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Physics-based vs data-driven constitutive modeling of granular media down an inclined plane

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Abstract. We present a numerical study of 3D granular flow down an inclined plane, using Discrete Element Method (DEM). The data of individual grains are used to compute the macroscopic density, velocity, and stress fields through a coarse-graining technique (CG). We begin by analyzing granular flows with the analytical rheology model $\mu(I)$, which has proven to be effective in describing dense, quasistatic, and inertial flow regimes. We also present a data-driven approach that utilizes machine learning methods to build constitutive models. This approach does not rely on predetermined balance equations; instead, the resulting constitutive model is trained directly on DEM-CG data to learn patterns and relationships. In general, our results suggest the potential of ML approaches in predicting stress distributions in dense granular flows. As expected, random forest and neural network analysis are more effective compared to simple linear regression. In particular, neural networks appear as a promising avenue for advancing predictive accuracy in future studies.

1 Introduction

Numerical modeling plays a crucial role in understanding the mechanical behavior of granular media. The Discrete Element Method (DEM) is a numerical technique specifically designed to simulate the motion of individual particles within a granular system [1]. Unlike continuous potential-based methods, DEM explicitly calculates contact forces between particles, making it well suited to capture both translational and rotational dynamics, even for particles with complex shapes [1–3]. In industrial applications, however, continuous modeling approaches are often preferred because of the computational challenge of DEM of tracking the motion of an enormous number of particles. Over time, researchers have developed accurate continuous models that solve the momentum balance equations for granular flows [4, 5]. These numerical schemes include constitutive models that describe how stress, shear rate, and other physical properties evolve in granular materials. In fact, granular media exhibit constitutive responses that significantly deviate from the behavior of conventional solids or fluids. For example, the Mohr-Coulomb constitutive model is based on classical soil mechanics and assumes that shear stress is proportional to normal stress through a friction coefficient. It typically works well for quasistatic granular flows, but struggles with highly dynamic or dense flows. In faster flows, such as landslides and hopper discharges, there is a model that relates the macroscopic friction coefficient of the material to the inertial flow movement. It introduces the inertial number $I = \frac{d\dot{\gamma}}{\sqrt{\sigma/\rho}}$, in terms of the local shear rate

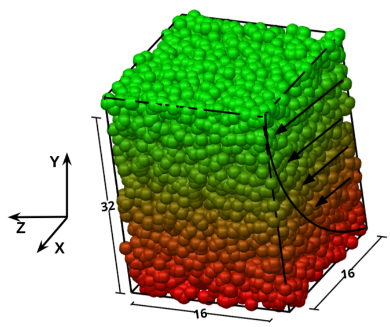

Figure 1. Sketch of the numerical setup. PBC are imposed on the x- and z- directions, and the particles move in the x-direction.

$\dot{\gamma}$ and stress (σ, τ), and prescribes a constitutive relation $\tau = \mu(I)\sigma$ [6, 7]. Furthermore, the kinetic theory of granular gases describes the behavior of rapid granular flows [8, 9]. This framework assumes that grains undergo inelastic collisions, while their velocity distribution follows statistical mechanics laws [8, 9].

Artificial intelligence (AI) models are based solely on existing data to make predictions and generalize responses [10]. In science, they are currently very popular and are used in a number of applications, such as analyzing massive DNA datasets to identify disease-related genes [11], and manipulating satellite data for climate modeling [12]. AI method typically requires large datasets, while laboratory tests are costly and time-consuming. In contrast, DEM offers an efficient and flexible means of generating modeling data. Using DEM as a virtual model is a viable approach to support experiment-based constitu-

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Table 1. Features or predictors used in each model. In all cases, predicted variables are $Y = [\sigma_{xx}, \sigma_{xy}, \sigma_{yy}, \sigma_{zz}]$.

Model A	$X = [$	α	$\phi(\vec{r})$	$V_x(\vec{r})$	$V_y(\vec{r})$	$V_z(\vec{r})$	$\dot{\gamma}_x(\vec{r})$	$\dot{\gamma}_y(\vec{r})$	$\dot{\gamma}_z(\vec{r})]$
Model B	$X = [$	α	$\phi(\vec{r})$	$V_x(\vec{r})$			$\dot{\gamma}_x(\vec{r})]$		
Model C	$X = [$		$\phi(\vec{r})$	$V_x(\vec{r})$			$\dot{\gamma}_x(\vec{r})]$		

tive modeling. Recently, several groups have developed micromechanics-informed ML models that reproduce the mechanical response of a granular system under compression [13, 14]. In the present work, we hypothesize that ML could also be used to build constitutive models of rapid granular flows. We employ data-driven models [15], which do not rely on predetermined balance equations and micro-mechanical details. Instead, the resulting constitutive equations are trained directly on DEM-CG data. We provide a critical comparison between physics-based and data-driven approaches.

