Investigating numerical parameter uncertainty in discrete particle simulations

Background: Discrete particle methods (DPM) are widely used in civil, mining and pharmaceutical industries to model the collective behavior of particulate processes (e.g., fragmentation of rock, concrete flow, tableting) by simulating various physics between particles. While extensive research has been conducted to develop DPM models and their couplings to other numerical methods in multi-physical phenomena, little attention is paid on algorithmic aspects, rooted in the stochastic nature of the method. Questions need to be addressed are, for example, what parameters are purely numerical and how much they influence the predicted macroscopic behavior.

Objectives: Granular materials can behave like a gas (e.g., sandstorm), solid (e.g., rock) and fluid (e.g., landslide) (see Fig. 1). When using DPM to simulate these processes, the relevant physical and numerical parameters are surely different. In this project, you will use Bayesian inference and machine learning to help researchers understand their DPM models better. To this end, you will be asked to

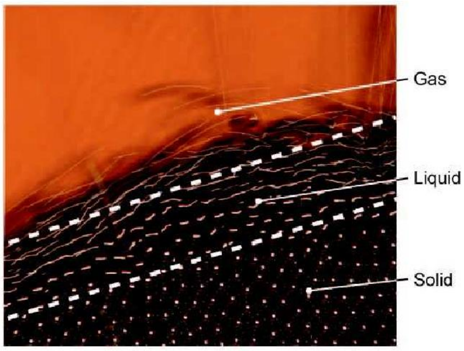

Figure 1 Granular materials in gas, fluid and solid states.

1. Identify parameters that are purely numerical in DPM simulations in gaseous, fluid and solid states,
2. Quantify the uncertainty of these numerical parameters conditioned on some reference data,
3. Propagate the uncertainty to macroscopic quantities of interest such as viscosity, elasticity, etc.

Method:

The open-source DPM code MercuryDPM [1] will be used to model granular materials at gaseous, fluid and solid states. After relevant numerical parameters are identified, such as the number of particles, you will use the Bayesian uncertainty quantification tool GrainLearning [2] to sample the parameter space. The method estimates the probability distribution with an adaptive resampling technique, thereby ensuring the efficiency of the uncertainty analysis.

Contributions:

The outcome of the assignment will be a deeper understanding of numerical parameters relevant to different physical states of granular materials. The quantification of their uncertainties is important to the reliability of DPM models and also to the reduction of computational cost. There is also a possibility to work with researchers in the group to further develop the Bayesian uncertainty quantification methods using state-of-the-art machine learning techniques.

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