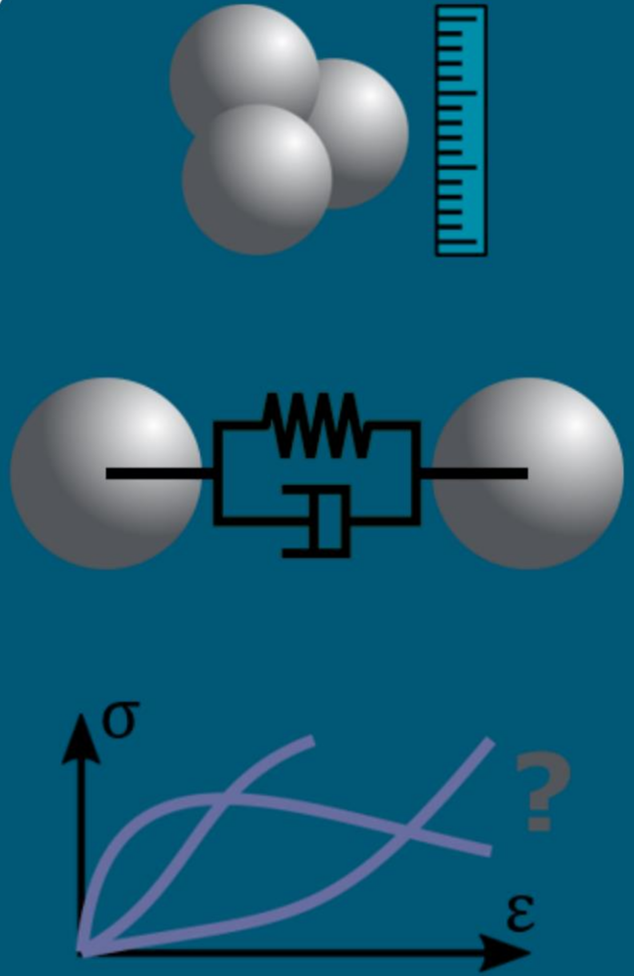
EBOOK

What is DEM

Theoretical background behind the Discrete Element Method (DEM)



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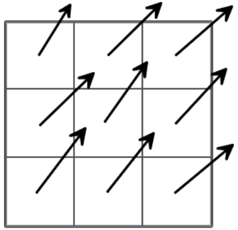
Modelling Approaches

When it comes to simulating particulate systems, two main modelling approaches can be identified – continuum (Eulerian) and discrete (Lagrangian).

Continuum

In the continuum approach, the constitutive behavior of granular matter is described by constitutive laws, commonly expressed in the form of differential equations which relate mechanical field variables (e.g. stress and strain).

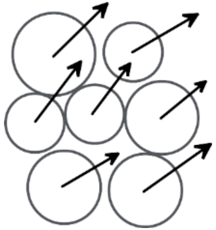
Modelling a substance with this approach assumes that it is continuous and completely fills the space it occupies. As a result, the behavior of individual particles is ignored. The resulting constitutive equations are solved numerically (e.g. Finite Element Method).



Discrete

In contrast to the continuum approach, discrete approaches model each single particle as a distinct entity and represent granular material as an idealized assembly of particles. The overall (macroscopic) system behavior results from individual particle interactions.

This makes the discrete approach very good for investigating phenomena occurring at the length scale of particle diameter and simulating bulk behavior of particles.



Discrete Approach for Granular Material Simulation

The critical issues in using continuum approaches for modelling of granular material are the proper formulations of constitutive behavior. Appropriate stress-strain laws for the material may often not exist or be excessively complicated. The particulate system phenomena are also very often highly dependent on particle level behavior.

As the micromechanics of granular material can be modelled more realistically with discrete approaches, they are better suited in modelling the flow and large displacements of discontinuous material.

