

The **basic DEM** (Discrete Element Method) can be described as a method for the integration of equations of motion for a collection of simple (spherical) rigid particles interacting via frictional Hertz contacts. The motion of each individual particle is incrementally calculated from the forces acting on it by other particles and bulk forces such as gravity. In basic DEM scale separation is assumed between contacts and particles and the contact scale is resolved. However, since only particle motions are of interest, the contact scale is generally described by a *force law* involving overlaps and relative velocities (strain variables attributed to the contacts and calculated from rigid-body motions of the particles). For this reason, in close analogy with the Molecular Dynamics method, the DEM is defined in terms of two major ingredients: 1) Equations of motion, and 2) Contact force laws.

During the 1990s, the DEM evolved into a common simulation tool adopted by researchers and engineers in various fields. With rapidly increasing power and memory of computers, the DEM was subsequently extended to simulate particle clumps of arbitrary shapes, adhesion forces, electrostatic forces, solid bonding/debonding, and rolling resistance. This **extended DEM** is still the most common simulation tool for granular materials.

Radically new features have, however, been developed more recently and evolved into **advanced DEM** codes. These developments have been mainly driven by industrial applications, requiring realistic simulations of complex granular processes. These advanced features comprise *aspherical particle shapes*, *hybrid* discrete-continuous modeling, *liquid bridging*, coupling with a *fluid phase*, coupling with a *scalar field* (temperature, humidity, charge, chemical species...) or *vector field* (electrostatic, magnetic), highly *deformable* particles, and *comminution*. In contrast to the common lower-level DEM, these features are not generic, require specialized techniques and allied methods, and are based on more sophisticated data-handling procedures. They also raise hard efficiency, accuracy, calibration and validation challenges. The allied methods include FEM (finite element method), CFD (computational fluid dynamics), MPM (material point method), SPH (smoothed particle hydrodynamics), LBM (lattice Boltzmann method), LEM (lattice element method), and Peridynamics.

It is useful to represent the advanced features, often involving physics and techniques **beyond DEM**, with respect to the dynamics of a single particle, as illustrated in Fig. 1. Nearly all these features involve subparticle length scales ranging from contact scale to particle scale: pressure exerted by a fluid phase, internal stresses governing deformation and fracture, torques developed at cohesive extended contacts (face-face, face-edge...), interstitial liquid or solid

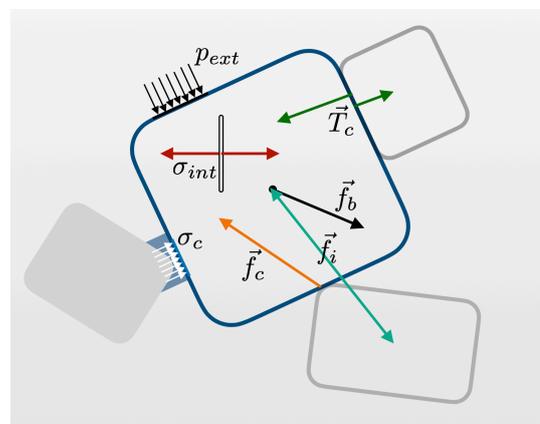


Fig 1. Schematic view of particle-scale and subparticle-scale forces acting on a particle.

phase stresses, long-range interbody forces (charged particles...), thermomechanical stress fields....

To account for multiple length scales and forces, four modeling strategies have been developed:

- 1) Subparticle resolution of particles, phases, fields and forces: The term DNS (direct numerical simulation) is often used for the methods of simulation of fluids at fine scales by solving Navier-Stokes equations or Boltzmann equation. This term can be generalized here to all other phases and fields such as cementing phase. Full resolution of particle shapes belongs to this category (for geometry).
- 2) Coarse-graining subparticle forces to the particle scale: Effects of subparticle forces are taken into account at the particle scale by averaging subparticle equations. The contact forces are excluded as they govern the collective behavior. Averaged subparticles forces become either contact forces or body forces acting on the particle centers. The interstitial phases can also be modeled at the pore scale and solved over the pore network.
- 3) Coarse-graining to a scale above the particle scale: The phase equations are solved on a grid containing several particles. Coarse-grained forces become body forces acting on the particles such as drag forces.
- 4) Coarse-graining both particles and forces to a scale above the particle scale: This leads to a continuum particle phase coupled with other continuum phases and fields.

