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UNSUPERVISED LEARNING BASED INTERACTION FORCE MODEL FOR NONSPHERICAL PARTICLES IN INCOMPRESSIBLE FLOWS

FE0031905

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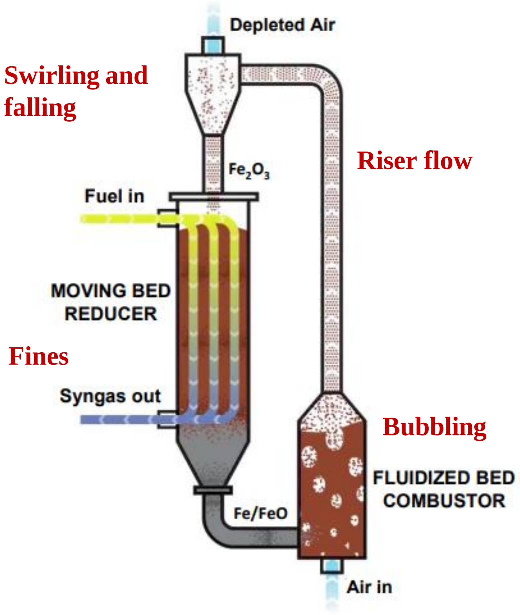
Outline

- **Project Description and Objectives**
- **Project Update**
  - Methods
  - Single particle
  - Multiple particle
  - High density
- **Concluding Remarks**

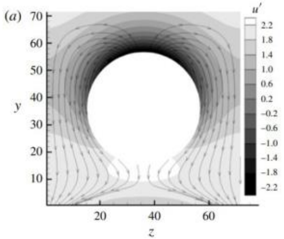
Project Description and Objectives

Gas-Solid Flows

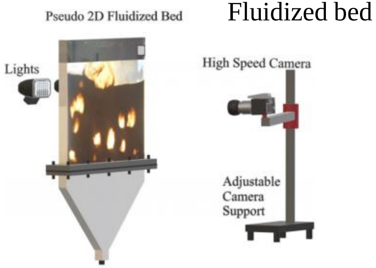


Interaction Forces

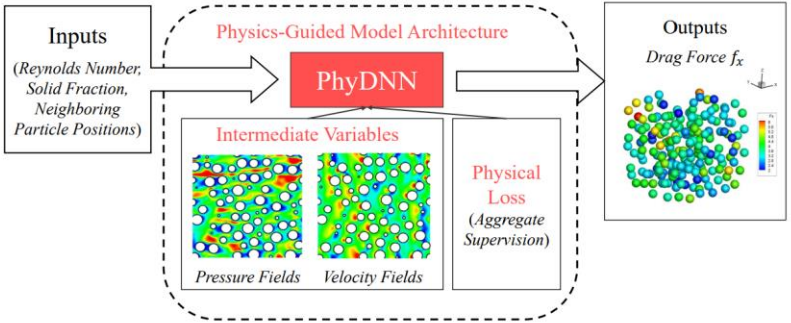
CFD



Fluidized bed



Machine Learning



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)

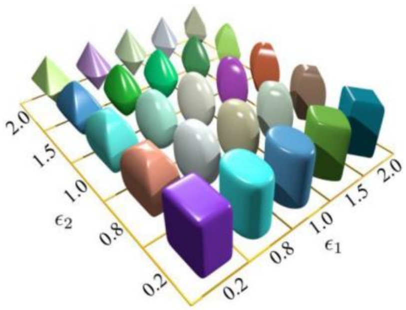
Project Description and Objectives

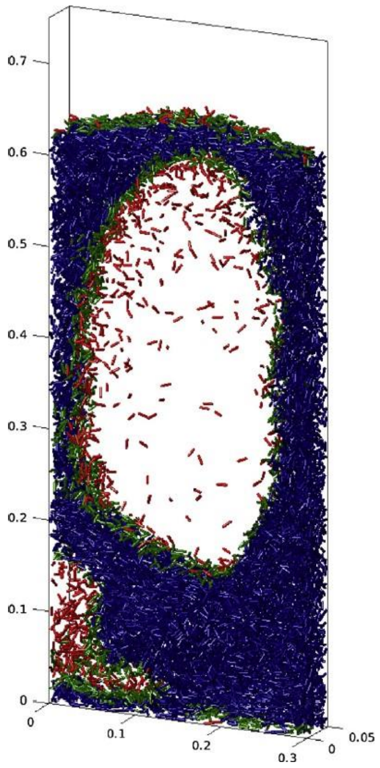
Non-spherical particle

- 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)