Continuum	*Discrete*
Continuous systems	Discontinuous, granular media
Assumes granular substance fills the space it occupies	Models *behavior of individual* particles
Relates stresses and strains through constitutive equation	Overall system behavior results from individual particle interactions
Suitable when length scale of importance is higher	Good for investigating phenomena occurring at particle length scale

Motivation and Background of DEM

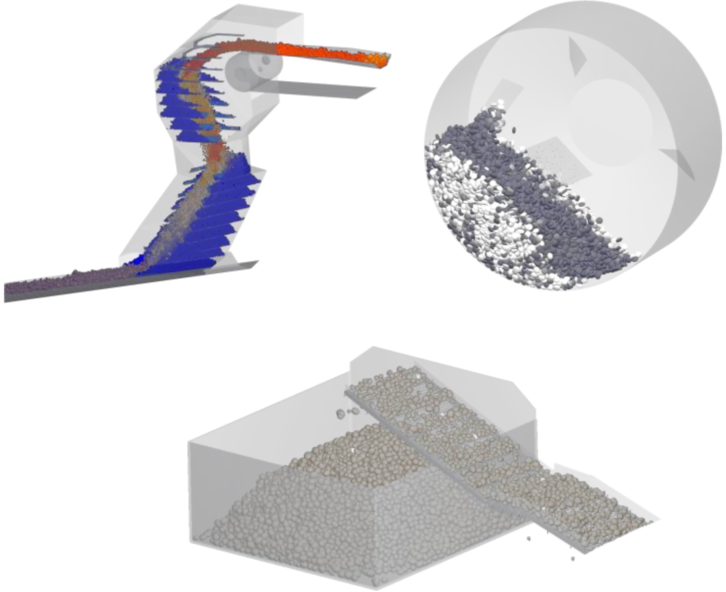
History

The theory of a discrete element model was introduced in 1956 (Alder and Wainwright) for the purpose of molecular dynamics studies. The principles of the discrete element method, also called the distinct element method, were then developed by Cundall and Strack in the 1970s.

The Discrete Element Method (DEM) can be precisely identified as a discrete approach having the ability to (i) numerically calculate finite particle displacements and rotations and to (ii) automatically perform contact detection for an assembly of particles.

Motivation

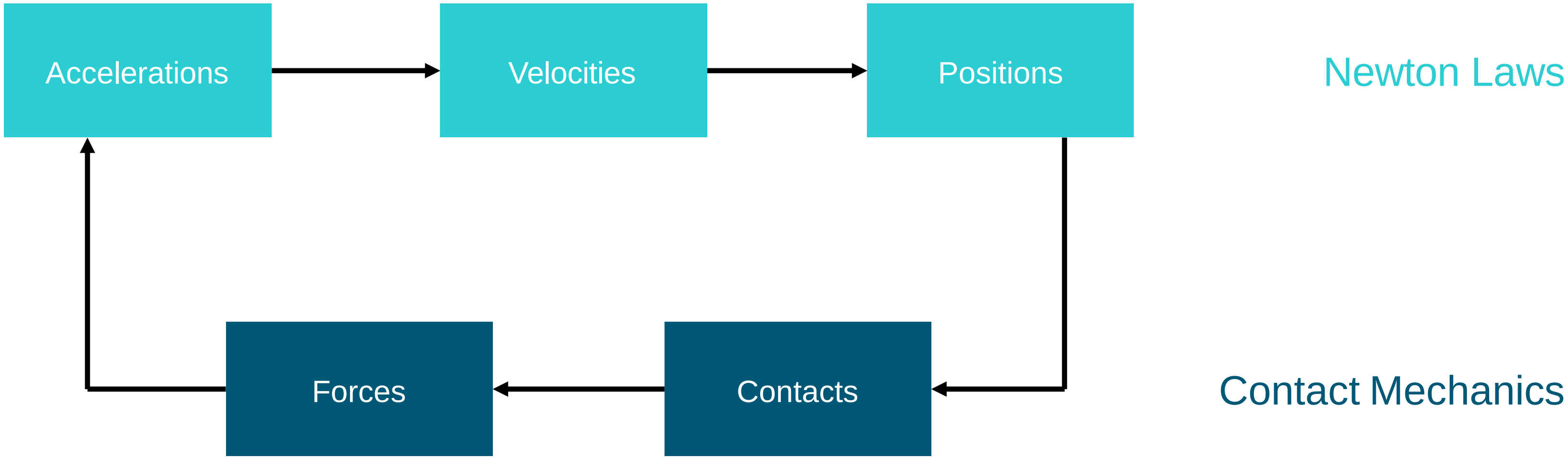
As DEM uses the discrete approach, it is very suitable for modelling the bulk behavior of materials. The simulations of discontinuous media provide enhanced understanding of the processes and often reduce the number of physical experiments required.



