Computer-aided calibration of *PFC3D* coal samples using a genetic algorithm

R. Garvey & U. Ozbay
Colorado School of Mines, Golden, CO, USA

ABSTRACT: Bonded-particle models (BPM) may be developed in *PFC3D* to represent rock samples with pre-determined material properties. Numerous particle and bond input parameters are required when constructing a BPM and the calibration of an advanced model is a non-trivial task. A routine was written in the FISH language to iteratively calibrate a simulated laboratory sample of coal to match a set of desired material properties: Young's modulus, Poisson's ratio, uniaxial compressive strength (UCS), and the slope of the UCS stress-strain curve after failure. This calibration method was developed using a Genetic Algorithm (GA) to search for an optimal set of input variables through a process of random variation, selection based on fitness, and a recombination of inputs. The Genetic Algorithm simultaneously modified 9 independent input parameters to calibrate the test results of a simulated specimen of coal to within 1% of the desired results.

1 INTRODUCTION

1.1 *Discrete element method for modeling rock*

Numerical models are frequently developed to model rock in unfailed and failed states. Continuum models such as the finite difference method are well suited to analyze a rock mass in a stressed state up to the point of failure. However, when excess stress is applied to rock to cause major damage in the form of fractures, the influence of the fractures and internal discontinuities begin to dominate the behavior of the rock. An alternate and perhaps more suitable approach to capturing the behavior of rock during failure is to apply the discrete element method (DEM) to directly model discrete fractures within a simulated rock sample.

The three-dimensional particle flow code, or *PFC3D,* was the DEM code adopted for use in this paper. The *PFC3D* code, by Itasca Consulting Group, can be used to connect an assemblage of spherical particles with breakable, elastic bonds between particles. The process of progressive failure is then demonstrated as bonds continue to break throughout an overly stressed rock specimen. If the properties of the model are calibrated suitably, then this collection of masses (balls) and springs (bonds and ball-ball interactions) can provide a realistic representation of rock during simulated laboratory tests (Potyondy & Cundall 2004).

1.2 *FISHTank inputs*

To aid in the task of generating samples and running generic *PFC* simulations, Itasca has included a library of FISH functions known as FISHTank (Itasca 2008). With this library, the user can generate samples with basic geometries using parametric inputs in FISH. A suite of uniaxial compressive strength (UCS), triaxial confinement, and Brazilian tensile strength tests are included with the FISHTank. The user is provided a wide range of possible inputs during the model generation process. Roughly 10 user defined input parameters are required to develop the

reasonably advanced model known as bonded-particle model, or BPM. Within a BPM, the rock is modeled by assembling spherical particles with parallel bonds between spheres initially in contact. Parallel bonds act between particles by transmitting a shear force, normal force, and generated moment between particle centers. The bonds can be assigned both normal and shear strengths at which the bond is removed.

1.3 *Coal sample properties*

For the purposes of this paper, a BPM was adopted to simulate a laboratory sized coal specimen with in-situ strength and elastic properties. Several macroproperties were chosen to assess how well a BPM sample compared to the idealized representation of the coal specimen. These properties were Young's Modulus, Poisson's Ratio, Uniaxial Compressive Strength (UCS), and the slope of the post-failure stress-strain curve in uniaxial compression. Most of these properties are commonly identified as important qualifiers of a material's response; however the slope of the post-failure stress-strain curve is a non-obvious measurement which was identified by the authors as a key means of classifying the relative energy stored within a sample during and after failure. Due to DEM's ability to more accurately model fracturing rock, these post-failure characteristics of the sample should also be identified through the calibration process for a more complete understanding of rock behavior during and after failure.

   A series of recommended calibration steps have been developed by Itasca and others (Wang & Tonon 2009, Yoon 2007) to provide a sensible means of determining sets of BPM inputs which generate models with appropriate material responses. These steps include guidelines on the relationships between input parameters and macroproperties of the simulated sample. Some detailed studies have added insight into the effects of input parameters using artificial neural networks (Tawadrous et al. 2009), statistical Central Composite Design method (Yoon 2007), and dimensional analysis (Fakhimi & Villegas 2006). Due to confounding variables and a complex design space, the difficulty of calibrating a BPM becomes compounded as a greater number of inputs are considered. Non-linear effects between inputs and responses only add to the difficulty of developing a satisfactorily calibrated model.