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Project Update

Tasks	Year 1				Year 2				Year 3			
	10/20	1/21	4/21	7/21	10/21	1/22	4/22	7/22	10/22	1/23	4/23	7/23
PR-DNS development												
Particles Generation & VAE												
Low Re data Collection											Current stage	
High Re data Collection												
MLP Training												

Spherical Harmonic (SH)

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\varphi^2} = 0.$$

$$f(r,\theta,\varphi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} f_\ell^m r^\ell Y_\ell^m(\theta,\varphi)$$

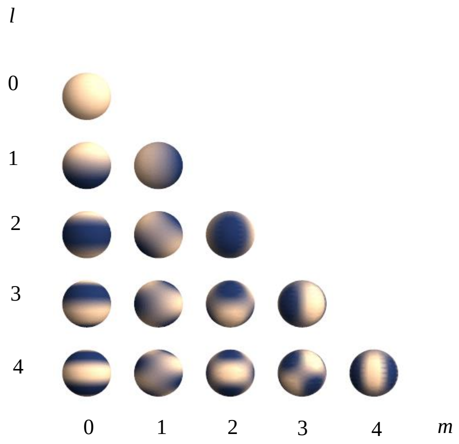
$$\boldsymbol{X} = (x,y,z) = \sum_{l=1}^{l=8}\sum_{m=-l}^{l}\boldsymbol{C}_l^m Y_l^m(\varphi_1,\varphi_2)$$

$$\boldsymbol{C}_l = \begin{pmatrix} C_{x,l}^{-l} & \cdots & C_{x,l}^{0} & \cdots & C_{x,l}^{l} \\ C_{y,l}^{-l} & \cdots & C_{y,l}^{0} & \cdots & C_{y,l}^{l} \\ C_{z,l}^{-l} & \cdots & C_{z,l}^{0} & \cdots & C_{z,l}^{l} \end{pmatrix}$$

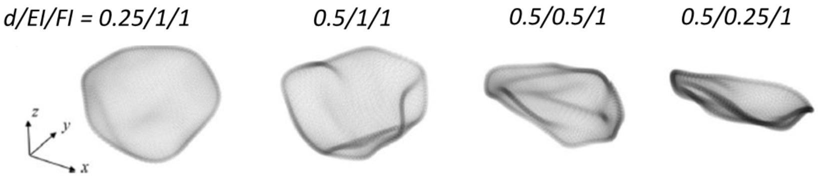
$$= \begin{pmatrix} k_{x,l}(\alpha_{x,2l}-\alpha_{x,2l+1}i) & \cdots & k_{x,l}\alpha_{x,1} & \cdots & k_{x,l}(\alpha_{x,2l}+\alpha_{x,2l+1}i) \\ k_{y,l}(\alpha_{y,2l}-\alpha_{y,2l+1}i) & \cdots & k_{y,l}\alpha_{y,1} & \cdots & k_{y,l}(\alpha_{y,2l}+\alpha_{y,2l+1}i) \\ k_{z,l}(\alpha_{z,2l}-\alpha_{z,2l+1}i) & \cdots & k_{z,l}\alpha_{z,1} & \cdots & k_{z,l}(\alpha_{z,2l}+\alpha_{z,2l+1}i) \end{pmatrix}$$

$$k_{i,l} = \sqrt{\frac{d_{i,l}^2}{\alpha_{i,1}^2 + 2\sum_{j=2}^{2l+1}\alpha_{i,j}^2}},\quad i \in (x,y,z)$$

$$d_{i,l} = \frac{d\sqrt{\frac{\pi}{3}(1+EI^2+EI^2FI^2)}}{\sum_{k=2}^{8}\left(\frac{2}{k}\right)^{1.387}}\left(\frac{2}{l}\right)^{1.387}$$