Various types of material can be simulated with DEM: ores, tablets, crop and others.

Main Principles of DEM

By using contact detection algorithms and applying suitable contact models, DEM software is capable of calculating forces acting on particles. Accelerations, velocities and positions are then computed using Newton's laws of motion and numerical integration.



Accelerations

Velocities

Positions

Newton Laws

Forces

Contacts

Contact Mechanics

Two Discrete Simulation Approaches

There are two main methods of discrete simulations: hard-sphere and soft-sphere approach.

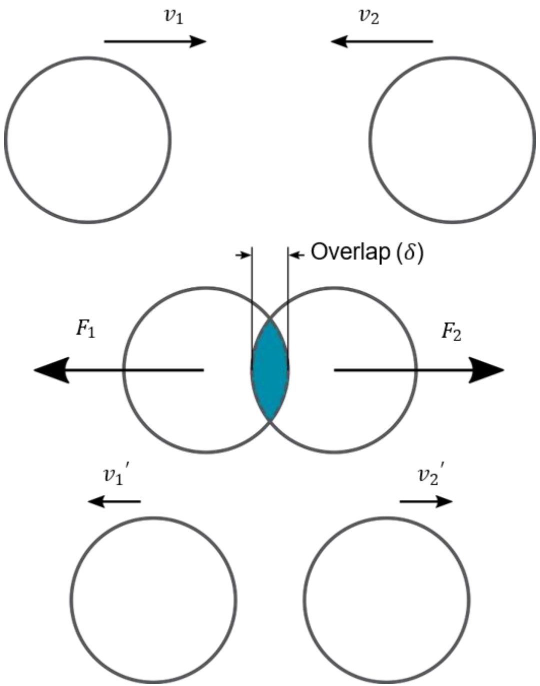
Hard-sphere

In a hard-sphere approach, the interaction forces are assumed to be impulsive and particles only exchange momentum through collisions. Forces between particles are not explicitly considered.

Soft-sphere

Another method is a soft-sphere approach in which particles are also assumed to be rigid but small overlaps are allowed to represent deformations during contact.

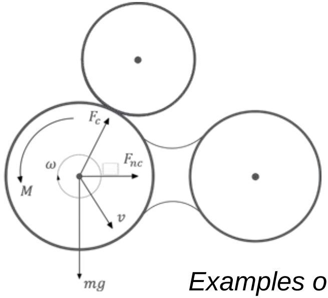
Soft-sphere method is the most common and accurate approach. It is used in most DEM packages, including EDEM.



The soft-sphere approach allows for small overlaps which are used to calculate magnitudes of the forces acting on particles.

Particle Motion Calculations

Each particle within a granular flow has 6 degrees of freedom and as a result can have two types of motion: translational and rotational. In DEM simulations, Newton's second law is used to calculate the translational and rotational accelerations, which are then numerically integrated over a time step to update particle velocities and positions.



Examples of forces acting on a 2D discrete particle. Same principles govern 3D DEM simulations with 6 d.o.f.

Rotation

The rotational motion is calculated based on the following equation:

$$I\frac{d\omega}{dt} = M$$

where

I is the moment of inertia

ω is the angular velocity

M is the resultant contact torque acting on the particle

t is time

Translation

The translational motion is calculated based on the following equation:

$$m\frac{dv}{dt} = F_g + F_c + F_{nc}$$

where

v is the translational velocity of the particle

m is the mass of the particle

Fg is the resultant gravitational force acting on the particle

FC and Fnc are the resultant contact and noncontact forces between the particle and surrounding particles or walls.

