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Applied Mathematical Modelling 30 (2006) 116–128
APPLIED MATHEMATICAL MODELLING
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An integrated mechanistic-neural network modelling for granular systems

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Received 1 May 2003; received in revised form 1 February 2005; accepted 15 March 2005
Available online 4 May 2005

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

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0307-904X/$ - see front matter
doi:10.1016/j.apm.2005.03.010

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 uniformly, even for an isotopic and homogeneous assembly of particles subjected to homogeneous applied load. This important qualitative observation of stress distribution can be seen in photoelastic studies of two-dimensional disks reported by several investigators [6–9]. The inhomogeneous distribution of optical fringe patterns in these studies, even for a homogeneous applied load, reveals that the load is transmitted by relatively rigid, heavily stressed chains of particles which form a relatively sparse network of greater than average normal contact force. The groups of particles separating the strong force chains are only lightly loaded. Although a consensus on the nature of the distribution of contact forces in granular media and a 'perfect' physi- cal model to capture the force distribution is far from achieved, recent numerical simulations on a two-dimensional [10–13] and three-dimensional system of particles [13–17] under quasi-static shearing have revealed some exciting features. It has been shown that the normal force contribution is the major contribution to the total stress tensor and the spatial distribution of normal contact forces can be divided into two sub-networks, viz., (i) the contacts carrying less than the average force (forming 'weak force chains') and (ii) the contacts carrying greater than the average force (forming 'strong force chains'). The contacts that slide are predominantly in the weak force chains and they contribute only to the mean stress while their contribution to the deviator stress (shear strength) is negligible. The contribution of the strong force chains to the deviator stress is the dominant contribution. Hence, the weak force chains play a role similar to a fluid surrounding the solid backbone composed of the strong force chains [15,16]. The 'fluidity' of the particles increases with an increase in size ratio of the particles (size of the particle in relation to their surrounding particles) [17]. These findings clearly show that the macroscopic shear strength of granular materials is not an independent entity, rather it strongly depends on the interplay between different variables of the granular assembly such as packing condition, individual properties of the particles, nature of force distribution within the assemblies and the network of contacts that develop an anisotropic fabric structure during shearing. Hence, in the present work, we trained the neural network to capture the above mechanical characteristics of granular materials using DEM, originally developed by Cundall and Strack [18]. However, the interaction between the neighbouring particles in the DEM modelling employed here is based on theoretical contact mechanics provided by Thornton and Yin [19,15].

3. Mechanistic neural networks

3.1. *Soft-sensor*

Soft-sensor is a technique for estimating variables usually difficult to measure on-line. In general, soft-sensor technique is to construct some mathematical model (i.e., soft-sensor model) for estimating the primary variable, on the basis of a group of secondary variables selected according to some optimal criterions, which are closely related to the primary variable [20]. There are two basic approaches for soft-sensor modelling, i.e., mathematical modelling and identification modelling. To build a mathematical model of a system, one can use the physical laws that govern the system's behaviour. Alternatively, one can observe the signals produced by the system to known inputs and find a model that best reproduces the observed data [21].

3.2. Back propagation neural networks

Back propagation neural networks are analogous to the computational models of the brain. The modelling based on neural network is one of the identification techniques to determine a model of a system according to the observed inputs and outputs signals to the system [21]. Identification is necessary when there is not sufficient information about the system for it to be accurately modelled by mathematical modelling approaches.

A neural network for identification generally consists of an input layer which receives input signals, an output layer which generates output signals, and some hidden layers which include a number of interconnected neurons, i.e., processing elements (Fig. 1). If the connections are unidirectional, the network is called a feed-forward network. Other types of the neural network are feedback network, self-organizing network and etc. Each neurons in the hidden layers or the output layer sums up its input signals after weighing them with the strengths of the respective connections from the input layer or the former hidden layer, and compute its output as a transfer function (usually nonlinear function) of the sum plus a bias.

