



THE OHIO STATE UNIVERSITY

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

FE0031905

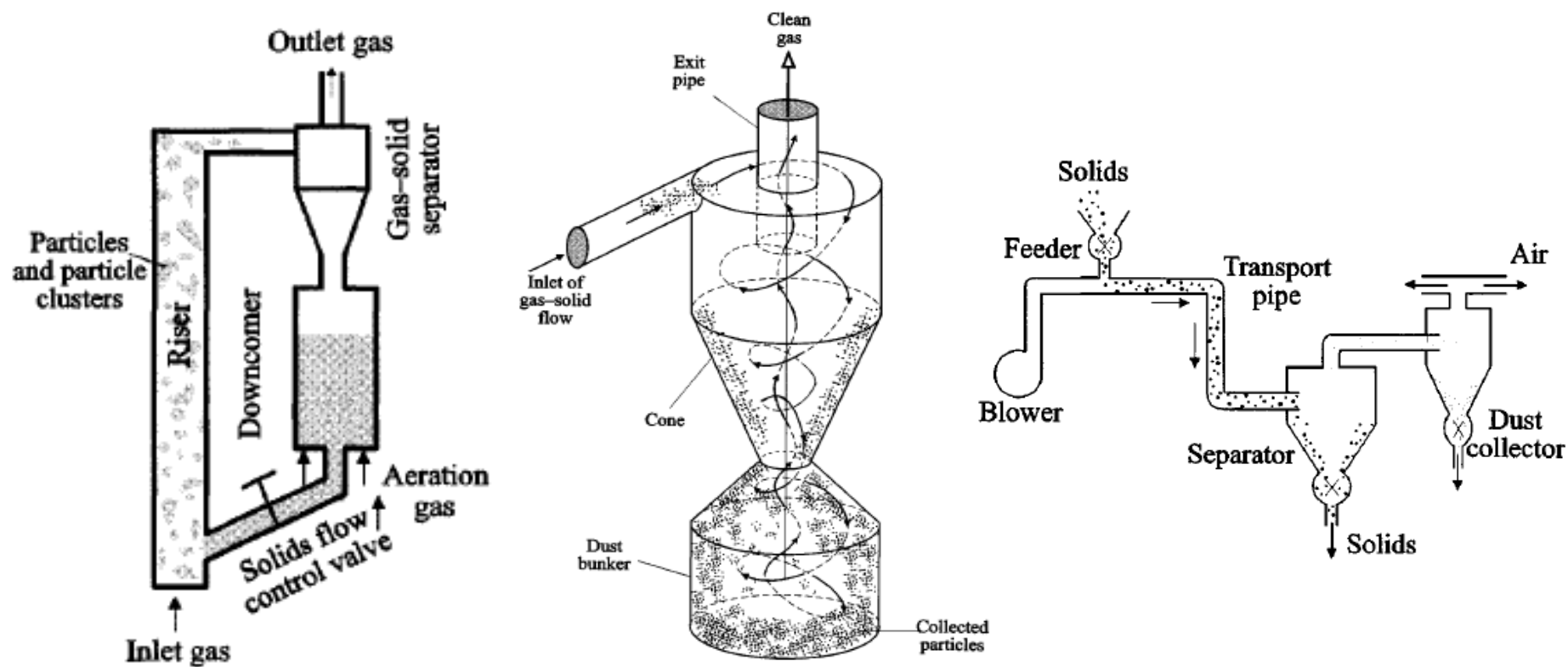
Soohwan Hwang, Jianhua Pan, Liang-Shih Fan