Particle Motion Calculations

Numerical Integration

The accelerations are numerically integrated over a time step to update particle velocities and positions.

$$\boldsymbol{x}\,(\boldsymbol{t} + \Delta\boldsymbol{t}) = \boldsymbol{x}\,(\boldsymbol{t}) + \boldsymbol{v}\,(\boldsymbol{t})\,\Delta\boldsymbol{t}$$

$$\boldsymbol{v}\,(\boldsymbol{t} + \Delta\boldsymbol{t}) = \boldsymbol{v}\,(\boldsymbol{t}) + \boldsymbol{a}\,(\boldsymbol{t})\,\Delta\boldsymbol{t}$$

where

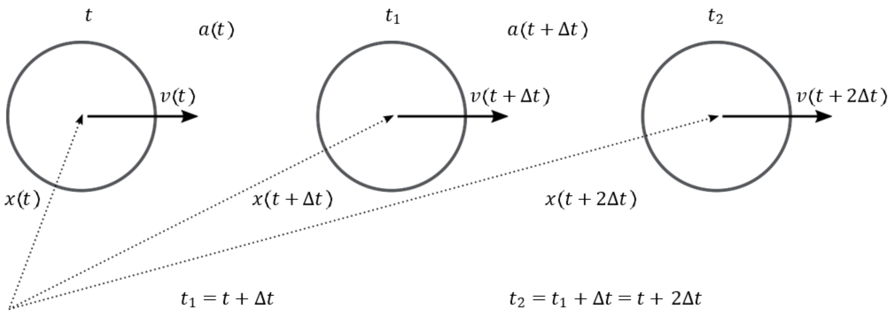
$\boldsymbol{v}(t)$ is velocity

$\boldsymbol{x}(t)$ is the position

$\boldsymbol{a}(t)$ is the accelerate of a particle at a given time $\boldsymbol{t}$

Δt is the time step

Rotational velocity and particle orientations are updated in a similar manner.



Single element motion calculation in terms of acceleration, velocity and position in DEM.

Importance of Time Steps

Time step (Δt) choice is of critical importance in DEM simulations. It has to be chosen sufficiently small for two main reasons: prevent excessive overlaps which result in unrealistically high forces and avoid effects of disturbance waves (Rayleigh waves). A typical time step range for DEM is in the range of 1e-4 to 1e-6 s, which is 10 or 100 times smaller than what is often seen in computational fluid dynamics (CFD).

Rayleigh surface waves

Movement of a particle within granular flow is affected not only by contacts with its immediate neighbors but also by disturbance propagations from particles far away.

By choosing a small enough time step in DEM, disturbance waves from each particle are prevented from propagating further than its neighboring partners.

Suitable time step (Rayleigh time step) is approximated from Rayleigh surface wave propagation speed. Usually a fraction of this time step is taken to ensure realistic force transmission rates and prevent numerical instability.

