AUTOMATIC CALIBRATION OF DISCRETE ELEMENT MODELS

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ABSTRACT

Calibration means the determination of parameters governing the mechanical interaction of the individual particles and walls making up our discrete element model (DEM). Since the elaboration of DEM [1], calibration is the most difficult part of the DEM modeling process.

INTRODUCTION

Direct measurement of the parameters governing the particle–particle, particle–wall interactions would be the best solution, but in most of the cases it is impossible. It can also happen that even the measured parameters would not be suitable for modeling purposes, as the applied constitutive equations in the numerical calculations are only approximations. In most of the cases the proper measured values of these parameters are not needed, but a combination of parameters ensuring the modeled macro behavior to be the same as the measured one.

Standard shear testing technique

The standard shear technique [2] is one of the most commonly used calibration method [3], [4]. The standard shear testing technique for particulate solids is based on the so called Jenike shear cell (see fig.1). Material sample is placed into the shear apparatus and before shear a vertical force F_N is applied to the upper plate and hence to the particulate solid within the cell to pre-compress the material sample. A horizontal force is applied to the bracket by a mechanically driven measuring stem which is driven forwards at a steady rate of 1-3 $\frac{\mathrm{mm}}{\mathrm{min}}$. This stem is attached to the drive system through a force transducer which measures the shear force F_T. During the shear operation the shear ring moves from the original offset position to the opposite. During shear a shear zone develops inside the sample, and in this way we can create a shear stress shear strain plot. By knowing the shear stress values corresponding to a given compressive normal stress, the parameters of the failure line can be determined in the form of $T = \varphi N + c$, where T is the shear stress, N is the normal stress, φ is called the internal friction of the assembly and c is the cohesion (see fig. 2). Naturally, the failure curve of the material is not always linear, but the linear approximation of the failure curve is a common method in the practice[5].

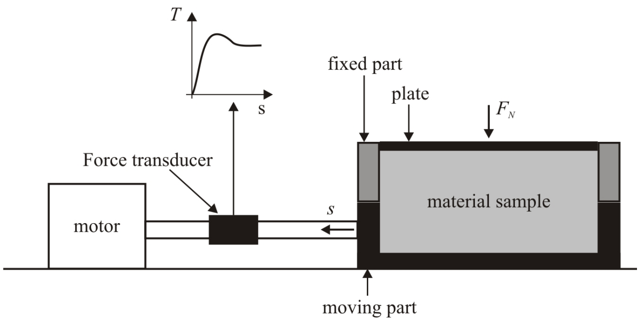

Fig. 1. Shear cell

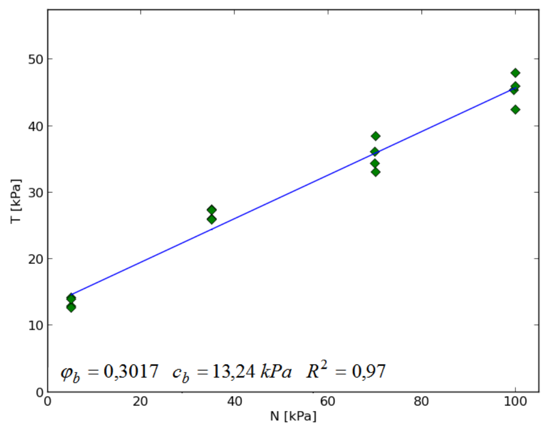

Fig. 2. Typical failure line

Discrete element modeling

DEM models the mechanical behavior of bulk materials by applying and solving the equation of motion on each singular particle of the bulk material assembly. The out of balance forces arising during particleparticle and particlewall interactions are calculated during the simulation circle, which is a cycle with repeated application of the Newtonian laws of motion to obtain the acceleration, velocity and displacement. The displacement is then used to evaluate the contact forces and moments acting due to the interactions between

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the particles in their new position. In this article, we use Yade discrete element method software for numerical modeling [6]. In YADE the approximate collision detection filters out the impossible collisions, and after this step, a more computationally expensive collision detection algorithm evaluates the possible interactions between these individual particles.

