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A methodical calibration procedure for discrete element models

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ABSTRACT

Researchers and engineers have widely adopted the discrete element method (DEM) for simulation of bulk materials. One important aspect in such simulations is the determination of suitable material and contact law parameters. Very often, these parameters have to be calibrated because they are difficult to measure or, like rolling friction, do not have a physical analogue. Moreover, coarse-grained particle models are commonly used to reduce computational cost and these always require calibration. Despite its disadvantages, trial and error remains the usual way to calibrate such parameters. The main aim of this work is to describe and demonstrate a methodical calibration approach which is based on Latin hypercube sampling and Kriging. The angle of repose and bulk density are calibrated for spherical glass beads. One unique feature of this method is the inclusion of the simulation time-step in the calibration procedure to obtain computationally efficient parameter sets. The results show precise calibration outcomes and demonstrate the existence of a solution space within which different parameter combinations lead to similar results. Kriging meta-models showed excellent correlation with the underlying DEM model responses. No correlation was found between static and rolling friction coefficients, although this has sometimes been assumed in published research. Incorporating the Rayleigh time-step in the calibration method yielded significantly increased time-step sizes while retaining the quality of the calibration outcome. The results indicate that at least particle density, Young's modulus and both rolling and static friction coefficients should be used for calibration; trial-and-error would be highly inefficient for this number of parameters which highlights the need for systematic and automatized calibration methods.

1. Introduction

Although the discrete element method (DEM) was developed in the 1970s [1], it is only recently that researchers and engineers have been able to run DEM simulations of sufficiently large size and complexity to be practically useful. This has caused a rapid growth in the adoption of DEM [2], enabled by continual advances in affordable computational power. Huge numbers of studies have shown the usefulness of DEM for modelling the behavior of bulk solids in industrially relevant systems such as fluidised beds, silos, mixers or mills.

One major benefit of DEM is that the simulations require specification of a relatively small number of microstructural parameters. However, it can be difficult to establish suitable values for all of these model inputs. For example, input parameters cannot be obtained by laboratory testing for coarse-grained simulations in which the particle diameters are increased beyond their physical values to reduce the computational requirements of a simulation, e. g., [3–5]. Even if particle diameters are simulated accurately, other parameters can be difficult to relate to physical measurements, e. g., numerical damping coefficients [6] or rheological parameters required in the force–displacement laws [7]. The interparticle friction coefficient is often increased to unphysically large values in an attempt to capture particle irregularity [8]. Additional parameters which lack a physical basis are usually needed when grain crushing [9] or rolling resistance [10] are considered in the model.

When the foregoing limitations of laboratory experiments to supply model input parameters are considered, it is unsurprising that most DEM simulations contain parameters which can be obtained only by calibration. Calibration involves varying the unknown parameters until a satisfactory match has been achieved between the simulation results and the corresponding physical measurements for the response(s) of interest. Calibration is often done in an inefficient manner based on trial and error. Trial-and-error calibration has many obvious disadvantages [7]: it is not known in advance how many simulations will be needed for calibration; the success

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of the method depends on the modeller's experience; little, if any, mechanistic insight is gained; the calibrated parameters may be suboptimal; and using a trial-and-error approach rapidly becomes impractical as the number of parameters increases. Furthermore, DEM simulations can be very computationally expensive so running more simulations than essential for calibration is undesirable.

The significant disadvantages associated with trial-and-error calibration of DEM input parameters have motivated research into alternative approaches based on design of experiments (DoE) methods. Yoon [11] uses response surface analysis and a Plackett–Burman experimental design to identify suitable parameters to simulate uniaxial compression of bonded rock. Favier et al. [12] and Johnstone [13] both use DoE methods to calibrate DEM models based on experimental measurements. Benvenuti et al. [14] train an artificial neural network for DEM simulation parameter identification. However, none of these calibration approaches are widely used in industry where *ad hoc* trial-and-error methods remain predominant.

In this paper, a novel calibration procedure is described which is based on Latin hypercube sampling and Kriging [15]. This workflow was designed to be automated, i. e., to run efficiently with minimal user intervention. It was implemented using purely open-source software including LIGGGHTS [16] and GNU Octave [17]. Both the open-source implementation and the high level of automation are intended to encourage the widespread adoption of this calibration method. Another novel aspect is the inclusion of the simulation time-step in the calibration process. In most cases, DEM adopts an explicit, conditionally-stable time-stepping algorithm. The size of the largest time-step which maintains numerical stability is strongly dependent on the particle density and stiffness. Considering the simulation time-step during calibration means that optima requiring small time-steps to maintain stability are disfavoured. This ensures that the calibration process is prevented from converging to a solution which causes the simulation to run prohibitively slowly.