It is believed that with sufficient hidden neurons and using some special training or learning algorithm based on the known input and output data set for adjusting or training the strengths of the connections and the biases to the neurons until a stopping criterion is met, a neural network can approximate arbitrary mapping or function [21,22].

3.3. Mechanistic-neural network modelling

Fig. 2 shows the block diagram of a mechanistic neural network modelling approach. The network is initially trained to capture the micro-mechanics of particulate assemblies, by feeding the soft signals obtained using mechanistic three-dimensional DEM 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 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.

In the present study, we consider the case of granular system consisting of mono-sized spherical particles. To obtain the soft-sensor signals, the DEM simulations were carried out in a

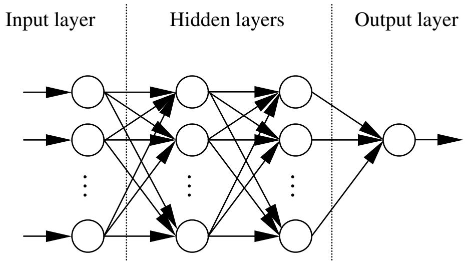

Fig. 1. The structure of neural network model.

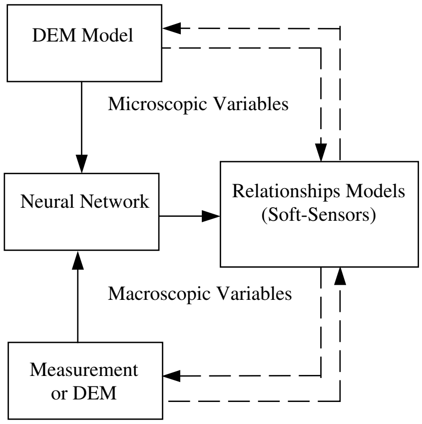

Fig. 2. The block diagram of the mechanistic (hybrid) neural network modelling.

three-dimensional cuboidal periodic cell. The periodic cell consisted 5000 randomly generated spherical particles with diameter 0.1 mm. All the particles were given the following properties: Young's modulus, $E = 70$ GPa, Poisson's ratio $v = 0.3$, coefficient of inter-particle friction $\mu = 0.3$ and interface energy $\Gamma = 0.6$ J/m^2. After the particles were initially generated, the system was isotropically compressed until a mean stress $p = 20$ kPa was obtained. At the end of the isotropic compression, the microstructure of the sample was isotropic. At this stage, the solid fraction and mechanical coordination number (average number of load bearing contacts) of the sample considered in this study were 0.61 and 4.8, respectively. For shearing, a strain rate of 10^{-5} s^{-1} was employed in the simulations. The samples were subjected to the axi-symmetric compression test ($\sigma_1 > \sigma_2 = \sigma_3$) [15]. During shearing, the mean stress $p = (\sigma_1 + \sigma_2 + \sigma_3)/3$ was maintained constant at 20 kPa using a servo-control algorithm. The detailed description and numerical methodology of the DEM simulations carried out here can be found elsewhere [15–17]. For the

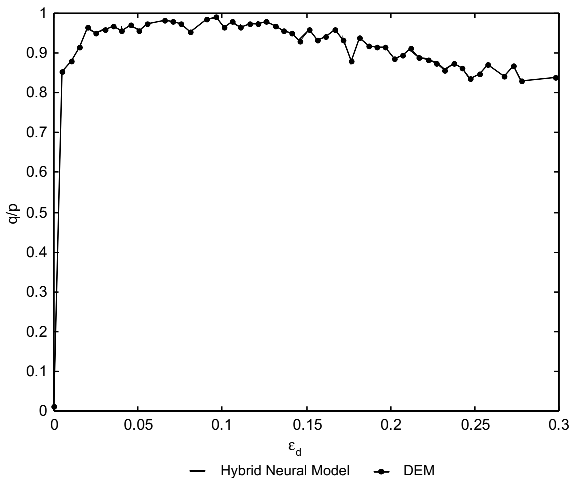

Fig. 3. Results for mapping $q/p = F_1(\varepsilon_d, P(f))$.