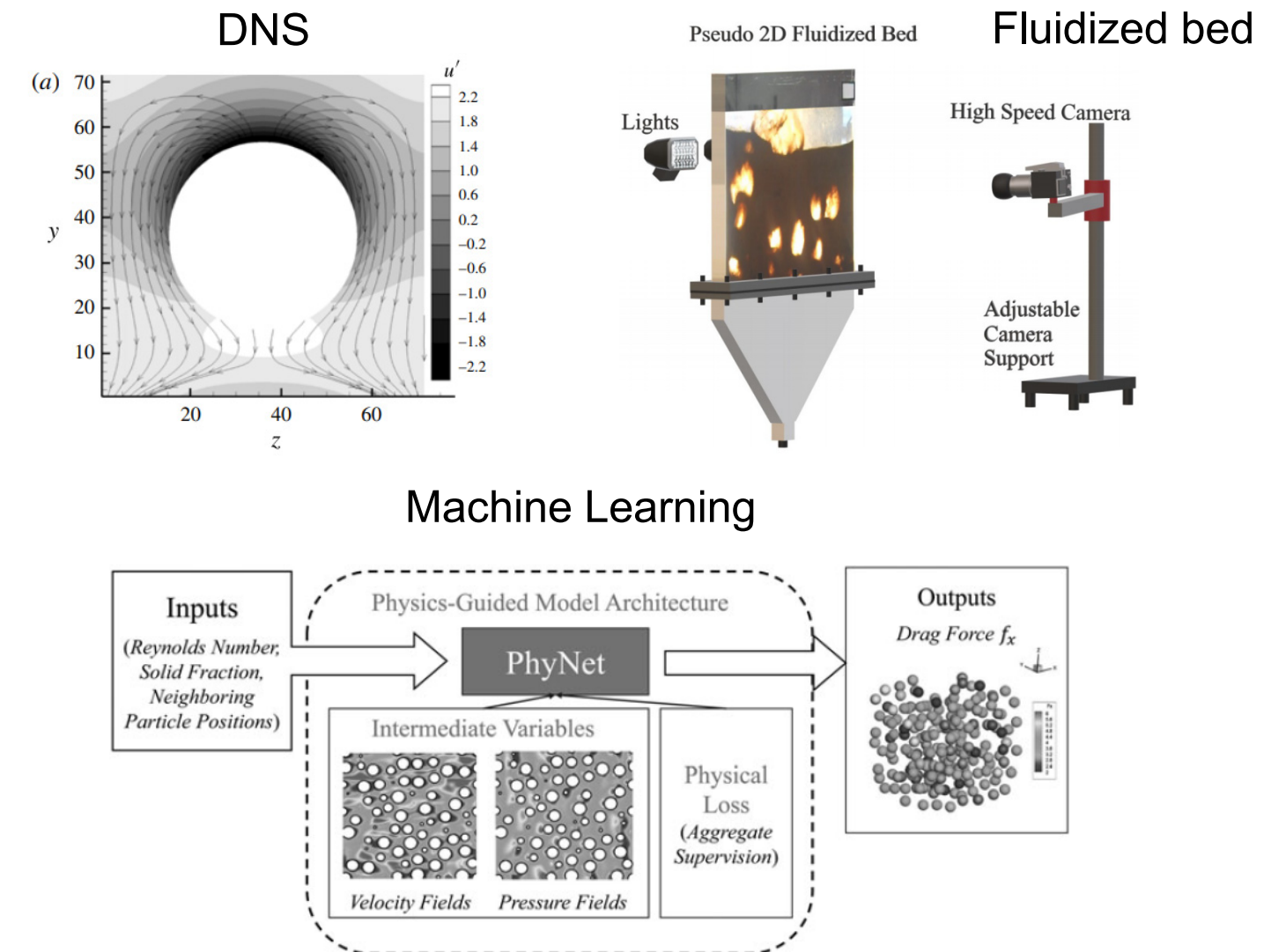
- **Project Description and Objectives**
- **Project Update**
- **Preparing Project for the Next Steps**
- **Concluding Remarks**



## Gas-Solid system



## Interaction forces



Liang-Shih Fan, Principles of gas-solid flows (1999)

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)