$$T_R = \frac{\pi R(\rho/G)^{1\ 2}}{0.1631\nu + 0.8766}$$

where

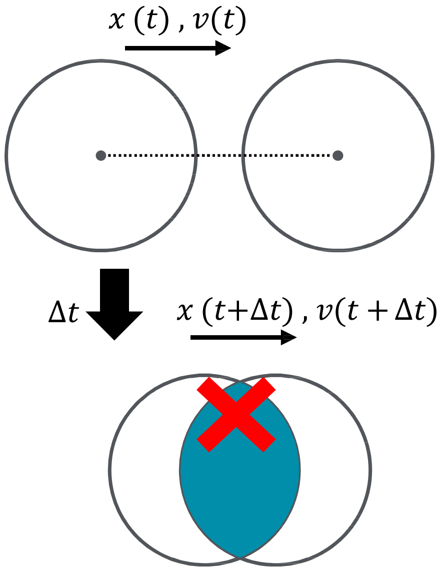
TR is the Rayleigh time step

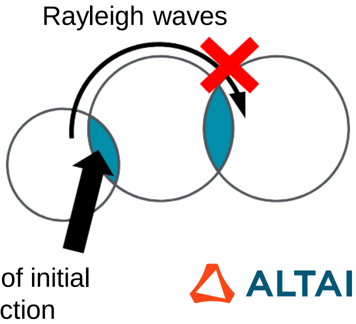
R is the particle radius

ρ is the density

G is the shear modulus

v is the Poisson's ratio of the particle





Force and Contact Force Models

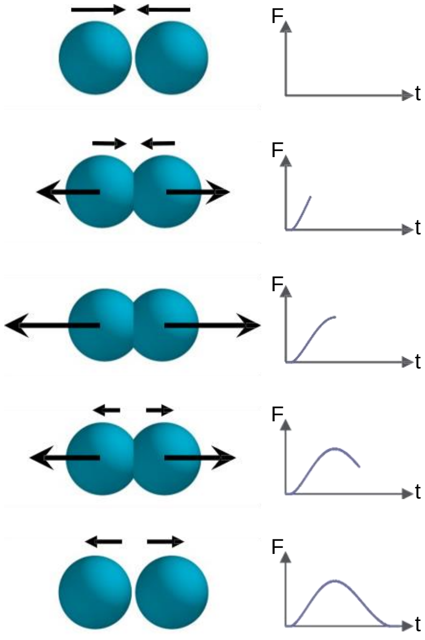
Contact force models

The particle deformation during collisions is modelled as overlap. The contact models relate the amount of overlap (tangential and normal) between two objects to determine the magnitudes of forces. The material and interaction properties (e.g. shear modulus, restitution, friction coefficients) defined by the user are used in the calculations.

The contact models are based on theories of contact mechanics and are mostly developed for spherical contacts. A number of them exists and they are capable of modelling elastic or plastic collisions for both non-cohesive and cohesive materials.

Other forces

Forces resulting from particle collisions are not the only ones present in DEM. The effects of particle body forces like gravity or noncontact forces like electrostatics or Van der Waals can also be simulated.



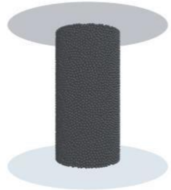
A typical dependence of normal force on the normal overlap is depicted with an example of two colliding spheres. Hertz-Mindlin (no slip) contact model is used.

Models for Various Material Behavior

In DEM, different types of material behavior can be simulated by a range of well-established models.

Dry granular material

This type of material can be simulated in DEM by a variety of linear or nonlinear models. The most common ones include Linear Spring or Hertz-Mindlin (no slip), which is a default contact model in EDEM.

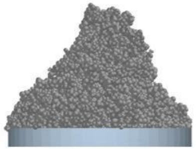


Bonding

Particles in DEM can be bonded together to resist tangential and normal movement up to a maximum value (defined by the user) at which the bond breaks. This model is particularly useful in modelling concrete and rock structures.

Electrostatics

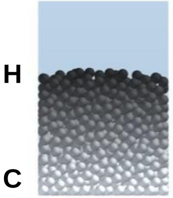
Longer-range electrostatic interactions can also be modelled in DEM. Particles are assigned a charge and experience forces based on the Coulomb's law. Applications like laser printer behavior can be simulated with such a module.



Cohesion

The cohesion models in DEM can simulate the influence of Van der Waals forces within the contact zones and allow the user to model strongly adhesive systems, such as dry powders or wet materials.

Heat transfer



For dense particulate systems, contacts between particles are substantial and heat conduction can be of significant importance. DEM simulations allow for modelling this inter-particle heat transfer and provide insight into variety of applications ranging from multi-phase reactors to kilns and calciners.

