

Probabilistic calibration of discrete particle models for geomaterials

Calibration probabiliste des modèles discrets de particules pour les géomatériaux

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ABSTRACT

This paper introduces the use of a probabilistic inverse model method to calibrate numerical models based on Particle Flow Code in three dimensions (PFC^{3D}). The main aim is to fully define the parameters of the particle models through a joint probability density function conditioned on experimental observations obtained from triaxial rock testing. The discrete particle model built for the rock specimen simulation is comprised of an assembly of spheres of specified stiffness bonded together with specified strengths. A case study is presented where the probabilistic calibration method is applied to experimental results of triaxial compressive tests of Vosges sandstone specimens tested at the L3S-R (Grenoble, France). Calibration results will serve for simulating likely rock specimens' behaviour when matching not only the global stress-strain and volumetric responses of jointed rock for different confining pressures, but also the fracture modes observed in the laboratory. Additionally, probability descriptions of the models' performance at different levels of axial strain are also retrieved, enhancing the quantity and quality of inferences that are obtained traditionally by optimization methods for inverse problems. Preliminary results include in-progress trends and model relationships as the probabilistic calibration is currently being computed.

RÉSUMÉ

Ce papier présente une méthode de modélisation inverse probabiliste pour calibrer les modèles numériques basés sur le logiciel 'Particle Flow Code' en trois dimensions (PFC^{3D}). L'objectif principal est de définir entièrement les paramètres du modèle de particules par une fonction de densité de probabilité commune conditionnée pour différentes pressions de confinement obtenues à partir d'essais triaxiaux sur roche. Les modèles discrets de particules établis pour la simulation des échantillons de roche sont composés d'un ensemble de sphères de rigidité spécifique reliées entre elles par des liens de résistance spécifique. Une étude de cas est présentée où la méthode probabiliste est appliquée aux résultats expérimentaux d'essais triaxiaux de compression sur des échantillons de grès des Vosges menés au L3S-R (Grenoble, France). Les résultats de calibration serviront pour la simulation de roches spécimens comportement lors de la recherche non seulement la contrainte-déformation volumétrique et réponses de jointed rock pour les différentes pressions de confinement, mais aussi les modes de rupture observés dans le laboratoire. De plus, une description probabiliste de la performance du modèle à différents niveaux de déformation axiale est également obtenue, augmentant la quantité et la qualité des inférences qui peuvent être traditionnellement obtenues par les méthodes d'optimisation pour les problèmes inverses. Les résultats préliminaires en cours, notamment les tendances et les relations que le modèle probabiliste de l'étalonnage est en cours de calcul.

Keywords : Probabilistic calibration, discrete element modelling, Vosges sandstone

1 INTRODUCTION

Discrete element methods (Cook and Jensen, 2002) are emerging as very powerful tools for understanding and simulating kinematic effects that correspond better to the mechanistic nature of geomaterials. However, a major limitation is the lack of testing capabilities as to determine the particle model parameters at the element scale. Consequently, scale assumptions are required for utilizing meso-scale testing results such as triaxial data, which are translated at the element level assuming that the material of interest is homogeneous. This process imposes significant uncertainties since material testing at a larger scale is used to parameterize a discrete model with unknown element parameters. To account for the uncertainty on the parameters of the discrete element model, it is proposed to solve the inverse problem defined as the probabilistic parameterization of the model conditioned on the meso-experimental data.

This paper introduces the use of a probabilistic inverse model method based on the Bayesian paradigm to calibrate geomaterial models (Medina-Cetina, 2006), when applied to a numerical model of a Particle Flow Code in three dimensions (PFC^{3D}). Herein, the main aim is to fully define the parameters

of the particle models through a joint probability density function conditioned on experimental observations obtained from triaxial rock testing.

The discrete particle model built for the rock specimen simulation is comprised of an assembly of spheres of specified stiffness bonded together with specified strengths. A case study is presented where the probabilistic calibration method is applied to experimental results of triaxial compressive tests of Vosges sandstone specimens tested at the Laboratory 'Sols Solides Structures-Risques' L3S-R (Grenoble, France).

Calibration results will serve for simulating likely rock specimens' behaviour when matching not only the global stress-strain and volumetric responses of jointed rock for different confining pressures, but also the fracture modes observed in the laboratory. Additionally, probability descriptions of the models' performance at different levels of axial strain are also retrieved, enhancing the quantity and quality of inferences that are obtained traditionally by optimization methods for inverse problems. Preliminary results include in-progress trends and model relationships as the probabilistic calibration is currently being computed. Finally, a section discussing expected failure mechanisms is included.

