# GrainLearning: A Bayesian uncertainty quantification toolbox for discrete and continuum numerical models of granular materials

Hongyang Cheng ®[2], **Luisa Orozco** ®[1¶], **Retief Lubbe**[2], **Aron Jansen** ®[1], **Philipp Hartmann** ®[3], **and Klaus Thoeni** ®[3]

1 Netherlands eScience center, Amsterdam, The Netherlands **2** Soil Micro Mechanics (SMM), Faculty of Engineering Technology, MESA+, University of Twente, Enschede, The Netherlands **3** University of Newcastle, Callaghan, NSW, Australia ¶ Corresponding author

Summary

How to keep dikes safe with rising sea levels? Why are ripples formed in sand? What can we prepare for landing on Mars? At the center of these questions is the understanding of how the grains, as a self-organizing material, collide, flow, or get jammed and compressed. State-of-the-art algorithms allow for simulating millions of grains individually in a computer. However, such computations can take very long and produce complex data difficult to interpret and be upscaled to large-scale applications such as sediment transport and debris flows. GrainLearning is an open-source toolbox with machine learning and statistical inference modules allowing for emulating granular material behavior and learning material uncertainties from real-life observations.

To understand what GrainLearning does, let us consider a mechanical test performed on a granular material. The macroscopic response of such material, in terms of stress-strain evolution curves, is obtained from the test. It would be interesting to have a digital equivalent material to further investigate, using numerical simulations such as the discrete element method (DEM), how such material would behave under other mechanical constraints. To do so, the first step is defining a contact model governing interactions between grains in DEM. This involves multiple a-priori unknown constants, such as friction coefficients or Young's modulus, whose chosen values will determine the macroscopic behavior of the simulation. By repeatedly comparing the simulation results with provided experimental data, GrainLearning allows one to calibrate or infer these values such that the mechanical response in the DEM simulation is the closest to that observed in the real-world experiment.

While it was initially developed for DEM simulations of granular materials, GrainLearning can be extended to other simulation frameworks such as FEM, CFD, LBM, and even other techniques such as agent-based modeling. In the same vein, the framework is not exclusive for granular materials.

Statement of need

Understanding the link from particle motions to the macroscopic material response is essential to develop accurate models for processes such as 3D printing with metal powders, pharmaceutical powder compaction, flow and handling of cereals in the alimentary industry, grinding and transport of construction materials. Discrete Element Method (DEM) has been used widely as the fundamental tool to produce the data to understand such link. However, DEM simulations are highly computationally intensive and some of the parameters used in the contact laws
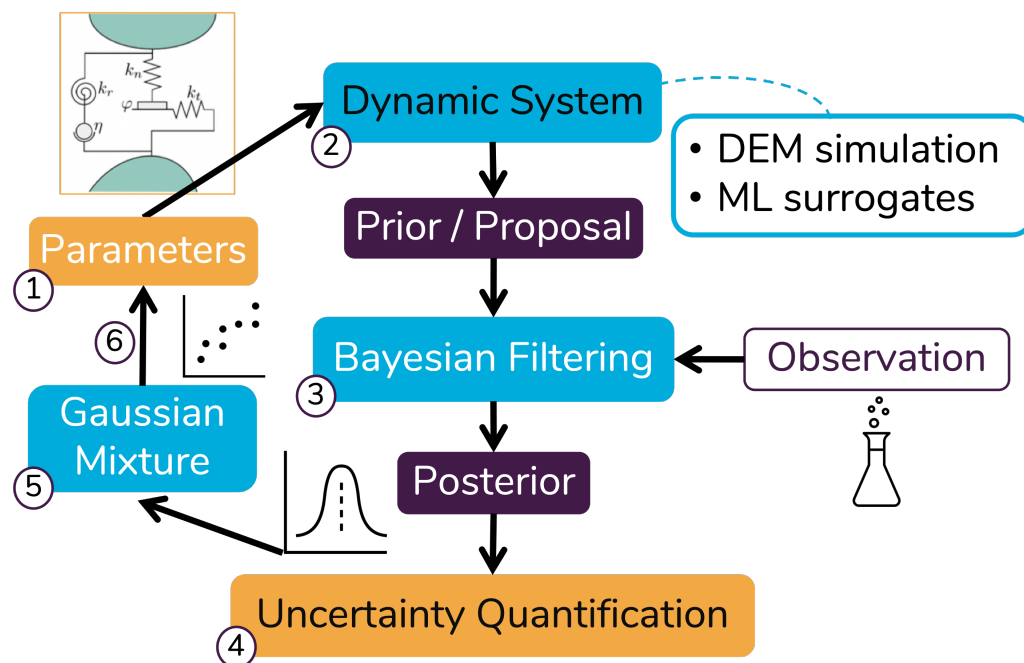
cannot be directly measured experimentally.

GrainLearning (Cheng et al., 2023) arises as a tool for Bayesian calibration of such computational models, which means the model parameters are estimated with a certain level of uncertainty, constrained on (noisy) real-world observations. Effectively, this makes the simulations digital twins of real-world processes with uncertainties propagated on model outputs, which then can be used for optimization or decision-making.

Conventionally, the calibration of contact parameters at the grain scale is accomplished by trial and error, by comparing the macroscopic responses between simulation and experiments. This is due to the difficulty of obtaining precise measurements at the contact level and the randomness of grain properties (e.g., shape, stiffness, and asphericity). In the last decade, optimization (Do et al., 2018) and design-of-experiment (Hanley et al., 2011) approaches such as Latin Hypercube sampling and genetic algorithms have been used. However, the amount of model runs is still too large. For this reason, Gaussian process regression (Fransen et al., 2021) or artificial neural networks (Benvenuti et al., 2016) were tested as surrogate- or meta-models for the DEM. GrainLearning combines probabilistic learning of parameter space and sampling to achieve Bayesian optimization efficiently.