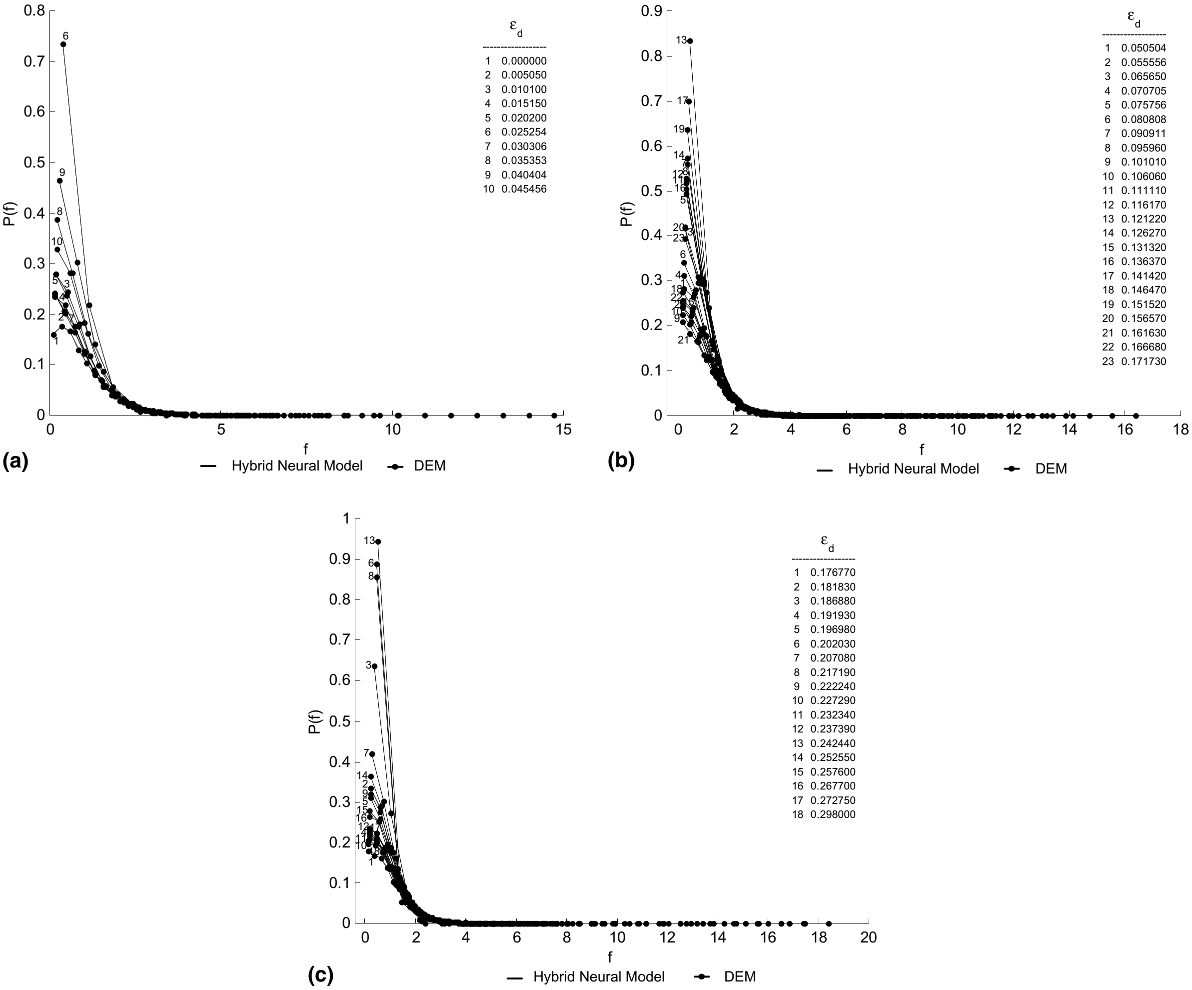

Fig. 4. Results for mapping: (a) $P(f) = F_2(\varepsilon_d, q/p, f)$ (Table 2, sub-model 1); (b) $P(f) = F_2(\varepsilon_d, q/p)$ (Table 2, sub-model 2); (c) $P(f) = F_2(\varepsilon_d, q/p)$ (Table 2, sub-model 3).