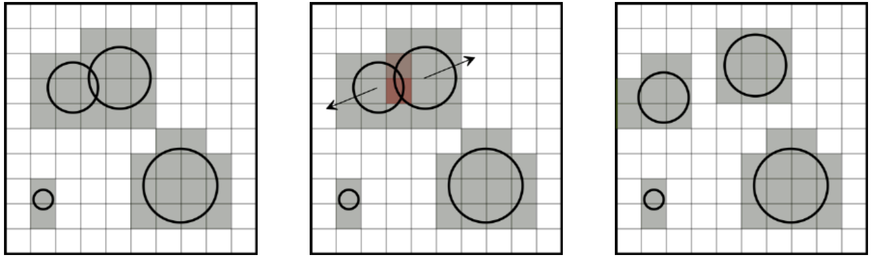
Contact Detection Algorithms

Importance

For spherical particles, a contact is detected if the distance between two spheres is less than summation of their radii. Therefore, the contact detection involves checking the distance between all the particles in the system. This process is computationally expensive and together with the force calculations takes about 70- 80% of the DEM computational effort.

Steps

In DEM simulations, the calculation domain is usually discretized into 3D cells to help the contact detection algorithms to be applied on a smaller scale and reduce the computational time. The grid size must be chosen based on the particle size distribution, dynamics and others. A grid size of 3-5 times the smallest particle radius is usually found be optimum. Once the domain has been discretized, the cells containing particles are marked active and are checked for contacts. The forces acting on each colliding particle are then calculated. Finally, the elements are repositioned as the result of the forces acting upon them and the active cells are again identified. The process repeats until the last time step of the simulation.



Steps of a typical contact detection algorithm: discretize domain and identify active cells, check for contacts and calculate forces, update particle positions and add/remove active cells. Similar principles are applied in 3D and for particle-geometry contacts.

Particle Shape Representations

Among all 3D shapes, spheres require the simplest and most efficient method of contact detection which significantly decreases simulation time. However, in some applications it is necessary to model particle irregularities as the shape of the particles affects the bulk material behavior (e.g. via mechanical interlocking).

Polyhedrons

This particle shape is defined in terms of corners, edges and faces. Its advantage is that complex flat-faced particles can be accurately represented. However, it requires massive computational power to detect contacts and recompute the coordinates of each corner and face during collisions. Also, simple and non-verified linear contact models are used for the interaction between polyhedrons.

Continuous superquadratic functions

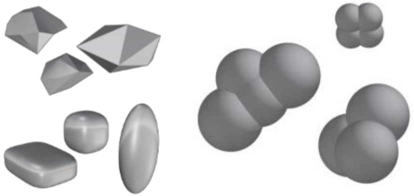
Particle shapes is described by the following equation:

$$\left(\frac{x}{a}\right)^m + \left(\frac{y}{b}\right)^m + \left(\frac{z}{c}\right)^m = 1$$

The contact detection process for those particles is more efficient than for polyhedrons but still computationally expensive due to nonlinear equations. Similar to polyhedral particles, the main disadvantage is the lack of well-defined contact models for this shape.

Multi-sphere method

Particle shape approximated by a number of overlapping or touching spheres whose centers are fixed in position relative to each other. The advantage of this method is that it provides an approximation to actual irregularities while maintaining the computational efficiency and accuracy of spheres.



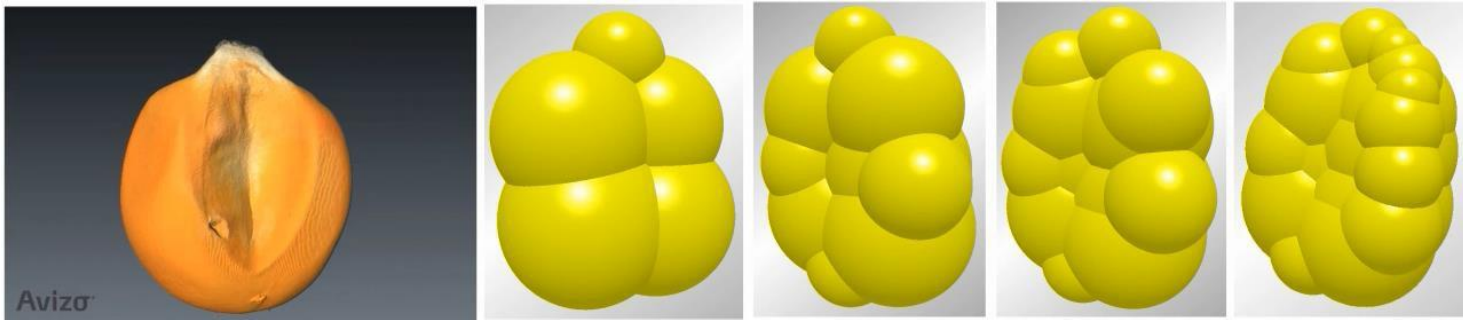
Three main irregular particle shapes used in DEM simulations. Clockwise from the top left: polyhedrons, multi-spheres and superquadratic functions. Other approaches which make use of combination of those also exist (e.g. spheropolyhedra).

