A review of the Discrete Element Method/Modelling (DEM) in agricultural engineering

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Abstract

With the development of high-performance computing technology, the number of scientific publications regarding computational modelling of applications with the Discrete Element Method/Modelling (DEM) approaches in agricultural engineering has risen in the past decades. Many granular materials, e.g. grains, fruits and soils in agricultural engineering are processed, and thus a better understanding of these granular media with DEM is of great significance in design and optimization of tools and process in agricultural engineering. In this review, the theory and background of DEM have been introduced. Some improved contact models discussed in the literature for accurately predicting the contact force between two interacting particles have been compared. Accurate approximation of irregular particle shapes is of great importance in DEM simulations to model real particles in agricultural engineering. New algorithms to approximate irregular particle shapes, e.g. overlapping multi-sphere approach, ellipsoid, etc. have been summarized. Some remarkable engineering applications of the improved numerical models developed and implemented in DEM are discussed. Finally, potential applications of DEM and some suggested further work are addressed in the last section of this review.

Introduction

The Discrete Element Method/Modelling (DEM) is a numerical technique proposed by Cundall et al. (Cundall and Strack, 1979), which has been widely used to model and understand the behaviour of granular materials during the past decades. Xia et al. proposed an approach coupling DEM to the Finite Element Method (FEM) to understand the impact-induced deformation of screen mesh and the numerical approach developed in this work can be used to optimize the screen machines (Xia et al., 2017). Another application of DEM is to model the screening process for a linear screening machine, and the underlining physics regarding particle looseness has been investigated (Li et al., 2016; Wu et al., 2018). An optimization algorithm has been developed by Chen et al. to optimize the elliptically vibrating screen, and discrete element simulations have been used to model the virtual screening process to validate the prediction of the hybrid MACO-GBDT algorithm (Chen et al., 2021). In addition to these applications in processing engineering, DEM can also be used to model complex mechanical behaviour in geotechnical engineering, e.g. Xia et al. investigated the crushing of brittle materials with an extended DEM and three different particle packing patterns (Xia et al., 2019). DEM is also widely used in understanding complex physics in chemical engineering, e.g. modelling viscosity of particle suspensions (Kroupa et al., 2016), aggregation of suspended micro-sized particles (Peng et al., 2010), and various forces due to, e.g. DLVO theory, Brownian motion and Hooke's law implemented in DEM are used to model the agglomeration of polymer particles (Kroupa et al., 2012). A more general and comprehensive review can be found via (Zhu et al., 2008).

Particle shape is of great significance in the motion and contact behaviour of granular media (Coetzee, 2016; Lu and McDowell, 2007). In agriculture, many irregular particle shapes, such as bulk wheat particles, corn kernel and soil powders can be found. In recent years, both conventional and extended DEM approaches have been increasingly used in agriculture to model and investigate various processes involving granular materials, such as soil (Qi et al., 2019; Huang et al., 2023), seeds (Pasha et al., 2016), and fertilizers (Bangura et al., 2020). The effect of particle shape on the seed motion and mixing has been investigated by Pasha et al. (Pasha et al., 2016). The X-ray microtomography was used to scan the surface of natural seeds (as shown in Figure 1) and then approximate the shape of real seeds with a certain number of overlapping spheres with difference diameters, as shown in Figure 2.

Figure 1: Surface morphology of a natural corn seed particle obtained by the X-ray microtomography (Pasha et al., 2016).
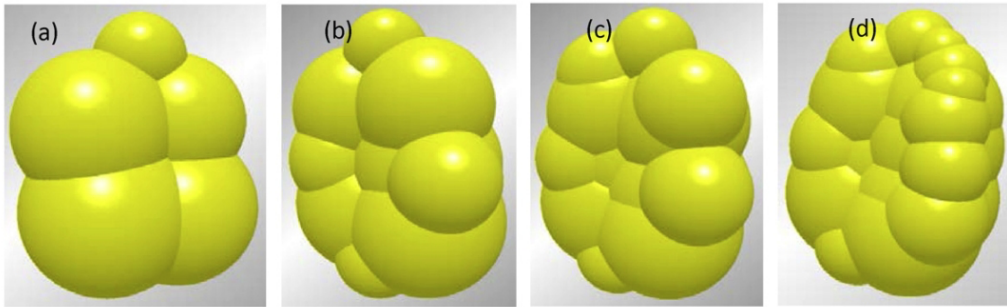

Figure 2: Representation of a real corn seed with overlapping sub-spheres in DEM with: (a) five, (b) ten, (c) fifteen and (d) twenty overlapping sub-spheres (Pasha et al., 2016).

The main focus of this review is to summarize the recent significant progress of these applications of DEM in modelling and optimizing some critical processes in agriculture. One of the primary applications of DEM in agriculture is to model the complex behaviour of soil particles. Soil is a typical granular media with irregular particle shape, poly-disperse radius ratio, and different compositions, as shown in Figure 3. Understanding the behaviour of soil particles is of great importance in designing and optimizing high-performance soil-engaging tools in agriculture as presented in (Qi et al., 2019). The flowability of soil powders was modelled via DEM, and this numerical model was validated with experimental studies.

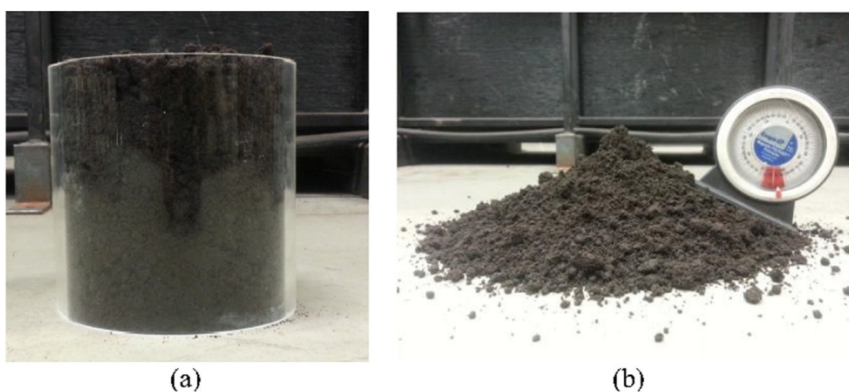Figure 3: (a) A cylinder filled with soil particles is used to measure the angle of repose, (b) accumulations of soil particles on a wall (Qi et al., 2019).

