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Original Research Paper

A calibration framework for discrete element model parameters using genetic algorithms

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ABSTRACT

In this research, a universal framework for automated calibration of microscopic properties of modeled granular materials is proposed. The proposed framework aims at industrial scale applications, where optimization of the computational time step is important. It can be generally applied to all types of DEM simulation setups. It consists of three phases: data base generation, parameter optimization, and verification. In the first phase, DEM simulations are carried out on a multi-dimensional grid of sampled input parameter values to generate a database of macroscopic material responses. The database and experimental data are then used to interpolate the objective functions with respect to an arbitrary set of parameters. In the second phase, the Non-dominated Sorting Genetic Algorithm II (NSGA-II) is used to solve the calibration multi-objective optimization problem. In the third phase, the DEM simulations using the results of the calibrated input parameters are carried out to calculate the macroscopic responses that are then compared with experimental measurements for verification and validation.

The proposed calibration framework has been successfully demonstrated by a case study with two-objective optimization for the model accuracy and the simulation time. Based on the concept of Pareto dominance, the trade-off between these two conflicting objectives becomes apparent. Through verification and validation steps, the approach has proven to be successful for accurate calibration of material parameters with the optimal simulation time.

1. Introduction

The discrete element method (DEM) [1] has become a widely accepted numerical technique for computing the behavior of granular materials. However, a major barrier to effective uses of DEM is selecting appropriate input parameters so that simulations can accurately reproduce the behavior of real systems. Furthermore, efficient parameter sets to reduce computational cost are required for industrial applications. Some microscopic input parameters can be determined directly from experiments, while others can be obtained only or more practically by calibration of macroscopic responses [2–14]. Calibration is traditionally carried out by "trial and error" in which an iterative process of adjusting unknown input parameters until the DEM simulated results match the given measured bulk behavior. "Trial and error" is a purely forward, primitive methodology and is hence limited by the parametric multi-dimensionality and computational expense of performing DEM simulations.

From a mathematical point of view, DEM calibration is classified as an inverse problem [15,16]. The process aims at searching for input parameters such that the model response best matches experimental data. An inverse procedure of calibration can be divided into two steps. In the first step, DEM simulations are carried out to construct an objective function that indicates the discrepancy between the solution profile of the model and the experimentally measured profile. To reduce the number of simulations required, approaches such as design of experiment/simulation [17–19], artificial neural network training [20], and Latin hypercube sampling and Kriging [21], have been used. In the second step, optimization is used to search for the optimal parameter set that minimizes the objective function. Several different optimization methods are used for DEM calibration, *e.g.*, Levenberg-Marquardt residual minimization [21], Nelder-Mead simplex [22], weighted least squares [23], Gauss-Newton algorithm [24], and genetic algorithms [25]. In many practical cases, if the profile consists of more than one bulk property to be considered, it is formulated as a multi-objective optimization problem (MOOP). In

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earlier work on DEM calibration [17,21–24], MOOPs have been solved using single-objective optimization. In that work, MOOP is converted to a single objective function, with different weight factors assigned to the corresponding objectives. However, the drawbacks of using single-objective optimization techniques to solve MOOP are evident, not only because the solution obtained cannot capture the tradeoff between the different objectives, but also because the determination of the weight factors tends to substantially influence the solution. Moreover, gradient-based search techniques [21–24] may converge to a local optimum.

For more than four decades, multi-objective evolutionary genetic algorithms (MOEAs) [26–29] have been proven to be an efficient method to overcome the foregoing problems. In this paper, a DEM calibration framework is presented. In the framework, after choosing the calibration setup, an optimization process based on MOEAs is carried out. The framework offers novel aspects that have not been addressed yet in the literature on DEM calibration. The first novelty is the ability to handle any number of objective functions with a unified formulation and accommodate the discrete nature of the design parameters. Secondly, since MOEA is based on the notion of Pareto dominance, visualizations of tradeoffs among conflicting objectives provide essential information for decision making during the optimization process. Thirdly, evolutionary algorithms search for a broad portion of the decision space, and they are hence more likely to reach a set of solutions close to a global optimum.

The paper is structured as follows: Section 2 presents the novel DEM calibration framework based on MOEAs. Section 3 describes the case study for calibration composed of three DEM simulation setups that replicate numerically the experiments. A two-objective optimization problem of calibration, in which both the model error and simulation time are simultaneously minimized, is defined. In Section 4, the numerical calibration results, verification, and validation, are discussed and evaluated. Finally, Section 5 gives conclusions on the performance of the calibration framework.

