A discrete-continuum particle method for complex deformation and fracture events

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Complex fracture events take place in many materials and applications.In this context, discrete particle methods are an attractive computational methodology since they can easily accommodate complex and arbitrary discontinuities. The added value of particle methods to capture intricate fracture behaviour of elastic-brittle materials such as glass and concrete, has been widely demonstrated in the literature. Beyond linear elasticity and the small strain fracture regime, the ability of current particle methods such as the Discrete Element Method (DEM), Smoothed Particle Hydrodynamics (SPH) and Peridynamics to account for the underlying material behaviour remains questionable. Most of the discrete constitutive formulations are not consistent with their continuum counterparts. The origin of this limitation stems from the adopted mathematical formulation that only yield approximate deformation tensors.

This contribution introduces an innovative particle method that relies on a dedicated averaging scheme that determines the deformation gradient tensor at each particle based on the relative positions of the particle's nearest neighbours [1]. The adopted scheme reveals similarities with the volume weighted nodal averaging procedure used in the Finite Element Method (FEM) [2]. The novel particle routine, referred to as the Continuum Bond Method (CBM), preserves the constitutive flexibility of continuum methods while maintaining the powerful fracture properties of discrete particle methods. Within a general context, two numerical examples are presented to demonstrate the discrete-continuum consistency and its complex fracture capabilities: (i) an elasto-plastic tensile bar subjected to large deformations and (ii) a dynamic crack branching problem. The first example relies on a finite strain J_2 plasticity model with non-linear hardening law. The local and global mechanical response obtained with CBM is assessed in direct comparison with a FEM reference solution and further compared to SPH results. The second numerical example demonstrates the CBM's capability to account for complex fracture events, which are naturally driven by the dynamics in the simulation. The need for specific criteria and tailored domain enrichments that would allow for crack branching in dynamic fracture simulations is hereby obsolete, which is one of the major merits of particle methods.

The methodology is next applied to the micro-scale scratching of mono-crystalline silicon. Two ingredients are important for this model: (i) a three-dimensional CBM implementation in LAMMPS and (ii) constitutive model that accounts for pressure-induced phase transformations in silicon (based on [3], extended to finite strains). the LAMMPS-CBM scratch setup will be used to evaluate the global and local response from a modified continuum plasticity model designed to phenomenologically capture silicon phase transitions under contact conditions. In the future, this will be extended beyond the ductile-to-brittle transition point, which can be easily achieved with CBM using a bond breakage criterion.

References

[1] S.O. Sperling, J.P.M. Hoefnagels, K. van den Broek, M.G.D. Geers, A continuum consistent discrete particle method for continuum-discontinuum transitions and complex fracture problems, Comp Meth Appl Mech Engng 390 (2022) article 114460.

[2] C. R. Dohrmann, M. W. Heinstein, J. Jung, S. W. Key, W. R. Witkowsk, Node-based uniform strain elements for three-node triangular and four-node tetrahedral meshes, Int Jnl Num Meth Engng 47 (2000) 1549-1568.

[3] M. Budnitzki and M. Kuna, A thermomechanical constitutive model for phase transformations in silicon under pressure and contact loading conditions, Int Jnl Sol Struc 49 (2012) 1316-1324.