2 PFC^{3D} MODEL

As a preliminary application of the probabilistic inverse modelling method, the macro-mechanical behaviour of Vosges sandstone has been chosen for calibrating the PFC^{3D} model. A series of triaxial compression tests were experimentally carried out on cylindrical samples of Vosges sandstone under different confining pressures to study the onset of localisation of deformation, shear band orientation and patterning (Bésuelle, 1999). Only the results of a confining pressure of 10 MPa were calibrated.

A cylindrical model of synthetic rock sample measuring 40 mm in diameter and 80 mm in length was created to simulate the experimental triaxial test. Owing to the small grain size of this rock type (0.2 mm in average radius), it was infeasible to produce a PFC^{3D} model in which every spherical particle represented as a single mineral grain. Therefore each particle is assumed to represent a small representative volume of about 6-10 mineral grains. By this way, a model was created as shown in Figure 1, composed of 1122 particles with a range of artificial radii from 2.0 to 3.3 mm, randomly distributed, and packed so as to approach a measured porosity of 0.22, and a bulk density of 1960 kg/m³. A process analogous to physical compaction is followed (Itasca 2005). Note that the average particle size is 2.6 mm.

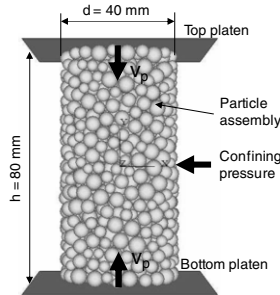


Figure 1. PFC^{3D} model of Vosges sandstone. Thick vertical arrow shows the direction of applied velocity.

The top and bottom platens are assumed to be rigid and frictionless. The specimen was loaded by moving two platens toward one another at a constant velocity v_p . The sleeve wall, controlled by a servo-mechanism algorithm, was used to maintain the constant confining pressure on the specimen. Note that the sleeve wall is also frictionless.

Since Vosges sandstone is a cemented material (Bésuelle, 1999), the parallel bond model provided in PFC^{3D} has been used for the synthetic rock. The parallel bonds can be seen as a set of elastic springs with constant normal and shear stiffnesses uniformly distributed over a circular disc lying on the contact plane. The readers are referred to Potyondy and Cundall (2004) for more details of the parallel bond model.

Figure 2 lists two set-up micro mechanical parameters (named Mat 1 and Mat 2) used for reproducing the Vosges sandstone behaviour with a PFC^{3D} model. In general, the micro mechanical stiffnesses influence the global stiffness of the sample, and the measured Poisson's ratio of the PFC^{3D} will be affected by the ratio of normal to shear micro-stiffness. The bond strengths are related to the strengths of the simulated material. The ratio of standard deviation to mean tensile bond strength, $\sigma_{sdev}^n/\sigma_{mean}^n$, affects the threshold of the microcracks nucleation (i.e. crack initiation stress). Increasing this ratio lowers the crack initiation stress and vice versa. The ratio of tensile to shear bond strength, σ^n/σ^s , affects the failure mode (ductile or brittle) by controlling the relative numbers of shear and tensile cracks. A material with a small ratio σ^n/σ^s will fail in a brittle mode (predominated by tensile cracks) while it will fail in a ductile mode (predominated by shear cracks) when σ^n/σ^s is large.

Table 1. Micro mechanical parameters used in PFC^{3D} model.

Micro-parameter	Symbol	Unit	Mat 1*	Mat 2**
Contact Young's modulus	$\theta_1=E_c$	GPa	12.0	12.1
Ratio of contact normal to shear stiffness	$\theta_2=k^n/k^s$	-	7.5	4.5
Inter-particle friction coefficient	$\theta_3=\mu$	-	3.0	3.0
Parallel bond Young's modulus	$\theta_4=E$	GPa	12.0	12.1
Ratio of bond normal to shear stiffness	$\theta_5=k^n/k^s$	-	7.5	4.5
Average bond tensile strength	$\theta_6=\sigma_{mean}^n$	MPa	50	68
Standard deviation in bond tensile strengths	$\theta_7=\sigma_{sdev}^n$	MPa	5.0	6.8
Average bond shear strength	$\theta_8=\sigma_{mean}^s$	MPa	50	38
Standard deviation in bond shear strength	$\theta_9=\sigma_{sdev}^s$	MPa	5.0	3.8

(*) initial micro parameters used during the application of the probabilistic calibration method.

(**) micro parameters used for investigating the damage mechanisms.