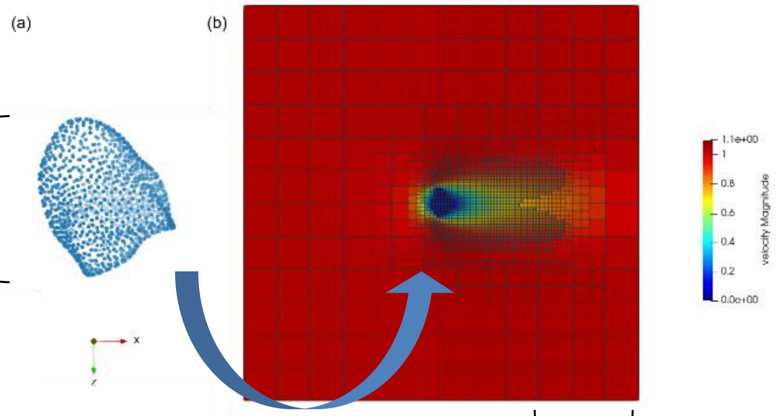
Combine linearly,
Higher weight on higher $l \rightarrow$ high ***d***
d ~ roughness



Wei, D., Wang, J., & Zhao, B. (2018). *Powder Technology*, *330*, 284-291.
https://en.wikipedia.org/wiki/Spherical_harmonics

Particle-Resolved Direct Numerical Simulation (PR-DNS)

Lagrangian points



$$F^{n+1} = \frac{\widetilde{U}_p^n - \widetilde{U}^{n+1}}{\Delta t}$$

Direct forcing scheme

$\widetilde{U}_p^n = 0$ for fixed particles

Adaptive mesh refinement based on:

$$\Omega = \frac{b}{a+b}$$

$$a = \mathrm{trace}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}) = \textstyle\sum_{i=1}^{3}\sum_{j=1}^{3}\left(\boldsymbol{A}_{ij}\right)^2, \qquad \nabla \boldsymbol{V} = \frac{1}{2}(\nabla \boldsymbol{V} + \nabla \boldsymbol{V}^{\mathrm{T}}) + \frac{1}{2}(\nabla \boldsymbol{V} - \nabla \boldsymbol{V}^{\mathrm{T}})$$

$$b = \mathrm{trace}(\boldsymbol{B}^{\mathrm{T}}\boldsymbol{B}) = \textstyle\sum_{i=1}^{3}\sum_{j=1}^{3}\left(\boldsymbol{B}_{ij}\right)^2. \qquad = \boldsymbol{A} + \boldsymbol{B},$$

Gas Kinetic Scheme

$$\frac{\partial f}{\partial t} + v \cdot \nabla f = \frac{g-f}{\tau}$$

$$f(0,t) \approx g(0,t) + \frac{\tau}{\delta t}\left(g(-v\delta t, t-\delta t) + g(0,t)\right)$$

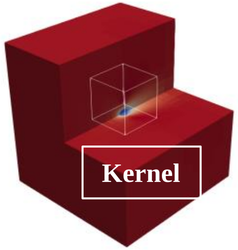
$$\boldsymbol{F} = \int f(0,t) v_x \Xi d\boldsymbol{v}\ ,\ \Xi = \begin{pmatrix} 1 \\ \boldsymbol{v} \end{pmatrix}$$

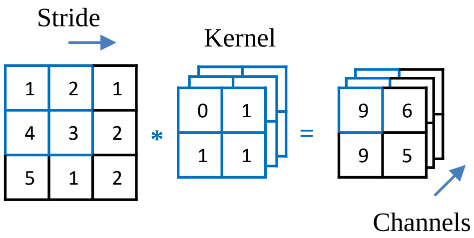
$$\frac{\partial \boldsymbol{W}}{\partial t} + \nabla \cdot \boldsymbol{F} = 0,\ \boldsymbol{W} = \begin{pmatrix} \rho \\ \rho \boldsymbol{u} \end{pmatrix}$$