It is found that the diameter of soil particles influences the kinetic energy of particles significantly. However, particle diameter has less influence on the angle of repose in these numerical simulations as found in this literature (Qi et al., 2019).

Another promising application of numerical approaches based on DEM in agriculture is the computational modelling of seed particles. Seed particle is another typical granular material widely processed in agriculture. The mechanical behaviour of seed particles can be influenced by various factors, e.g. particle shape (either convex or concave), moisture, and some other physical properties (Zhou et al., 2020). In agricultural engineering, one goal is to disperse seeds efficiently and accurately. The DEM method can be used to model the dispersal of seeds, which is an essential process in crop production. For instance, DEM simulations can be used to study the effect of pressure airflow on the transport of seeds in the seed tube (Lu et al., 2022). A summary of promising applications of numerical methods and models based on DEM is outlined in Table 1.
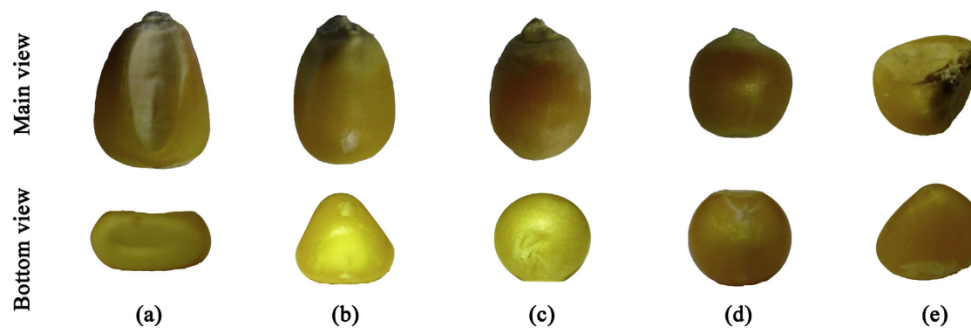

Figure 4: Different particle shapes of maize seeds: (a) horse-tooth shape, (b) truncated triangular pyramid shape, (c) ellipsoid cone shape, (d) spheroid shape and (e) irregular shape (Zhou et al., 2020).

Table 1: Summary of remarkable applications of DEM approaches in engineering.

Authors (publication year)	Applications
Lu et al. (2007) (Lu and McDowell, 2007)	Effect of particle shape on heterogeneous stresses
Peng et al. (2010) (Peng et al., 2010)	Aggregation of suspended nanoparticles
Kroupa et al. (2012) (Kroupa et al., 2012)	Agglomeration of polymer particles
Li et al. (2016) (Li et al., 2016)	Particle looseness in screening process
Kroupa et al. (2016) (Kroupa et al., 2016)	Viscosity in concentrated suspensions
Pasha et al. (2016) (Pasha et al., 2016)	Simulations of rotary seed coater
Xia et al. (2017) (Xia et al., 2017)	DEM-FEM coupling for vibrating screen
Podlozhnyuk et al. (2017) (Podlozhnyuk et al., 2017)	DEM simulations with superquadric particles
Soltanbeigi et al. (2018) (Soltanbeigi et al., 2018)	DEM simulations with irregular particles
Wu et al. (2018) (Wu et al., 2018)	Parameter optimization of a linear vibrating screen
Qi et al. (2019) (Qi et al., 2019)	Properties of soil flow
Xia et al. (2019) (Xia et al., 2019)	Particle crushing and particle packing
Bangura et al. (2020) (Bangura et al., 2020)	Discharge of fertilizer particles
Chen et al. (2021) (Chen et al., 2021)	Optimization of an elliptical vibrating screen
Schramm et al. (2022) (Schramm and Tekeste, 2022)	Modelling flexible wheat straw
Lu et al. (2022) (Lu et al., 2022)	Transport of seed particles in a tube

| Sharaby et al. (2022) (Sharaby et al., 2022) | Modelling sesame seed particles |
| Huang et al. (2023) (Huang et al., 2023) | Movement of soil particles |

Theory and mathematical formulation

The underlying physics behind DEM is governed by Newton's and Euler's second law of motion for translational and rotational motions, respectively. These equations are given by

$$m_i \frac{d^2 \mathbf{x}_i}{dt^2} = \sum_{i=1}^{N_p} \mathbf{F}_{ij} + m_i \mathbf{g}, \qquad (1)$$

$$I_i \frac{d^2 \boldsymbol{\theta}_i}{dt^2} = \sum_{i=1}^{N_p} \mathbf{M}_{ij}. \qquad (2)$$

Here, Eqn. 1 and Eqn. 2 are the governing equations for translational and rotational motions, respectively (Cundall and Strack, 1979). Additionally, m_i is the mass of the particle i, N_p is the number of particles contacting with particle i, and $\mathbf{F}_{ij}$ is the interaction force acting on the particle i by its neighbouring particles interacting with it.

