, D. Jauffrès, P. Lhuissier and C.L. Martin. *International Journal of Mechanical Sciences*, 110:14-21, 2016.

[4] C. Kloss, C. Goniva, A. Hager, S. Amberger and S. Pirker. *Progress in Computational Fluid Dynamics, An Int. J*, 12(2/3):140-152, 2012.