Simplified Sphere function for incompressible flows

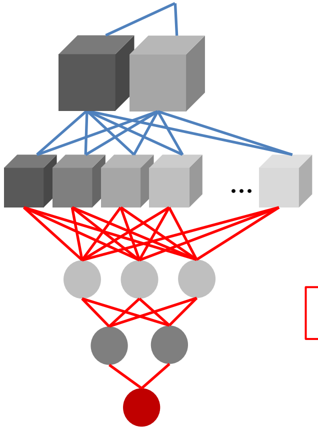
$$g = \begin{cases} \frac{\rho}{4\pi}, & if\ (\boldsymbol{u}-\boldsymbol{v})^2 = c^2 \\ 0, & otherwise \end{cases}$$

Neural Networks





(transposed) convolutional layers (CNN)



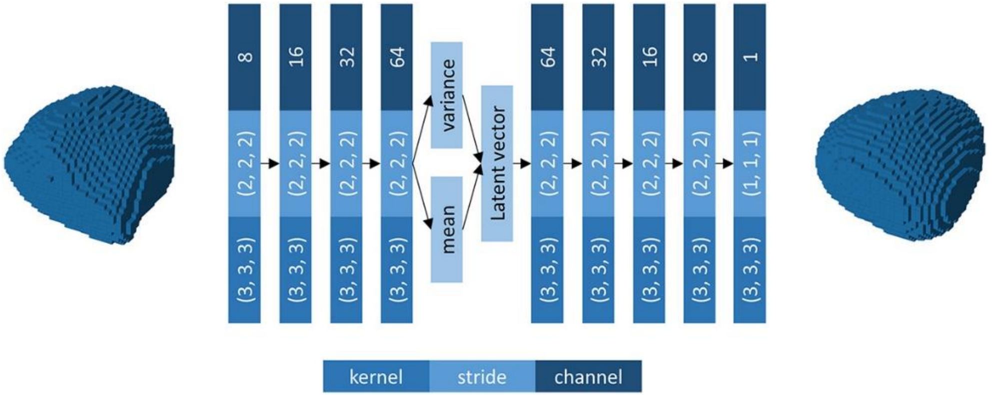
Regressed features

Reduce features with multiple channels

$$\boldsymbol{y} = \sigma(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

Multi-layer perceptron (MLP)

Variational Auto-Encoder (VAE)



- Encoder

$48^3 \rightarrow 24^3 \times 8 \rightarrow 12^3 \times 16 \rightarrow 6^3 \times 32 \rightarrow 3^3 \times 64 \rightarrow 27$

- MLP/Regularization

$27 \rightarrow 128 \times 2 \rightarrow$ **128 (latent)**

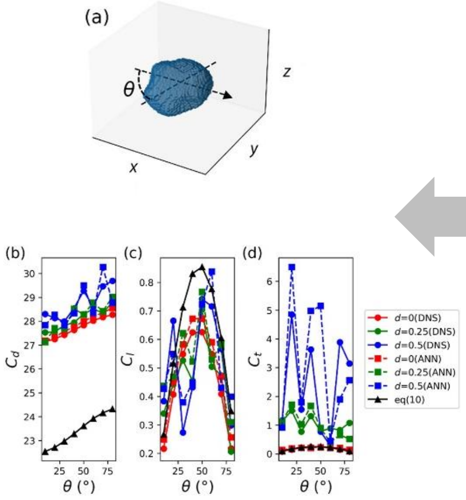
Vertices (Decoder, TCNN)

Force coefficients (MLP)

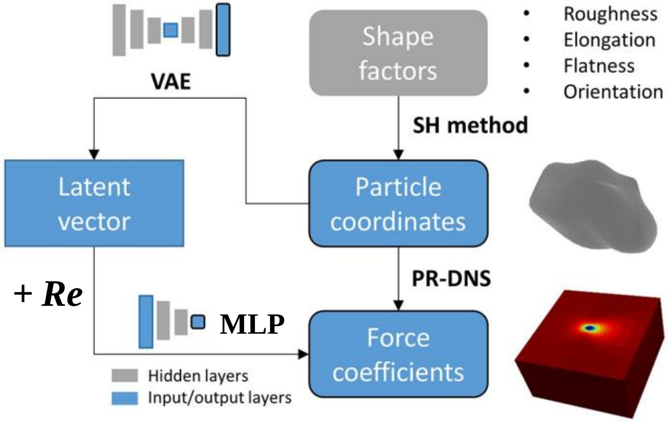
Flow fields (PIEP, TCNN)