In principle, the interaction force $\mathbf{F}_{ij}$ consists of two components, namely, forces in normal and tangential directions. $\mathbf{F}_{ij}$ is given by

$$\mathbf{F}_{ij} = \mathbf{F}_{ij}^n + \mathbf{F}_{ij}^t, \qquad (3)$$

where $\mathbf{F}_{ij}^n$ and $\mathbf{F}_{ij}^t$ are the interaction forces in normal and tangential directions, respectively (Goniva et al., 2012; Norouzi et al., 2016). The normal contact force $\mathbf{F}_{ij}^n$ is calculated by

$$\mathbf{F}_{ij}^n = (k_n \delta_n - \gamma_n \mathbf{u}_n^r)\mathbf{n}_{ij}, \qquad (4)$$

where $\mathbf{n}_{ij}$ is the unit normal vector pointing from particle i to particle j. Some other terms in Eqn. 4 are explained in the coming sections. Furthermore, the tangential contact force $\mathbf{F}_{ij}^t$ is computed by

$$\boldsymbol{F}_{ij}^t = \min \left\{ \left| k_t \int_{t_0}^{t_c} \boldsymbol{u}_t^r \, dt + \gamma_t \boldsymbol{u}_t^r \right|, \mu_c \boldsymbol{F}_{ij}^n \right\}, \qquad (5)$$

where μ_c is the coefficient of friction. This is the so-called history-dependent tangential contact force model which is implemented in the open-source DEM code LIGGGHTS (Computing, 2015).

In Eqn. 2, I_i is the moment of inertia of particle i, θ_i is the angular displacement of particle i and $\mathbf{M}_{ij}$ the moment acting on particle i. Numerical integration with the Verlet integration scheme (Verlet, 1967) is adopted to solve and update the particle position vector $\mathbf{x}_i$ and angular displacement $\boldsymbol{\theta}_i$ from Eqs. 1 and 2. The numerical scheme to obtain and update the particle velocity $\mathbf{u}$ from Eqn. 1 is given by:

$$\mathbf{u}\left(t + \frac{\Delta t}{2}\right) = \mathbf{u}(t) + \frac{\Delta t}{2}\frac{d\mathbf{u}(t)}{dt}, \qquad (6)$$

$$\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \Delta t\mathbf{u}\left(t + \frac{\Delta t}{2}\right), \qquad (7)$$

$$\mathbf{u}(t + \Delta t) = \mathbf{u}\left(t + \frac{\Delta t}{2}\right) + \frac{\Delta t}{2}\frac{d\mathbf{u}\left(t + \frac{\Delta t}{2}\right)}{dt}, \qquad (8)$$

where Δt is the size of the time step. For such an explicit numerical scheme, the maximum time-step size must be smaller than the Rayleigh time-step size R_{ts} calculated by

$$R_{ts} = \frac{\pi\bar{R}\sqrt{\frac{2\rho_p(1+\nu)}{E}}}{0.1631\nu + 0.8766}, \qquad (9)$$

where $\bar{R}$ is the average particle radius, ρ_p the particle density, E the Young's modulus and ν the Poisson's ratio (Norouzi et al., 2016).

In addition to the second-order velocity Verlet integration scheme, the other two integration schemes are introduced for completeness. The first-order Euler integration scheme (also called the forward Euler method) is simple and easy to implement. It can also be used to update particle position and velocity. The basic idea for updating particle position and velocity is given by

$$\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \mathbf{u}(t)\Delta t, \qquad (10)$$

and

$$\mathbf{u}(t + \Delta t) = \mathbf{u}(t) + \frac{d\mathbf{u}(t)}{dt}\Delta t, \qquad (11)$$

respectively (Atkinson, 1991).

The Leapfrog integration scheme is another second-order scheme, and it is a variant of the Verlet integration scheme. In Leapfrog integration scheme (Skeel, 1993), the position and velocity are updated by

$$\mathbf{x}\left(t + \frac{\Delta t}{2}\right) = \mathbf{x}(t) + \mathbf{u}(t)\frac{\Delta t}{2}, \qquad (12)$$

$$\mathbf{u}(t + \Delta t) = \mathbf{u}(t) + \frac{d\mathbf{u}\left(t + \frac{\Delta t}{2}\right)}{dt}\Delta t, \qquad (13)$$

$$\mathbf{x}(t + \Delta t) = \mathbf{x}\left(t + \frac{\Delta t}{2}\right) + \mathbf{u}(t + \Delta t)\frac{\Delta t}{2}. \qquad (14)$$

More detailed discussion regarding these contact models in Eqs. 1 and 2 and numerical details can be found in the literature (Goniva et al., 2012; Blais et al., 2016; Norouzi et al., 2016). During the past several decades, some open-source and commercial software have been developed for conducting DEM simulations. These software and code are listed in Table 2. Table 2 provides valuable guidance for engineers to select code/software for conducting DEM simulations.

Table 2: Summary of the open-source and commercial software/code for DEM simulations.

Code/Software	Parallel	Open-source	Description
LIGGGHTS	MPI	Yes	Modified from the open-source code LAMMPS
EDEM	Shared memory	No	Commercial code, can be coupled to Adams, Ansys, etc.
PFC	Multi-threaded	No	Commercial code, can conduct 2D and 3D simulations
Yade	OpenMP	Yes	Can be coupled to OpenFOAM, Escript, etc.
ESyS-Particle	MPI	Yes	Can be coupled to Escript, etc.
MFiX-DEM	MPI	Yes	Can be coupled to fluid simulation code
Woo	MPI	Yes	A fork of Yade DEM code
GranOO	OpenMP	Yes	Excellent in the bonded particle model
MercuryDPM	MPI	Yes	Large simulations with wide size distributions
BECKER 3D	MPI	No	Multiphase simulations with GPU acceleration

3. Model development and applications

During the past decades, many promising applications regarding the understanding of processes in agricultural engineering have been presented in the literature. In this section, these applications are classified into the following subsections: contact models and algorithms for DEM, approximations of irregular natural seed particle shapes, and fancy applications of DEM in optimizing the design of tools for agricultural engineering.