3 PROBABILISTIC CALIBRATION

A first approach for the assessment of the model performance is to assume that the model parameters are random variables. In order to fully quantify the uncertainty of the proposed model conditioned on the observations included in the full data-set, a Bayesian analysis is developed. This not only define the probability density function (PDF) of each model parameter but of the correlation between them, allowing for the possibility of simulating the model beyond the mean estimates given by the traditional least square calibration approaches LS.

3.1 Bayesian Analysis for the solution of inverse problems

The probabilistic calibration of the proposed model is performed using the Bayesian paradigm, which is defined as (Papoulis, 1991):

$$\pi(\theta | \mathbf{d}_{obs}) = \frac{f(\mathbf{d}_{obs} | \theta, g(\theta))\pi(\theta)}{\int f(\mathbf{d}_{obs} | \theta, g(\theta))\pi(\theta)d\theta} \quad (1)$$

where the prior $\pi(\theta)$ introduces the *a priori* state of information associated to a set of parameters θ by defining the proper PDF, which in this case is defined as the vector of the model parameters $\theta = \{\theta_i\}$, with $i=1 \dots 9$ according to Table 1.

The likelihood $f(\mathbf{d}_{obs} | \theta)$ represents the *a priori* state of information defined by a PDF representing the potential of the parameters θ to match the vector of observations $\mathbf{d}_{obs}$ (deviatoric stress and volumetric strain), or to help to match them if they are embedded into a predictive model $g(\theta)$, represented by the PFC^{3D} numerical simulator. The posterior $\pi(\theta | \mathbf{d}_{obs})$ is thus the joint probability function between the *a priori* states of information associated to both the prior and the likelihood.

For the parameterization of the proposed model, it is assumed that the coefficients included in the vector θ follow vague priors, and that the likelihood $f(\mathbf{d}_{obs} | \theta)$ follows a Gaussian-type behavior (Press, 2003). This hypothesis can be verified by plotting the CDF of the residual and compared it with its corresponding Gaussian model. It is worth mentioning, that the prior can be further refined as more experience is gained in the model calibration, and similarly the likelihood, if the model formulation generates more accurate results.

For estimating the mean and the covariance (first and second moments), or for estimating marginal statistics for each parameter included in θ , it is required to integrate the posterior with respect to the parameters domain. This integral is solved numerically, yielding a full description of the uncertainty associated to the model parameters θ conditioned on the available data.

An efficient way to solve the posterior integral is using Markov Chain Monte Carlo (MCMC) (Robert and Casella, 2004). A useful property of the MCMC is that it converges to the target joint density as the sample integration grows. For this work, the decision rule that determines which samples are 'accepted' or 'rejected' is the Metropolis-Hastings (MH) criteria measured by α or the probability of accepting or rejecting a candidate point or set of parameters used to run the numerical model. Under these premises, the posterior integration at the MH 'state' of the chain $s + 1$ iteration is obtained by sampling a candidate point Y from a proposal distribution $q(\cdot | \hat{\theta}_s)$, where the candidate point Y is accepted or rejected as the next step of the chain with probability given by:

$$\alpha(\hat{\theta}_s, \mathbf{d}_{obs}) = \min \left\{ 1, \frac{\pi(Y | \mathbf{d}_{obs}) q(\hat{\theta}_s | Y)}{\pi(\hat{\theta}_s | \mathbf{d}_{obs}) q(Y | \hat{\theta}_s)} \right\} \quad (2)$$

The value of α is compared to a random uniform value u for each simulation and the acceptance of the proposed set of parameters is thus defined when $\alpha \leq u$.

3.2 Preliminary results

Due to the computational effort to run the PFC^{3D} simulations, a testing phase was designed to corroborate the efficiency of the probabilistic inversion approach. Results corresponding to this phase are discussed in this section, which considers only the effect of the deviatoric stress as a starting point.

The testing phase considered the use of the material response in the form of the global axial strain vs. deviatoric stress as the target or reference values for any combination of the model parameters. A measure of uncertainty corresponding to deviatoric stress was given by a Gaussian-type behavior along the strain domain to reproduce typical variations of the same material tested under similar conditions. Figure 2 shows the reference and the uncertainty bands indicated by a standard deviation SD proportional to the deviatoric stress (10%).

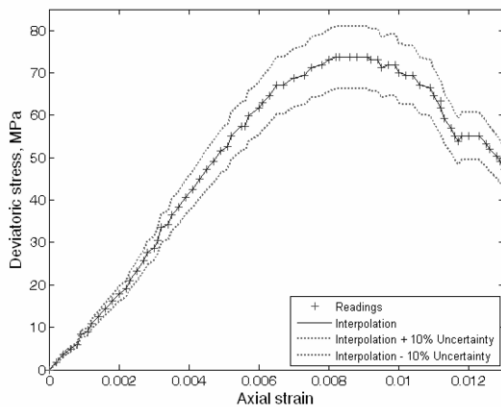


Figure 2. Experimental evidence (target) showing the specimen's response and proportional measures of uncertainty.

