Grain Learning: Bayesian Calibration of DEM Models and Validation Against Elastic Wave Propagation

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1 Introduction

The estimation of micromechanical parameters of discrete element method (DEM) models is a nonlinear history-dependent inverse problem. In order to reproduce the experimental measurements with high accuracy, this work aims to develop a *machine learning*-based calibration toolbox named "*Grain* learning", which can extract grains from X-ray computed tomography (CT) images and perform Bayesian parameter estimation for DEM models of dry granular materials.

2 Bayesian Calibration

We first introduce a feature-based watershed algorithm which performs multi-phase image segmentation and analysis empowered by the WEKA *machine-learning* library [1]. A novel iterative Bayesian filter is developed to estimate the posterior probability distribution of the micromechanical parameters of a DEM model, conditioned to history-dependent experimental data. The iterative application of conventional sequential Bayesian estimation [2,3] allows the virtual granular material to *learn* from all previous experimental measurements of the physical system being modeled in a fast and automated manner.

Bayesian calibration is conducted for DEM modeling of glass beads under cyclic oedometric compression. Using the particle configuration resulting from the CT images, the representative volume of a glass bead packing is

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reconstructed in DEM simulations. The DEM packing governed by the simplified Hertz-Mindlin contact law and rolling resistance is then calibrated through a iterative Bayesian filtering process, which is able to focus increasingly on highly probable parameter subspaces over iterations. Three iterations are needed to obtain excellent agreement between posterior predictions and experimental data as well as accurate approximation of the posterior probability distribution as shown in Fig. 1a. From the posterior probabilities, micro–macro correlations can be obtained with known uncertainties (see Fig. 1b), which also help understand the uncertainty propagation across various scales.

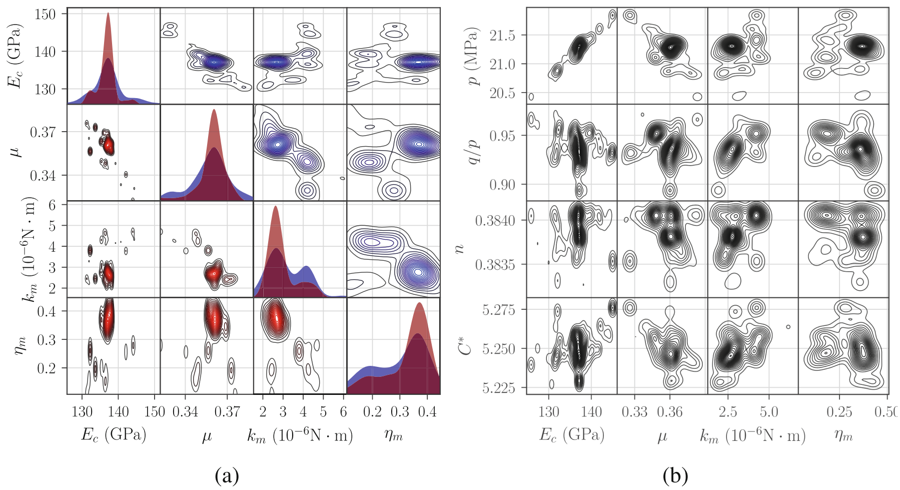


Fig. 1. (a) Posterior PDF estimated at the beginning (blue) and the end (red) of the sequential Bayesian filtering. 2D projections of the posterior PDF in the above- and below-diagonal panels are colored by the posterior probability densities. (b) Approximated posterior distributions for pairs of micromechanical parameters and macroscopic quantities of interest at the maximum stress ratio state.

3 Validation

To demonstrate that the grains are successfully trained by the experimental data, DEM modeling of elastic waves propagating through a long granular column is considered for model validation. The elastic moduli are experimentally measured from ultrasonic traces received along the oedometric compression path. The elastic moduli can be numerically calculated by (1) static probing: load the representative volume with a small strain increment, and (2) dynamic probing: agitate elastic waves through a long granular column constructed with the same representative volume. The wave velocities obtained at different pressures using the two approaches quantitatively agree with those measured in experiments,

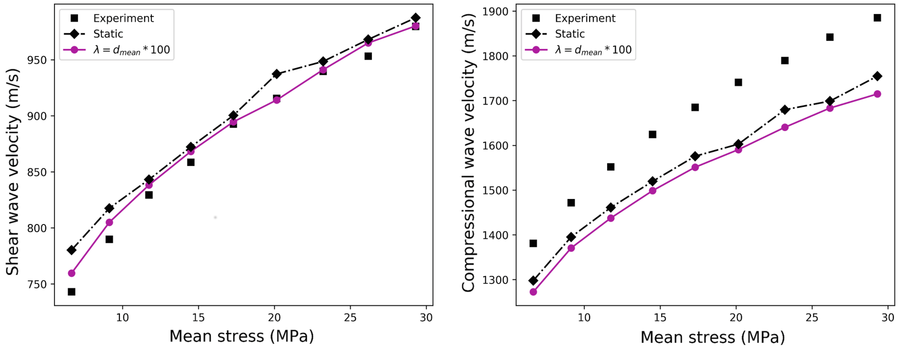
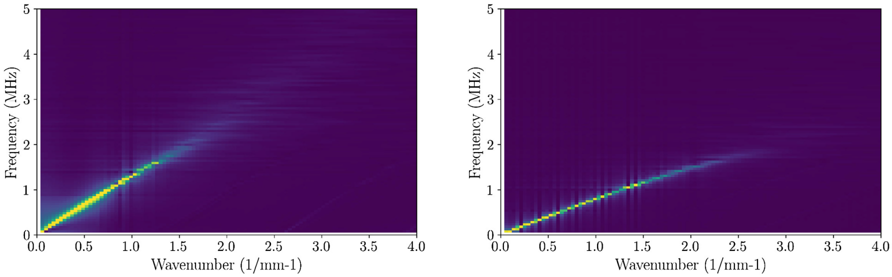


Fig. 2. Comparison of elastic wave velocities predicted by the two probing methods and measured in ultrasonic experiments. A wavelength of 100 times the mean particle diameter is used as the source for agitating elastic waves



(a) P-wave

(b) S-wave

Fig. 3. Dispersion relations obtained by applying two-dimensional fast Fourier transform to layer-averaged particle velocities.

having errors less than 10% for the former and 16% for the latter, as shown in Fig. 2.

In addition to the good agreement between numerical predictions and experimental data, the dispersion relation, namely elastic P- or S-wave velocities as functions of frequency and wavenumber, can be obtained from the DEM simulations as shown in Fig. 3, which is rather difficult in experiments. The initial slopes that correspond to elastic moduli of a continuum agree well with the experimental values, thus validated the robustness of the calibrated DEM model. Although not shown here, a variety of input frequencies and waveforms are considered during the dynamic probing to investigate their effect on the dispersion relations. While the dispersion curves are mostly unaffected by the source, the activated frequency bands show dependency on the characteristics of input signals.

4 Conclusions

The present study show the capability of the *Grain* learning toolbox for calibrating DEM models of granular materials. The new iterative Bayesian filter facilitates a fast and automated search in parameter space from coarse to fine scales. The wave propagation simulations performed with the calibrated DEM model agree well with the ultrasonic experiments conducted during the oedometric loading. It is worth noting that although static and dynamic probing give similar predictions for the elastic moduli of granular materials, the latter generally takes less computational time and provide more useful information than the former.

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