After having exact collision detection, it is possible to model the interaction between the particles in contact. DEM interaction model uses two stiffnesses: K_N normal stiffness and K_T shear stiffness. K_N is related to the Youngs modulus of the particles material, and K_T is defined as a given fraction of K_N. Yade evaluates the K_N stiffness by modeling the two particles in contact as a serial connection of two springs having length equal to the radius of particles in contact:

$$k_N = 2\frac{E_1 r_1 E_2 r_2}{E_1 r_1 + E_2 r_2}.$$

The kinematic variables (displacements) of the contact are called as strains in Yade terminology. To evaluate the normal strain, there is a reference distance d_0 (or equilibrium distance) used to convert the evaluated displacements to dimensionless strain: $d_0 = |\mathbf{C}_2 - \mathbf{C}_1|$, where $\mathbf{C}_1$ and $\mathbf{C}_2$ are the initial position vectors of the two contacting spheres centers. Because of the possible overlap between the two contacting spheres, there are reduced distances $d_1 = r_1 + \frac{1}{2}(d_0 - r_1 - r2)$ and $d_2 = d_0 - d_1$ used for further strain evaluations. For the constitutive laws Yade uses an equivalent cross-section $A_{eq} = \pi \min(r_1, r_2)^2$ to convert stresses into forces. By knowing the normal and shear displacements u_N , u_T, normal and shear forces are computed in the following way:

$$F_N = K_N u_N,$$

$$F_T = \begin{cases} F_N \tan\varphi & \text{if } |K_T u_T| > F_N \tan\varphi, \\ K_T u_T & \text{otherwise.} \end{cases}$$

If we have cohesive model, cohesive interactions bonds between particles are used to represent the materials cohesive properties. The normal force is $F_N = \min(K_N u_N, a_N)$, where a_N is the normal adhesion. The tangential shear force is $F_T = K_T u_T$, the plasticity condition defines the maximum value of the shear force, by default $F_T^{\max} = F_N \tan\varphi + a_S$, where a_S is the shear adhesion. If the maximum tensile or maximum shear force is reached, the cohesive link is broken.

The forces and torques evaluated above are used to integrate the equations of motion (linear- and angular momentum theorem) of the particles in contact. From the equations of motion by integration the new particle positions can be determined, and based on the new particle positions, the simulation circle can start again from collision detection.

In case of simulating quasi-static phenomena, the kinetic energy of the particle assembly must be dissipated in some way. Since the constitutive law does not include velocity dependent damping, Yade uses artificial numerical damping: the forces, which increase the particle velocities are decreased by $(\Delta F)_d$. Yade uses for the artificial damping the following:

$$\frac{(\Delta F)_{dw}}{F_w} = -\lambda_d \mathrm{sign} F_w \left(\dot{u}_w (t - \Delta t) + \frac{1}{2} \ddot{u}_w (t) \Delta t \right).$$

For numerical stability reasons, there is an upper limit Δt_{crit} on the simulation timestep calculated from the highest eigenfrequancy of the system. The so called unbalanced force is used to keep the modeling process to be close to quasistatic conditions, the unbalanced force ratio will tend to zero as simulation stabilizes.

Discrete element model of the shear test

We used a slightly modified version of Jenike shear cell for the discrete element modeling purposes, as in our case the lid is rectangular (see fig. 3). We evaluated

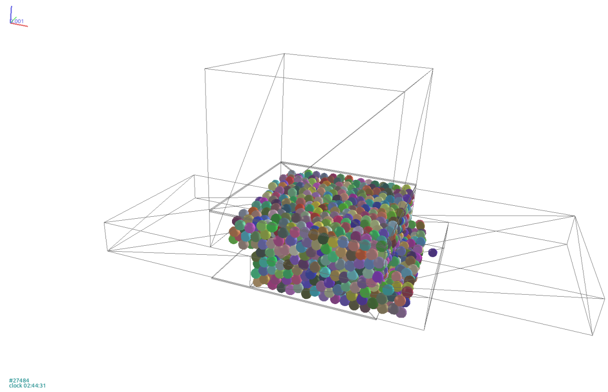

Fig. 3. DEM model of the shear apparatus

the normal-force shear force diagrams in case of four different pre-compressing forces four times (16 simulations for one failure line) to get one failure line similar to the example showed in fig. 2. The block diagram of the shear test can be seen on fig. 4. It can be seen, there, that the compression of the material sample starts only after the granular material poured into the shear box is in a state of rest. The constant compressive force value is maintained by up- and downwards motion of the compressing plate.