2 DEM and AI Data Analysis

We perform DEM simulations of a chute flow of spheres with diameter $d = 1/16$ m. The simulations mimic particles made of glass, $\rho = 2600\,kg/m^3$, friction coefficient $\mu_p = 0.5$, and restitution coefficient $e_n = 0.88$. We used a simple linear spring-dashpot model to compute the interaction force between two contacting particles. The chute is inclined at an angle θ such that gravity acts in the direction $[\sin(\theta), -\cos(\theta), 0]$. In all the cases reported here, the dimensions of the system were $L_x = L_z = 16d$ and $L_y = 32d$, and periodic boundary conditions were imposed in the $x-$ and $z-$ directions. The bottom surface consists of a layer of fixed particles (see [16] for more details). To extract continuum data from DEM, we use the coarse-graining (CG) method for granular flows [17, 18].

The chute flows are characterized by two critical angles; in the regime $\alpha < \alpha_{c1}$ friction dominates gravity and the material is at rest. In addition, there is a critical value and for $\alpha > \alpha_{c2}$ the material accelerates uncontrolled, since in this regime gravity dominates over the frictional forces. Controlled steady-flow situations develop in the regime $\alpha_{c1} < \alpha < \alpha_{c2}$. As a first step, we measured the angle of repose of the system, resulting in $\alpha_{c1} = 21.5°$. As a second step, we examine fully developed steady-state situations with $\alpha > \alpha_{c1}$ and duration of 120 seconds. Note that the steady-state momentum balance requires $\frac{\sigma_{yx}}{\sigma_{xx}} = \tan(\alpha)$, which was carefully checked in all cases. The value of $\mu = \tan(\alpha)$ is the macroscopic friction.

Using the CG methodology, we calculate all relevant fields, that is, the packing fraction $\phi(\vec{r}, t)$, the velocity field $\vec{V}(\vec{r}, t)$, and the stress fields $\sigma(\vec{r}, t)$. We find that the variations of the fields in the x and z directions are diminished. Thus, mean field profiles ($\bar{\phi}(y)$, $\bar{V}_x(y)$, and $\bar{\sigma}(y)$) were obtained by sampling the fields every $\Delta t = 4\sqrt{2d/g}$. The values of $\bar{V}(y)$, are used to calculate the macroscopic shear rate by central finite differencing. The data is then reasoned in terms of the $\mu(I)$-rheology framework.

In addition, we implemented data-driven models to predict the mechanical behavior of granular materials under fluid-like conditions. The goal was to relate the stress components to macroscopic quantities such as the packing fraction, velocity, and shear rate. Three supervised learning algorithms were evaluated: linear regression, Random Forest, and a multilayer perceptron (MLP). The linear model served as a baseline, while the Random Forest captured nonlinear dependencies. The MLP, consisting of three hidden layers (128, 64, 32 neurons) with ReLU activations, was trained using the Adam optimizer and mean squared error loss. These models aimed to predict the main components of the stress tensor, $[\sigma_{xx}, \sigma_{xy}, \sigma_{yy}, \sigma_{zz}]$, based on various input feature sets, as detailed in Table 1. The datasets were filtered to retain only regions with $\partial_z v_x < 0$, representative of active shearing. From these, either 10% or 25% of the entries were randomly sampled, depending on the case. A standard 80/20 train-test split was used, with a 5-fold cross-validation applied in selected runs to assess generalization. The training set consisted of data from the first half of the simulation, while the second half was reserved for testing. The input features included geometric descriptors, local velocities, shear rates, and stress-related quantities. Reduced input sets were also tested, showing that richer descriptors generally improved performance. The precision and power of the model were evaluated using the Root Mean Squared Error RMSE, and the adjusted coefficient of determination R^2.

