Air-induced defect formation during powder compaction

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Project Overview: This work focuses on developing new simulation capabilities to improve the manufacturing of pharmaceutical tablets using powder compaction processes. Specifically, we concern ourselves with the expulsion of air during the compaction, which is initially trapped in voids between powder particles and at the die-powder interface. A desire to increase throughput of tablet forming requires high speeds of compaction. High compaction speeds lead to turbulent flow and high air pressures within the voids between particles that can cause cracking or capping/lamination after ejection from the die. Defective tablets must then be thrown out leading to wasted material. The objective of this research is to use a mechanics-based approach to create models capable of predicting the conditions under which defect formation will occur during powder compaction. The research has two major branches. The first is to create a discrete model capable of capturing the compaction process. To accomplish this an improved contact model for powders undergoing high deformations is being developed. Coupling of the discrete element method with the improved contact models and computational fluid dynamics will then lead to high resolution numerical "experiments". These can then be used as a guide for the second branch of the research–developing a (computationally cheaper) continuum mixture model suitable for powder compaction. When complete, the two branches will provide a robust complementary toolkit for predicting defect formation during powder compaction that properly considers the coupled mechanics between the air and powder.

Current Research Thrust–Towards continuum accuracy at low computational cost: a dimensionally reduced contact model for elastic-plastic particles: We present a contact model able to capture the response of interacting elastic-plastic particles. The model makes use of the *Method of Dimensionality Reduction* which allows for the problem of 3D axisymmetric contact to be mapped to a semi-equivalent simpler 1D problem of a rigid indenter penetrating a bed of springs. By assuming a generic elliptical displacement profile, small and large deformation is properly captured through simply adjusting the indenter shape. Importantly, our model distinguishes itself from previous large deformation contact models in that it allows pointwise variation of the plastic displacement and hence curvature along the contact rather than assuming a new constant radius of curvature after plastic deformation, an assumption that leads to a non-physical stress profile.

To validate the model, we compare it to finite element simulations of elastic-plastic contact. These comparisons show that the proposed contact model is able to accurately capture the total force at the contact and the plastic deformation upon unloading. The end result is a powerful and robust contact model that is easily adaptable to many contact problems. Moreover, the contact model allows pointwise evaluation of stresses and plastic displacement across the contact, counter to typical contact models which lack pointwise evolution of quantities. This property moves the contact model closer to the more robust solutions provided by the continuum mechanics of solids without sacrificing computational efficiency.