The DEM refers essentially to the first three modeling strategies. Obviously, numerical efficiency increases from (1) to (4) at the expense of decreasing accuracy. The first strategy, despite its high computational cost, is needed for understanding the physical processes at fine scales and supports the elaboration of other strategies. The second strategy is closest to the spirit of DEM and it provides the best compromise between accuracy and efficiency. It can be compared to the *Potential of Mean Force* (PMF) used for mesoscopic simulations of nanoparticles (e.g. CSH cement particles and clay particles). For granular materials, this amounts to the elaboration of *enhanced force laws* based on both overlaps and interstitial or intercenter distance and involving stable minima (for cohesion), potential barriers (e.g. combination of capillary force and electric repulsion), evolving strength..., coupled with locally averaged fields (humidity, temperature, ionic species...). The four strategies have been extensively applied in powder technology for gas-particle flows. More recently, hybrid approaches have been designed to describe different parts of a granular material alternatively as discrete or as a continuum depending on a criterion, allowing therefore to benefit from the advantage of accuracy for regions where high resolution is needed (for example at the outlet of a silo) and the advantage of efficiency where a spatial low resolution is sufficient (for example in the core of a silo flow).

Many recent developments concern *particle shape*. Different fully analytic particle shapes, digitalized real shapes and general representations based on spherical harmonics have been considered with smooth surface. However, common overlap-based force laws have mostly been used without properly accounting for the changes of curvature. Consistent contact force laws accounting for the geometry should be formulated based on energy considerations. A special case concerns force laws for extended contacts, e.g. face-face and face-edge contacts between polyhedral particles. Such contacts require at least two (for face-edge) or three (face-

face) contact points since a line is parametrized by two points and a surface by three points. Without this description adhesive extended contacts cannot transmit torques.

Simple reversible or irreversible *cohesive force laws* have been used to investigate the rheology of cohesive or cemented granular materials. It is often assumed that the effects of cohesion are uniquely controlled by the maximum tensile force sustained by the contact. However, it happens that the effective cohesive action of forces crucially depends on both contact stiffness and damping coefficients. This means that the contact stiffness cannot be downscaled (for the sake of numerical efficiency) raising therefore a difficult scaling problem for the simulation of cohesive powders. Such a dynamic effect is also relevant for *liquid bridges* in the pendular state where an approximate solution of the Young-Laplace equation in equilibrium is generally used. Extending the capillary force law to dynamic situations is necessary for the simulation of wet granular flows even in the pendular state.

Regarding rough particle surface states, the general understanding is that they can be coarse-grained into enhanced friction force. However, *elastic asperities* lead to enhanced stress concentration and significant deviation from the Hertz regime. The asperities can be fully included as part of particle shape (first strategy), but a coarse-grained contact force law accounting for roughness size and angles can provide an interesting shortcut for DEM simulations. This is more specifically important for *plastic asperities*. The effect of damageable asperities can even be more complex with effects depending on how debris particles move inside the granular materials. They can lead to enhanced dissipation or solid lubrication with adverse effects for friction.

Particle fracture and deformation involve *internal texture* and stresses inside particles. A fine treatment (first strategy) can be achieved by incorporating *fracture mechanics* in a continuum representation of each particle. This approach has been applied by means of FEM, MPM, LEM and Peridynamics in 2D and 3D. Two major issues arise for the simulation of contacts between meshed particles: 1) The usual overlap-based or penalization approach makes no more sense, and 2) fine meshing in the volume does not imply a fine meshing of the surface. Hence, a specifically fine meshing of particle surface is required and the contact needs to be enforced as a *unilateral constraint*. This aspect strongly moves the method away from the spirit of DEM, which is based on contact force laws, although the particles remain discrete entities and their contacts bear friction forces. A coarse-grained approach (second strategy) is possible to particle fracture and large deformations by “making soft from hard”, i.e. by subdividing each particle into rigid cells interacting through force laws. This *bonded particle method* has been applied and characterized, with several promising results. However, the interactions between primary particles should be further worked out in the light of what was discussed previously about the interaction laws between particles in order to implement correctly the material behavior (elastic, plastic...) and *dynamic fracture* (involving second law of thermodynamics).