3 Results and Discussion

We compute all relevant macroscopic fields, which show uniform behavior in the x and z directions within our numerical uncertainties. Figure 2 (see panel I) displays the mean macroscopic packing fraction $\bar{\phi}(y)$, obtained after averaging in the x and z directions. The graph includes numerical data corresponding to several inclinations, namely, $\alpha = [23° - 25°]$. As expected for the chute-flow configuration, the packing fraction of the particle flow is practically constant in the bulk region. Moreover, we also reproduced that the velocity profile $V_x(y)$ agrees with a Bagnold-type velocity profile (data not shown), and the maximum velocity increases with increasing chute inclination. As expected, it also induces the system's dilatancy. Furthermore, we find that the mean velocities in the y and z directions practically diminish as a result of the absence of forces in those directions. Next, the values of $V_x(y)$, are used to calculate the macroscopic shear rate $\dot{\gamma} = dV_x(y)/dy$ by central finite differencing. We calculate the $I(y) = \dot{\gamma}(y)d/\sqrt{\sigma_{yy}(y)/\rho_p}$ profiles (see Figure 2 (Panel II)). The values of $I(y)$ correspond to average over the x and z directions. Note that the $I(y)$ profiles are practically constant in the bulk region, with larger variations only in the bottom and surface layers. It justifies the depth averaging and the use of a $\mu(I)$-rheology scheme, which postulates that the macroscopic friction follows,

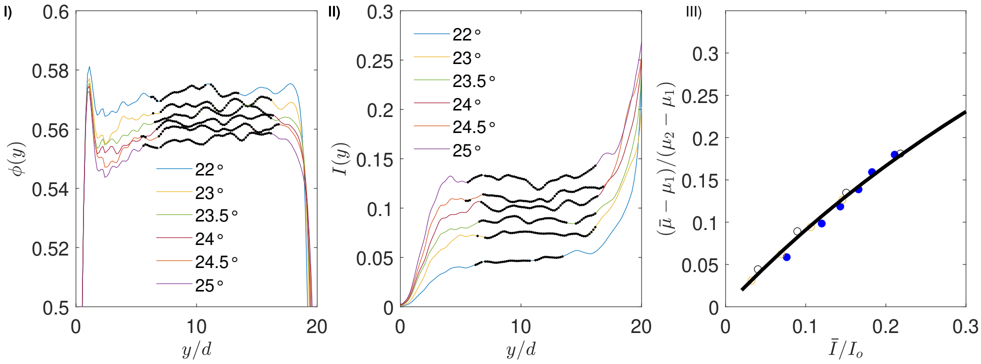

Figure 2. Vertical profiles of CG fields, panel I illustrates the packing fraction $\bar{\phi}(y)$, in panel II the inertial number $\bar{I}(y)$, varying the inclination. Panel III shows the data collapse obtained when plotting the relative friction versus the depth-averaged inertial number $\bar{I}$. The continuous lines represent the $\mu(I)$-rheology equation [6, 7]. Results for glass (filled circles) and steel (empty circles) particles with different friction are also shown.

$\mu(I) = \mu_1 + (\mu_2 - \mu_1)\frac{I}{I+I_o}$, where $\mu_1 = \tan(\alpha_{c1})$ and $\mu_2 = \tan\alpha_{c2}$. Figure 2 (Panel III) shows the depth-averaged macroscopic friction $\bar{\mu}$ against the depth-averaged inertial number $\bar{I}$, obtained for different inclinations. For convenience, the μ data have been scaled to compare with the physics-based theoretical expression. Remarkably, the behavior of the internal friction μ agrees very well with the theoretical prediction, estimating $I_o = 0.62$. For generalization, the figure also includes data corresponding to particles with higher density ($\rho = 7250\ kg/m^3$; $\mu_p = 0.5$) and friction ($\rho = 2600\ kg/m^3$; $\mu_p = 0.7$). Our results corroborate and highlight that the $\mu(I)$-rheology framework is an appropriate continuum theory to describe dense granular flows [6].

We also examine data-driven constitutive models that are trained directly on DEM-CG data. A shallow inspection of the data in Figs. 3 and 4 indicates that the three ML procedures produce similar results when predicting the target stress tensor components. The values of R^2 are in the range $[0.73 - 0.89]$, while the $RMSE$ in $[0.22 - 0.35]$, in terms of maximum values. These performances would be acceptable for engineering applications, but there is room for further improvement. A closer inspection indicates that Neural Networks outperform Linear Regression but underperform comparably to Random Forest. As expected, Linear Regression performs the worst in all scenarios. In principle, it is expected, due to its inability to capture complex non-linear relationships. In addition, the results indicate that the Random Forest is the best model for explaining variance (highest R^2), while Neural Networks achieve the lowest RMSE in most cases, suggesting that they provide more precise predictions.

