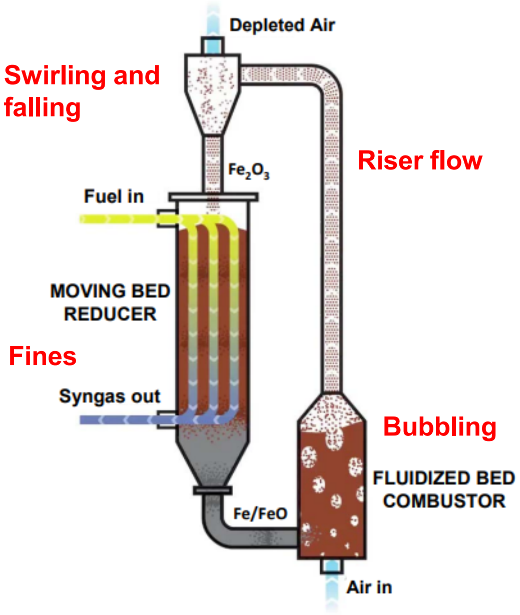
THE OHIO STATE UNIVERSITY

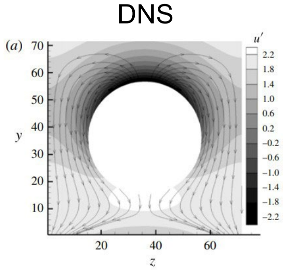
# MACHINE LEARNING-BASED FORCE MODELS FOR IRREGULAR PARTICLES IN GAS-SOLID FLOWS

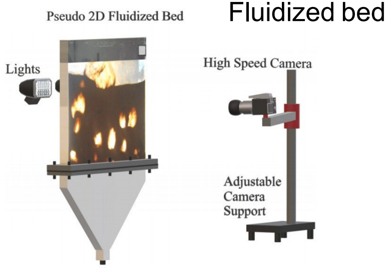
Soohwan Hwang, Liang-Shih Fan

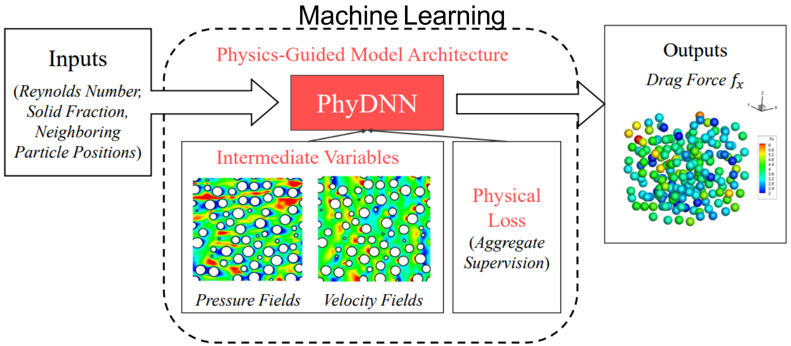
## Gas-Solid systems




## Interaction forces



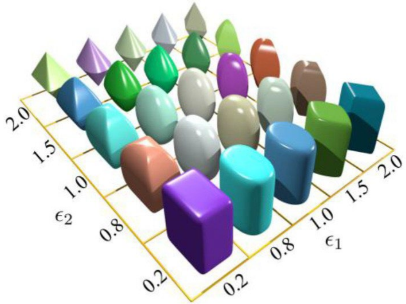

Qiang Zhou et al., Journal of Fluid Mechanics, 765 (2015)
Cesar Martin Venier et al. International Journal of Numerical Methods for Heat and Fluid Flow (2019)
Long He et al., Powder Technology 345 (2019)

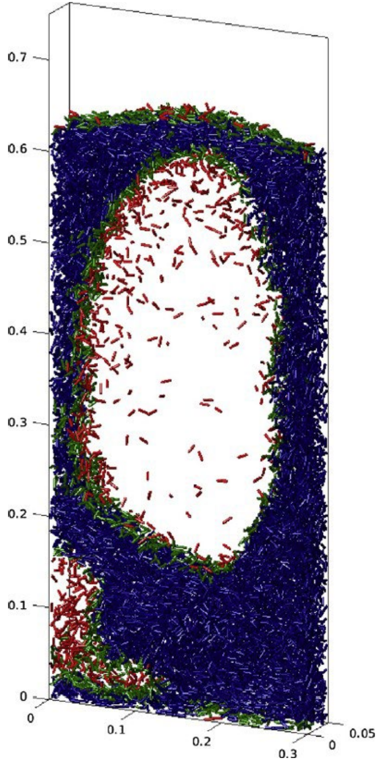
## Non-spherical particle

- Difficult to define the geometrical factors sphericity, flatness, elongation and circularity, etc.
- Data for the interaction force between non-spherical particles and the fluids are limited.
- Correlation may be highly-nonlinear.