Initial values for the vector of model parameters θ are obtained from the meso-scale triaxial testing. The first simulation given by these values is presented in Figure 3, illustrating that a first move towards the target values is likely to be given by an increase of the Young's modulus. This effect is showed in Figure 4, representing a 'pan' view of subsequent

MCMC samples of global deviatoric stress responses of a series of numerical simulations plotted with respect to the axial strain domain. From this figure it is observed a transition of upward leveling of the linear response and a general uplift of the deviatoric stress looking for accommodating the target experimental response based on the simultaneous sampling of the model parameters. Figure 4 also indicates a threshold where the sampling becomes 'stationary' or stable.

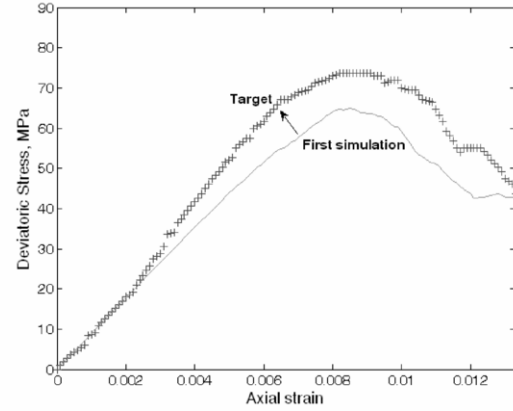


Figure 3. First simulation obtained using parameter values from the triaxial test.

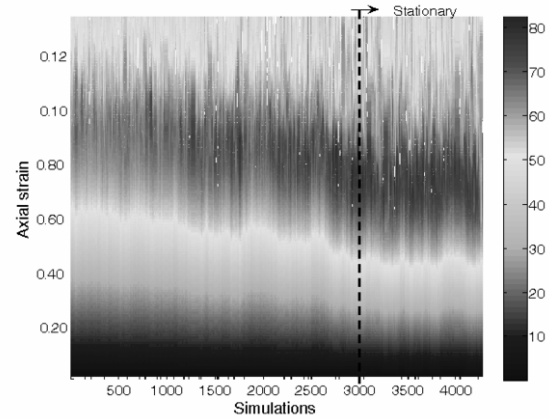


Figure 4. Deviatoric stress values of a series of numerical simulations with respect to the axial strain.

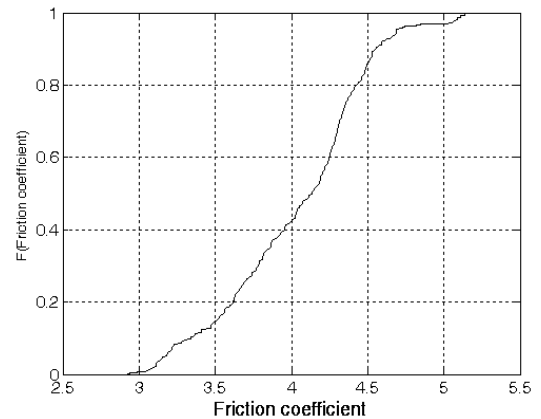


Figure 5. Cumulative density function of the friction coefficient (preliminary results).

Once the stationary condition is reached, it is possible to generate inferences about the posterior. For instance, Figure 5 shows a preliminary description of the inter-particle friction coefficient. Further investigations are required to achieve

conclusive inferences from the joint probability function integrated after the burn-in point.

4 AN EXAMPLE OF INVESTIGATION OF DAMAGE MECHANISMS

A parallel effort to the testing of the probabilistic inversion consisted in looking at potential failure mechanisms. Figure 6 shows the comparison of global stress-strain responses between PFC^{3D} synthetic rock and Vosges sandstone. It can be seen that overall responses for stress-strain are well reproduced. It should be noted that the rock sample fails without need to incorporate any constitutive macro failure criteria.

Four stress states (A, B, C and D) as shown in Figure 6 have been chosen for investigating the development of the microcracks during the triaxial compression loading. It can be seen that at state A being close to the peak stress a few microcracks (tensile and shear) locally initiate at the top platen. Whilst continuing to increase the compressive load up to the peak stress (state B), more cracks are observed around the top platen and also in the middle right side of the specimen. After the peak stress, at state C, a clear inclined zone containing numerous microcracks (failure pattern) is formed in the sample. This damage zone at this state is seriously weakening the sample which results in a significant reduction of the deviatoric stress. Final distribution of cracks at state D shows significant enlargement of microcracks along the inclined failure zone.