2. Methods

The flowchart of the calibration approach consists of three phases, as illustrated in Fig. 1. In the first phase, calibration setups are chosen. The calibration setups should reflect the important physics aspects of final target problems, *i.e.*, material behaviors in industrial applications. The calibration setups should also be large enough in relation to particle dimensions to demonstrate realistically material behaviors as on a large-scale (industrial) case. In addition, contact force models should be chosen that properly reflects the nature of the material behaviors. DEM simulations are then carried out on a user-defined, multi-dimensional grid of sampled values of the input parameters being calibrated. The simulated macroscopic outputs and their corresponding experimental data are used as the database to interpolate the objective functions with respect to an arbitrary set of parameters. In the second phase, the Non-dominated Sorting Genetic Algorithm II (NSGA-II) [30], one of MOEAs, is used to solve the multi-objective optimization problem. In the third phase, DEM simulations using the calibrated input parameters obtained from the optimization are carried out to calculate bulk properties that are then compared with experimental measurements for verification.

2.1. Simple genetic algorithm

Genetic algorithms (GAs) are search and optimization methods inspired by Darwin's theory of evolution of natural selection and genetics. In a simple genetic algorithm [31], an initial population of candidate solutions evolves through generations (iterations) towards individuals with better fitness by applying genetic operators such as selection, crossover, and mutation. The fitness is measured by an objective function of the optimization problem being solved. In each iteration, the better fit individuals are stochastically selected from the current population for breeding to create a new generation. The population is then replaced by a new generation and used for the next iteration of the process. The algorithm terminates when fitness values of the individuals satisfying a predefined criterion have been found, a predefined maximum number of generations has been reached, or the best fitness value has reached a plateau such that successive iterations no longer produce any improvement.

A single-objective optimization problem for a typical calibration is given as:

$$\underset{\text{such that } \mathbf{x}\in\mathbf{S}}{\arg\min}\ O(\mathbf{x}), \tag{1}$$

where: the design variable vector $\mathbf{x} = (x_1, x_2, \ldots x_n)^{\intercal}$ is a set of input parameters varying within a search space $\mathbf{V} \subset \mathbb{R}^n$, and intervals $S_i = [l_i, u_i]$ (for $i = 1, 2, .., n$) are the given lower and upper bounds of parameter x_i. O is the objective function to be minimized, which is the fitness function of GAs and defined as the discrepancies between DEM model results and experimental measurement data.

To represent input parameters by means of a binary alphabet, a function $cod_i : S_i \rightarrow \{0 \vee 1\}$,has to be specified, which codes each parameter x_i in interval S_i using binary strings of length L_i characters. An input parameter set, a so called individual in GAs, is represented by linking together the coded binary strings of all parameters as $cod(\mathbf{x}) = cod_1(x_1)cod_2(x_2)\ldots cod_n(x_n)$.

For example, a calibration problem involves $n = 2$ input parameters: rolling and sliding friction coefficients, $\mathbf{x} = (x_1, x_2) = (\mu_r, \mu_s)$, in ranges [0.1,0.5] and [0.2,0.7], respectively. If, for instance, 4 and 5 binary bits defining ranges of 0000–1111 and 00000–11111 are used to encode μ_r and μ_s, respectively, the encoding functions cod_1 and cod_2 map the continuous solution space into the numerical discrete solution space. The discrete solution space consists of $2^4 \times 2^5 = 512$ possible values and each value is presented by a string of 9 binary bits. This encoding provides a numerical precision of $\frac{0.5-0.1}{2^4-1} \times \frac{0.7-0.2}{2^5-1} = 0.02666 \times 0.01613$. A parameter set (μ_r, μ_s) with real values, *e.g.*, (0.2862, 0.5387), can be encoded by an individual as (01110101), in which the first four digits are used for μ_r and the last five digits for μ_s. At the beginning of the GA process, an initial population $\mathbf{P}$ with $|\mathbf{P}|$ individuals, is randomly generated.

In the next phase of GAs, selection techniques are used to choose the new population of individuals for the next generation. Selection is an important part of GAs since it affects significantly their convergence. The basic strategy follows the rule: the better fit an individual, the larger the probability of its survival and mating. In this study, the most widely used selection type, the so-called binary tournament selection [31], is applied. It assumes that the probability of selection for crossover is proportional to the fitness of an individual.

The crossover operator mimics the natural process in biology whereby genes from two parents meet to produce new offsprings that are a mix of the parent's genes. Crossover is vitally important in introducing new possible solutions by exploring new domains of the search space. Individuals, as a result of the selection process, are randomly selected and mated in pairs using a single-point crossover [31].

The mutation operator is used to promote genetic diversity from the current population to the next, aiming at introducing new genetic information in the search. Analogous to biological mutation, this operator alters one or more gene values in randomly

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