## Objectives

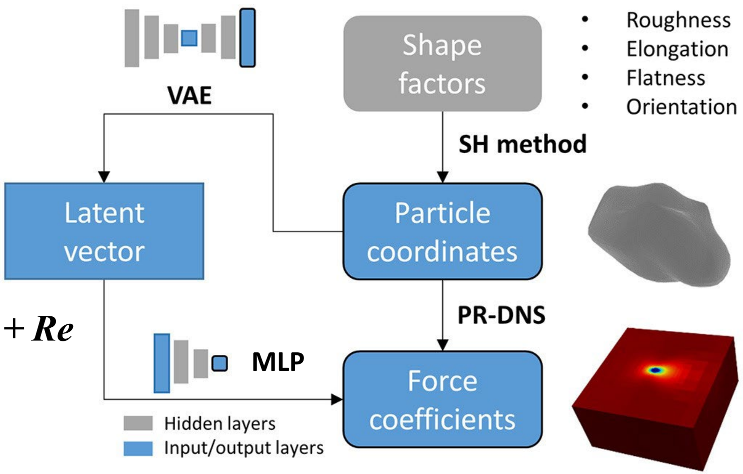
- Developing a neural network-based force model for a diversity of non-spherical particles.
- From low O(1) to moderate O(100) Reynolds number.
- From low to high volume fraction.



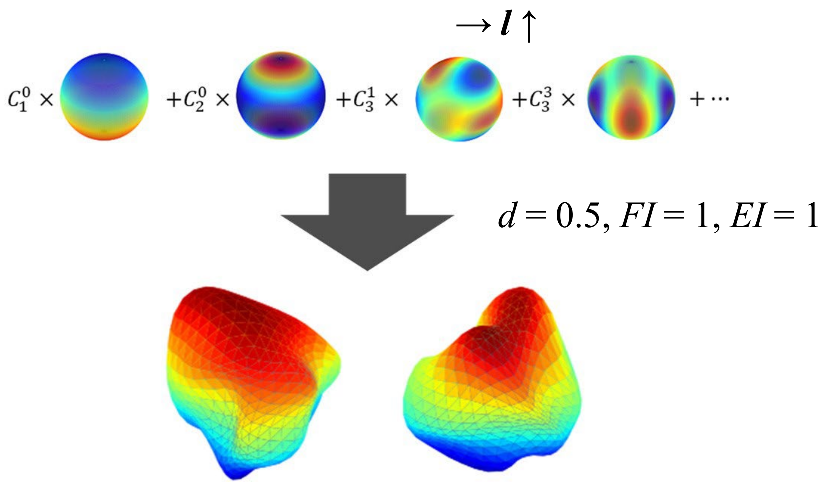




Shiwei Zhao et al., Int J Numer Anal Methods Geomech., 43 (2019)
Vinay V. Mahajan et al., Chemical Engineering Science, 192 (2018)

## Strategy for MLP




## Spherical Harmonic (SH) Methods

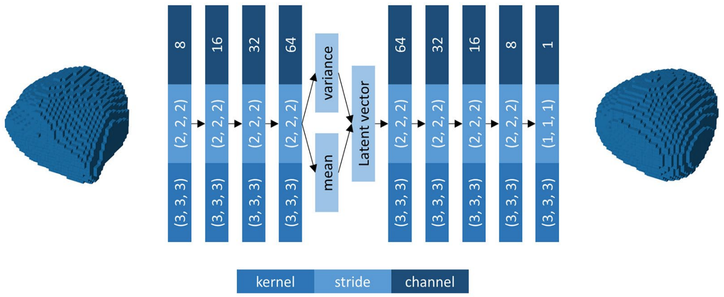



The SH method includes random numbers so the outputs have different shapes

Soohwan Hwang et al., Powder Technology, 392 (2021)
MLP : Multi-Layer Perceptron
PR-DNS : Particle Resolved Direct Numerical Simulation

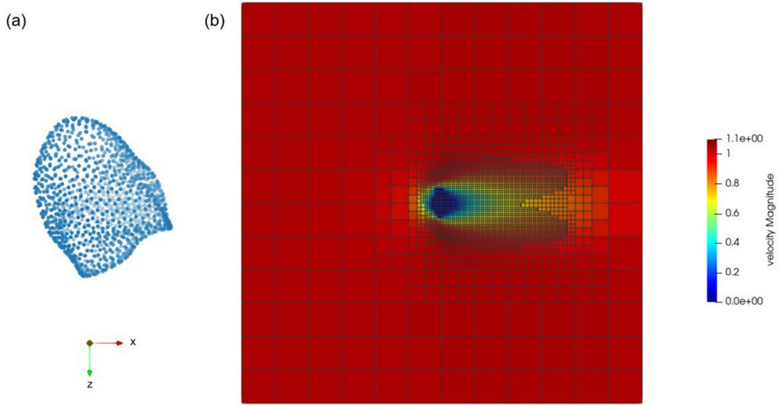
## VAE

- Deep CNN layers with ELUs
- 2,000 data to train, 400 data to validate, 10400 data for DNS
- Less than 1% reconstruction error