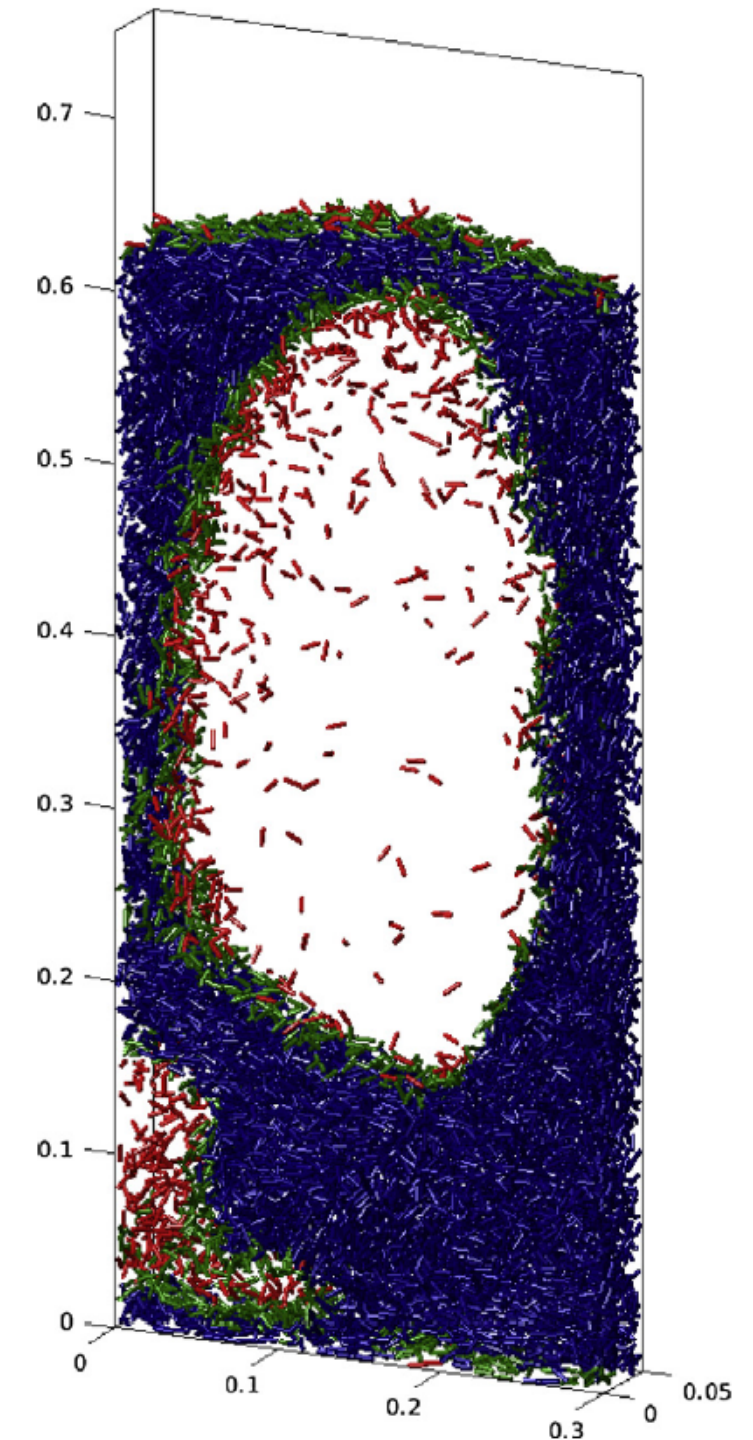
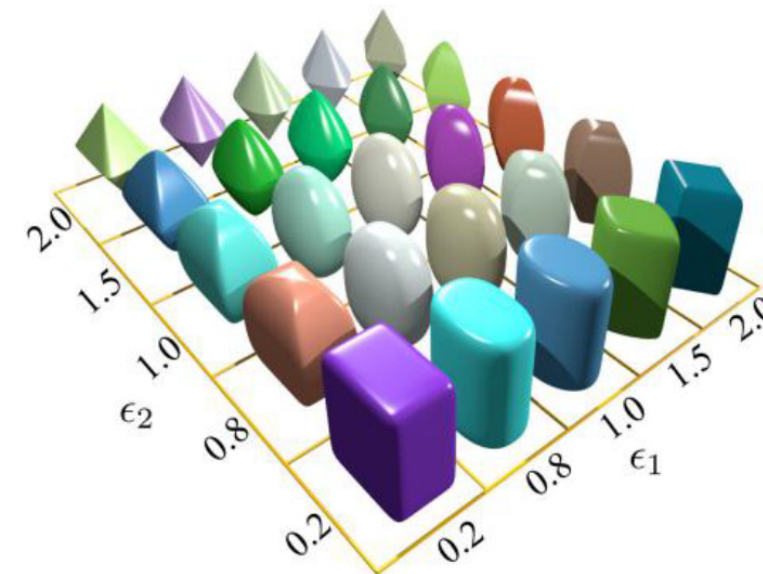


## Non-spherical particle

- 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-nonlinearity.

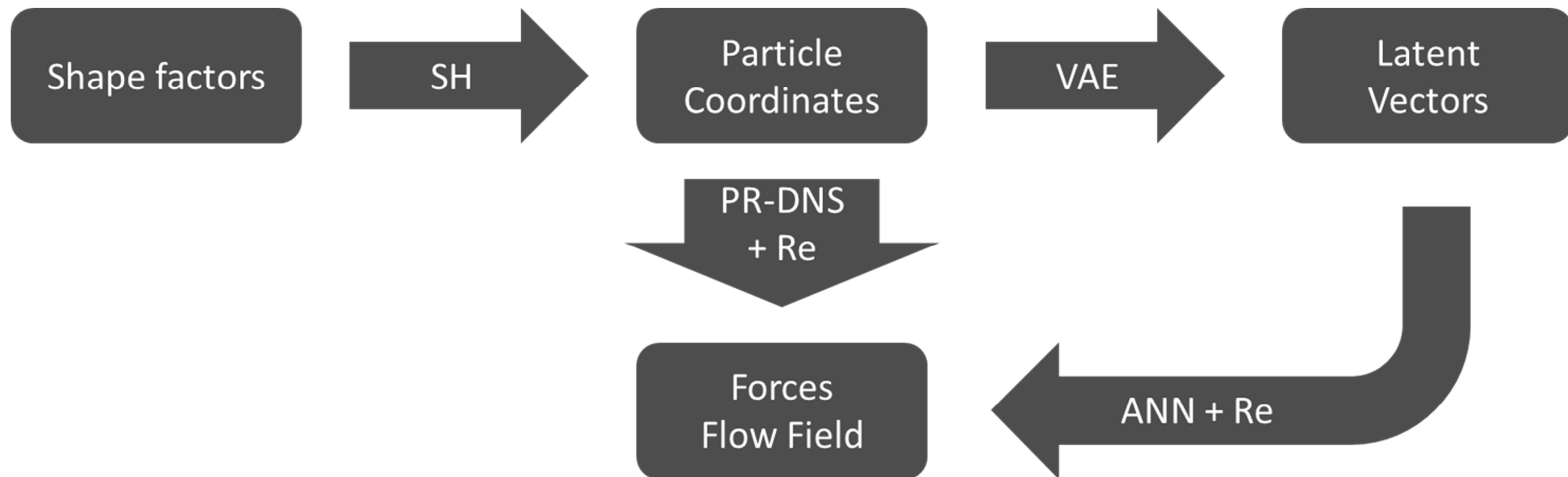
## Objectives

- 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)