3.1. Contact models and algorithms for DEM

3.1.1. Contact models of DEM

The contact model is of great significance in accurately predicting contact forces between two particles or a particle and a wall. During the past few years, several improved contact models have been developed for calculating contact forces accurately and accelerating numerical calculations. The Hertzian contact model is a simple yet efficient contact model to compute the contact force between two particles (Goodier and Timoshenko, 1970). The normal contact force $\mathbf{F}_n$ is given by

$$\mathbf{F}_n = k_n \Delta x^{\frac{3}{2}}, \qquad (15)$$

where Δx is the normal overlap between two particles, and k_n is the spring stiffness. k_n is calculated by

$$k_n = \frac{4}{3} E^* \sqrt{R^*}, \qquad (16)$$

where E^* and R^* are the equivalent Young's modulus and radius, respectively. The two quantities are given by

$$E^* = \frac{E_i E_j}{E_i(1-\nu_j^2) + E_j(1-\nu_i^2)}, \qquad (17)$$

and

$$R^* = \frac{R_i R_j}{R_i + R_j},$$ (18)

respectively (with E_i, R_i, and v_i being the Young's modulus, radius and Poisson's ratio of particle i, respectively).

The hertzian contact model only accounts for the contribution of the spring model as shown in Eqn. 15. Visco-elastic contact model is extended to model the visco-elastic behavior of two interacting particles by adding the contribution of a dash-pot. The normal contact force calculated by the visco-elastic contact model is given by

$$\mathbf{F}_n = k_n \Delta x^{\frac{3}{2}} + c k_n \Delta x^\alpha \mathbf{U}_n,$$ (19)

where c is the damping coefficient of the dash-pot, α is the exponent (α can be 0.5 as suggested in the literature) and $\mathbf{U}_n$ is the relative velocity in the normal direction (Kuwabara and Kono, 1987; Seville et al., 2000). Additionally, the first force term in Eqn. 19 is due to the elastic deformation between two particles, and the second term is non-linear and known as the viscous dissipative force term. Regarding the damping coefficient in the visco-elastic model, it is defined by

$$c = 2K^* \sqrt{R^*},$$ (20)

where K^* is the equivalent curvature of two interacting particles whose curvatures are K_i and K_j, respectively.

Thornton et al. proposed an adhesive contact model to model the stick/bounce behavior of granular media (Thornton and Ning, 1998). The force-displacement relationship is demonstrated in Figure 5, and the detailed derivation of this model can be found via (Thornton and Ning, 1998; Horabik and Molenda, 2016).
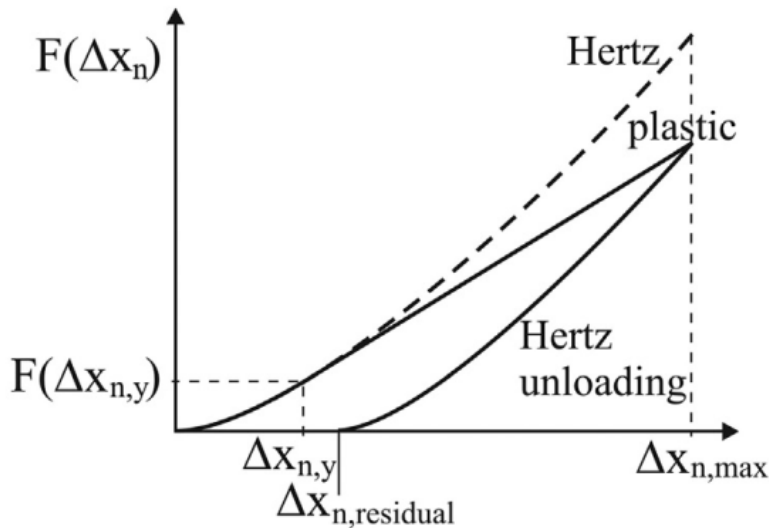

Figure 5: Force versus displacement of the Thornton model (Horabik and Molenda, 2016).

Luding et al. proposed a very simple contact model for cohesive and frictional granular materials in the range of $0.1 - 10 \ \mu m$ (Luding, 2008). This model is known as the adhesive and elastic-plastic contact model, and the force-displacement relationship can be found in Figure 6. The contact force of the adhesive and elastic-plastic Luding model is given by
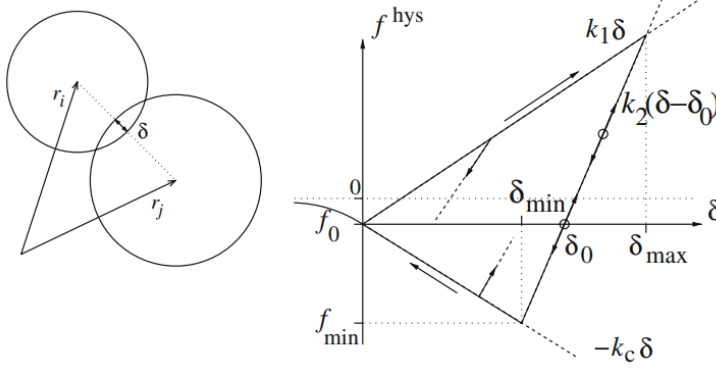

Figure 6: Left image: two interacting particles with overlap δ; Right image: force-displacement diagram (Luding, 2008).

$$\mathbf{f}_{hys} = \begin{cases} k_1\delta, & \text{if } k_2(\delta - \delta_0) \geq k_1\delta, \\ k_2(\delta - \delta_0), & \text{if } k_1\delta > k_2(\delta - \delta_0) > -k_c\delta, \\ -k_c\delta, & \text{if } -k_c\delta \geq k_2(\delta - \delta_0). \end{cases} \quad (21)$$

In addition to these aforementioned contact models for calculating the contact force. In DEM, another promising model called the Bounded Particle Model (BPM) has been used to model continuous media within the framework of DEM. The basic idea of BPM is to generate virtual beams for every particle-particle pair and set parameters for beams. These beams fail and break when external forces acting on beams are larger than their strength threshold. A simple BMP implemented in the open-source DEM code YADE was conducted by Xia et al. to model the continuous media, namely, a rectangular rock sample and its crushing behavior was numerically investigated (Xia et al., 2019). In agricultural engineering, the BPM is extended to model the failure of flexible straw steams by Shi et al. (Shi et al., 2023). In this study, two different types of virtual bonds have been proposed, as shown in Figure 7. Simulation results are found to be in good agreement with corresponding experimental validations. It proves that the BMP proposed by Shi et al. (Shi et al., 2023) is feasible and promising in modelling flexible straw steams.