2 GENETIC ALGORITHM

2.1 *Calibration limits*

To aid in the process of calibration, a new tool was developed in FISH programming language to interact with existing FISHTank functions. The tool calibrated BPMs by iteratively changing inputs to match desired macroproperties for the samples. This tool included an option to apply a Genetic Algorithm (GA) to calibrate the sample. The 9 independent inputs listed in Table 1 were considered for the case of coal specimen calibration.

Table 1. Input limits for genetic algorithm.

Inputs	GA limits	
	Lower	Upper
Young's modulus of balls (ba_Ec)	4 GPa	8 GPa
Young's modulus of bonds (pb_Ec)	4 GPa	8 GPa
Normal:shear stiffness of balls (ba_krat)	0.5	2.5
Normal:shear stiffness of bonds (pb_krat)	0.5	2.5
Parallel bond normal strength (pb_sn_mean)	20 MPa	30 MPa
Parallel bond shear strength (pb_ss_mean)	20 MPa	30 MPa
Friction between balls (ba_fric)	0.25	0.75
Max:min ball size (mg_Rrat)	1.5	2.0
Remaining floaters ratio (mg_nfrat)	0.00	0.01

The GA routine written in FISH iteratively provided inputs for *PFC³D* FISHTank to generate a bonded-particle model and ran a series of simulated tests to determine macroproperties of the model. These inputs were varied within the user-defined limits according to an evolutionary process of random variation, natural selection based on fitness, and a recombination of successful inputs to calibrate the desired macroproperties. Wide limits were set based on past trials which had produced successful results. However, new users would be able to apply limits using little prior knowledge due to the algorithm's ability to search large ranges of input values with no reduction in precision during the calibration.

2.2 *Genetic algorithm*

Several choices were considered during the design of the Genetic Algorithm to significantly reduce the number of trials required to obtain a calibrated sample. The final structure of the GA with these modifications is described below:

1. Generate initial population. Create forty sets of random inputs and generate forty BPMs using these inputs.
2. Perform uniaxial compressive stress tests on each sample. Compute E, ν, UCS, and post-peak modulus for each sample based on these tests. Approximate the post-peak modulus by using a linear fit between two points on the stress-strain curve. For convenience these points may be taken when the stress within the sample is reduced by 25% and 50% after failure. Assess the fitness of the population as a measure of relative error of N number of BPM macroproperties. This fitness can be found from the relationship shown in Equation 1.

$$\text{Individual fitness} = 1 - \frac{1}{N}\sum_{i=1}^{N}\left|\frac{\text{desired - actual}}{\text{desired}}\right|_i = 1 - \left|\text{relative error}\right| \qquad (1)$$

3. Identify 3 samples which most closely fit the desired macroproperties.
4. Breed the 3 fittest samples for a total of 10 times. During breeding, the input values for each child are selected randomly from a uniform distribution of values which lie between the parent inputs. The parents are chosen randomly for each child, with a possibility existing that one of the fittest samples is selected to be both parents for a single child. In this instance, only random mutation will create a new combination of inputs.
5. Randomly select inputs from these new child inputs to mutate with a frequency determined by Equation 2. If the fitness of both parents is high, then the likelihood that a child input will be mutated is higher. A suitable value for the maximum mutation rate was found to be 15%.

$$\text{Mutate rate} = \text{max mutation rate} - [1 - (\text{parent1 fitness} + \text{parent2 fitness})/2] \qquad (2)$$

6. Mutate randomly selected inputs with a magnitude inversely proportional to the average fitness of the parents. This is achieved by creating a Gaussian distribution with a mean equal to the input before mutation and with a standard deviation equal to the relative error of the parents multiplied by the mean.
7. Repeat process starting on Step 2 for the new generation of inputs.

An all-inclusive library was compiled which listed input parameters and corresponding sample macroproperties from all of the populations generated within the Genetic Algorithm. This library was then used in subsequent tests to determine appropriate input limits based on past trials. A filter was applied to find all samples with a high overall fitness and determine the maximum range of their input parameters. These limits were then applied for future calibrations with the Genetic Algorithm. A complete flow diagram of the recommended calibration process for a BPM is shown as Figure 1.