SH : Spherical Harmonic method

VAE : Variational Auto-Encoder

PR-DNS : Particle Resolved Direct Numerical Simulation

ANN : Artificial Neural Network





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												
High Re data Collection												
MLP Training												

Current stage

Preliminary tests

## Spherical Harmonic Method

- Spherical harmonic functions

$$\begin{pmatrix} x(\theta, \phi) \\ y(\theta, \phi) \\ z(\theta, \phi) \end{pmatrix} = \begin{pmatrix} \sum_{l=1}^{l_{max}} \sum_{m=-l}^l C_{x,l}^m Y_l^m(\theta, \phi) \\ \sum_{l=1}^{l_{max}} \sum_{m=-l}^l C_{y,l}^m Y_l^m(\theta, \phi) \\ \sum_{l=1}^{l_{max}} \sum_{m=-l}^l C_{z,l}^m Y_l^m(\theta, \phi) \end{pmatrix}$$

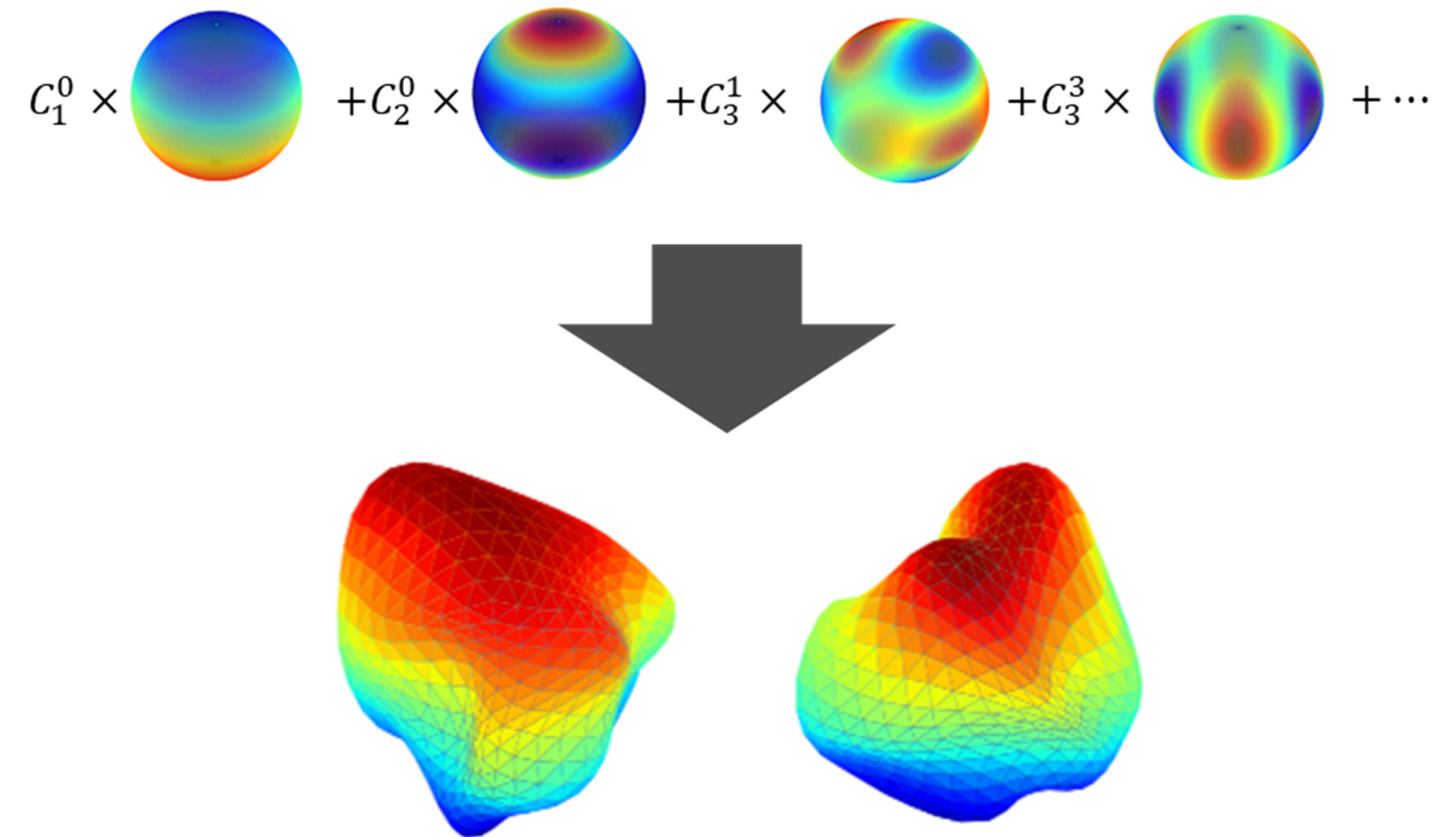
- Few shape factors

$d$  : spherical descriptor, roughness

$El$  : elongation index

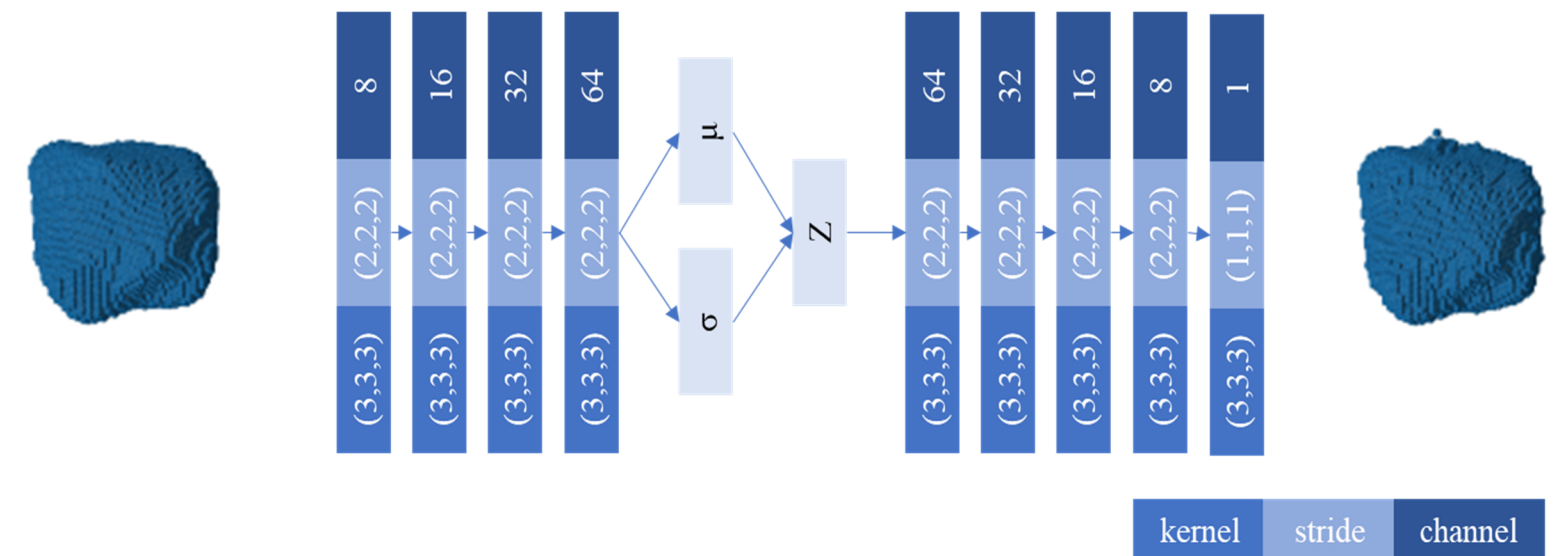
$Fl$  : flatness index

- Randomness



## Variational Auto-Encoder

- Voxel input
- Deep CNN layers with ELUs
- Latent vectors with 128 dimension
- 1,200 datasets to train, 400 datasets to validate
- Less than 1% reconstruction error
- For the DNS, new 5,200 particles were generated (error < 1%)