## PR-DNS Development

- Simplified Spheric Gas Kinetic Scheme (GKS)
- Immersed boundary Method (IBM) / Direct Forcing
- Adaptive Mesh Refinement (AMR)

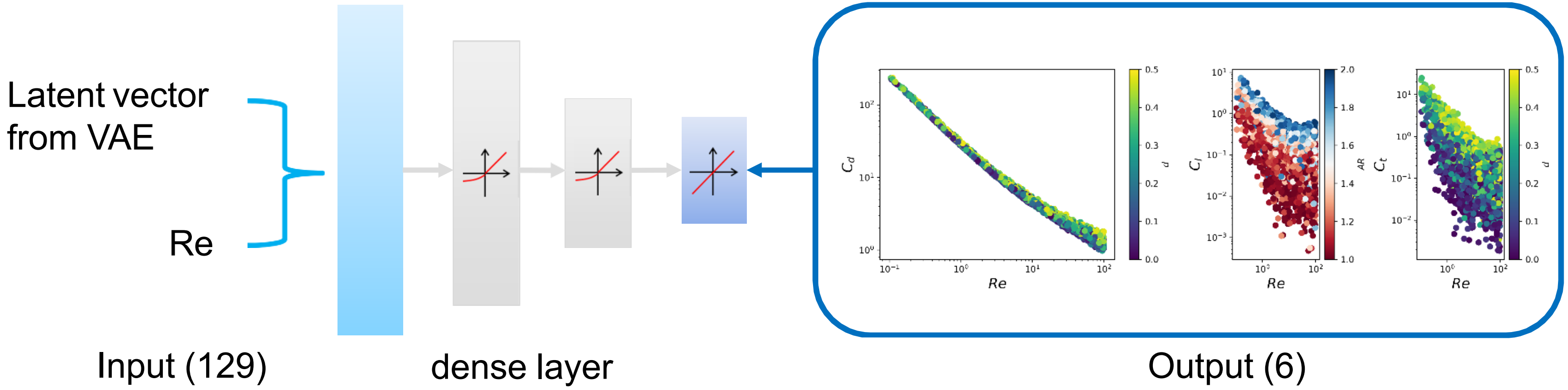


# PR-DNS Results / MLP

- Re = 0.1~100, 10400 single particles
- Two fully connected hidden layers with 32 and 8 nodes with ELUs, and an output layer with linear function

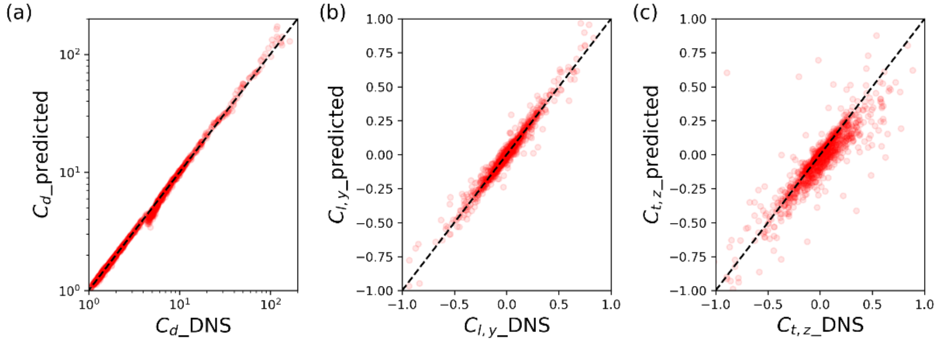
**Eq. (1)**

$$C_f = \frac{-\sum_l F_l \Delta V_l}{\frac{1}{2}\rho u_\infty{}^2 (\frac{Deq}{2})^2 \pi}, \quad C_t = \frac{-\sum_l r \times F_l \Delta V_l}{\frac{1}{2}\rho u_\infty{}^2 (\frac{Deq}{2})^3 \pi}$$



# MLP results

- MSEs of ANN 1 for evaluation data are:
  - $C_d$ : 7.97
  - $C_l$ : 0.00546
  - $C_t$ : 0.0647
- MAPE of $C_d$ is 2.8%