AUTONOMOUS CALIBRATION ALGORITHM

The inputs of the calibration algorithm are the desired values of the shear failure line φ and c, and the micromechanical parameters related to a starting point. As a first step, the slope of the failure line is calibrated (see fig. 5), and then the calibration of the cohesion is done (see fig. 6). A sensitivity test is important part of the calibration, because we have to decide, which parameters should be changed to reach the desired parameters of the failure line. The details of the sensitivity test are available in [3].

To calibrate by hand the micromechanical parameters related to the desired cohesion and internal friction values presented in fig. 2, we needed 312 hours of computation time. The automatic calibration algorithm managed to reach the desired micromechanical values in 60 hours.

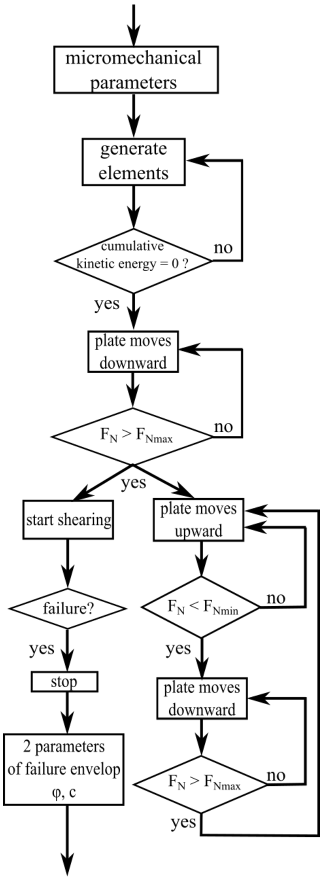

Fig. 4. Block diagram of shear test

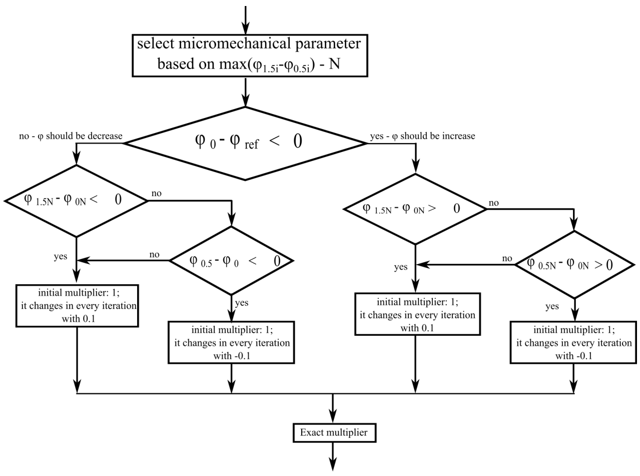

Fig. 5. Automatic calibration for φ

CONCLUSIONS

Calibration of discrete element based models is still a challenging question of the engineering practice. It would be preferable to have a standard calibration method available for use. Our opinion is that the standard shear testing technique is a well-grounded method applicable to ensure properly calibrated discrete element models. The calibration itself is a time consuming, monotonic process which is (in many cases) based on trial and error methods. We suppose that this process can be automatized. For the automatization, the process must be rigorously controlled; the trial and

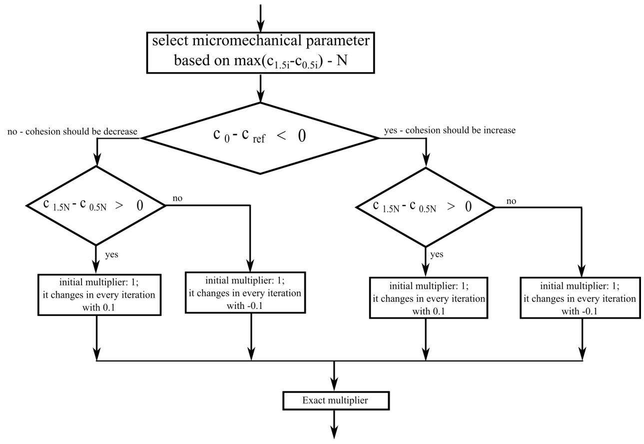

Fig. 6. Automatic calibration for c

error process must be superseded by sensitivity test based gradient methods. In this article, we demonstrated, that this is possible. The discrete element calibration can be automatized. A highly autonomous algorithm can be constructed, which is capable to find desired macromechanical behavior by systematic modification of micromechanical parameters. The change of micromechanical parameters must be based on initial sensitivity analysis to realize relatively short calibration time.

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