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DEM prediction of industrial and geophysical particle flows☆

Paul W. Cleary

CSIRO Mathematical and Information Sciences, Private Bag 33, Clayton South 3169, Australia

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ABSTRACT

Simulation of industrial particle flows using DEM (Discrete Element Method) offers the opportunity for better understanding of the flow dynamics by the inclusion of particle scale physics that often determine the nature of these flows. Increased understanding from the models can lead to improvements in equipment design and operation, potentially leading to large increases in equipment and process efficiency, throughput and/or product quality. Industrial applications are typically large and involve complex particulate behaviour in complex geometries. This paper explores the critical influence of particle shape on granular system behaviour and then discusses examples of DEM applied to several large industrial problems.

1. Introduction

Historically, the use of DEM for the simulation of industrial particle flow processes began with Cundall and Strack (1979) modelling very small systems. In the 15 years following, modelling was restricted to simple two dimensional geometries, such as chute flows, small hoppers and shear cells, primarily with a view to understanding the flow fundamentals of granular materials (see Campbell, 1990; Haff & Werner, 1986; Walton, 1992, chap. 25 as examples).

This work led to early studies of industrial applications. As before, these were typified by small scale problems (in the order of 100–1000s of particles), in two dimensions using highly idealised particles. Examples include ball mills (Mishra & Rajamani, 1992, 1994) and hoppers by Langston, Tuzun, and Heyes (1995), Potapov and Campbell (1996a) and others. Early geophysical modelling using DEM also started with small scales and idealised particles. Examples include ice pack modelling by Hopkins, Hibler, and Flato (1991) and landslide modelling by Cleary and Campbell (1993).

As the power of computers steadily increased through the 1990s, the computational sizes of DEM models have increased in a corresponding fashion. Models used were typically in the 10,000–100,000 range. In general, most were either two dimensional (such as Campbell, Cleary, & Hopkins, 1995; Cleary, 1998a, 1998b, 1998c, 2000; Holst, Rotter, Ooi, & Rong, 1999; Pöschel & Buchholtz, 1995; Potapov & Campbell, 1996a; Ristow, 1994; Thornton, Yin, & Adams, 1996 and many others) or three dimensional but with very simple geometries (such as for fracture by Potapov & Campbell, 1996b).

More recently DEM has been able to be used for large scale industrial applications in complex three dimensional geometries (Cleary, 2004; Cleary & Sawley, 2002; Herbst & Nordell, 2001). It has now progressed to the point where large scale industrial and geophysical systems can be modelled with increasing realism. Quantitative prediction accuracy is now feasible for dry cohesionless granular flows when the particle shape and boundary geometry are well represented and realistic material properties are used.

Challenges remain including adequately representing progeny from particle breakage and cohesion arising from disparate mechanisms ranging from liquid bridges, electrostatics through to cohesive quasi-continuum materials such as clay. Despite the large increase in the model sizes to date, many systems such as silos, stockpiles and hoppers containing smaller grains and pellets remain beyond DEM with real particle numbers being up to 9 orders of magnitude larger than that which is now feasible.

2. Summary of the DEM method

The DEM methodology is now well established and is described in many papers including older review articles by Barker (1994), Campbell (1990) and Walton (1992, chap. 25). In the modelling reported here we use a linear-spring and dashpot collision model, which is described in more detail in Cleary (1998a, 2004). The particles are allowed to overlap and the amount of overlap Δx, and normal v_n and tangential v_t relative velocities determine the

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E-mail address: Paul.Cleary@csiro.au.

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collisional forces via a contact force law. The normal force

$$F_n = -k_n \ \Delta x + C_n v_n \tag{1}$$

has a linear spring to provide the repulsive force and a dashpot to dissipate a proportion of the kinetic energy. It is restricted to being positive to prevent unphysical attractive forces at the end of collisions when the spring component is small and the dashpot component is larger and negative. The tangential force is given by

$$F_t = \min\left\{\mu F_n, k_t \int v_t \, dt + C_t v_t\right\} \tag{2}$$

where the vector force F_t and velocity v_t are defined in the plane tangent to the surface at the contact point. The integral term represents an incremental spring that stores energy from the relative tangential motion and models the elastic tangential deformation of the contacting surfaces. The dashpot dissipates energy from the tangential motion and broadly represents the tangential plastic deformation of the contact. The total tangential force F_t is limited by the Coulomb frictional limit μF_n, at which point the surface contact shears and the particles slide over each other. Energy loss is produced by both the dashpot and slipping at the contact