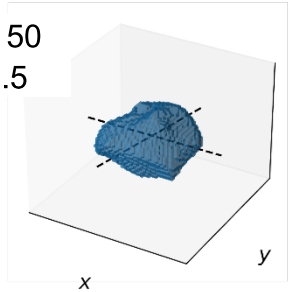

**Eq. (2)**

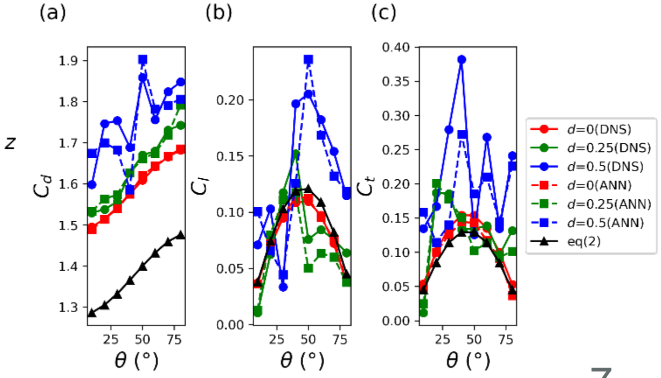
$$C_d = \frac{a_1}{Re^{a_2}} + \frac{a_3}{Re^{a_4}} + \left(\frac{a_5}{Re^{a_6}} + \frac{a_7}{Re^{a_8}} - \frac{a_1}{Re^{a_2}} - \frac{a_3}{Re^{a_4}}\right)sin(\theta)^{a_9}$$

$$C_l = \left(\frac{b_1}{Re^{b_2}} + \frac{b_3}{Re^{b_4}}\right)sin(\theta)^{b_5+b_6Re^{b_7}}cos(\theta)^{b_8+b_9Re^{b_{10}}}$$

$$C_t = \left(\frac{c_1}{Re^{c_2}} + \frac{c_3}{Re^{c_4}}\right)sin(\theta)^{c_5+c_6Re^{c_7}}cos(\theta)^{c_8+c_9Re^{c_{10}}}$$

*Re* = 50
*d* = 0.5

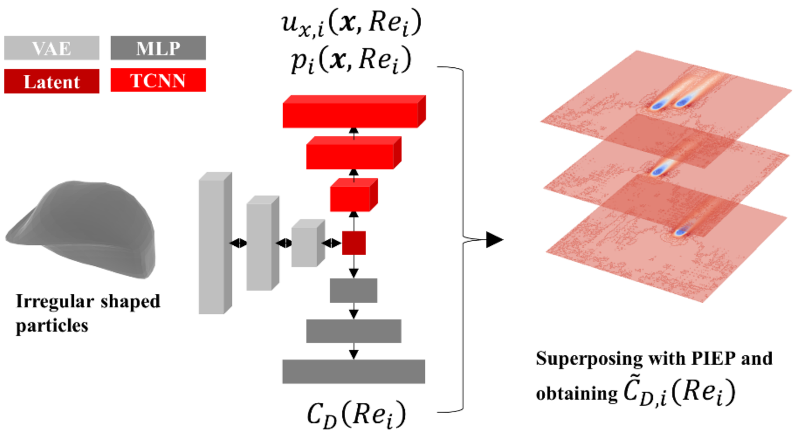



M. Zastawny, el al., International Journal of Multiphase Flow. 39 (2012)

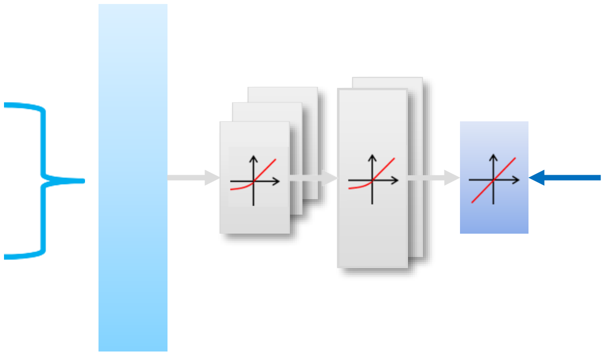
# Flow field prediction (TCNN)

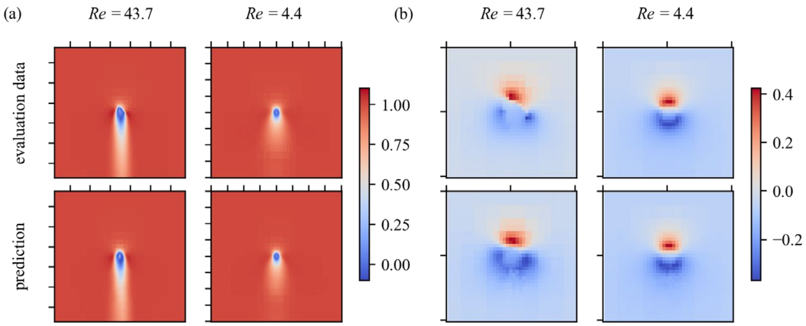
- 0.1 < Re < 100, *x*-direction velocity & pressure
- MSE : 0.00091/0.013
- Ignore the wake effect farther than 10 times $D_{eq}$