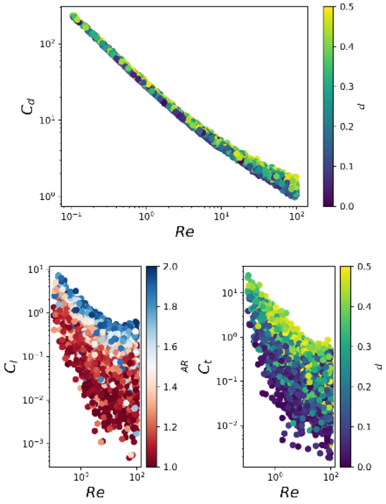
Re

Interaction Force Model for Single Particles



MLP results





CFD results

Soohwan Hwang et al., *Powder Technology*, 392 (2021)

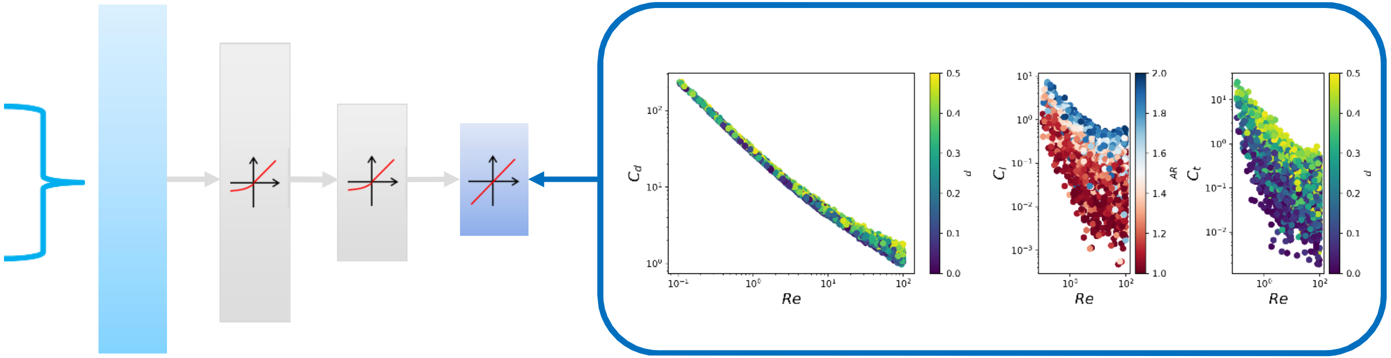
PR-DNS Results / MLP

- 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

$$\boldsymbol{C_f} = \frac{-\sum_l \boldsymbol{F}_l \Delta V_l}{\frac{1}{2}\rho \boldsymbol{u}_\infty{}^2 \left(\frac{Deq}{2}\right)^2 \pi}, \quad \boldsymbol{C_t} = \frac{-\sum_l \boldsymbol{r} \times \boldsymbol{F}_l \Delta V_l}{\frac{1}{2}\rho \boldsymbol{u}_\infty{}^2 \left(\frac{Deq}{2}\right)^3 \pi}$$