Training  
Input



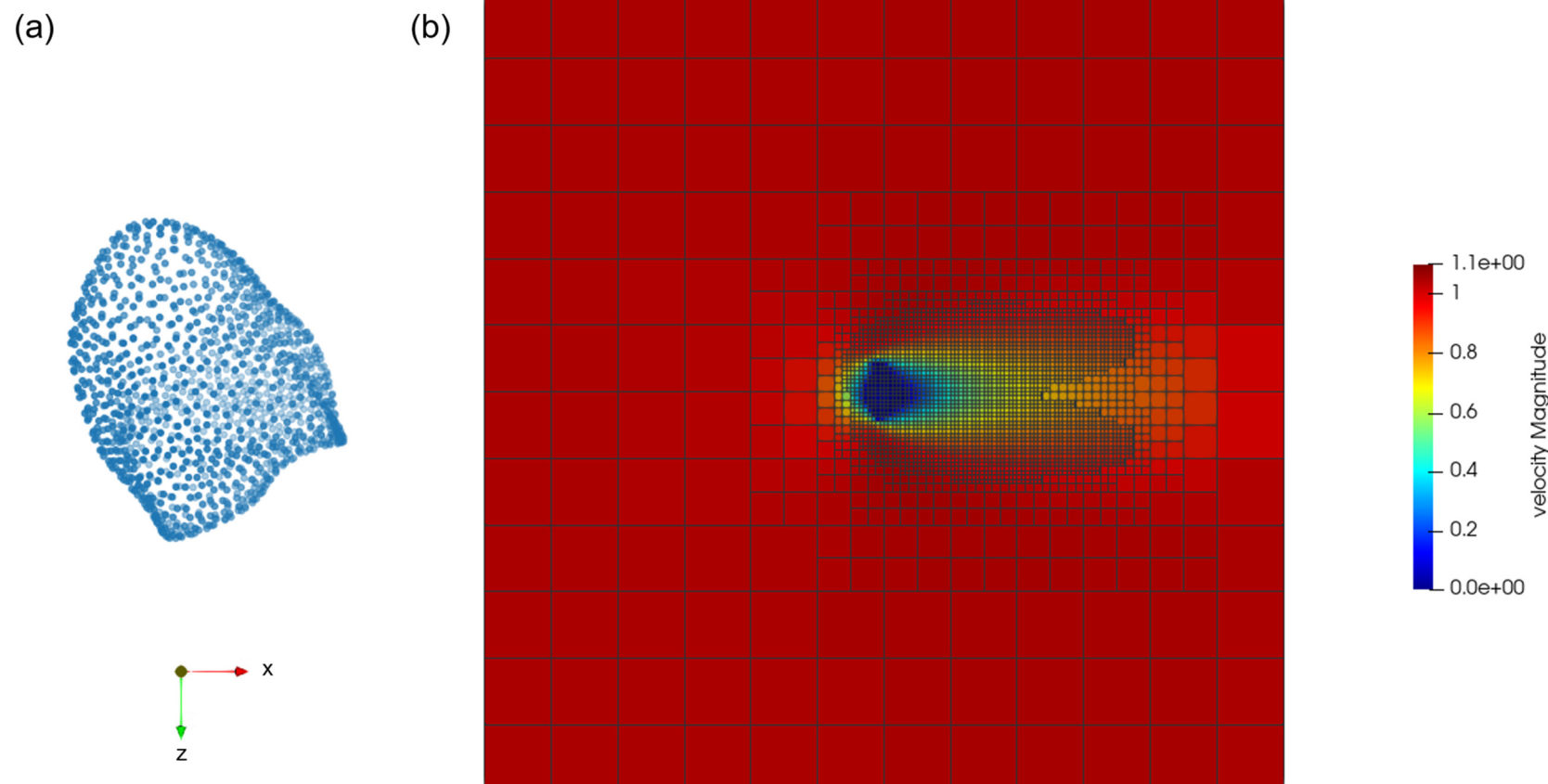
Decoded  
Output





## PR-DNS Development

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



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

$$f = g - \tau \frac{Df}{Dt} = g - \tau \frac{D}{Dt} (g + f^{neq})$$

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

