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# Particle Modelling with the Discrete Element Method
# A success story of PARDEM (www.pardem.eu)

## 1. General

Bulk handling, transport and processing of particulate materials such as powders and granules are integral to a wide range of industrial processes in many fields [1,2] or natural, geophysical phenomena and hazards like landslides [3]. Particulate systems are difficult to handle and display unpredictable behaviour, which represents a great challenge for both design and operation of unit operations and plants, but also for the research community of Powders and Grains [4,5].

Granular materials and powders consist of *discrete particles* such as individual sand-grains, agglomerates (comprising of many primary particles), or bonded solid materials like sandstone, ceramics, or some metals or polymers sintered during additive manufacturing. The primary particles can be as small as nano-metres, micro-metres, or millimetres [6] covering multiple scales in size and a variety of mechanical interaction mechanisms. Those interactions include friction and a variety of cohesive forces [7,8], which becomes more and more important the smaller the particles are. All these particle systems have a particulate, usually disordered, inhomogeneous and often anisotropic micro-structure, which is at the core of many of the challenges one faces when trying to understand powder technology and granular matter.

## 2. Fluid- and solid like behaviour

Particle system as a bulk shows a completely different behaviour as one would expect from the individual particles. Collectively, particles can either flow like a fluid or at rest like a solid. In the former case, in rapid flows, granular materials are collisional and inertia-dominated and compressible similar to gases. In the latter case, particle assemblies are solid-like and thus can form, for example, sandpiles or slopes that can remain static for a long time. In between is the dense and slow flow regimes that connect the extremes and is characterized by the transitions (i) from static to flowing (failure, yield) or vice-versa (ii) from fluid to solid (jamming).

At the particle and contact scale, the most special property of particle systems is their dissipative, frictional, and possibly cohesive nature. Here dissipation means that the fluctuating kinetic energy at particle scale is irrecoverably lost by a number of mechanisms including contact friction and contact plastic deformation. The transition from fluid to solid can be caused by dissipation alone, which tends to slow down motion. The transition from solid to fluid (initiation of flow) is due to failure and instability, when dissipation is not sufficient to prevent the system from yielding which then evolves into a flowing regime.

## 3. Particle simulation by DEM

Besides experiments, the methods used to explore the behaviour of particle systems involve continuum theory solvers, numerical particle simulations and micro–macro transition methods, where the latter in general attempt to connect the particle (micro) scale with the process (macro) scale that can usually, due to the enormous number of particles, only be modelled using continuum methods.

The complexity of particle systems as described above is such that the study of bulk flow behaviours at the scale of unit-operations or so-called element tests are often a considerable challenge. In order to understand and model the bulk behaviour using particle simulations, new particle-contact experiments need to be developed, for example, nano-indentation equipment becoming increasingly deployed [9]. However detailed contact information is only available for idealized materials such as glass spheres [9,10] or rather large particles with complex interactions [11], whereas realistic, industrially relevant fine powders can hardly be measured. They involve a multitude of shapes and structures that do not allow for conclusive data, but possibly can be modelled by the so-called meso-scale models [12–14] which catch the essential phenomenological features but are not directly related to the interaction parameters of the primary particles. These meso-scale models represent many particles as an entity, and as such allow for the modelling of much larger systems.

On the macro-scale, it is noted that the particulate nature and the salient details of the contact mechanics are not adequately captured in the constitutive relations that are needed to solve the continuum equations. The influence of the particles on the bulk behaviour has to be better understood to ultimately provide effective predictive tools for particulate flows. One promising development in bridging from micro-mechanical insights at particle- and contact-level to the next generation of superior continuum models will come from the coarse-graining methodologies.

In recent decades, the Discrete Element Method (DEM) [15] that models the motion and interaction of individual particles has become very popular as a computational tool to model granular systems in both academia and industry. To date, not only due to increasing computer power available, considerable scientific advances have been made in the development of particle simulation methods, resulting in an increasing use of DEM. However, careful verification of the various numerical codes and validation of the simulation results with closely matching experimental data is essential to establish DEM as a widely accepted tool able to produce satisfactory quantitative predictions with added value for design and operation of industrial processes. One fundamental step towards this goal is the determination of the simulation

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parameters for the DEM particle model. Contrary to the more established CFD codes [16], so far only very few examples and no best practice guidelines or norms are available for the verification, calibration and validation of DEM simulations [17].

## 4. Overview of the special issue

The papers within this special issue cover a significant effort by the authors, in the framework of the EU-FP7 Marie Curie ITN (Initial Training Network) PARDEM (see www.pardem.eu) in deploying various aspects of DEM. A range of industrial application examples are studied (silo flow [18], mixing [19], and segregation [20]); for large, granular particles as well as two-phase systems (fluidized beds [21] or pneumatic conveying [22]); and cohesive powders (cone penetration and unconfined strength testing [23], dosing of cohesive food powder [24]), as well as the more fundamental issues of fine powder testing with different devices and the extremely slow stress-relaxation in such systems [25]. On the macroscopic level several important questions are addressed, such as the effect of the particle size-ratio on the bulk stiffness of granular mixtures [26] as well as the asymmetry of stress tensor arising from a micropolar formulation [27]. Furthermore, DEM results are compared to the prediction of a micropolar hypoplastic continuum model [28]. Finally the critical issue of the scaling of model parameters with particle size for both cohesionless and cohesive systems is addressed [29], and the micro–macro transition parameters are studied in detail using a model silo flow of non-spherical particles [30] that involves stagnant/static zones, shear bands as well as the rapidly flowing core.

In all of these papers, the investigation of various element tests and model experiments, the calibration of DEM models, the micro–macro (coarse graining) transition and the understanding of the bulk flow behaviour based on particle and contact properties provide novel, deeper insights into the mechanics governing these granular and powder handling processes. These papers demonstrate clearly the considerable potential of this powerful numerical technique to provide answers to fundamental questions and innovative solutions to industrial problems. They also highlight some challenges that must still be overcome to transform DEM from a well established scientific tool into an efficient, reliable industrial predictive tool.

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