granular system under study, the DEM simulations provided (i) the normalised shear stress ratio q/p ($q = \sigma_1 - \sigma_3$), (ii) the evolution of force distribution in terms of the probability distribution of normal contact force $P(f)$ and (iii) evolution of fabric anisotropy tensor ϕ_d during shearing. These soft-sensor signals were used to train the neural network model. The specific objectives set for the mechanistic neural network are as follows:

(1) To predict the evolution of macroscopic shear stress ratio q/p (defined as the ratio of the deviator stress to the mean stress) as a function of the probability distribution of contact normal force $P(f)$ and deviator strain ε_d ($=\varepsilon_1 - \varepsilon_3$). It is known that the stress ratio q/p (Fig. 3) strongly depends on the probability distribution function of contact normal forces $P(f)$, where $f = N/\langle N \rangle$, N is the contact normal force and $\langle N \rangle$ represents the average contact

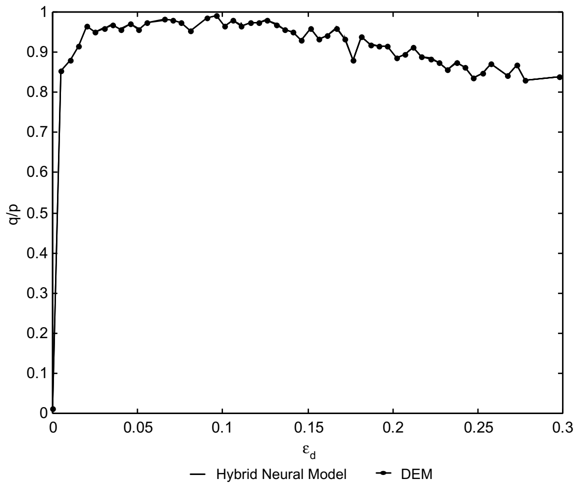

Fig. 5. Results for mapping $q/p = F_3(\varepsilon_d, \phi_d, P(f))$.

normal force in the system. A detailed physical analysis on the influence of the properties of individual particles on the distribution of $P(f)$ for granular packing has been reported elsewhere [16].

(2) To predict the contact normal force distribution $P(f)$ during shearing as a function of ε_d and q/p.
(3) To predict the evolution of q/p as a function of the deviator strain ε_d, the deviator fabric ϕ_d and contact normal force distribution $P(f)$. Recent studies show that the micro-macroscopic relations for granular media strongly depends on the way network of particle contacts develop during mechanical loading. The contact network can be defined by the distribution of contact orientations using the 'fabric tensor' ϕ_{ij}, as suggested by Satake [23]:

$$\phi_{ij} = \langle n_i \; n_j \rangle = \frac{1}{M} \sum_{1}^{M} n_i \; n_j,$$

where M is the number of contacts in the representative volume element and n_i define the components of the unit normal vector at a contact between two particles. Recent studies have proved that the macroscopic shear strength of granular assemblies strongly depend on the ability of the material to form a strongly anisotropic fabric network of contacts [13–16]. Hence, it would be appropriate to design the neural network to predict the evolution of q/p as a function of the deviator strain ε_d, the deviator fabric ϕ_d and contact normal force distribution $P(f)$. The deviator component of the fabric tensor is given by ϕ_d $(=\phi_1 - \phi_3)$.
(4) To predict $P(f)$ as a function of ε_d and ϕ_d.
(5) To predict $P(f)$ as a function of ε_d, ϕ_d and q/p.
(6) To predict ϕ_d as a function of ε_d and $P(f)$.