$$F = \int f(0, t) v \Xi dv, \quad \Xi = \begin{pmatrix} 1 \\ v \end{pmatrix}$$

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

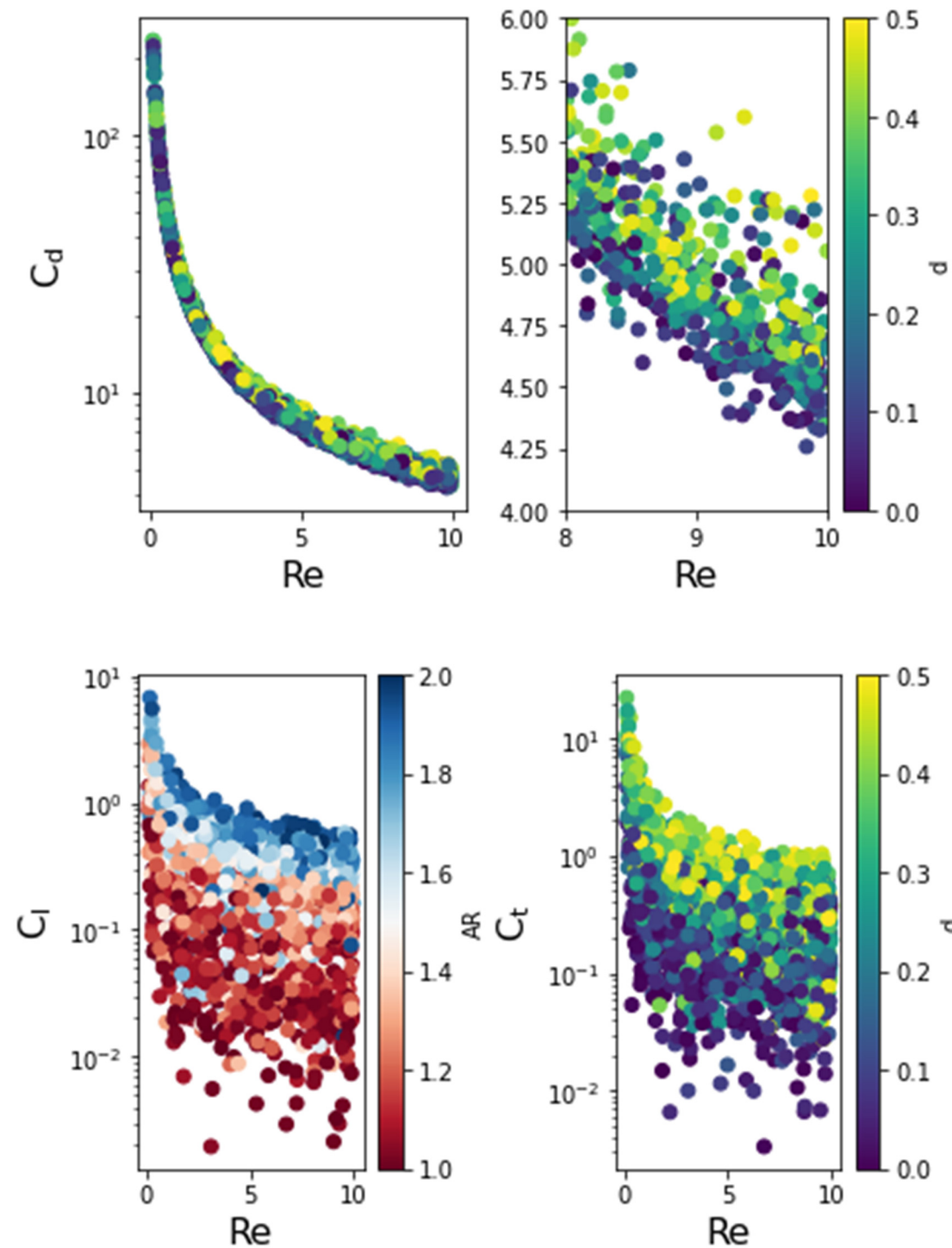
$$\frac{\partial W}{\partial t} + \nabla \cdot F = 0, \quad W = \begin{pmatrix} \rho \\ \rho u \end{pmatrix}$$