2.3 *Calibration results*

By following this basic process, the Genetic Algorithm successfully calibrated BPMs to represent coal to within 1% of desired results after approximately 500 trials. The inputs listed in Table 1 were manipulated during the calibration process to achieve the desired values for E, ν, UCS, and post-peak modulus. The resulting test results of a calibrated sample are shown in Table 2.

Table 2. Calibrated macroproperties for BPM coal sample after 100 and 500 trials.

Macroproperty	Test results				
	Desired	Calibrated (100 trials)	Error (%)	Calibrated (500 trials)	Error (%)
Young's modulus	6.00 GPa	5.77 GPa	3.77	5.89 GPa	1.89
Poisson's ratio	0.20	0.21	4.13	0.20	1.15
Peak UCS	25.0 MPa	24.8 MPa	0.82	24.9 MPa	0.39
Post-peak modulus	-6.00 GPa	-6.03 GPa	0.50	-6.02 GPa	0.35
		Average	2.31		0.95
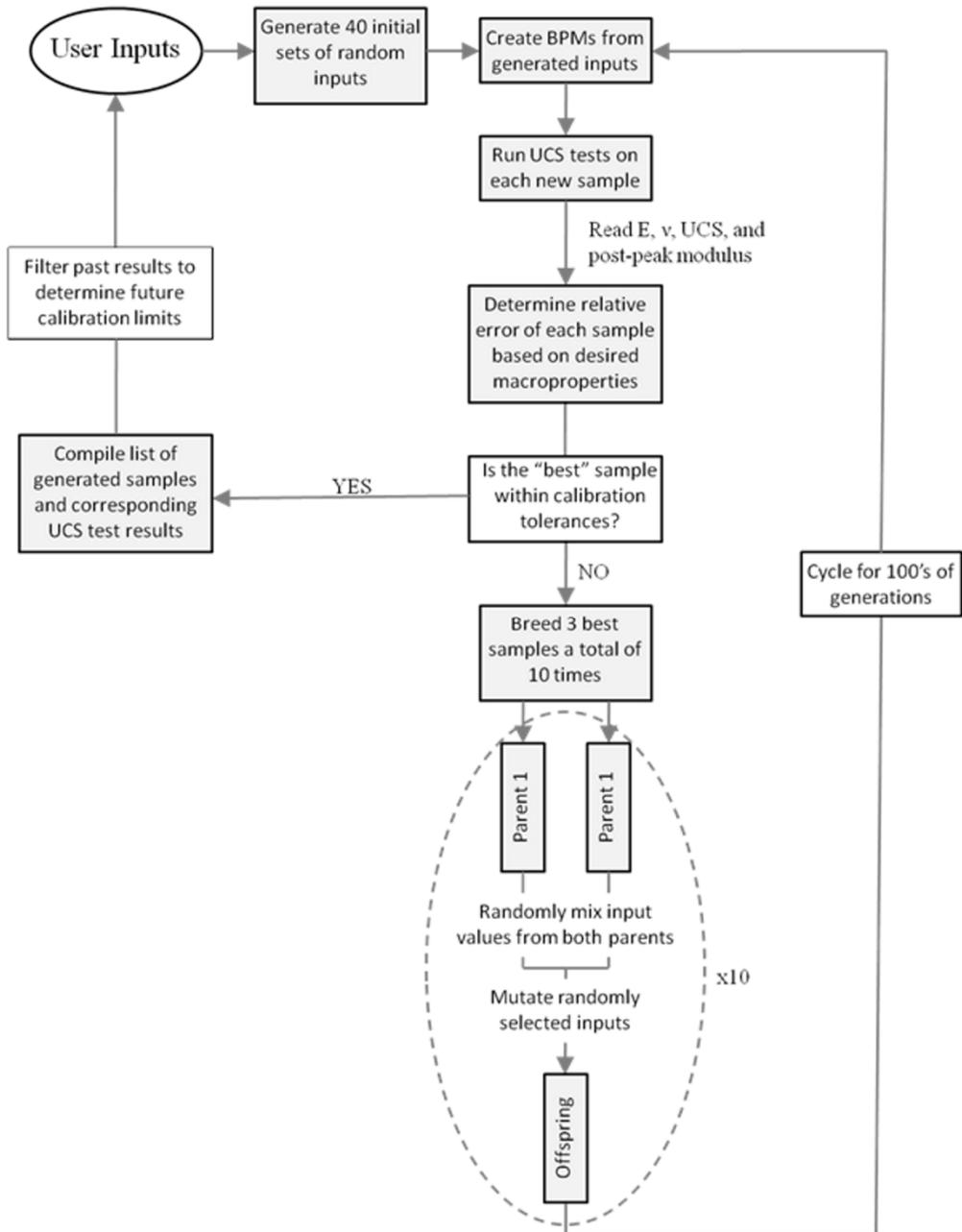
Figure 1. Cycle of iterations within the genetic algorithm.

