Developing a physics-informed machine learning model to predict granular flow in a rotating drum

Yaoyu Li[1,*] and Runyu Yang[1]

[1] School of Materials Science and Engineering, University of New South Wales, Sydney, 2052
Corresponding author's E-mail: yaoyu.li@unsw.edu.au

Abstract

Predictions of granular flows in the tumbling mill are one of the main challenges in the grinding process. Discrete Element Method (DEM) has been widely used for better understanding mechanisms of granular materials. However, this method cannot be directly applied in the real industry due to unaffordable computational cost associated with detecting and computing contacts. In the work, we propose a physics-informed machine learning model based on continuous convolution neural network (CCNN) to replace the direct calculation of particle–particle and particle-boundary collisions. The DEM simulation was used to generate the training and testing dataset at different rotation speeds. The data was used to train the model and test the prediction results. A loss function based on distance was instructed to guide model learning. The modelling of a lab scale ball mill demonstrated the accuracy and efficiency of the machine learning in comparison with DEM in the simulation of granular flows.

Keywords: DEM simulation, Machine learning, Granular flow, Continuous convolution neural network, ball milling

1. INTRODUCTION

Granular materials, range in size from nanometers to centimeters, are widely used in in many industries such as milling, pharmaceuticals, and chemicals (Levy and Kalman, 2001). Understanding granular flow behavior is critical for process control and optimizations. However, their collective movements are very complex and difficult to predict without considering contact mechanisms.

Discrete element method (DEM) is a numerical simulation method, has been widely applied in studying granular flow (Zhu et al., 2008). It can predict the collective dynamics of the granular flow based on simulation of movements of each particle by well-defined contact mechanisms, following Newton's second law. However, its computation cost is unaffordable for full-scale system and long-time scales even using existing acceleration methods like GPU parallel computing and coarse-grained method, since particle contacts are explicitly resolved with small timesteps.

Machine learning (ML) could be a complementary technology for numerical simulations of large systems. The ML technology, based on large dataset, is capable of strong non-linear approximations and rapid predictions. Recently, it has been increasingly applied in the physics mechanism areas, such as molecular dynamics, fluid dynamics, and granular materials (Zhu et al., 2022). There are three main applications areas where ML can contribute: First, the ML-based data-driven model was used to direct rapid predictions of collective dynamics based on process measured data. The advantage of this type of model is rapid predictions, easily trained and applications. However, it may sacrifice prediction precisions and the model is often back-box with less interpretability. and Example of this includes but not limited to particle size, ball load predictions in the ball milling process (Li et al. 2022), flow regime detections in multi-phase flows (Liu and Bai, 2019). Second, the ML technology will improve/accelerate the numerical simulation by replacing sub-models or constants/coefficients of computation framework. For example, He and Tafti (He and Tafti, 2019) used neural networks to develop more accurate predictions of the drag force, replacing the conventional mean drag correlations based on the Reynolds number and void functions. Similar contributions in the derivation of drag models for gas–solid flows can also be found in (Zhu et al., 2022). In molecular dynamics, the deep learning models were recently applied to replace solving density function theory (DFT) to accelerate MD simulations in 10^3 scales (Jia

et al. 2020).

Third, emerging physics-informed ML technology can be used to directly simulate particle movements and fluid mechanics, which can integrate/learn the classical physics laws, and boundary conditions as constraints into the architecture of ML algorithms. The role of such constraints is to teach the ML models about the prior knowledge, which can not only greatly improve its approximation ability but also boost the interpretability that the ML does not have. For example, Ummenhofer et al. (Ummenhofer et al., 2019) first proposed a network model based continuous convolution to learn the fluid particle movements from Smooth Particle Hydrodynamics (SPH) simulations. The advantage of continuous convolution, rather than using traditional graphs-based representations, is taking the fluid as point cloud and computing each point's movements according to spatial convolution kernel in the neighboring area. Lu et al. (Lu et al., 2021) applied the continuous convolution neural network (CCNN) to predict granular flows in a rotating drum and hopper, replacing the direct time consuming calculation of the particle-particle and particle-wall contacts in DEM simulation. The model takes the particle positions, velocities, and static boundary conditions as model inputs to predict the particle position at next timestep. The particle velocity is then updated based on the variations of particle positions over the timestep. Xu and Shen (Xu and Shen, 2022) took a further step. They altered the computation framework to instruct the CCNN model to predict particle acceleration firstly following Newton's second law and upgraded the model to consider the particle-particle and particle-wall collision separately to have better prediction performance in the packing.