Since for advanced DEM we are concerned with realistic simulations at the industrial level (and not only with a better understanding of physical mechanisms and qualitative description of phenomena), the calibration issues are of paramount importance. Clearly, the DEM is an intrinsically predictive method with physical parameters fed into the system at the particle scale to predict the overall behavior emerging from the collective interactions of the particles. This *bottom-top approach* faces the challenge of measuring the relevant parameters at fine scales. There are not many examples in the literature based on this type of calibration and validation. In contrast, in many examples can be found with a *top-down approach* based on

the adjustment of particle-scale and contact parameters to fit to a macroscopic descriptor of the material.

There are several major issues that need to be solved in this respect: 1) There has not been enough fundamental research reported on the sensitivity of macroscopic (or effective) properties to the micro-scale (particle-scale and contact) parameters. Most parameters considered so far describe static packings of grains rather than *dynamic properties*; 2) Some micro-scale parameters have no influence on the (known) macroscopic parameters. For example, the interparticle friction coefficient bears on the angle of repose only for values below 0.5; 3) Furthermore, some micro-scale parameters may well be ineffective in steady states or in static equilibrium but effective in dynamic transients. This is the case for the restitution coefficient, which controls the compaction rate but not the solid fraction in the final stages of compaction; 4) Last, but not the least, we are used to assume that the particles have well-defined parameter values. In practice, however, one often observes high *variability*. This variability is well known, for example, in the case of particle fracture and characterized by the Weibull distribution. For other parameters, such as friction coefficient, no information is available. Such a variability can be included in the DEM, but the corresponding parameters should be provided from measurements. It is also important to note that finite numerical precision is a source of variability in normal restitution coefficient.

As mentioned previously, *gas-particle flows* have been modeled through the four modeling strategies in connection with applications to chemical and pharmaceutical processes. The first approach is known as particle-resolved DNS. The multicomponent LBM is increasingly used as a volatile method with improved treatment of no-slip condition and momentum exchange at the particle surface using methods such as immersed boundary. The second approach consists in considering gas flow through the pore network and a *pore-scale finite volume* scheme. In the third approach (Euler-Lagrange or *CFD-DEM*) the equations of fluid are averaged and solved together with expressions of effective fluid stress and forces between particles and fluid in a Eulerian framework. In the fourth approach (Euler-Euler or two-fluid model) transport equations are applied to averaged variables of both fluid and particles. This approach needs models of phase stresses and the interface between the two phases.

Advanced DEM simulations with resolved or partially resolved fields and phases involve much larger numbers of degrees of freedom than the basic DEM. Fully resolved simulations even for a few thousands of particles are possible only with *parallelized codes* or *GPU* techniques. Moreover, the huge amount of simulation data requires smart strategies for storage, access and analysis. For example, a single gas-particle simulation using a coupled DEM-LBM approach produces several terabytes of information. Future developments can benefit from progress in data science and *Machine Learning* techniques to manage both run-time data flows and post-processing procedures to extract meaningful information from raw data.

This review will expand and illustrate all the aspects mentioned in this brief outline. Here is a list of major topics that will be covered:

Gas-particle flows

Highly deformable particles

Particle fragmentation

Particle shapes and contacts

Generalized force laws  
Cohesive interactions  
Tribocharging  
Cementing bonds  
Capillary bridges  
Transport of scalar and vectorial variables by particles and contacts

Coarse-graining  
Data-driven approaches  
Hybrid discrete-continuum approaches  
Upscaling particle size  
Calibration issues  
Validation strategies