## PR-DNS Results

- $Re = 0.1 \sim 10$
- 5,200 datasets in low Re regime
- Show the typical  $Re-C_D$  trend
- MSEs for drag, lift, torque coefficients 380, 0.15, 0.61, respectively
- $C_d$  and  $C_t$  depend on  $d$
- $C_l$  depends on AR

$$C_d = \frac{24}{Re} + \frac{4}{\sqrt{Re}} + 0.4 \quad (1)$$

A.A. Kaskas, dissertation (1970)





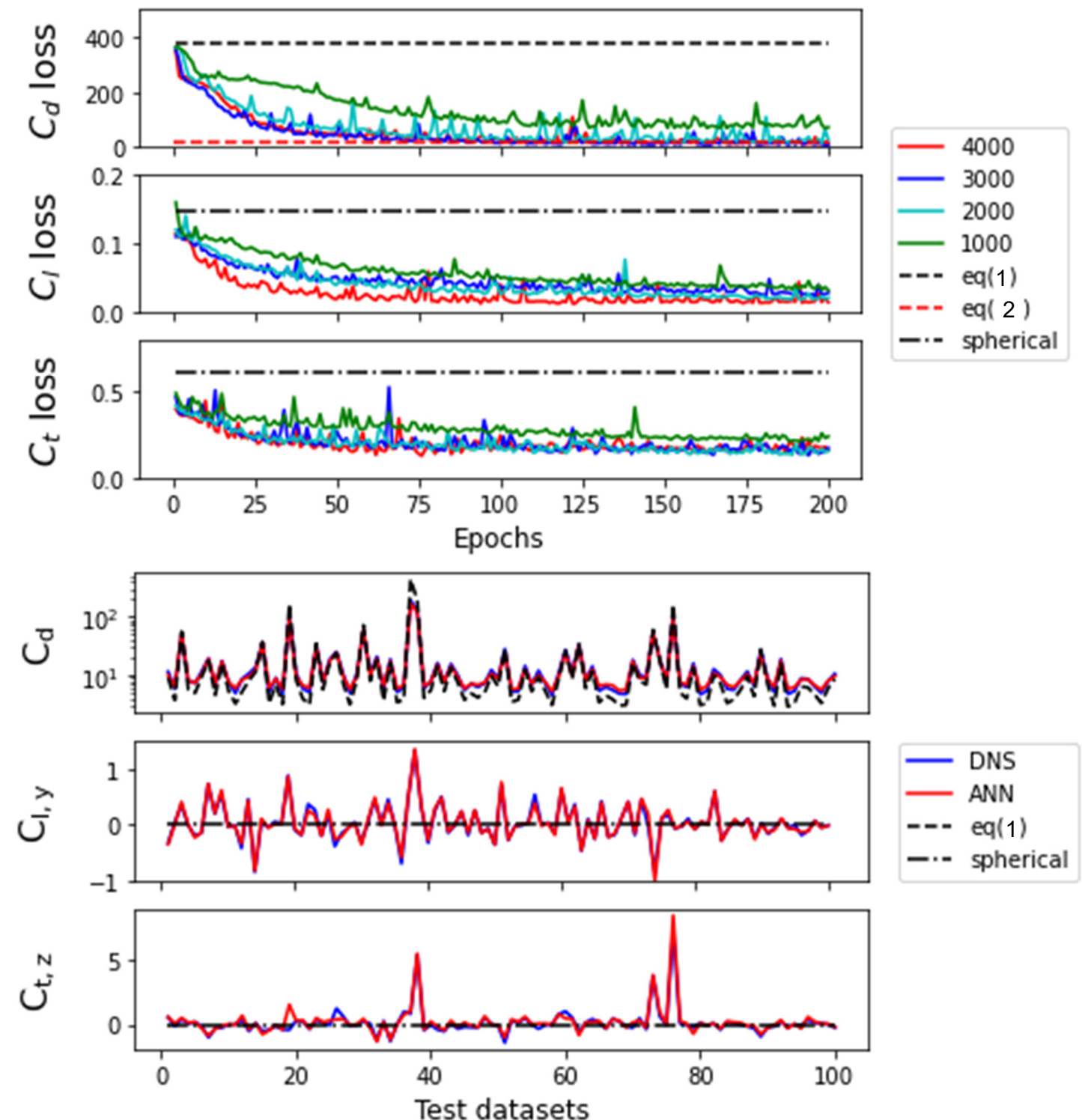
## ANN results

- 1,000~4,000 datasets for training and 600 datasets for validation and evaluation
- Two hidden layers with 32, 8 nodes