Latent vector from VAE

Re



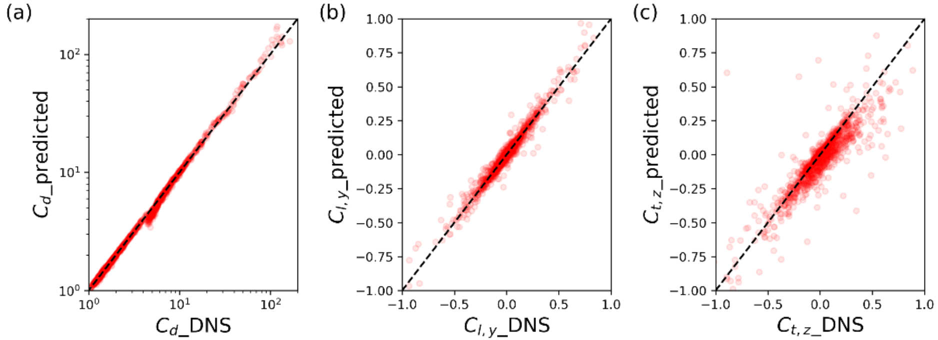
Input (129)

dense layer

Output (6)

MLP results

- MSEs of evaluation data are:
  - C_d : 7.97
  - C_l : 0.00546
  - C_t : 0.0647
- MAPE of C_d is 3.3%

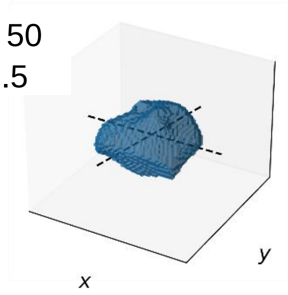


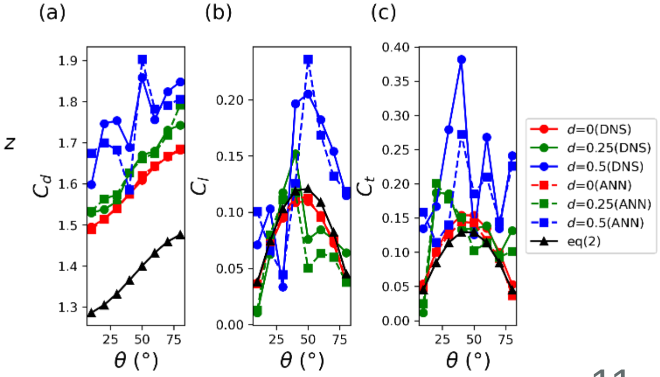
$$C_d = \frac{a_1}{Re^{a_2}} + \frac{a_3}{Re^{a_4}} + \left(\frac{a_5}{Re^{a_6}} + \frac{a_7}{Re^{a_8}} - \frac{a_1}{Re^{a_2}} - \frac{a_3}{Re^{a_4}}\right) sin(\theta)^{a_9}$$

$$C_l = \left(\frac{b_1}{Re^{b_2}} + \frac{b_3}{Re^{b_4}}\right) sin(\theta)^{b_5+b_6 Re^{b_7}} cos(\theta)^{b_8+b_9 Re^{b_{10}}}$$

$$C_t = \left(\frac{c_1}{Re^{c_2}} + \frac{c_3}{Re^{c_4}}\right) sin(\theta)^{c_5+c_6 Re^{c_7}} cos(\theta)^{c_8+c_9 Re^{c_{10}}}$$