The main aim of this paper is to describe and demonstrate a novel calibration method. Spherical glass beads are used as the bulk material. Two responses are calibrated, angle of repose and bulk density, while simulation time-step is also considered during calibration. Subsidiary aims are as follows: (i) to demonstrate that significantly larger time-steps can be achieved by explicitly including the time-step as a factor in the calibration process, while still achieving an excellent match between the experimental data and the model; (ii) to show that parameter sets which differ substantially can yield similar outcomes; (iii) to explore interactions among the DEM input parameters being calibrated.

This calibration approach is generally applicable to all types of DEM simulation. The example presented in this paper is for a conventional DEM simulation in which each simulated particle represents one physical particle. However, the method has even greater potential for coarse-grained simulations for which the number of parameters requiring calibration can be very large.

2. Materials and methods

This section contains a brief overview of DEM, followed by a more detailed description of the specific model considered in this study.

2.1. Discrete element method

Both hard-sphere and soft-sphere DEM simulations are possible; the latter are more frequently used and are the focus of this paper. The particle geometry is idealized to reduce the computational requirements: often spheres are used in three-dimensional simulations. The density and stiffness of each particle can differ. The particles are not permitted to deform during the simulation; instead deformation is captured by allowing the particles to overlap at contacts with surrounding particles and boundary walls. DEM is driven by a time-stepping algorithm, often a central difference, velocity–Verlet scheme. During each time-step [18], interparticle forces are evaluated at contact points based on a defined force–displacement law. This contact model is almost always based on either a linear, Hookean spring or a nonlinear, Hertzian spring along the contact normal. The interparticle contact forces are summed, along with body forces such as gravity, to calculate resultant forces for each particle. Then Newton's Second Law is applied to determine the translational and angular particle accelerations which are numerically integrated to find particle velocities and displacements. These displacements are used to update the particle positions at the end of each time-step. Individually, these calculations are very straightforward. However, as millions of particles may be simulated using time-steps of the order of nanoseconds, the computational effort can be very considerable to simulate a short time period.

2.2. Investigated DEM model of this study

All simulations were run using the public version of the LIGGGHTS [16] DEM code. A Hertz–Mindlin contact model was chosen for these simulations along with an elastic–plastic spring–dashpot (EPSD) rolling friction model. This model incorporates viscous damping in its formulation [19]. The critical time-step for each simulation was computed using Eq. (1) where G is the shear modulus, ρ is particle density, ν is Poisson's ratio and r is the radius of the smallest particle.

$$dt_r = \frac{\pi r\sqrt{\frac{\rho}{G}}}{0.1631\nu + 0.8766} \tag{1}$$

The time-step used for the DEM simulations was taken as a quarter of this critical Rayleigh time-step. For this paper, it is assumed that the time-step is solely a function of the parameters used in Eq. (1). Although it is known that the simulation time-step must be reduced to ensure stability when particle relative velocities are large, the nature of this reduction is currently unquantified. In cases where the relative velocities are large, it is noted that the factor by which Eq. (1) is multiplied (0.25) may need to be reduced to maintain stability.

The effect of this time-step on the calibration was controlled by means of a weighting factor. This weighting factor, WRL, was one of the seven factors adjusted in the calibration process. Apart from the Rayleigh time-step, two responses were calibrated: bulk density and angle of repose. The system shown schematically in Fig. 1 was simulated to obtain these responses. It consists of a horizontal steel plate with a steel cylinder of diameter 100 mm resting on top so that the plate obstructs the bottom of the cylinder. A rigid ring of height 3 mm and diameter 100 mm is affixed to the steel plate to prevent particles from rolling away on the flat surface. Each simulation is run in the following manner. Particles of diameter 5 mm are poured into the cylinder under gravity (g=9.81 m s^{-2}) to a height exceeding 50 mm

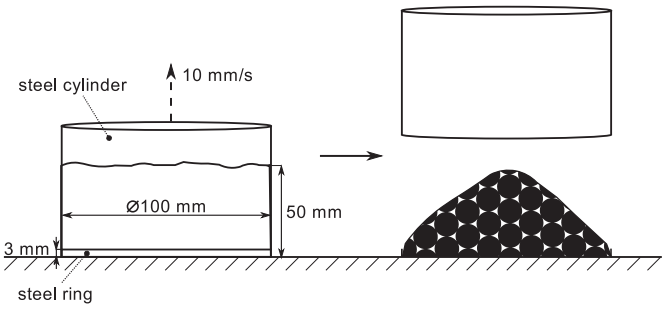

Fig. 1. Schematic of the three-dimensional simulated system used to measure bulk density and angle of repose.