Latent vector from VAE

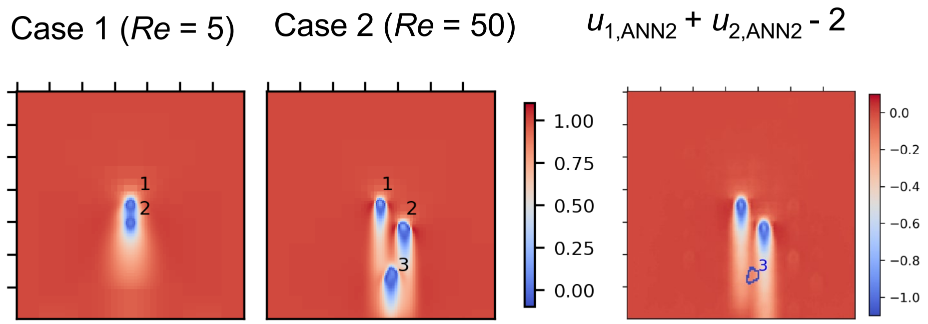
Re






Input (129) transposed-convolutional layers Output (160, 160,160)

# PIEP with MLP and TCNN




**Eq. (3)**

velocity perturbation due to *j* th neighbor

$$\tilde{F}_{qs,i} = \bar{F}_{drag}(Re_i,\varphi) + \left\{3\pi\mu d_i \sum_{\substack{j=1\\ j\neq i}}^{N} \boxed{\overline{u_{j\to i}}^{S}} \left(1+0.15\,{Re_i}^{0.687}\right)\right\}$$

**Eq. (4)**

TCNN

MLP

$$\tilde{C}_{D,i} = \boxed{C_D(Re_i)} \left\{ f(\varphi,Re_i) + \frac{\boxed{\sum_{\substack{j=1\\ j\neq i}}^{N} \overline{u_{x,j\to i}}^{S}(\boldsymbol{r}_i)}}{u_{mac}} \right\} - \frac{4 d_{eq,i}\left[\sum_{\substack{j=1\\ j\neq i}}^{N} \boxed{\overline{\nabla_x p_{j\to i}}^{V}(\boldsymbol{r}_i)} - \frac{1}{Re_i}\sum_{\substack{j=1\\ j\neq i}}^{N} \boxed{\overline{\nabla^2 u_{x,j\to i}}^{V}(\boldsymbol{r}_i)}\right]}{3\rho {u_{mac}}^2}$$

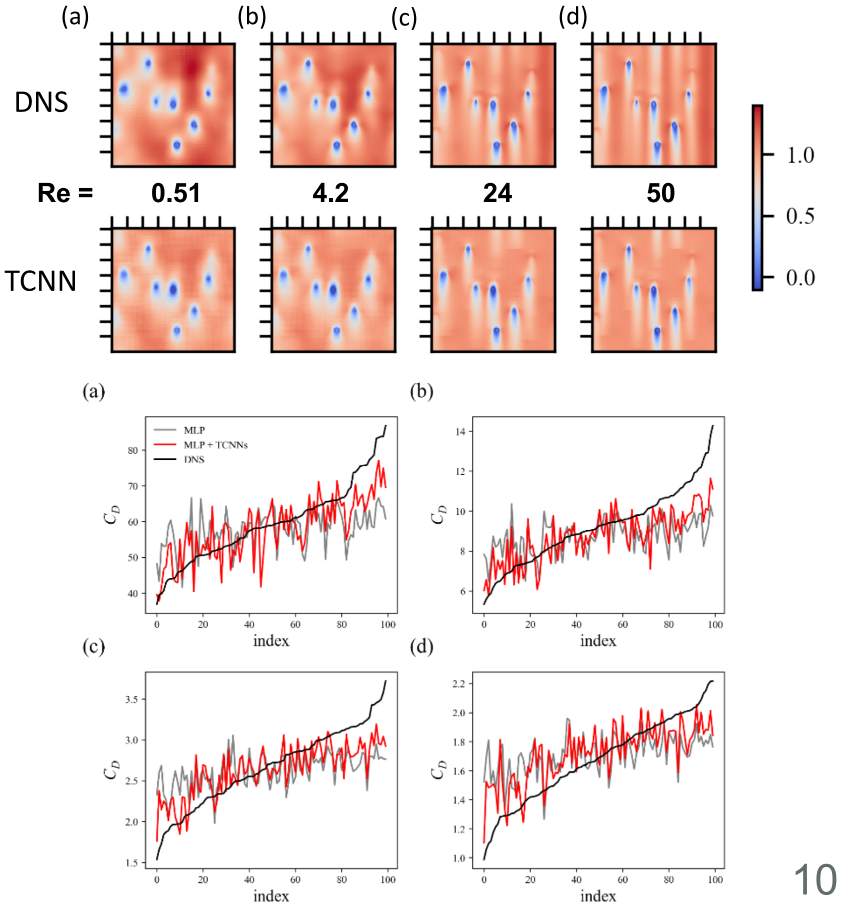
| $C_D$ / error | Case 1 | | Case 2 | | |
|---|---|---|---|---|---|
| | 1 | 2 | 1 | 2 | 3 |
| DNS (multi-particle) | 6.66 | 4.48 | 1.73 | 1.68 | 1.40 |
| DNS (single particle) | 7.48 | 7.21 | 1.75 | 1.71 | 1.63 |
| ANN 1 | 7.53/ 13.1% | 7.37/ 64.5% | 1.75/ 1.11% | 1.71/ 2.3% | 1.62/ 16.3% |
| ANN 1+ ANN 2/PIEP | 6.64/ 0.2% | 4.23/ 5.6% | 1.73/ 0.1% | 1.70/ 1.7% | 1.38/ 1.0% |

