What is Discrete Element Method?

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With large-scale processes in many industries handling particulate material, or bulk solids, there is the necessity to understand their behavior without expensive trial-and-error experiments that can be both time and cost restrictive. The use of first principle computational methods, such as Discrete Element Modeling (DEM), is becoming increasingly common and is playing a very critical role in efforts to gain insight into these processes. With the steadily increasing speed of computer hardware, the virtual design of complex multi-phase systems (solid-liquid-gases) is also fast becoming a reality.

A calibrated DEM model can obtain insight into many industrial processes. A few examples include: granular material mixing and drying in food & pharmaceutical industries; sorting and screening systems such as those used in mining and agriculture; handling equipment during upstream oil and gas production; transfer chute designs; pneumatic conveying systems; comminution processes such as crushing and grinding; storage and handling systems of biomass materials such as feedstock, wood chips, and saw dust.

DEM is a numerical technique with the theoretical basis of the method originating from Sir Isaac Newton’s laws of motion. The total force experienced by individual grains or particles in a granular system is modeled and the subsequent accelerations, velocities, and positions are tracked over a period of time. The total force is the summation of contact forces (particle/particle and particle/boundary), and body forces, such as gravity, fluid, magnetic, or electrostatic forces. The major distinction between DEM and molecular dynamics (MD) is that in DEM, the finite particle collisions and rotations play a dominant role.

Although DEM is emerging as a very powerful tool to study bulk materials, there still exist significant challenges and common misconceptions. This article describes the basic principles, applications, limitations, and challenges of the method. It also provides guidance when choosing DEM for it to be a useful design tool.

Basic Principles

Model Description

The behaviors of individual particles in the system are modeled using a mesh-free method and the behavior of the bulk is predicted. A flow chart showing the sequence of a DEM simulation is shown in Figure 1. The first step is the creation of the geometry using a standard CAD package and then to define the boundary motion of the moving parts. For example: a screw mixer can have a fixed outer cylinder and moving internal screw blades; a belt conveyor can have the belt moving at a given velocity. The bulk materials are then released in the system within the domain at certain initial coordinates. The simulation advances using small incremental time steps, and the total force on each particle is determined at every instant in time. The total force is the sum of all mechanical contact and body forces.

$$\sum F = F_{\text{contact}} + F_{\text{body}} = m \ddot{a}$$

The body force in the model can include gravity, fluid drag, adhesion/cohesion due to liquid bridging, electrostatics, and magnetic forces. A time integration scheme is used to predict each particle’s linear and angular velocities (spin) along with its displacements.

Mechanical Contact Forces

Although many mathematical models have been proposed to approximate the physical behavior of true impacts, the most commonly used in a DEM simulation is a spring-dashpot (damped harmonic oscillator) model (Figure 2).
For oblique collisions, the force is decomposed into normal and tangential impact directions with separate spring-dashpot elements. A slider element representing Coulomb friction also acts in the tangential direction. A general force-displacement law \[ F_{\text{contact}} = -K\delta^n - D\delta^{\prime n} \] where \( \delta \) is the overlap between the particles, \( \delta^{\prime} \) is the relative impact velocity (the prime represents the time derivative of the overlap), and \( K \) and \( D \) are the spring stiffness and damping constant respectively.

**Material Properties**

The spring stiffness, \( K \), is a function of particle size and material properties, such as Young's Modulus and Poisson's ratio. The damping constant, \( D \), is related to the coefficient of restitution, which is a lumped parameter quantifying the energy loss during a collision. The choice of the contact model and its parameters is dependent on the system and measurements of interest. Determination of material properties and contact interaction parameters is pivotal and needs to be calibrated in order to produce accurate results.

**Particle Shapes**

Particle shape representation in the DEM model is critical in many applications. Most DEM models use spherical particle shapes, not due to its accuracy, but due to the benefits of straightforward contact detection and overlap (used for contact force calculation). However, this ideal shape representation fails to accurately model most phenomenon exhibited by real granular materials, such as mechanical interlocking, predicting the performance of sorting systems, vibrating feeders, and communication devices. Several different methods have been proposed to represent non-spherical shapes. The simplest and most commonly used is the glued-sphere or multi-sphere method [4, 5]. In this approach, the shape is approximated by rigidly bonding a cluster of spheres that may or may not overlap. An advantage of using this technique is that the simplicity of contact detection associated with spheres is retained while increasing computational bookkeeping. Although any arbitrary shape can be modeled, a significant drawback is the difficulty in approximating shapes having sharp edges and large aspect ratios. In addition, the ‘bumpy’ nature of the surface causes artificial friction between contacts. Another approach to represent non-spherical particles is a mathematical approximation of their shape using continuous functions, e.g. superquadrics [6, 7]. In comparison with the glued-sphere method, superquadrics can algebraically model a wide variety of shapes with increased accuracy (Figure 3).