Re = 50
d = 0.5

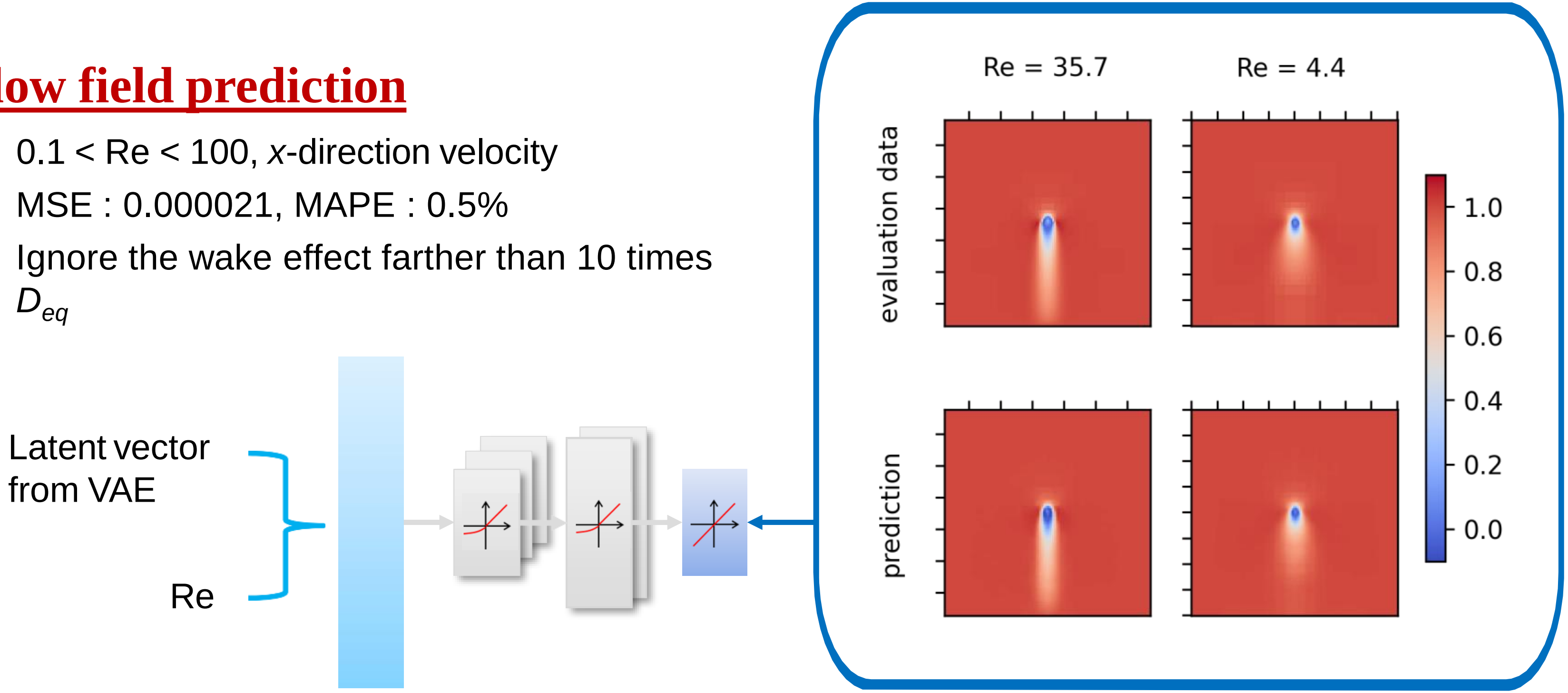




M. Zastawny, el al., International Journal of Multiphase Flow. 39 (2012)

Flow field prediction

- $0.1 < Re < 100$, *x*-direction velocity
- MSE : 0.000021, MAPE : 0.5%
- Ignore the wake effect farther than 10 times D_{eq}

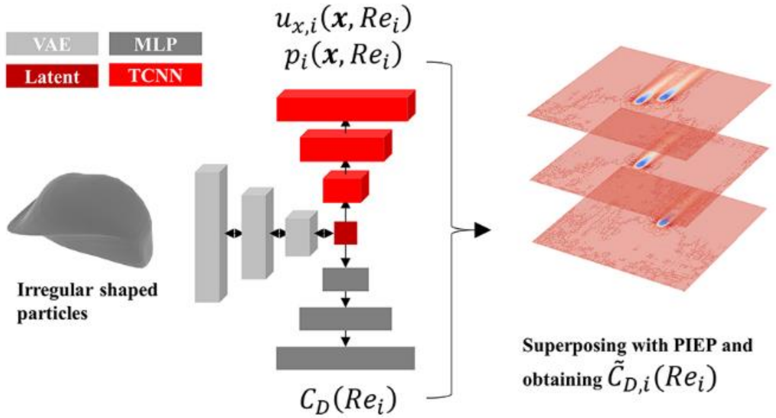


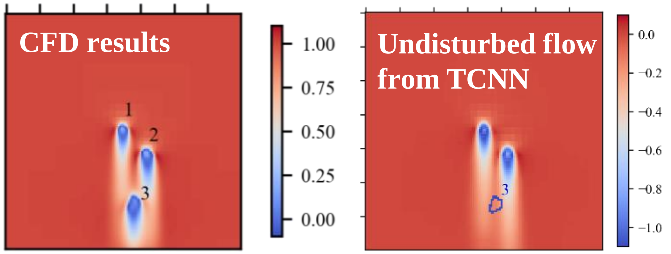
Input (129)

