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An integrated mechanistic-neural network modelling for granular systems

S.J. Antony *, C.H. Zhou [1], X. Wang

Institute of Particle Science and Engineering, School of Process, Environmental and Materials Engineering, University of Leeds, Leeds LS2 9JT, UK

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Abstract

A hybrid neural network model is designed to predict the micro-macroscopic characteristics of particulate systems subjected to shearing. The network is initially trained to understand the micro-mechanical characteristics of particulate assemblies, by feeding the results based on three-dimensional discrete element simulations. Given the physical properties of the individual particles and the packing condition of the particulate assemblies under specified loading conditions, the network thus understands the way contact forces are distributed, the orientation of contact (fabric) networks and the evolution of stress tensor during the mechanical loading. These relationships are regarded as soft sensors. Using the signals received from soft sensors, a mechanistic neural network model is constructed to establish the relationship between the micro-macroscopic characteristics of granular assemblies subjected to shearing. The macroscopic results obtained form this hybrid mechanistic neural network modelling for data that were not part of the training signals, is compared with simulations based on discrete element modelling alone and in general, the agreement is good. The hybrid network responds to their inputs at a high speed and can be regarded as a real-time system for understanding the complex behaviour of particulate systems under mechanical process conditions.

Keywords: Particulate materials; Granular materials; Neural network; Hybrid modelling

* Corresponding author. Tel.: +44 113 233 2409; fax: +44 413 502 3689.
E-mail address: s.j.antony@leeds.ac.uk (S.J. Antony).
[1] Present address: Beijing Creative Century Information Technology Co. Ltd., 6th Floor, Kunxun Building, 9 Zhichuan Road, Haidian District, 100083 Beijing, PR China.

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1. Introduction

Granular materials and granular flows are everywhere in nature, in various industrial processes, in everyday life. We find them in landslides and avalanches, erosion, raw minerals extraction and transport, cereal storage, powder mixing in chemistry or pharmaceutics, on our table as sugar, salt or pepper, just to cite a few examples. Granular materials are sometimes considered as a fourth state of matter, different from the classic solid, liquid and gas. They exhibit specific phenomena that call for better understanding. To this end, experimental studies have been and are being conducted, but numerical simulation is increasingly seen as a means to understand both the internal mechanics and macroscopic behaviour of granular materials under actual process conditions. The recent surge in the computer power has attracted several researchers to study the underlying mechanics and physics of granular materials using advanced computational modelling tools such as discrete element modelling (DEM), e.g., [1–5]. However, DEM analysis, even for a simple particulate assembly requires simulating several thousands of individual particles and their complex particle–particle contact interactions. The numerical algorithms for contact detection and contact laws governing the inter-particle force–displacement relations are generally complex, thus require a large amount of computational time to handle the simulations. At the moment, DEM simulations can handle granular assemblies with the number of particles ranging from a couple of thousands to a few million particles, depending on the nature of the inter-particle contact interaction laws employed; some simulations define the contact interaction of particles using simple spring-dashpot systems while others use algorithms based on theoretical contact mechanics. In the present work, we have employed an alternative strategy, using a mechanistic neural network modelling to predict the micro-macroscopic behaviour of dense granular systems, subjected to quasi-static shearing. The network is initially trained to understand the internal mechanics of particulate assemblies subjected to shearing, using DEM. Once trained, the neural network does not require any further input from DEM to predict the micro-macroscopic characteristics of particulate assemblies (under mechanical loading) outside the range of data used to train the model. The network derives the advantages of both a conventional neural network and discrete element modelling, thus could be used as an efficient, hybrid modelling tool to analyse the behaviour of granular materials without compromising on the accuracy of the predictions. In the present work, we restrict our predictions to certain micro-macroscopic characteristics of three-dimensional, mono-dispersed granular system subjected to quasi-static shearing. Using the mechanistic neural network model, we present results for the evolution of macroscopic shear strength ratio, contact normal force distribution $P(f)$ and the contact networks characteristics (fabric tensor) of three-dimensional granular assemblies during shearing. The results obtained using the mechanistic neural network have been verified with simulations based on DEM alone and in general, the agreement is good.

2. Micro-macroscopic characteristics

In granular media, the transmission of forces from one boundary to another can occur only via the inter-particle contacts. Hence the distribution of contacts will determine the distribution of forces within the system of particles. These forces will not be necessarily distributed