Another remarkable study conducted by Wang et al. (Wang et al., 2019) is to investigate the effect of particle size ranging from 3 to 19 mm on soil-subsoiler interactions with a Hertz-Mindlin Bonding (HMB) model implemented in the commercial DEM software EDEM. In this study, soil rupture distance ratio, height of accumulated soil, and soil disturbance area were investigated by varying the particle radius. It found that particles with a radius of 7 mm are recommended for numerical simulations with the HMB model (Wang et al., 2019). An extended Hertz–Mindlin model with the bonding contact was developed by Zhao et al. for modelling the cotton stalk as shown in Figure 8 (Zhao et al., 2023). The experimental study was used to validate the bonded model implemented in EDEM and found that the Hertz–Mindlin model with bonding contact is suitable for modelling the cot-ton stalk (Zhao et al., 2023).
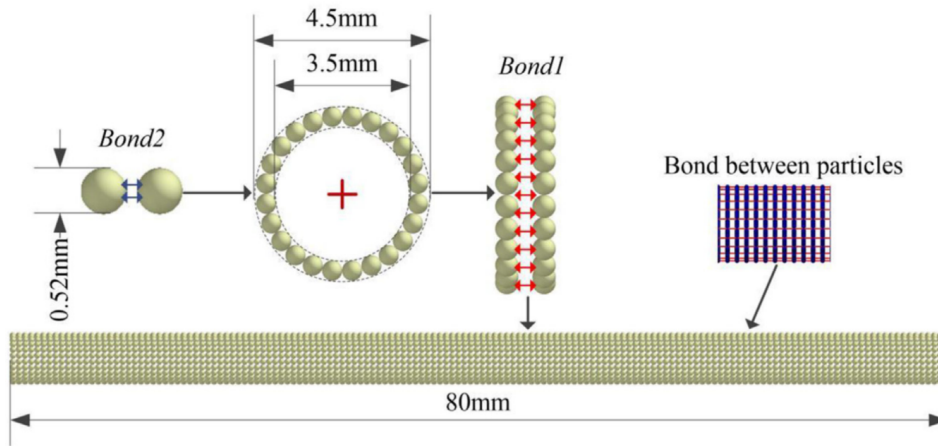
Figure 7: The schematic diagram of modelling a flexible straw steam with DEM (Shi et al., 2023).
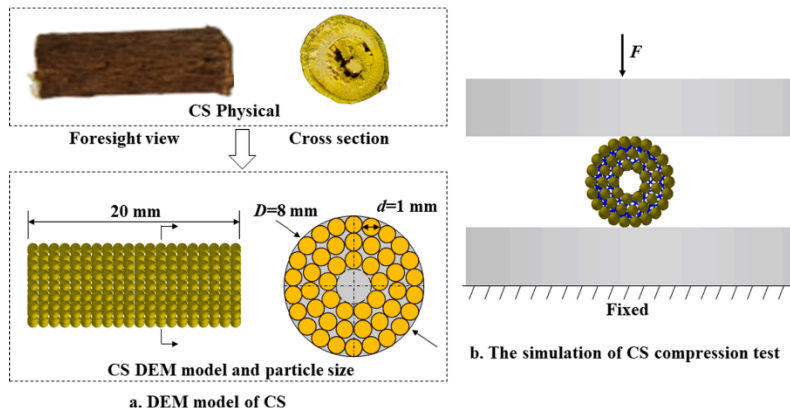

Figure 8: (a) numerical approximation of a cotton stalk in DEM, (b) the numerical set-up of the compression test (Zhao et al., 2023).

A better understanding of the tensile behaviour of tobacco leaf is of importance to design and optimize tobacco harvesting machines. An extended DEM model with virtual bonds was proposed to model the flexible tobacco leaf under tensile conditions as shown in Figure 9. The particle packing pattern does influence the mechanical behaviour of the continuous media, as discussed in the literature (Xia et al., 2019). As shown in the magnified sub-figure of Figure 9, the packing pattern is the so-called modified hexagonal close packing with some initial gap between every two particles.
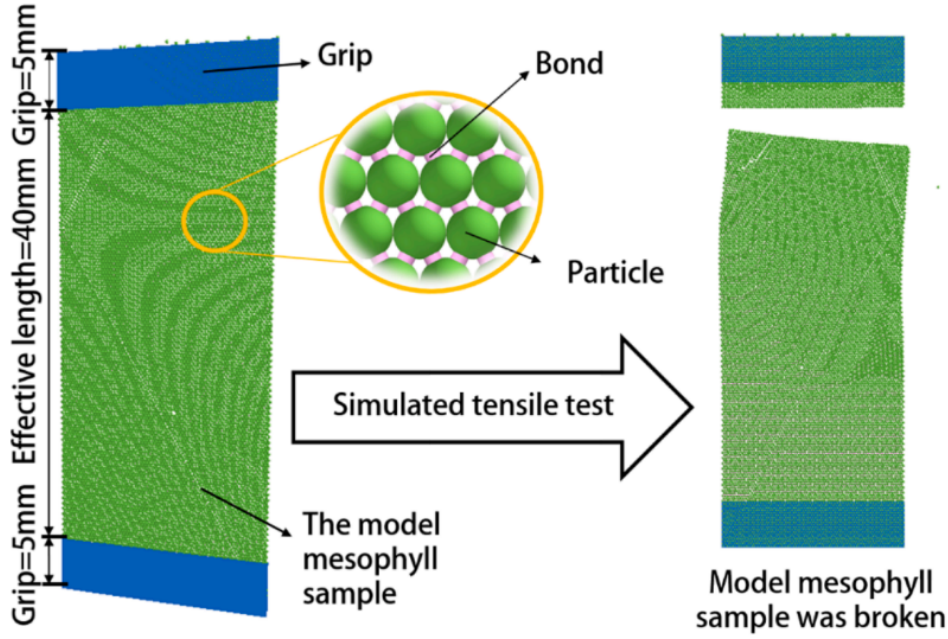
Figure 9: The numerical set-up for DEM simulations of the tensile test (Tian et al., 2023).