Despite recent pioneer works about machine learning model has shown potentials in understanding physics mechanisms and accelerating granular flow simulation, the research in this area is still lacked and applications are quite limited. For example, models in literature works (Lu et al., 2021; Xu and Shen, 2022) only consider static boundary points, while moving boundaries is more prevalent in real process. In addition, these models might only predict particle movements in a very strict operation condition and device design, which could not be extrapolated to different conditions (e.g. rotation speeds) and large scale.

In this study, this research is aimed to simulating granular flows by a physics-informed model in the milling process. The model used CCNN trained by DEM simulation data, explicitly considering moving boundary conditions with different mill rotation speeds. In the following sections, the details of models and methods are firstly introduced. Then the results are presented and analyzed. Finally, the applications potentials and limitations are discussed.

2. MODELS AND METHODS

2.1. DEM simulations and data generation

An in-house developed DEM model was used in the study. The theory and applications of DEM modelling have been reviewed extensively and are not discussed in detail here. In this work, the same Hertz-Mindlin force model was applied. The force model has been proved effectively in our previous work (Wang et al. 2012).

In the work, particle flows in a horizontal mill of diameter 1m, length 1m was simulated. The mill was firstly partially filled with 3000 particles with particle size 50mm and density 2500 kg/m^3 and formed a stable packing until the average particle velocity is zero at 1.5s. After that, the mill started to rotate at different rotation speeds (20 – 60 rpm) and data (particle positions and velocities) were collected each 10ms until to time 5.5 s. Table 1 shows key parameters in DEM simulations.

We simulated a total seven cases with different rotation speeds (20 – 60 rpm), where six cases were used into training process and one case (30 rpm) was used for validations. Each case had 400 frames (data sampling 100 Hz) over the period of 4 s (t = 1.5 s to 5.5 s).

2.2. Physics-informed model

In order to accelerate simulation of particle movements in a rotating drum, it is necessary to integrate the mechanistic model from DEM simulations and machine learning model based on knowledge established from multiscale study of grinding process. Specifically, Newton's second laws should be incorporated into the framework of physics-informed model. The direct calculation of particle–particle and particle-boundary collisions from DEM simulation in a very small timestep will be replaced by the machine learning model to approximate particle collisions more quickly in a larger time scale.

In the model, the intermediate positions and velocities of particles are firstly updated by gravity without considering particle-particle and particle wall interactions. Next, the intermediate velocities and positions are passed to the model to derive the particle accelerations $\mathbf{a}^{n+1}$ from the particle-particle and particle-wall collisions. The predicted acceleration is then used to calculate velocities and positions of the next machine learning timestep following the Newton's second law.

The key to this computation framework is predictions of accelerations $\mathbf{a}_{ext}^{n+1}$ by the physics-informed model. Fig. 1 shows the structure of the model. The structure is composed of two parts, namely the prediction of particle-particle collision $\mathbf{a}_{pp}^{n+1}$ and the particle-wall $\mathbf{a}_{pw}^{n+1}$. In each part, there are three hidden layers. For the first part (particle-particle collision), the input features include positions, velocities of moving particles. In each layer, a combination of continuous convolution and fully connected neural network are used to construct 64 latent features, which means the character of each moving particle is described by 64 float values (Lu et al., 2021). A ReLU activation function is used to transform these features non-linearly, represented as * in Fig. 1. They are then passed to the next layer for the next feature operations.

A similar forward calculation procedure also happens in the second part (particle-wall collision) where the input features include velocities of moving particles, positions, normal directions and velocities of boundary spheres In the output of layer 1, there are 96 hidden features where 32 features come from velocities of moving particles through fully connected network, 32 features come from normal directions of boundary particles, and the last 32 comes from velocities of boundary particles. The following feature operations in part 2 are exactly same as part1.