Note that the post-peak modulus of the UCS stress-strain curve is also taken into account in the calibration process using the GA. The genetic algorithm had the flexibility of design to be able to calibrate this macroproperty with no prior knowledge on how to achieve the desired material behavior in the post-failure stress-strain response. The calibrated PFC^{3D} coal sample and the resulting stress-strain curve are shown as Figure 2. The sample was constructed as a BPM of 3372 particles, with each BPM taking approximately 2 minutes to generate and test. This coarse resolution was selected to reduce overall runtime of the simulation, but was found to be appropriate at producing repeatable results with a coefficient of variation less than 5%. To eliminate this added variation, the random number seed was reset before each test so the packing configuration between samples remained the same.

Figures 3 & 4 show the progression of the genetic algorithm for 500 simulated trials over 47 total generations. The first generation contained 40 samples while any subsequent generation included 10 newly created samples.
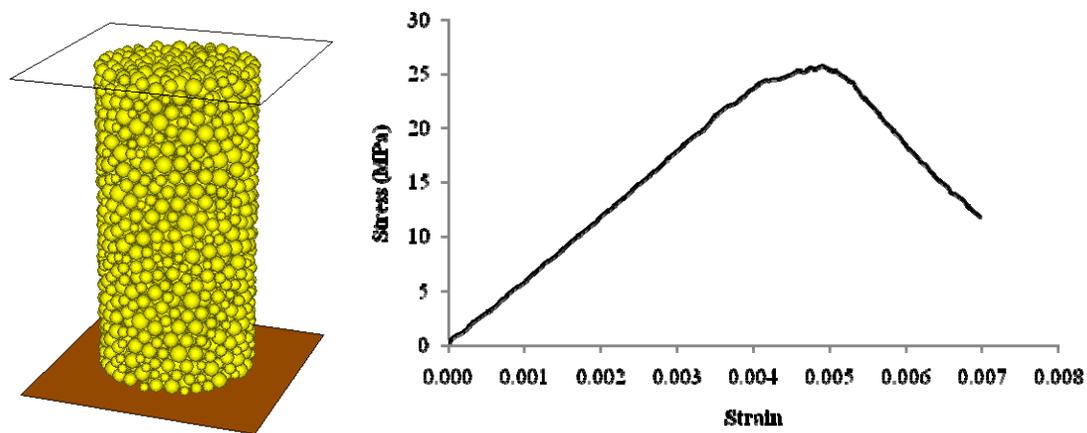

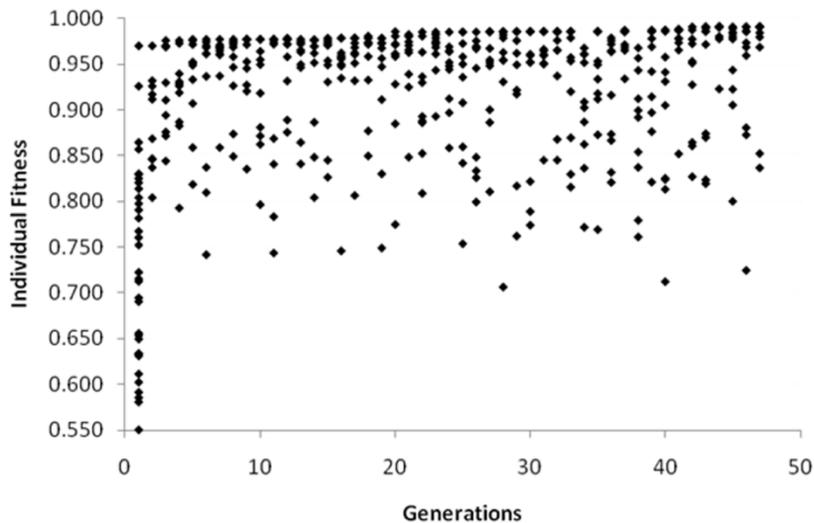Figure 2. BPM sample and resulting stress-strain curve during simulated UCS test.