Why do we use multi-sphere in EDEM

Why multi-sphere?

Spheres offer the most efficient method of contact detection as well as very accurate evaluation of contact overlap. This provides fast and reliable calculation of contact forces. Multi-spheres allow for modelling particle irregularities while maintaining the efficiencies mentioned above.

Theoretically, any particle shape can be modelled by increasing the number of overlapping spheres as long as the computations are within a reasonable range of complexity. If required, CAD templates can also be used for visualization purposes in the post - processing stage.



Representation of a seed using 5, 10, 15 and 20 spheres. Changing the number of spheres controls the induced surface roughness (Courtesy of Leeds University).

How to Represent Real Material

Single sphere representation

Precise particle shape representation

Although it is always of interest to simulate particulate systems with single spheres due to their efficiency, they may not be a good representative for irregular particles in some cases.

Characteristics of single sphere representation:

Simple and effective contact detection

Lacks mechanical interlocking properties of real materials

Rotation can only result from tangential forces

Real material particle shapes can be precisely modelled with numerous clumped-spheres, complex polyhedron and others. However, such precise models are usually computationally expensive or even impossible to achieve.

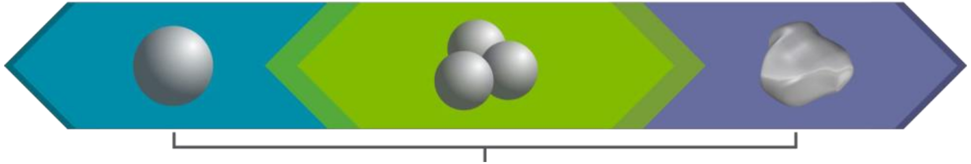
Characteristics of precise particle shape representation:

Very computationally expensive

May be impossible to obtain (e.g. very small particles in powder-like material)

Not necessary to model bulk behavior realistically

How to Represent Real Material



Representative calibrated model

The final material model is usually a balance between a detailed real particle representation and computational efficiency.

Characteristics of a representative calibrated model:

Models particle irregularities

Maintains computational efficiency and reasonable simulation times

Realistically and accurately represents properties and behavior of real bulk material

In order to realistically represent the bulk behavior of material, material calibration is needed for any particle shape.

Material Calibration

Overview

In order to have confidence to make design decisions based on DEM simulation results, there needs to be a link between material represented in the simulation and the real-world bulk flow behavior. This is achieved via material calibration.

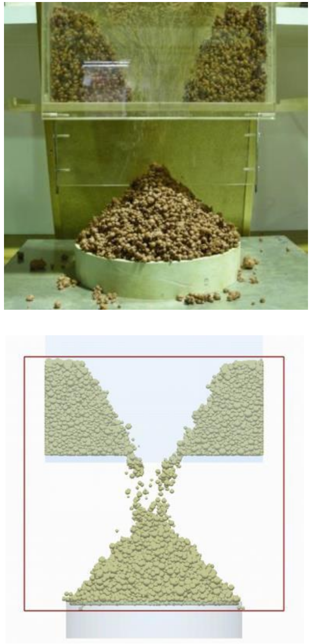
The material in many industrial applications can include large number of particles, variety of shapes or very fine particles. It is computationally expensive or even virtually impossible to exactly model the detailed structure of single material particles in DEM simulations. Hence, the most common approach involves creating a calibrated representation of the real material.