The Cconv in Fig. 1 represents the continuous convolution. For a system with total N particles, the continuous convolution at particle positions **x** is defined as:

$$(f * g)(\mathbf{x}) = \sum_{i \epsilon N(\mathbf{x},R)} a(\mathbf{x}_i, \mathbf{x}) f_i g(\Lambda(\mathbf{x}_i - \mathbf{x})) \tag{1}$$

Where f_i is the input features of neighbor particle i. For moving particles, the intermediate velocities and positions are used features. For boundary mesh, mesh positions, velocities, and normal directions are used as features. The convolution at position **x** is based on a set of particles within a radius R around x, defined as N(**x**,R). The contribution of each particle is weighted by a window function:

$$a(\mathbf{x}_i, \mathbf{x}) = \begin{cases} (1 - \frac{\|\mathbf{x}_i - \mathbf{x}\|_2{}^2}{R^2})^3 & \|\mathbf{x}_i - \mathbf{x}\|_2 < R \\ 0 & \|\mathbf{x}_i - \mathbf{x}\|_2 \geq R \end{cases} \tag{2}$$

The filter function g is a continuous function as the particles move to any location within the simulation domain. In practice, the values of this continuous function are stored at discrete locations and linear interpolation is used to calculate its values at given location. Λ is a function mapping a unit sphere to a unit cube as the filter domain is a sphere while the values of the filter function are stored on regular lattices. FC in Fig. 1 represents fully connected layer.

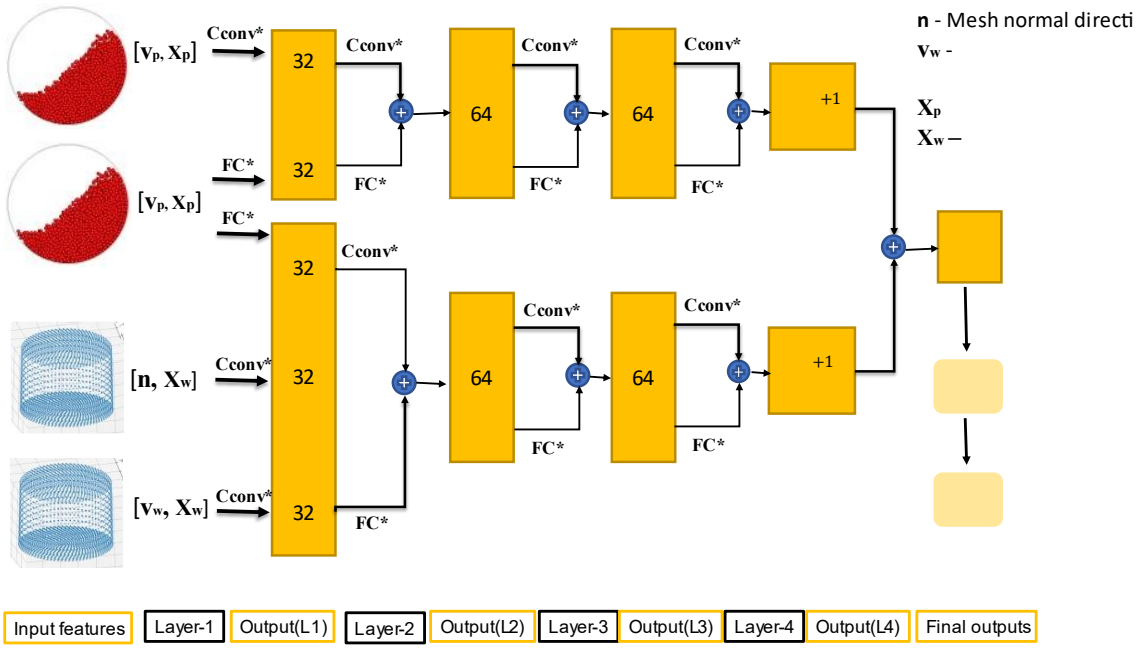


Figure 1 Structure of Physics-informed model (Cconv represents continuous convolutions; FC represents fully connected layer; * the ReLU function).