Transpose convolutional Layers (TCNN)

Output (160, 160,160)

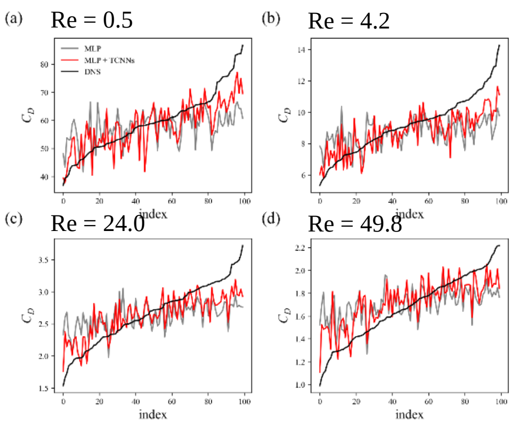
PIEP with MLP and TCNN





$$\tilde{F}_{qs,i} = \bar{F}_{drag}(Re_i, \varphi) + \frac{\rho {u_{mac}}^2 A}{2} C_{D,i} \left\{ \frac{1}{u_{mac}} \sum_{\substack{j=1 \\ j \neq i}}^{N} \overline{u_{j \to i}}^S \right\}$$

100 different particles with 0.5%
(1 < AR < 2, 0 < d < 0.5)



PIEP: Pairwise Interaction Extended Point-particle model
Soohwan Hwang et al., *Chemical Engineering Science* 266, 118299 (2023)

PIEP for dense systems

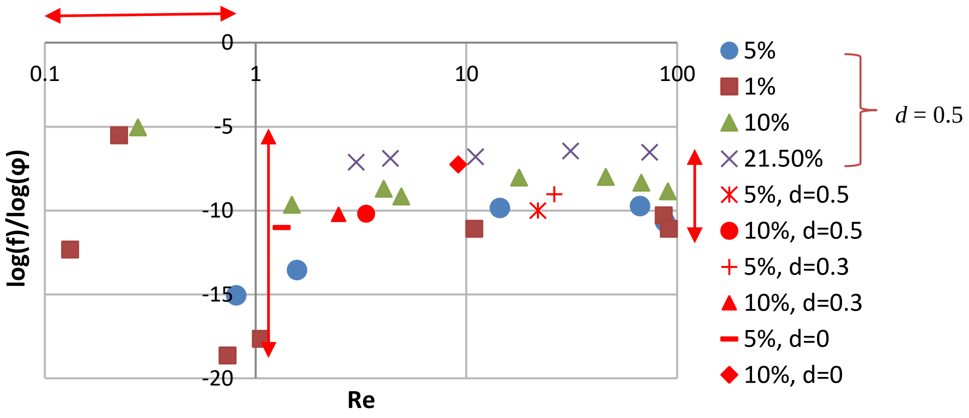
- Solid fraction factor needs to be determined.
- The factor need to consider particle irregularity and inhomogeneity.

$$\overline{F_D} = F_D f(Re, \varphi, d)$$

$$= F_D \varphi^{-3.7+0.65\exp(-0.5(1.5-\log(Re))^2)}$$

$$\frac{\log(f)}{\log(\varphi)} = (-3.7 + 0.65\exp(-0.5(1.5 - \log(Re))^2))$$

PR-DNS results for homogeneous, irregular particles (d = 0 ~ 0.5)



R. Di Felice, Chem. Eng. Sci., 50 (8) (1995), pp. 1213-1245

Concluding Remarks

- This study provides the interaction force model for the irregular shaped particle which is practical in industry.
- The NN based model can predict the neighboring effect of multi-particle systems.
- The solid fraction effect will be investigated further to make the model predict a wider range of flow conditions

Acknowledgement

Acknowledgment: "This material is based upon work supported by the Department of Energy Award Number DE-FE0031905."