Four-layer (including 2 hidden layers) feed-forward neural networks, as shown in Fig. 1, are used to approximate the six mappings discussed above. The transfer functions for neurons in

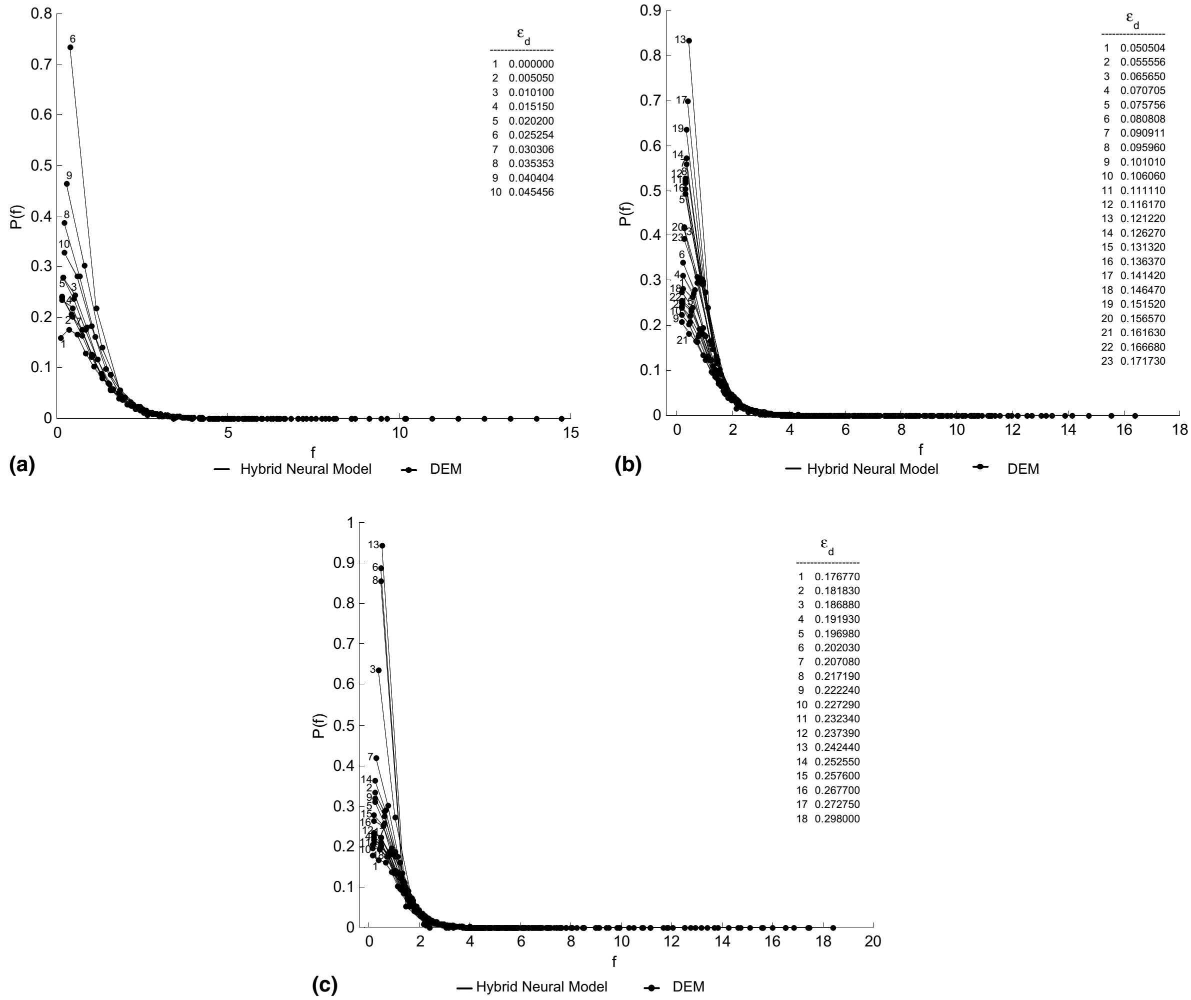

Fig. 6. Results for mapping: (a) $P(f) = F_4(\varepsilon_d, \phi_d)$ (Table 4, sub-model 1); (b) $P(f) = F_4(\varepsilon_d, \phi_d)$ (Table 4, sub-model 2); (c) $P(f) = F_4(\varepsilon_d, \phi_d)$ (Table 4, sub-model 3).