The maximum overlap between particles is controlled by the stiffness k_n of the spring in the normal direction. Long experience has shown that average overlaps of 0.1–0.5% are required to ensure that the flow behaviour is not dependent on the spring stiffness. The spring stiffness required for this depends on the size of the particles (principally the largest ones) and the magnitude of the maximum forces (controlled by the nature of the flow). Typically they are of the order of 10^4–10^6 N/m in three dimensions, but can be as low a 1 N/m for micron size particles and up to 10^8 N/m for crushers and landslides where the forces are substantial. The normal damping coefficient C_n is chosen to give the required coefficient of restitution ε (defined as the ratio of the post-collisional to pre-collisional normal component of the relative velocity). The equations relating the damping coefficients to the spring stiffness and the coefficient of restitution are given in many references including Cleary (1998a). The linear-spring–dashpot equation of motion can be solved analytically for a binary collision which gives the collision timescale and way to simply choose a time step that gives both stable and accurate explicit integration.

DEM is able to produce many types of quantitative output which can be used to gain insight into industrial particulate flow processes (Cleary, 1998a, 2004) including:

- Transient flow visualization and understanding of flow fundamentals
- Torque and power consumption
- Breakage rates, mill throughput and charge composition
- Collisional and cohesion force distributions
- Energy loss spectra/spatial and frequency distributions
- Wear rates and distributions and the interaction of evolving boundary geometry
- Dynamic boundary stresses (e.g. on lifters and liner plates)
- Segregation and/or mixing rates
- Axial flows rates and residence time distributions
- Sampling statistics and flow rates.

3. Particle shape: importance to flow and approaches to modelling

3.1. Approaches for modelling shape in DEM

In DEM, particles are traditionally approximated by discs or spheres, in two and three dimensions, respectively. These shapes are preferred because of their computational efficiency. The contact is always on the line joining the center of each particle and is as simple as comparing the distance between their centers to the sum of their radii. However, such particle assemblies do not usually reproduce the behaviour of real materials because their shapes have been over-idealised. Circular (spherical) particles differ from real particles in at least four major ways:

1. Material shear strength (essentially the resistance to shear forces and failure)
2. Dilation during shear (due to the volume of revolution)
3. Realistic voidage distributions (circular particles pack very efficiently but more extreme shapes pack poorly which affects porosity)
4. Partitioning of energy between linear and rotational modes is completely different.

Depending on the flow, some combination of these is generally very important. Cleary, Metcalfe, and Liffman (1998) showed that rates predicted for the mixing of non-round real material in a rotating drum when using round particles was substantially in error by more than an order of magnitude. This resulted from predicting the wrong flow pattern because the model bed material was too weak and slumped continuously instead of avalanching down along the free surface.

Methods commonly used to try to treat some of the symptoms produced by using spheres include the use of unphysically large “rolling friction” (which is really just an arbitrary tuned torsional resistance) and moving the center of mass of the particle away from its geometric center. The use of very high friction coefficients is sometimes considered, but this is based on the mistaken belief that high friction contributes to the strength of the material. In reality, it only controls the point where sliding at the contacts occurs and this only influences the rate at which the failure of the particle structure occurs rather than whether it will fail. The strength of the microstructure principally arises from the geometric inter-locking of the particles and this cannot be well captured by any of these approaches.

There are many other choices of approaches for representing particle shape. Rothenburg and Bathurst (1991) used elliptical particles to explore shape effects. Cundall (1988) and Hopkins et al. (1991) used polygonal particles to represent rocks and sea ice blocks. Potapov and Campbell (1996b) used bonded assemblies of polygonal particles to model brittle fracture during impact. Numerous authors have used the clustering approach of gluing overlapping circular or spherical particles together to make simple non-round shapes. This has the disadvantage of being very expensive in representing many particles with high curvature and aspect ratios.

Another approach is to represent the particles as super-quadrics. These shapes were first used in DEM in two dimensions by Williams and Pentland (1992). More recently they were introduced in three dimensions by Cleary (2004). Super-quadrics, in their principle reference frame are given by

$$\left(\frac{x}{a}\right)^m + \left(\frac{y}{b}\right)^m + \left(\frac{z}{c}\right)^m = 1 \tag{3}$$

The super-quadric power m determines the roundness or blockiness of the particle shape. The ratios of the semi-major axes b/a and c/a are the aspect ratios of the particle and control whether it is elongated or platey or roundish. For $m = 2$ and aspect ratios of unity spherical particles are obtained, so this shape class has the advantage of being asymptotically spherical (i.e. matching the traditional DEM shape representation). For $m = 2$ and non-unit aspect ratios then elliptical particles are obtained. As m increases, the