2.3. training conditions

The training process was to learn the values of model parameters by minimizing the error between network prediction and the ground truth provided by DEM simulation. In the training process, the results from every five steps were used to calculate the loss and update the values of the trainable parameters. The learning rate decayed with multiple steps from 1.0×10^{-4} to 2.0×10^{-6}.

In each training step, the trainer fetched the data of frame n and let the model predict the results of the next three frames. A loss function is needed to quantify the error between the predicted results and the ground-truth. In the research, a loss function considering particle position errors is proposed to reduce the influence of training epochs on the model:

$$L^{n+1} = \frac{1}{N}\sum_{i=1}^{N}\left\|\mathbf{x}_i^{n+1} - \hat{\mathbf{x}}_i^{n+1}\right\|_2 \tag{3}$$

Where $n+1$ represents frame $n+1$, N is the number of particles, $\mathbf{x}_i^{n+1}$ is the predicted position of particle i, and $\hat{\mathbf{x}}_i^{n+1}$ is the ground-truth. The first term is the mean square distance loss. It calculates the distance between predicted positions and ground-truth positions at the particle scale.

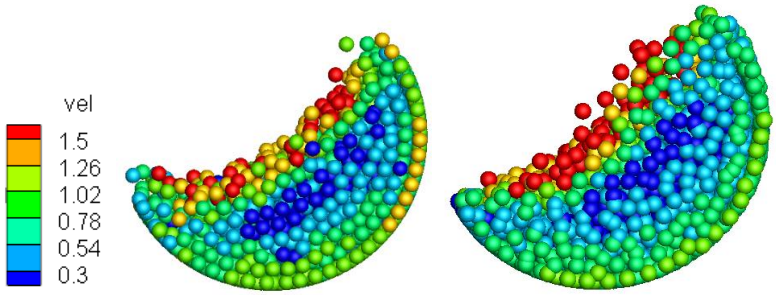
The predicted results of frame $n+1$ were then used to predict the results of frame $n+2$. This process was repeated until the predefined number of frames was reached. The total loss in this training step was calculated as a sum of the loss from all the predicted frames:

$$L = \sum_{i=1}^{F} w^i L^{n+i} \tag{4}$$

Where $F = 3$ is the total number of frames used to calculate the loss in each training step. $w^i = 1$ is the weighting factor of the loss calculated from frame $n + i$.

3. RESULTS AND DISCUSSIONS

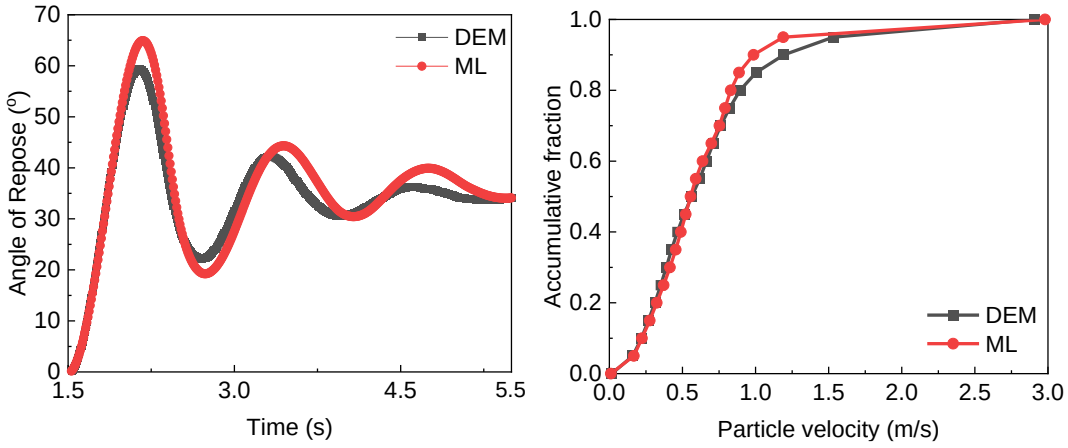
Fig. 2 shows comparisons of flow patterns of granular flow between DEM simulations and the proposed physics-informed model after rotation at time 2.5 s . It can be found the flow pattern are similar where a thin layer of fast-moving particles (velocity > 1.5 m/s) rolls down the flat surface and small velocity particles (< 0.5 m/s) are in the middle of particle flow.



