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# From Discrete Particle Simulations towards Continuum Theory and Applications

Lecture of

**Prof. Dr. Stefan Luding**

Multiscale Mechanics  
Faculty of Engineering Technology  
University of Twente

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Okerhochhaus, Pockelsstraße 3,  
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The dynamic behavior of particulate and granular matter – like sand, powder, suspended particles or molecules, often with a wide distribution of particle sizes – is of considerable interest in a wide range of industries and research disciplines since they can behave both solid-like and fluid-like. The related mechanisms/ processes in particle systems are active at multiple scales (from nano-meters to meters), and finding the reasons for, e.g., the reasons for natural disasters like avalanches or plant problems like silo-failure, is an essential challenge for both academia and industry.

In order to understand the fundamental micro-mechanics one can use particle simulation methods, where often the fluid between the particles is important too. However, large-scale applications (due to their enormous particle numbers) have to be addressed by coarse-grained models 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, nonclassical fields are needed to describe the micro-structure (fabric, force-chains) or the statistical fluctuations, e.g. of the kinetic energy, before one can reach the ultimate goal of solving application problems.

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 elastoplastic material mechanics related to the failure of cohesive, frictional solids [1-4].