PIEP : pairwise-interaction extended point-particle

G. Akiki et al., Journal of Computational Physics (2017)

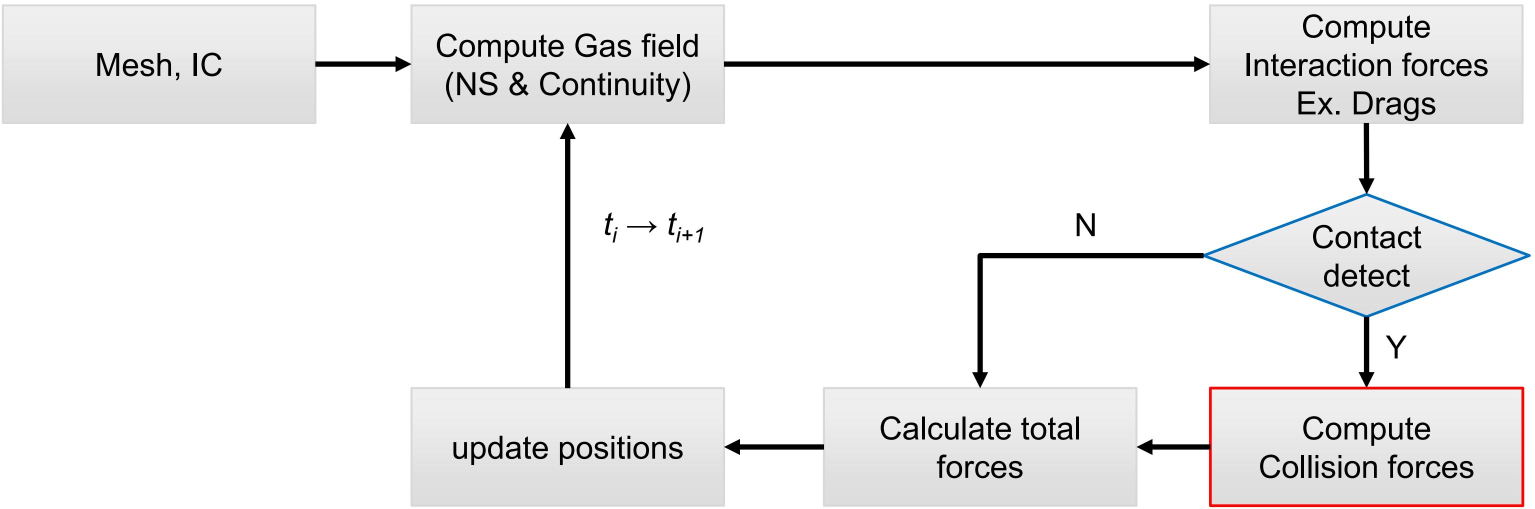
## PIEP with MLP and TCNN

- Poly-dispersed 100 irregular particles
- Solid volume fraction = 0.5%
- MAPE ≈ 10%, 0.56 < $R^2$ < 0.62
- Underestimated correction for the particles with strong neighboring effects
- Higher computational efficiency and flexibility