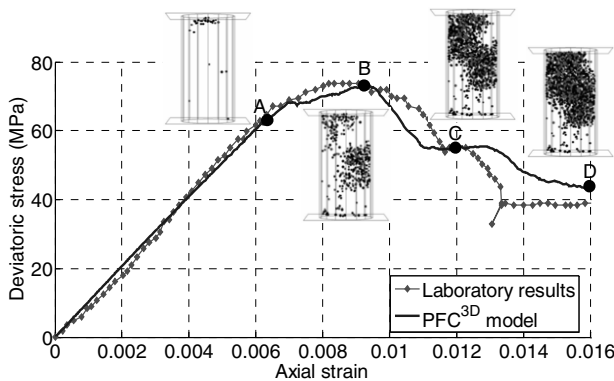


Figure 6. Development of the damage, represented by bond breakages, of the Vosges sandstone sample during triaxial compressive loading path with confining pressure of 10 MPa. Shear cracks are denoted by red color and tensile cracks by black.

Figure 7 presents the comparison of final damage (i.e. at the axial strain of 0.016) between the PFC^{3D} model and the laboratory test in the Vosges sandstone sample. It would appear from the figure that there is clear correlation between the formation of the microcracks and the displacement field in the PFC^{3D} results. The PFC^{3D} model can reproduce very well the inclination of shear band observed from the experimental tests. The thickness of shear band in PFC^{3D} model is, however, significant larger. This is clearly due to the much larger grain (particle) size used for the synthetic rock since there is ample experimental evidence that shear band thicknesses in granular materials depend on grain size. A shear band thickness of about 10 times the average particle diameter obtained in PFC^{3D} model agrees very well with the proposition of Roscoe (1970) which has been based on direct experiment observations.

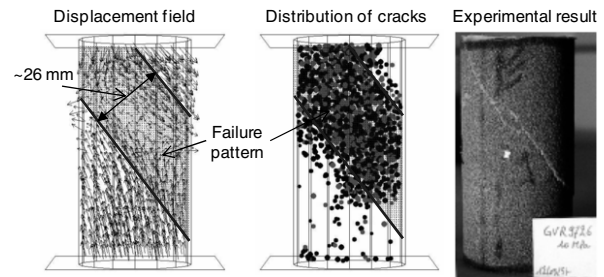


Figure 7. Comparison of damage in the Vosges sandstone sample between the PFC^{3D} model and the laboratory test (Bésuelle 1999) after failure under triaxial compressive loading path with confining pressure of 10 MPa. Shear cracks are denoted by red color and tensile cracks by black.

5 CONCLUSIONS

This paper introduces the use of a probabilistic calibration methodology for assessing a full description of discrete element model parameters and a qualitative evaluation of likely failure mechanisms for geomaterials. A case study is presented based on experimental data obtained from a triaxial test performed on a Vosges sandstone specimen. A testing phase was designed to corroborate the efficiency of the probabilistic inversion method showing successful results. Likely failure mechanisms were discussed as a way to understand the physics behind the model parameters and their corresponding association to actual behavior of

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REFERENCES

- ASCE, 2002. Discrete Element Methods: Numerical Modeling of Discontinua, Benjamin K. Cook and Richard P. Jensen (Editors), Special Publication Number 117, Proceedings of the Third International Conference on Discrete Element Methods, Santa Fe NM, September 23-25.
- Bésuelle, P. 1999. Déformation et rupture dans les roches tendres et les sols indurés: comportement homogène et localisation, PhD Thesis, Université de Grenoble I, Grenoble, France.
- Itasca 2005. PFC^{3D}-Particle Flow Code in three-dimensions, version 3.1, User's manual, Vol. I & II. Itasca Consulting Group, Inc., Minneapolis, USA.
- Medina-Cetina Z. 2006. Probabilistic calibration of a soil model. PhD Dissertation, The Johns Hopkins University, Baltimore MD USA.
- Papoulis A. 1991. Probability, Random Variables and Stochastic Processes, Mc-Graw Hill, USA.
- Potyondy D.O. and Cundall, P.A. 2004. A bonded-particle model for rock, Int. J. Rock Mech. Min. Sci., 41, 1329-64.
- Robert C. P. and Casella G. 2005. Monte Carlo Statistical Methods, Springer, New York.
- Roscoe, K.H. 1970. The influence of strains in Soil Mechanics. Géotechnique, 20, 129-170.