the two hidden layers and the output layer are hyperbolic tangent, hyperbolic tangent and sigmoid respectively, defined as

$$f(x) = \frac{1 - e^{-2x}}{1 + e^{-2x}}, \tag{1}$$

$$f(x) = \frac{1}{1 + e^{-x}}. \tag{2}$$

The training algorithm is the back-propagation (BP) algorithm with a momentum coefficient and an adaptive learning rate [22]. The stopping criterion for training is that the differences between the actual and target outputs of the network model achieve a minimum (acceptable value).

Considering the complexity of these mappings, a relatively large numbers of the data (obtained from DEM simulations) are employed in the network training, including about 840 data of ε_d and the same size of data for the corresponding f, $P(f)$, q/p and ϕ_d. In this work, no noise was added to the data produced by the DEM model. The impact of noise on neural network training has been studied by many researchers, for instance the work of An [24] and more recently of Seghouane et al. [25], who found that adding a certain degree of noise to the inputs can improve the generalization capability of the neural network performance. However, if the noise to signal ratio is too high, it may adversely affect the training. In the past, research has been conducted to use experimental design to determine the minimum number of training data sets, e.g., the work of Lanouette et al. [26]. In the present study, the number of datasets used for training each network is sufficiently large (about 840) and the perturbation in the input has been made through careful de-

