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SCIENTIFIC MACHINE LEARNING FOR GRANULAR MATERIAL SIMULATIONS ACROSS SCALES AND REGIMES

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ABSTRACT

Granular material behaviour is fundamental to many engineering problems: dikes can fail because sand grains lose stability and form failure zones under rising water levels; silo blockages can happen due to the cohesion of the material stored in them; the quality of construction materials such as concrete depends on appropriate mixing of the ingredients. All these problems are related to understanding how grains move and interact with each other. Computational methods, such as discrete element methods, can be used to simulate millions of grains individually and investigate how they influence the processes at the macroscale. However, these simulations are expensive to run, hard to interpret, and therefore difficult to use for practitioners from industry.

Machine learning (ML) can help interpret granular processes, and make fast and accurate predictions, after being trained with data generated from physics-based simulations and laboratory experiments. These ML surrogates make digital twinning affordable for real-life applications, including uncertainty quantification and optimization of industrial and natural processes involving powders and grains. This is a new field of research that requires a collaboration between numerical modelers, data analysts, experimentalists, and practitioners from various engineering disciplines.

This session brings together numerical modelling and machine learning experts who have worked on the following aspects of computational granular mechanics:

(1) Use of machine learning to improve our understanding of constitutive laws for granular materials from discrete particle data and granular experiments;

(2) Emulating the temporal and spatial response of granular materials in the solid-like and fluid-like regimes using deep learning models and operators;

(3) Integration of physics-based and ML surrogate models to enable computationally expensive digital twinning tasks such as uncertainty quantification and optimization; and

(4) Essential steps to develop an open software-data infrastructure/workflow where data from different packages can be easily connected and repurposed.