However, for these shapes, contact detection is computationally expensive and sometimes slow for certain applications. The advents of fast solvers using graphic cards and multi-core CPUs have made this method more practical than before. Although particle shapes play an important role in granular flow dynamics, the user needs to assess the benefits of improving a DEM model against the added complexity of contact detection and computational efficiency. Hogue [6] and Houlsby [8] discuss the implications and issues of different shape representations in DEM models.

**Applications**

DEM is currently used to study processes such as mixing, segregation, separation, storage and handling, transport and fluid-particle flows.

A few examples demonstrating the above strengths are include in these references [2, 9, 10]. Figure 4 on the next page shows prediction of flow patterns in a transfer chute handling iron ore. DEM predictions of mixing lengths of two chemical powders are shown in Figure 5 on the next page. The efficiency of different mixer designs can be analyzed using this approach. DEM can also be used to predict flow and segregation of fine powders in the pharmaceutical industry. It can be used as a tool to predict and troubleshoot content uniformity variations during powder handling. Although still in its early stages, studies involving heat transfer and/or reaction chem-
addition to the significant effect the number of particles has on the simulation time, technical complexities, such as non-spherical particle shapes, moving boundaries and contact force models also have an influence on computational time. Secondary forces, such as cohesion, coupling with CFD etc, also increase the computational time. However, with the advent of faster computers and processing units, the processing speed of DEM simulations is improving.

In addition to the above limitations, another major challenge with DEM models is validation of the results. DEM is ideal for systems where experimental measurements are difficult or cost prohibitive; however this becomes a detriment when validating model results. Another common concern is the representation of non-spherical particle shapes with perfect spheres. Although it is quite tempting to use spherical shapes for its computational efficiency and simplicity of model development, studies have shown that most applications are very sensitive to mechanical interlocking arising due to the representation of particle shape in a DEM model. A few examples include phenomena such as mixing and segregation in blenders and forces in a bladed mixer granulator. DEM predictions of performance of devices such as vibratory screen separators and sorters are also sensitive to the representation of particle shape.

**DEM Codes and Softwares**

There are many open-source and commercial DEM codes available (Table 1). Although all DEM codes use the same basic method, there can be significant differences between them based on their implementation details [12]. Hence accuracy of results can vary between different codes and every code needs to be validated independently.

A summary of factors to consider when choosing a DEM software or simulation over other potential tools to solve a problem is as follows:

**Cost and manpower**
- Number of licenses needed and their cost
- Cost associated with hardware
- Cost associated with hiring experienced personnel
- Ease of simulation set-up and flexibility with data analysis

**Return on investment**
- What will the DEM results predict? Will this lead to significant process understanding and an efficient design?
- Number of simulations (and hence licenses) needed to obtain reliable results

**Physics**
- Are the physics of the process modeled accurately? Can custom

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**Table 1 Examples of DEM codes**

<table>
<thead>
<tr>
<th>Codes</th>
<th>Few Examples</th>
<th>Pros</th>
<th>Cons</th>
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| **Open-source** | LIGGGHTS, YADE-OPEN, ESys-Particle, LMGC90 | • No license cost  
• Full control of source code implementation  
• Multiple users and simulations  
• Cost effective scaling for large organizations | • Programming and DEM expertise needed  
• Support group needed for multiple users  
• XML based inputs/outputs |
| **Commercial** | Rocky-ESS, PFC3D, EDEM, Chute Maven, Chute Analyst, PASSAGE | • No programming experience needed  
• Better graphic user interface  
• Support and training | • Expensive license cost, especially for multiple users and multi-core processor licenses  
• Limited control over implementation but code is thoroughly tested for quality  
• Custom defined force models and measurements might not be trivial to implement |
DEM is ideal for systems where experimental measurements are difficult or cost prohibitive; however this becomes a detriment when validating model results.

Discrete Element Modeling (DEM), Computational Fluid Dynamics, and Finite Element Analyses for industries such as pharmaceutical, chemical, agriculture, mining, oil & gas, etc. He received his M.S. in Mechanical Engineering from the University of Kentucky (2003) and a Ph.D. in mechanical engineering from Purdue University (2006). He was previously a senior scientist at Pfizer Global R&D, where he was responsible for the development of computational models of pharmaceutical processes. He is also an active member of the American Association of Pharmaceutical Scientists (AAPS) and is the past-chair of its Process Modeling and Simulation Focus Group. For more information, email rbharadwaj@jenike.com or visit www.jenike.com.

**Literature Cited**