(a) (b)

Figure 2 Flow pattern at time 2.5 s: (a) DEM simulations; (b) Physics-informed model predictions

Fig. 3a shows evolutions of Angle of Repose (AoR) from time 1.5 s to 5.5 s. The predictions of AoR by Physics informed model is consistent with DEM simulations. The AoR starts from 0° (packing) and then increase to around 60° and then drops down rapidly due to particle flow avalanche. As rotation time goes, the fluctuation is smaller as the particle flow becomes stable and AoR stays at around 35°. Fig. 3b shows velocity distributions at time 2.5s. The velocity distributions of physics-informed model are consistent with DEM simulations. Most particles have the velocity between 0.5 m/s to 1.0 m/s.



(a) (b)

Figure 3 (a) Variations of angle of repose t = 1.5 – 5.5 s; (b) velocity distributions at time 2.5 s.

4. CONCLUSIONS

We developed a physics-informed model based on continuous convolutions to predict the granular flow of ball milling process. The model was trained by DEM simulation data, considering moving boundary conditions of the ball mill at different rotation speeds. Results show the predicted granular flow was consistent with DEM simulation in terms of AoR and velocity analysis. While the proposed model has great potential in accelerating granular flow simulation, several obstacles need to be overcome to test the capability in predicting full-scale

granular flows in ball milling process. Firstly, the current model only considers the same device and same mill loadings. To generate a more applicable model, the model should be trained by more cases of different mill loading and larger scale mills. Secondly, dispersed particles and steel balls need to be considered in the physics-informed model. Thirdly, the current model can only predict mean particle velocity over the time 10ms which cannot reflect the instant particle velocity at DEM timestep. A potential mapping model might be developed to generate high-resolution velocity data based on low-resolution predicted data.

5. ACKNOWLEDGMENTS

The support from the Australia Research Council (ARC) ARC Research Hub on Computational Particle Technology (IH140100035) and Jiangsu Industrial Technology Research Institute (JITRI) is acknowledged. YL is also grateful to the Australian Government Research Training Program (RTP) Scholarship for financial support of his PhD study.

6. REFERENCES

He L, Tafti DK, (2019). A supervised machine learning approach for predicting variable drag forces on spherical particles in suspension. Powder Technology, 345, 379-389.

Jia W, Wang H, Chen M, Lu D, Lin L, Car R, Weinan E, Zhang L, (2020). Pushing the limit of molecular dynamics with ab initio accuracy to 100 million atoms with machine learning, SC20: International conference for high performance computing, networking, storage and analysis. IEEE, 1-14.

Levy A, Kalman H, (2001). Handbook of conveying and handling of particulate solids. Elsevier.

Li Y, Bao J, Chen T, Yu A, Yang R, (2022). Prediction of ball milling performance by a convolutional neural network model and transfer learning. Powder Technology, 403, 117409.

Liu L, Bai B, (2019). Flow regime identification of swirling gas-liquid flow with image processing technique and neural networks. Chemical Engineering Science, 199, 588-601.

Lu L, Gao X, Dietiker JF, Shahnam M, Rogers WA, (2021). Machine Learning Accelerated Discrete Element Modeling of Granular Flows. Chemical Engineering Science, 116832.

Ummenhofer B, Prantl L, Thuerey N, Koltun V, (2019). Lagrangian fluid simulation with continuous convolutions, International Conference on Learning Representations.

Wang M, Yang R, Yu A, (2012). DEM investigation of energy distribution and particle breakage in tumbling ball mills. Powder Technology, 223, 83-91.

Xu D, Shen Y, (2022). An improved machine learning approach for predicting granular flows. Chemical Engineering Journal, 450, 138036.

Zhu H, Zhou Z, Yang R, Yu A, (2008). Discrete particle simulation of particulate systems: a review of major applications and findings. Chemical Engineering Science, 63, 5728-5770.

Zhu L, Chen X, Ouyang B, Yan WC, Lei H, Chen Z, Luo ZH, (2022). Review of machine learning for hydrodynamics, transport, and reactions in multiphase flows and reactors. Industrial & Engineering Chemistry Research 61, 9901-9949.