Micro-macro: From particles to continuum-theory

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ABSTRACT The behavior of particulate and granular matter – like sand, powder, suspended particles, colloids or molecules – is of considerable interest in a wide range of industries and research disciplines. These materials are intrinsically disordered, often come with a wide distribution of particle sizes and materials/mixtures, and can behave both solid- or fluid-like. The related mechanisms/processes in particle systems are active at multiple scales (from nanometers to meters) and understanding them is an essential challenge for both science and application, i.e., finding the reasons for natural/industrial disasters like avalanches or silo-collapse.

In order to understand the fundamental micro-mechanics one can use particle simulation methods [1-6], where often the fluid between the particles is important too, but neglevted here. However, large-scale applications (due to their enormous particle numbers) have to be addressed by coarse-grained models [1,3,6] or by continuum theory. In order to bridge the gap between the scales, so-called micro-macro transition methods are necessary, which translate particle positions, velocities and forces into density-, stress-, and strain-fields. These macroscopic quantities must be compatible with the conservation equations for mass and momentum of continuum theory. Furthermore, non-classical fields are needed to describe the micro-structure [2,4] or the statistical fluctuations, e.g. of the kinetic energy [5], before one can reach the ultimate goal of solving application problems.

More examples of multi-scale simulations, involving particle- and continuum-methods, are flows of particles/fluids in narrow channels/pores, dosing of cohesive fine powders in vending machines, avalanche flows on inclined slopes, segregation, rheology testing in ring-shear cells, as well as the study of non-linear elasto-plastic material mechanics related to the failure of solids.

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