Computational Strategies for Predicting Granular Matter Response under Extreme Compaction

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ABSTRACT

Many industries rely on consolidation of granular materials as an essential operation on their manufacturing processes. In particular, the pharmaceutical industry produces more than 80% of all its therapeutically dosages in the form of tablets manufactured by powder consolidation. A predictive modeling and simulation framework provides a strategy for designing the compaction process in order to tailor tablet performance properties. The development of such a framework requires predictive constitutive models of inter-particle interactions that account for high levels of confinement and a variety of physical mechanisms, including elasto-plastic deformations, adhesion, bonding, friction, and fracture.

We present a new 'nonlocal contact formulation' that overcomes the typical, but unrealistic, assumption that contacts are independent regardless the confinement of he granular system. We also describe a particle mechanics strategy, which solves for contact forces at the granular scale, for nonlocal deformations at the mesoscale, and for static equilibrium at the macroscale. Furthermore, we utilize this simulation framework to explore multi-component mixtures, which are a common practice in the pharmaceutical industry. Specifically, we study the manufacturing of bilayer tablets, tracing the observed defects during manufacturing to the microstructural evolution during the compaction process, including force networks, distribution of contact areas, particle bonding and residual stresses.