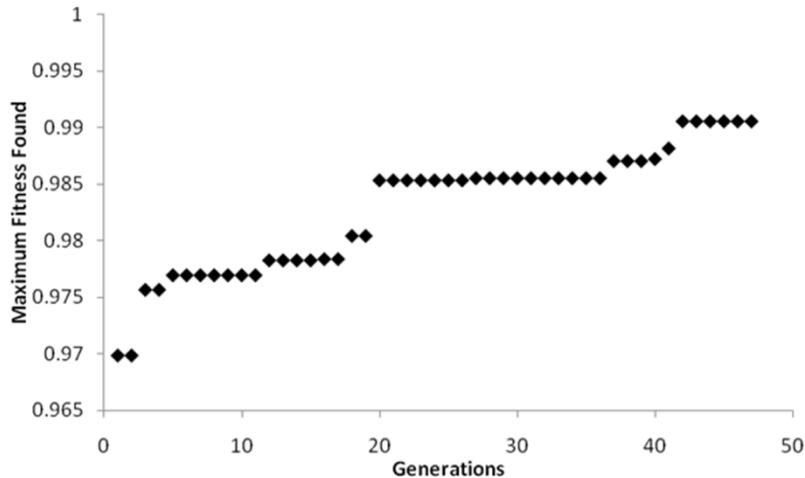Figure 3. Complete population results of genetic algorithm for 500 trials and 47 generations.

Figure 4. Calibration process using the genetic algorithm where fitness is found from Equation 1.

3 CONCLUSIONS

The Genetic Algorithm calibration developed for the generation of a Bonded-Particle Model could also be applied to more advanced rock models in PFC^{3D} such as the Synthetic Rock Mass model (Pierce et al. 2007) or cluster logic in the BPM (Cho et al. 2007). The Genetic Algorithm has the ability of calibrating PFC^{3D} samples for a wide range of desired macroproperties with little change to the structure of the algorithm. In this way the GA becomes a powerful tool for researching how to achieve specific material behaviors within the simulated rock sample. The calibration of post-peak modulus was one example of fitting a behavior with no prior knowledge of required input values.

In this study, the allowable ranges for input parameters were defined by the user at the onset of the experiment. To aid in the selection of appropriate ranges, a library of previous trials was compiled and analyzed. Roughly 25,000 individual PFC^{3D} samples were generated and tested. For such large data sets, an artificial neural network could be a valuable tool for analysis as is shown by (Tawadrous et al. 2009). Neural networks may be designed and trained to approximate the input values required to achieve desired macroproperties for the sample. The current Genetic Algorithm can be further improved by taking advantage of an artificial neural network to define better guess points for input parameters during a calibration.

Overall, the construction of the Genetic Algorithm was flexible enough to allow any FISHTank inputs to be modified through an evolutionary process to obtain a calibrated PFC^{3D} sample. This added flexibility was not without its costs, since the algorithm required a large number of trials to calibrate a sample appropriately. Roughly 500 UCS tests were required to fit 4 desired macroproperties using 9 adjustable inputs. The structure of the GA allows for parallel simulations to be run on multiple machines if this added runtime is prohibitive for a certain type of model. With these combined procedures the Genetic Algorithm could well be applied to calibrate a wide range of complex behaviors for a simulated PFC^{3D} sample.

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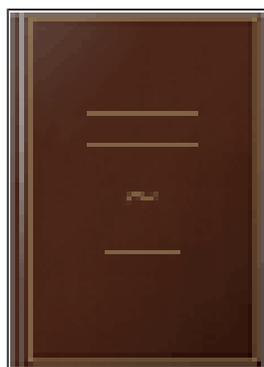Rent and save from the world's largest eBookstore. Read, highlight, and take notes, across web, tablet, and phone.

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