Additionally, simple cubic packing and some other packing patterns can also be used for the bonded particle model. In this study, two different regions, namely, a non-linear region and an elastic region have been found. This numerical model successfully predicted both the general trend and the data-yielding elastic behaviour (Tian et al., 2023). A brief summary of these aforementioned contact models are outlined in Table 3.

When particle shape matters

Accurate approximations of natural seed shapes are of great importance in the computational modelling of complex behaviour of seed particles with DEM.

Table 3: Summary of contact models in DEM.

Authors (publication year)	Formula/Applications
Goodier et al. (1970) (Goodier and Timoshenko,1970)	$$\mathbf{F}_n = \frac{4}{3} E^* \sqrt{R^*} \Delta x^{\frac{3}{2}}$$
Kuwabara et al. (1987) (Kuwabara and Kono, 1987)	$$\mathbf{F}_n = k_n \Delta x^{\frac{3}{2}} + c k_n \Delta x^{\alpha} \mathbf{U}_n$$
Luding et al. (2008) (Luding, 2008)	$$\mathbf{f}_{hys} = \begin{cases} k_1 \delta, & \text{if } k_2(\delta - \delta_0) \geq k_1 \delta, \\ k_2(\delta - \delta_0), & \text{if } k_1 \delta > k_2(\delta - \delta_0) > -k_c \delta, \\ -k_c \delta, & \text{if } -k_c \delta \geq k_2(\delta - \delta_0). \end{cases}$$
Xia et al. (2019) (Xia et al., 2019)	Crushing of rock samples
Wang et al. (2019) (Wang et al., 2019)	Soil-subsoiler interactions
Ucgul et al. (2020) (Ucgul and Saunders,2020)	Soil-mouldboard plough interaction
Zhao et al. (2023) (Zhao et al., 2023)	Compression test of the cotton
Shi et al. (2023) (Shi et al., 2023)	Stalk Flexible straw steams
Tian et al. (2023) (Tian et al., 2023)	Tensile behaviour of tobacco leaf

Constructing the irregular particles with several overlapping spheres has been adopted in the literature (Lu and McDowell, 2007; Wang et al., 2018; Song et al., 2021). Lu et al. proposed a simple procedure to represent real ballast particles by clumping some overlapping spheres together, as shown in Figure 10. The approximation of real ballast particles depends on the number of sub-spheres used to generate the clumps; namely, more particles guarantee a smooth representation of ballast particles (Lu and McDowell, 2007; Soltanbeigi et al., 2018).
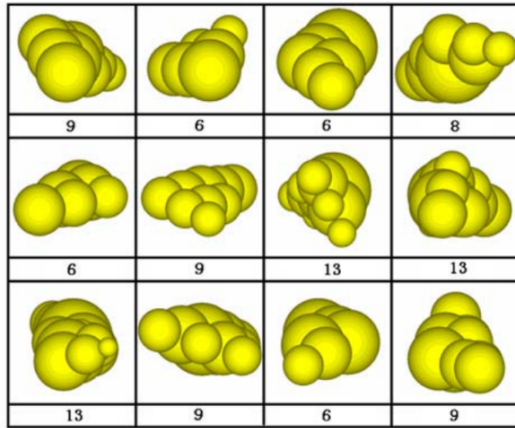

Figure 10: Constructions of irregular particles with overlapping spheres as clumps (Lu and McDowell, 2007).

Several numerical approaches have been proposed to model irregular seed particles with DEM. Zhou et al. proposed four different filling methods, namely horse-tooth shape, truncated triangular pyramid shape, ellipsoid cone shape, and spheroid shape for approximating maize seed particles as shown in Figure 11 (Zhou et al., 2020). Approximating the irregular shape of seed particles with clump methods as presented in (Lu and McDowell, 2007; Wang et al., 2018; Zhou et al., 2020) leads to coarse surface roughness. An improved approach called spherical harmonics was proposed by Radvilaite et al. to model three different agricultural grains, namely, bean, chickpea, and maize (Radvilaite et al., 2016). The main finding of this study is that a proper combination of low- and high-resolution harmonics can accurately represent either concave or convex shapes of particles. Li et al. used the rapid prototyping method to model the corn kernel particle, and this new method was proved to have a better representation of four common particle shapes, e.g. corn kernel, corncob, garlic, and wheat (Li et al., 2022a). The shape of wheat seeds does influence the complex behaviour of seed particles
and the accuracy of the numerical model. A robust and accurate ellipsoid modelling approach was proposed by Lu et al. (Lu et al., 2023). The general formula of the ellipsoid method for generating the ellipsoidal particles is given by

$$f(x, y, z) = \left(\left| \frac{x}{a} \right|^r + \left| \frac{y}{b} \right|^r \right)^{\frac{t}{r}} + \left| \frac{z}{c} \right|^t - 1 = 0, \tag{22}$$