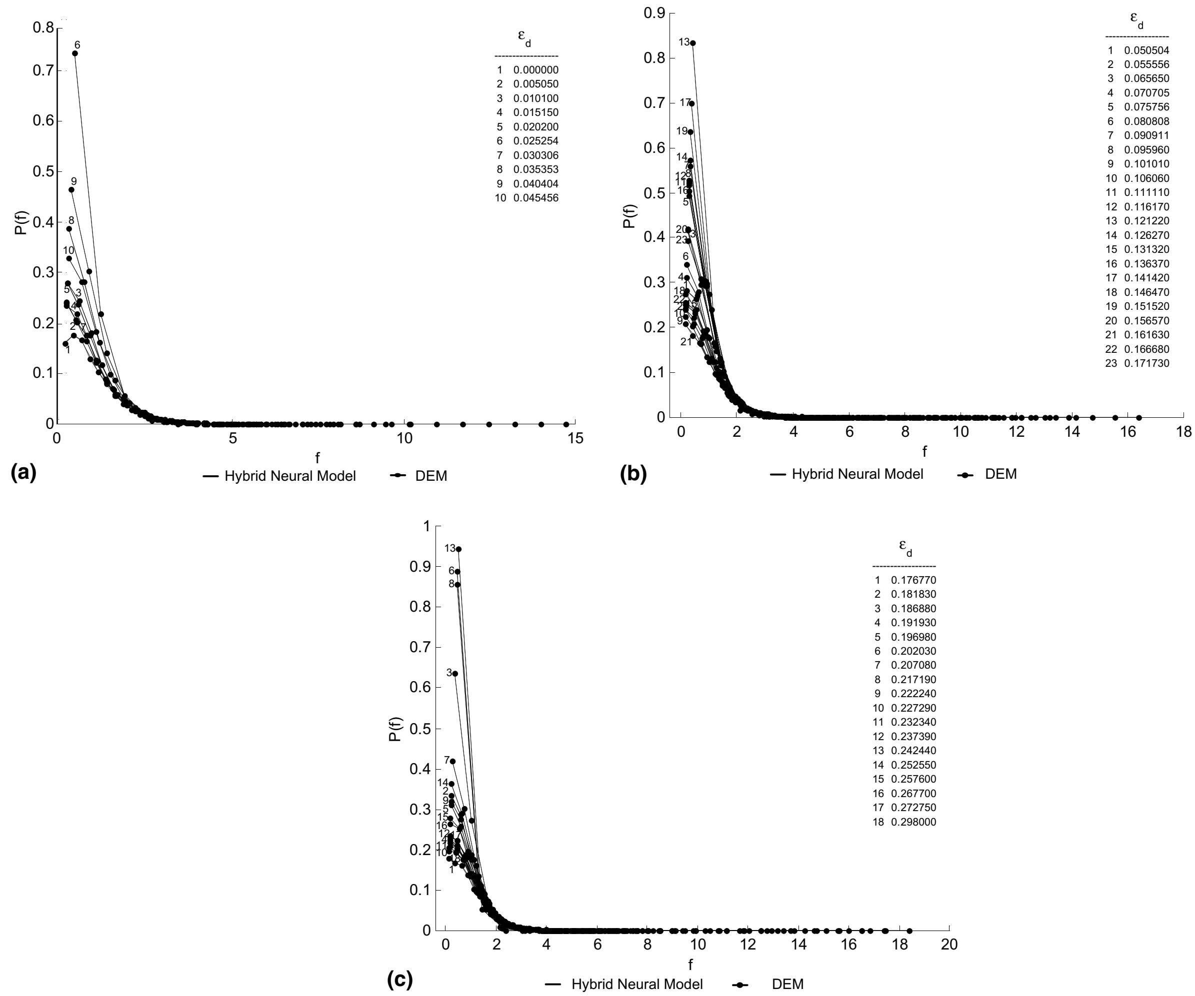

Fig. 7. Results for mapping: (a) $P(f) = F_5(\varepsilon_d,\phi_d,q/p)$ (Table 5, sub-model 1); (b) $P(f) = F_5(\varepsilon_d,\phi_d,q/p)$ (Table 5, sub-model 2); (c) $P(f) = F_5(\varepsilon_d,\phi_d,q/p)$ (Table 5, sub-model 3).

sign. For convenience, the training of the neural network model for each mapping is divided into three sub-models according to the effective range of ε_d as presented below. However, if the size of the network increases (e.g., number of hidden nodes) more data could be required. If the variables become more complicated such as size distribution, there are also techniques available in the literature to handle this, for example, to apply data dimension reduction using principal component analysis and independent component analysis before the neural network is trained [27–30].

4. Results and discussion

Figs. 3–8 show the results obtained by the mechanistic neural network, for mapping the functions F_1–F_6 (Tables 1–6). For comparison purposes, in these figures, we have incorporated the corresponding results obtained by three-dimensional DEM modelling alone. It is worth mentioning that the DEM results used for comparison purposes were not part of the training signals that were used to train the neural network model. It can be observed that the predicted results based on the mechanistic neural network compare very well with the results based on (independent) DEM simulations.

The comparison between the network model results, as shown in Figs. 3 and 5 and their corresponding mapping schemes presented in Tables 1 and 3 indicate that the introduction of the fabric tensor ϕ_d into the neural modelling for q/p is beneficial as the network structure tends to a smaller size. This confirms the ability of the mechanistic neural network to provide accurate predictions for the mechanical behaviour of granular materials as, the realistic mechanistic nature (for example the contact orientations could be fed in terms of ϕ_d, which is more sensitive to strain level ε_d) could be captured in the hybrid mechanistic neural network system. The hybrid neural network modelling allows fast prediction of the bulk behaviour of particulate system, and in the present case, by a factor of about 5–10 when compared with DEM simulations.

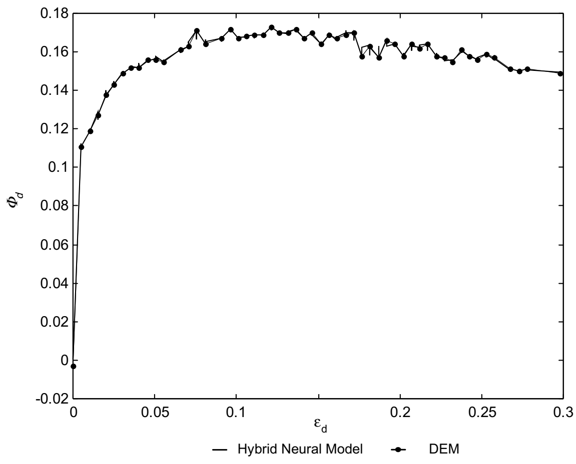

Fig. 8. Results for mapping $\phi_d = F_6(\varepsilon_d, P(f))$.