Suitable particle size distribution and shapes are chosen based on the real material samples. The material and interaction properties are then varied to match the real bulk behavior.

Calibration steps

The material samples for a site are first collected and prepared for testing. A suitable test is chosen (e.g. angle of repose, uniaxial compression) and a simple representative simulation of this test is created in a DEM software.

Appropriate characteristics of the bulk material are measured during the physical test. The material and interaction properties (e.g. shear modulus, restitution, friction coefficients) are then varied in the simulation software until the experimental bulk behavior is matched.



Experimental and DEM setups of a typical angle of repose test.

Geometries in DEM Simulations

Simple shapes

Simple shapes like boxes, cylinders or 2D polygons can be created in DEM. As they are usually defined using mathematical equations, the particle-geometry contact detection is very efficient.

Complex shapes

More complex geometry shapes are usually imported as a 3D surface-meshed files. Triangular mesh elements are typically used. Because the contact detection algorithms check for contacts with each individual mesh element, the amount of triangles may affect computational needs and simulation time.

Movement of the geometry

The geometries in DEM are also allowed to have dynamic motion. This includes translation, rotation or sinusoidal motions with or without accelerations. Similar to particles, the geometries are repositioned in small incremental displacements. Again, updating positions of complex geometries increases computational time.

In DEM, complex geometries can be imported as 3D surface-meshed files. The simulations also allow for assigning various types of motion to the geometry parts.

DEM Coupling and Co-Simulation

DEM-MBD

DEM coupling with multi-body dynamics (MBD) packages allows users to perform simulations with programmatic control of geometry motion and physics enabling implementation of complex, rigid body motion.

The bulk material forces acting on equipment surfaces calculated by DEM software can be retrieved by the coupled code to return realistic equipment kinematics.

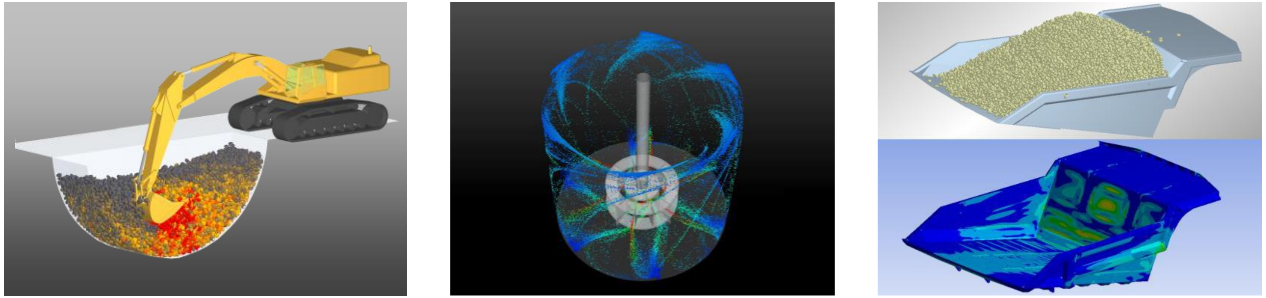
DEM-CFD

DEM can also be used in combination with computational fluid dynamics (CFD) in order to investigate particle behavior in fluid phase. The solid and fluid motion are solved through Newton's equations of motion for discrete particles and Navier-Stokes equations for the continuum fluid.

The coupling is based on continuous exchange of information between DEM and CFD software. Various drag models can be used for particle-fluid interaction.

DEM-FEA

DEM software can provide realistic forces and pressure distributions of material acting on equipment. These loads can then be used as inputs into structural or fatigue analysis in any finite element analysis (FEA) software.



DEM-MBD simulation of an excavator, DEM-CFD model of particle flotation dynamics (Courtesy of University of Utah) and DEM-FEA coupling used to analyze dump truck bucket loads (Courtesy of Austin Engineering).

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