where a, b, and c are the half-lengths along the coordinate axes, respectively. Additionally, t and r represent the sharpness indices of the particle surface (Lu et al., 2023). The comparison between numerical simulations with ellipsoids and simulations with irregular particles constructed with multi-sphere approaches (Xu et al., 2018; Binelo et al., 2019; Li et al., 2022b; Kafashan et al., 2021; Wang et al., 2022a; Boac et al., 2023) proves that the ellipsoid method is more accurate in representing the particle shape.
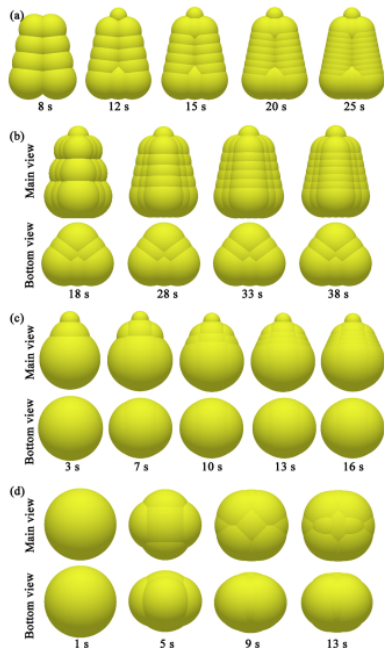
Figure 11: Constructions of irregular particles with overlapping spheres with four different methods: (a) horse-tooth shape, (b) truncated triangular pyramid shape, (c) ellipsoid cone shape, and (d) spheroid shape (Zhou et al., 2020).

Contact detection is of great importance in DEM simulations, especially for simulations with non-spherical particles as contact detection consumes the majority of computational time for a DEM simulation. The bounding volume method, namely, using a simple volume to encapsulate a more com-plex body (shown in Figure 12) was adopted by Podlozhnyuk et al. to reduce the number of detected potential contact pairs in a neighbour list (Podlozhnyuk et al., 2017). Once the contact pairs are detected, the next step is to further detect every contact for every two superquadrics. The so-called "midway" approach was developed by Soltanbeigi et al. to conduct the con-tact detection for superquadrics (Soltanbeigi et al., 2018).
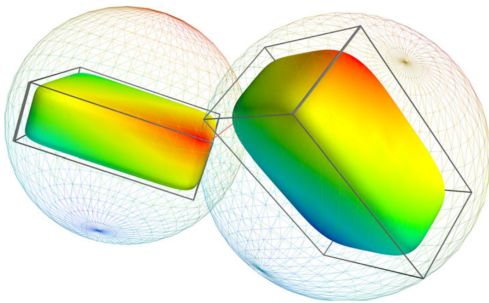

Figure 12: Schematic diagram of bounding spheres and oriented bounding boxes for su-perquadrics (Podlozhnyuk et al., 2017).

The basic idea is shown in Figure 13. Two superquadrics with centroids denoted by X_{CA} and X_{CB}, respectively. This algorithm is to find the midpoint denoted as X_0 between two intersection points X_A and X_B. More detailed numerical issues and algorithms can be found in the literature (Podlozhnyuk et al., 2017; Soltanbeigi et al., 2018).
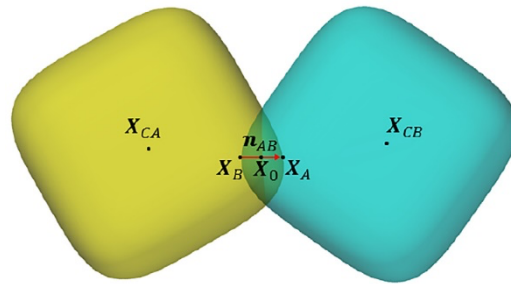

Figure 13: Schematic diagram of particle-particle contact for superquadrics (Soltanbeigi et al., 2018).

Modelling particle-tool interactions by DEM

In addition to these extended contact models and algorithms to approximate the complex irregular particle shape mentioned in the previous sections, some promising applications of DEM in agricultural engineering are discussed in this section.

Contact and interactions with neighbouring apples may lead to mechanical injury in the form of bruise damage when handling apples. A visco-elastic model has been developed and adopted for modelling bruise formations of apples which are approximated by the multi-sphere model as shown in Figure 14 (Scheffler et al., 2018). The agreement between the real shape of an apple and the numerical approximation becomes better by increasing the angle of smoothness. It demonstrates that this model can predict the dynamic bulk behaviour and mean bruise damage of an apple.

Understanding tool-particle interactions is of great significance in the optimization of tools used in agricultural engineering. DEM can capture the complex interactions between two particles, and a particle interacting with an agricultural tool. The influence of moisture contents, namely 7.5%, 21.5% and 38% on the traction force when modelling shoe-soil interactions with DEM was investigated by Shaikh et al. (Shaikh et al., 2021).
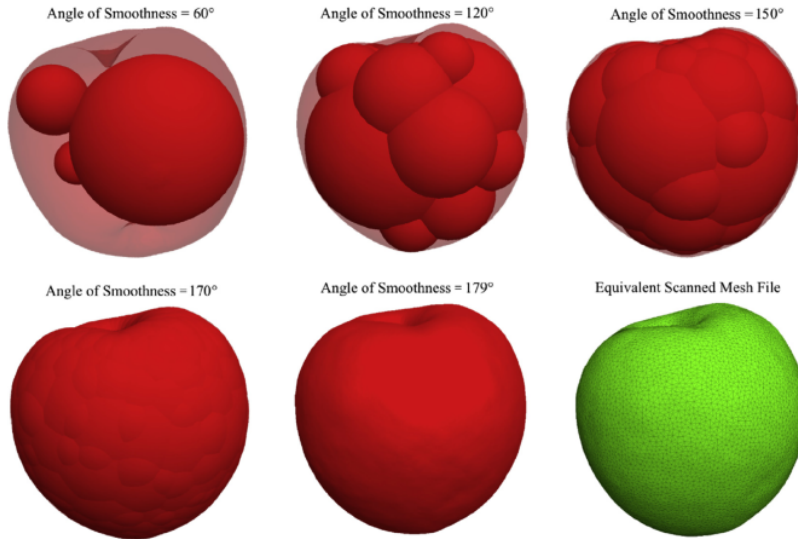
Figure 14: The effect of the angle of smoothness on approximations of a real apple with overlapping sub-particles (Scheffler et al., 2018).