Table 1
Model for mapping $q/p = F_1(\varepsilon_d, P(f))$

Sub-model no.	Range of ε_d	Number of hidden neurons		Training epochs[a]
		First layer	Second layer	
1	[0, 0.10)	60	60	120,000
2	[0.10, 0.20)	55	55	150,000
3	[0.20, 0.30]	50	50	150,000

[a] A training epoch is said to having been completed when the whole input and output data set for the training have been presented once to the network.

Table 2
Model for mapping $P(f) = F_2(\varepsilon_d, q/p)$

Sub-model no.	Range of ε_d	Number of hidden neurons		Training epochs
		First layer	Second layer	
1	[0, 0.050)	25	25	90,000
2	[0.050, 0.176)	40	40	120,000
3	[0.176, 0.298]	65	65	90,000

Table 3
Model for mapping $q/p = F_3(\varepsilon_d, \phi_d, P(f))$

Sub-model no.	Range of ε_d	Number of hidden neurons		Training epochs
		First layer	Second layer	
1	[0, 0.10)	50	50	150,000
2	[0.10, 0.20)	50	50	90,000
3	[0.20, 0.30]	50	50	60,000

Table 4
Model for mapping $P(f) = F_4(\varepsilon_d, \phi_d)$

Sub-model no.	Range of ε_d	Number of hidden neurons		Training epochs
		First layer	Second layer	
1	[0, 0.050)	25	25	60,000
2	[0.050, 0.176)	40	40	150,000
3	[0.176, 0.298]	55	55	60,000

Table 5
Model for mapping $P(f) = F_5(\varepsilon_d, \phi_d, q/p)$

Sub-model no.	Range of ε_d	Number of hidden neurons		Training epochs
		First layer	Second layer	
1	[0, 0.050)	25	25	150,000
2	[0.050, 0.176)	40	40	120,000
3	[0.176, 0.298]	55	55	120,000

Table 6
Model for mapping $\phi_d = F_6(\varepsilon_d, P(f))$

Sub-model no.	Range of ε_d	Number of hidden neurons		Training epochs
		First layer	Second layer	
1	[0, 0.10)	50	50	120,000
2	[0.10, 0.20)	60	60	120,000
3	[0.20, 0.30]	65	65	60,000

5. Conclusions

A hybrid mechanistic neural network method has been used to establish the relationships between the key variables (micro-macroscopic characteristics) involved in the mechanical behaviour of a slowly sheared (mono-dispersed) granular system. The possible correlation between the micro-macroscopic features and strength parameters in the granular material are investigated. Conceptually, the mechanistic neural network modelling is more reliable and efficient than the convention network models. The mechanistic neural network model employed here for granular systems is generic in nature, and can complement other analytical or modelling approaches, for approximating the desired mappings. However, just like any other identification modelling techniques, for more realistic granular systems, it may require rather long identification experiments. This may involve obtaining soft signals in terms of realistic particle shapes, size distributions, surface roughness, inter-particle forces etc. However, the generic nature of the hybrid network presented here provides the basis for further increasing the efficiency of soft sensors, once more realistic soft sensors are available. Furthermore, the possibility of obtaining soft sensors using rigorous theoretical analysis or experimental methods for granular media needs to be explored in future.

Acknowledgements

The research was supported by BNFL—Leeds Research Alliance in Particle Science and Engineering, UK. S.J.A and X.W. gratefully acknowledge Dr. D. Rhodes, Dr. D. Goddard and Mr. A. Milliken for their support to this study.

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