Next, we focus on the impact of the number of features on the models' predictive capabilities. In general, the three ML procedures produce results with similar trends when varying the number of features. In all cases, including more predictor variables increases the model's predictive power; *i.e.*, **Model A** shows better results. In the chute-flow geometry, the features $V_y(\vec{r})$, $V_z(\vec{r})$, $\dot{\gamma}_y(\vec{r})$, and $\dot{\gamma}_z(\vec{r})$ are very small compared to the rest of the components. However, **Model B** performs slightly worse than **Model A**. However, excluding the angle of inclination led to a decrease in predictive performance, highlighting its critical role in modeling granular flow dynamics. Despite the simplicity of the ML models used—trained with minimal hyperparameter tuning our results show that they are capable of capturing meaningful patterns from raw simulation data, without requiring prior assumptions about the underlying physics. This highlights the versatility of data-driven approaches and their potential for constitutive modeling of granular flows.

Summarizing: We numerically analyze a rough spheres chute flow, computing the packing fraction, velocities, and stress profiles, and deducing the inertial number profiles. By performing a depth average of these fields, we successfully reproduce the $\mu(I)$−rheology relationship between macroscopic friction and the inertial number. Our findings corroborated its applicability to dense granular flows across different particle densities and friction coefficients. Complementarily, we investigate data-driven constitutive models trained on DEM-CG data, finding that all three machine learning (ML) approaches produce comparable results in predicting stress tensor components. Finally, we explore the effect of feature selection on predictive performance. In all cases, increasing the number of predictor variables improved model's accuracy. Surprisingly, although the velocities and share rates in a direction perpendicular to the flow should have minimal influence due to their small magnitudes, models incorporating them consistently performed better. Finally, excluding the inclination angle from the analysis negatively impacts the predictive performance of the ML models. Overall, our results suggest the potential of ML approaches in predicting stress distributions in dense granular flows. As expected, Random Forest and Neural Networks analysis were more effective, compared to simple linear regression. Nevertheless, further improvements are expected with more systematic experimentation, such as testing alternative activation functions, exploring alternative neural network architectures, or tuning parameters like the number of estimators and tree depth in Random Forests. In particular,

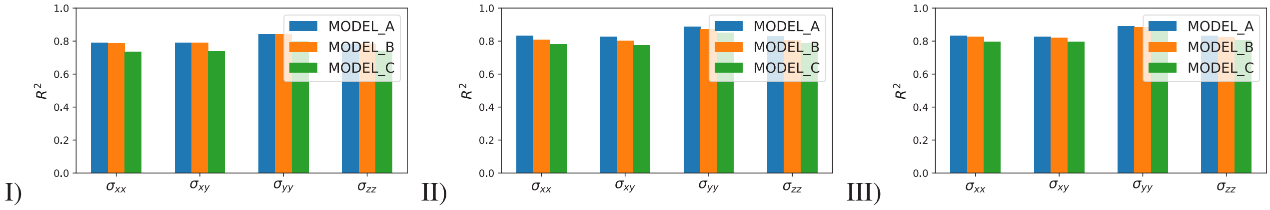

Figure 3. Values of the adjusted coefficient of determination, R^2, obtained after training each of the models (represented by different colors). Each group of three bars represents the value obtained for predicting each component of the mean contact stress tensor. Each panel includes: Panel I shows the results of the LR; Panel II the results of the RF; Panel III the results of the NNs.

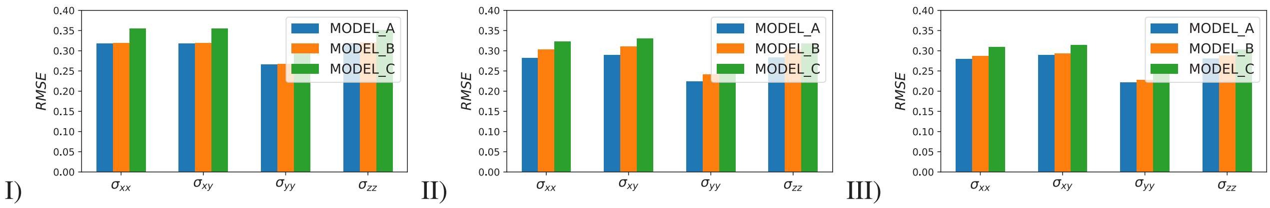

Figure 4. Values of the RMSE (Root Mean Squared Error), obtained after training each of the models (represented by different colors). Each group of three bars represents the value obtained for predicting each component of the mean contact stress tensor. Each panel includes: Panel I shows the results of the LRs; Panel II the results of the RFs; Panel III the results of the NNs.

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