The numerical error of around 10.09% is found when comparing numerical results obtained with the EDEM software against the experimental data. The complex motion of agricultural particles on the screen surface was numerically modelled by DEM in the literature (Ma et al., 2015, 2017). A variable-amplitude screening model was developed to understand the migration and dispersion of particles during the screening process. The main conclusion is that the frequency and turning angle influence the expansion of agricultural particles (Ma et al., 2017). Modelling cohesive soil particles with the hysteretic spring contact model coupling to the linear cohesion model, and the movement of tools on these cohesive soil beds was computationally modelled with DEM (Aikins et al., 2021). The motion patterns and dynamic response characteristics of sunflower seed particles were investigated by Wang et al., and the multi- sphere approach was used to represent the real sunflower seed particle as shown in Figure 15 (Wang et al., 2022b). The accuracy in approximating the shape of the sunflower seed is improved by increasing the number of sub-particles.
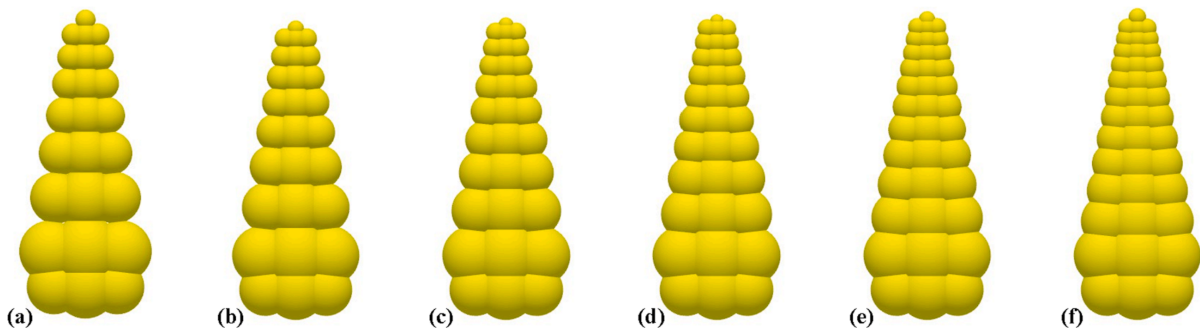

Figure 15: Representation of the sunflower seed with multi-sphere approach in DEM: (a) 25, (b) 28, (c) 31, (d) 34, (e) 37, (f) 40 sub-spheres (Wang et al., 2022b).

It turns out that the surface roughness of the numerical sunflower seed particles influences the accuracy of the numerical model, and a rough surface leads to poor simulation results (Wang et al., 2022b).

Summary and outlook

In this review, the application of the discrete element method in agricultural engineering during the past few years have been summarized. DEM is a promising numerical approach in modelling different irregular agricultural particles, e.g. wheat kernel, corn, apple, strawberry, etc. The multi-sphere approach, rapid prototype technology and ellipsoid approach have been used to approximate irregular particles. The existing contact models in DEM can be used to model the flow and cohesion of agricultural particles. The BMP has been used to model continuous and flexible agricultural particles, such as cotton stalks and tobacco leaves.

For future work, some potential applications and opening of the DEM method are outlined below:

- Approximations of natural agricultural particles

As seen in the most recent literature, superquadrics have been adopted in DEM to model irregular granular materials. Superquadric particles can be used to model a wide range of particle shapes, and this approach can be used to approximate many irregular agricultural particles.

- New contact models for very fine particles

Some non-contacting forces, e.g. Van der Waals force and electrostatic force can not be negligible when the size of particles becomes smaller (e.g., in micro-scale). In agricultural engineering, flour powders are widely processed. Modelling micro-sized flour powders with DEM can be enhanced by incorporating the non-contact Van der Waals force.

- Liquid bridge force model for long-range interactions

Granular materials containing some liquids demonstrate different behaviour from that of dry granular materials. Incorporating the liquid bridge model can be very helpful in further understanding the liquid-bridge-induced cohesion of agricultural particles.

- Coupling to some other numerical methods

DEM has been reported to couple to FEM for modelling contact-induced deformation, abrasion, etc. Computational Fluid Dynamics (CFD) has been extensively used to model compressive fluid in agricultural engineering. Accordingly, coupling DEM to CFD for modelling the gas-flow-induced motion of solid particles can be an interesting topic.

- GPU-based parallel computations for large-scale simulations

In agricultural engineering, large amounts of solid granular particles are processed. The scaling method has been proposed in the literature to scale the numerical model and to reduce the computational cost. The GPU-based parallel computational approach can be used to accelerate these computations when processing a considerable amount of irregular agricultural particles.

- Biologically inspired engineering

Biologically inspired structures have been used in mechanical engineering to enhance the mechanical properties under dynamic loads, e.g. energy absorption, lightweight structures, and the joint design Siddique et al. (2022); Zhang et al. (2022); Xu et al. (2022); Marquez-Florez et al. (2023). Accordingly, some structures from nature can inspire the design of some tools in agricultural engineering. Design and optimization of these biological-inspired structures and tools can be conducted with extensive DEM simulations.

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