Functionality

GrainLearning's core functionality is illustrated in Figure 1. GrainLearning started in the geotechnical engineering community and was primarily used for granular materials in quasi-static, laboratory conditions (Cheng et al., 2018, 2019). These include triaxial (Hartmann et al., 2022; Li et al., 2024) and oedometric (Cheng et al., 2019) compressions of soil samples. In the particle technology community, attempts with GrainLearning have been made to identify contact parameters for polymer and pharmaceutical powders against angle-of-repose (Nguyen, 2022), shear cell (Thornton et al., 2023), and sintering experiments (Alvarez et al., 2022). Satisfactory results have been obtained in simulation cases where the grains were in dynamic regimes or treated under multi-physical processes.

- **Calibration or parameter inference**: By means of Sequential Monte Carlo filtering GrainLearning can infer and update model parameters. By learning the underlying distribution using a variational Gaussian model, highly probable zones are identified and sampled iteratively until a tolerance for the overall uncertainty is reached. This process requires the input of: a time series reference data, the ranges of the parameters to infer and a tolerance. The software iteratively minimizes the discrepancy between the model solution and the reference data.

Figure 1: Elements of the trade in the calibration process. 1. Draw initial values of the parameters to calibrate. 2. Run the dynamic system with the parameters. 3. With the reference data or observation, estimate the posterior distribution via the Bayesian filtering. 4. Check convergence of the parameter inference, if the process has not converged: 5. Define a Gaussian mixture from the examples of this iteration and sample the parameters for the next iteration. 6. Next iteration step. For more details check the iterative Bayesian filter section of GrainLearning's documentation.

- **Surrogate modeling**: Besides using direct simulation results (e.g. DEM) GrainLearning offers the capability of building surrogates (e.g. recurrent neural networks) as an alternative to computationally expensive DEM simulations, effectively reducing the cost by several orders of magnitude.

Acknowledgements

Author contributions

All authors have contributed substantially to the development of GrainLearning. H. Cheng was responsible for the main idea and is the main contributor. R. Lubbe and H. Cheng designed the code structure, including the inference and sampling modules and tutorials and examples to facilitate understanding. A. Jansen and L. Orozco contributed to the conceptualization, implementation, testing and documentation of the machine learning module, as well as the improvement of best software practices.

References

Alvarez, J. E., Snijder, H., Vaneker, T., Cheng, H., Thornton, A. R., Luding, S., & Weinhart, T. (2022). Visco-elastic sintering kinetics in virgin and aged polymer powders. *Powder Technology*, *397*, 117000. https://doi.org/10.1016/j.powtec.2021.11.044

Benvenuti, L., Kloss, C., & Pirker, S. (2016). Identification of DEM simulation parameters by artificial neural networks and bulk experiments. *Powder Technology*, *291*, 456–465. https://doi.org/10.1016/j.powtec.2016.01.003

Cheng, H., Orozco, L., Lubbe, R., Jansen, A., Hartmann, P., & Thoeni, K. (2023). *Grain-Learning* (Version v2.0.2). Zenodo. https://doi.org/10.5281/zenodo.8352544

Cheng, H., Shuku, T., Thoeni, K., Tempone, P., Luding, S., & Magnanimo, V. (2019). An iterative bayesian filtering framework for fast and automated calibration of DEM models. *Computer Methods in Applied Mechanics and Engineering*, *350*, 268–294. https://doi.org/10.1016/j.cma.2019.01.027

Cheng, H., Shuku, T., Thoeni, K., & Yamamoto, H. (2018). Probabilistic calibration of discrete element simulations using the sequential quasi-monte carlo filter. *Granular Matter*, *20*. https://doi.org/10.1007/s10035-017-0781-y

Do, H. Q., Aragón, A. M., & Schott, D. L. (2018). A calibration framework for discrete element model parameters using genetic algorithms. *Advanced Powder Technology*, *29*, 1393–1403. https://doi.org/10.1016/J.APT.2018.03.001

Fransen, M. P., Langelaar, M., & Schott, D. L. (2021). Application of DEM-based metamodels in bulk handling equipment design: Methodology and DEM case study. *Powder Technology*, *393*, 205–218. https://doi.org/10.1016/J.POWTEC.2021.07.048

Hanley, K. J., O'Sullivan, C., Oliveira, J. C., Cronin, K., & Byrne, E. P. (2011). Application of taguchi methods to DEM calibration of bonded agglomerates. *Powder Technology*, *210*, 230–240. https://doi.org/10.1016/j.powtec.2011.03.023

Hartmann, P., Cheng, H., & Thoeni, K. (2022). Performance study of iterative bayesian filtering to develop an efficient calibration framework for DEM. *Computers and Geotechnics*, *141*. https://doi.org/10.1016/j.compgeo.2021.104491

Li, X., Kouretzis, G., & Thoeni, K. (2024). Discrete element modelling of uplift of rigid pipes deeply buried in dense sand. *Computers and Geotechnics*, *166*, 105957. https://doi.org/10.1016/j.compgeo.2023.105957

Nguyen, Q. H. (2022). *Machine learning in the calibration process of discrete particle model*. http://essay.utwente.nl/91991/

Thornton, A., Nguyen, Q., Polman, H., Bisschop, J., Weinhart-Mejia, R., Vesal, M., Weinhart, T., Post, M., & Ostanin, I. (2023, January). *Simulating industrial scenarios: With the open-source software MercuryDPM*. https://doi.org/10.23967/c.particles.2023.015