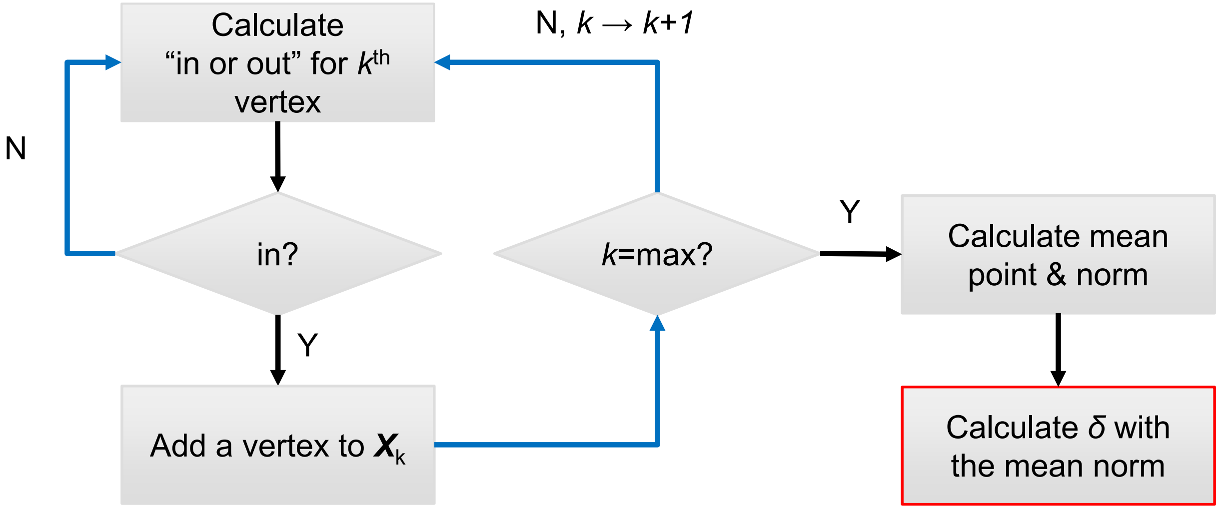
## Collision algorithms in CFD-DEM

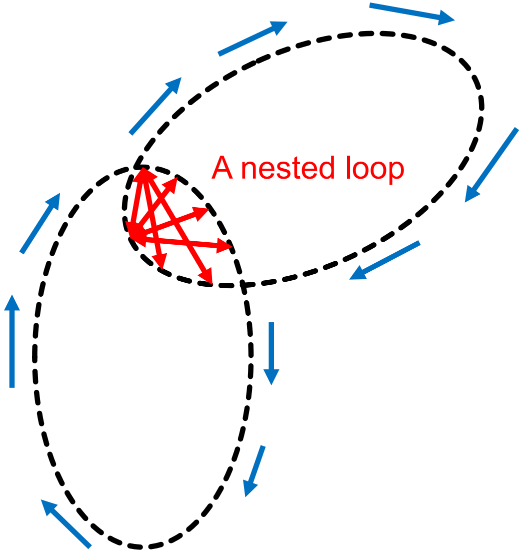
- DEM method involves iterative calculations for particles



## Collision algorithms in CFD-DEM

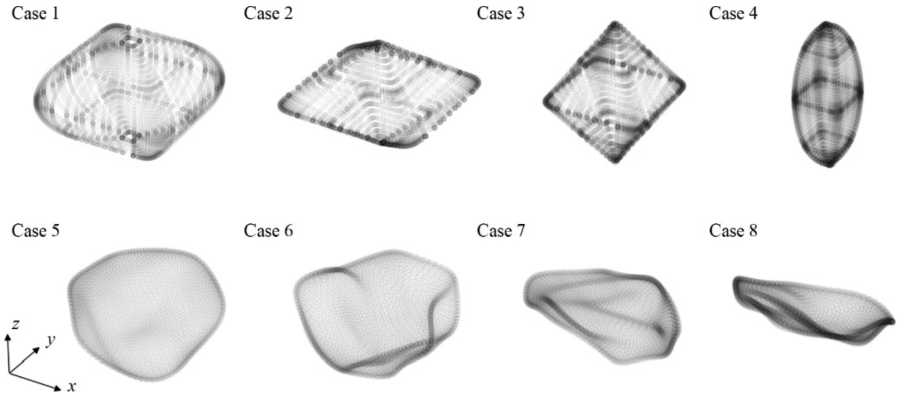
- At $t = t_i$ and for the $j^{th}$ particle,



## Non-spherical particles

- Regular & irregular particles




$$((\frac{x}{r_1})^{2/\varepsilon_1} + (\frac{y}{r_2})^{2/\varepsilon_1})^{\varepsilon_1/\varepsilon_2} + (\frac{z}{r_3})^{2/\varepsilon_1} = 1$$

$$x = r_1 sign(cos\varphi_1)|cos\varphi_1|^{\varepsilon_1}|cos\varphi_2|^{\varepsilon_2}$$

$$y = r_2 sign(sin\varphi_1)|sin\varphi_1|^{\varepsilon_1}|cos\varphi_2|^{\varepsilon_2}$$

$$z = r_3 sign(sin\varphi_2)|sin\varphi_2|^{\varepsilon_2}$$

$$\dot{x} = \frac{2}{\varepsilon_2}(\left|\frac{x}{r_1}\right|^{\frac{2}{\varepsilon_1}} + \left|\frac{y}{r_2}\right|^{\frac{2}{\varepsilon_1}})^{\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1}}|x|^{\frac{2-\varepsilon_1}{\varepsilon_1}}|r_1|^{-\frac{2}{\varepsilon_1}}$$

$$\dot{y} = \frac{2}{\varepsilon_2}(\left|\frac{x}{r_1}\right|^{\frac{2}{\varepsilon_1}} + \left|\frac{y}{r_2}\right|^{\frac{2}{\varepsilon_1}})^{\frac{\varepsilon_1-\varepsilon_2}{\varepsilon_1}}|y|^{\frac{2-\varepsilon_1}{\varepsilon_1}}|r_2|^{-\frac{2}{\varepsilon_1}}$$

