Implementation of MCA in the framework of LIGGGHTS

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ABSTRACT

The Movable Cellular Automata (MCA) method was first introduced by Psakhie, Horie et al in 1995 [1] as a simulation tool within the framework of mesomechanics. It is a hybrid particle-based method based on the classical cellular automata (CA), discrete element (DEM) and molecular dynamics (MD) methods; combining their advantages. This method allows the modelling of complex materials behaviour and processes, such as crack generation and growth, mass mixing, phase transformation, etc. Many developments in MCA have been made since 1995, and the latest description of the method can be found in [2]; where MCA is presented as a discrete approach to model the behaviour of materials on different scales and is used as multi-scale modeling approach.

This paper focuses on the implementation of the MCA method within the framework of the open-source code LIGGGHTS; which stands for LAMMPS Improved for General Granular and Granular Heat Transfer Simulations [3]. LIGGGHTS is based on DEM to simulate granular materials, MCA is implemented to simulate complex solid behaviour, most importantly plastic deformation. The main difference between MCA and DEM is that the interaction between the particles is based on many-body forces of inter-automata interactions; similar to the embedded atom method used in molecular dynamics; because pair-wise interactions between elements are insufficient to simulate irreversible strain accumulation (plasticity) in ductile consolidated materials. LIGGGHTS was chosen as a framework due to its massive parallel computing capabilities, giving MCA the capability of simulating more complex systems on higher scale levels.

The testing and verification of the code includes 1- showing the macroscopic isotropic mechanical response for the simulated material by simulating loading and unloading of uni-axial compression, tension and shear loading of 3D material samples, 2- nano-indentation and scratching models similar to the ones simulated in [4]. Nano-indentation simulations will show the capability of modeling plastic deformation in contact interaction, and scratching simulations will show the capability of modeling fracture. The results show good corrolation with analytical solutions. The code could potentially be used in many different applications on different scales; such as the modeling of wear.

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