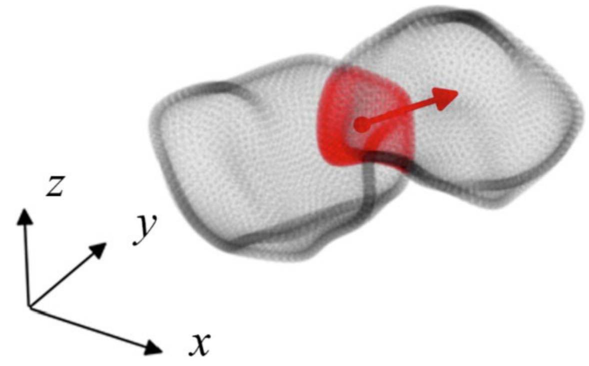
$$\dot{z} = \frac{2}{\varepsilon_2}|z|^{\frac{2-\varepsilon_2}{\varepsilon_2}}|r_3|^{-\frac{2}{\varepsilon_2}}$$

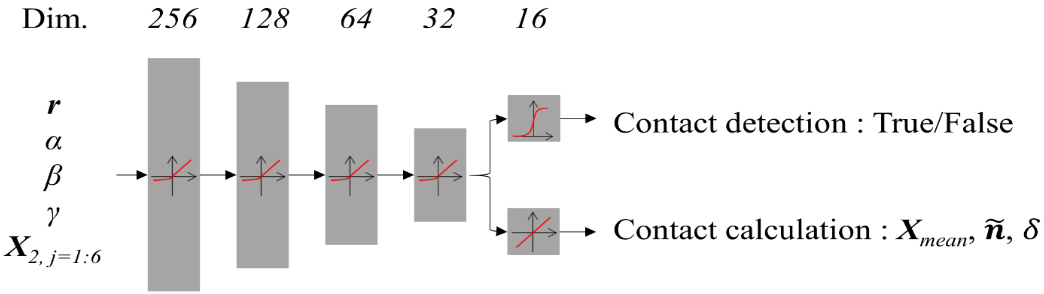
$$\tilde{\boldsymbol{n}} = (n_x, n_y, n_z) = \frac{\boldsymbol{n}}{|\boldsymbol{n}|} = \frac{1}{2|\boldsymbol{n}|}(\frac{1}{N_1}\sum_{i=1}^{N_1}\dot{\boldsymbol{X}}_{1,i}\frac{A_{1,i}}{A_1} + \frac{1}{N_2}\sum_{j=1}^{N_2}\dot{\boldsymbol{X}}_{2,j}\frac{A_{2,j}}{A_2})$$

Soohwan Hwang et al., Chemical Engineering Science, 251 (2022)

## ANN model

- Correlate the relative position, rotational angle and vertices to contact properties.
- Two ANN models for the detection and to properties.



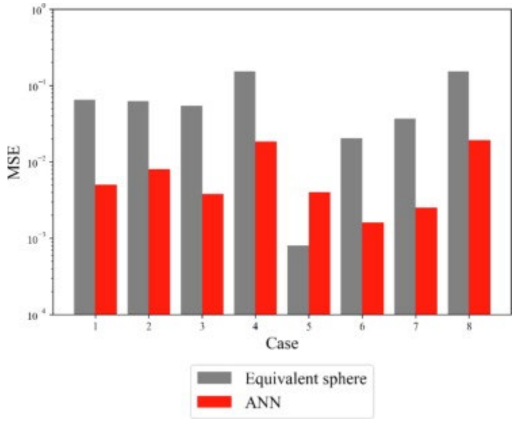



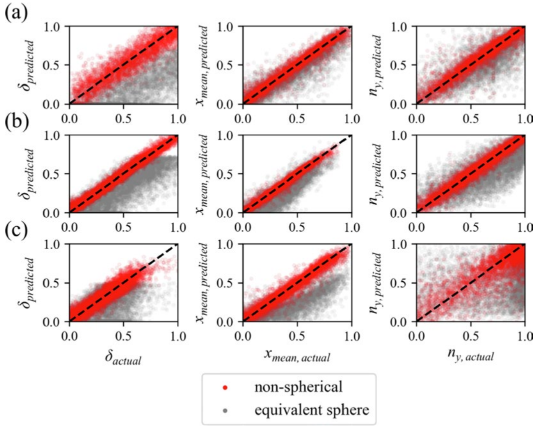

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot log(1 - p(y_i))$$

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2$$

## ANN results

- 80,000 datasets for each cases (< CFD-DEM)
- Rapid calculations : < 1 sec for thousands of cases
- More accurate prediction compared to volume equivalent sphere
- Applicable to screening tests



# Conclusion

- This study provides the interaction force and collision models for the non-spherical particles.
- In DEM, the NN based models can be implemented to obtain the interaction forces and collision forces.
- Both models show high accuracy of prediction on the forces and collision properties.
- The collision model can improve the computation efficiency.

# Acknowledgement

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