- MSEs for drag, lift, torque coefficients are reduced to 3%, 7%, 25%, respectively
- MSEs for eq (2) is 21.8 which is comparable to the ANN result ( $12.7 \pm 2.7$ )

$$C_d = \frac{24}{ReK_1} \{1 + 0.1118(ReK_1K_2)^{0.6567}\} + \frac{0.4305K_2}{1 + \frac{3305}{ReK_1K_2}} \quad (2)$$

$$K_1 = \left[ \left( \frac{d_n}{3D_{eq}} \right) + 2/3\psi^{-0.5} \right]^{-1}, \quad K_2 = 10^{1.8148(-\log\psi)^{0.5743}}$$

G.H. Gamer, Powder Technology. 77 (1993)





## ANN results

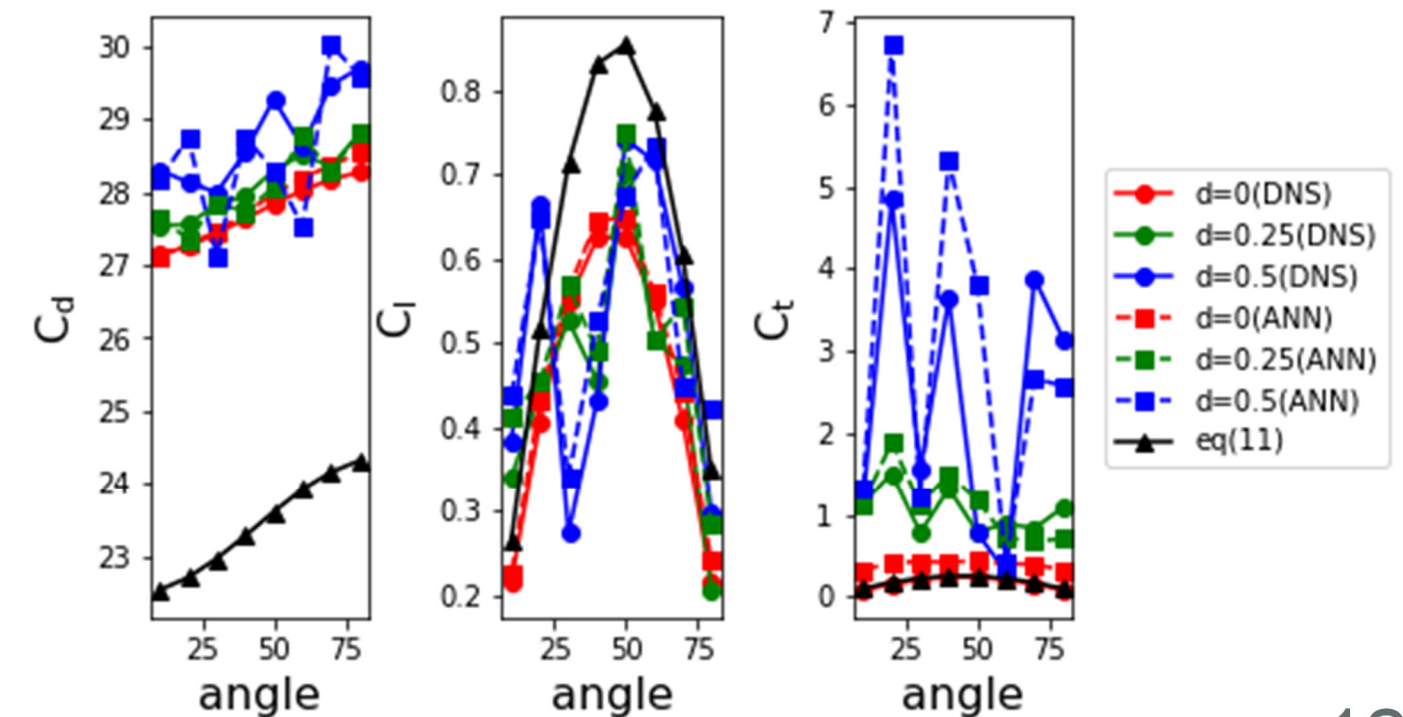
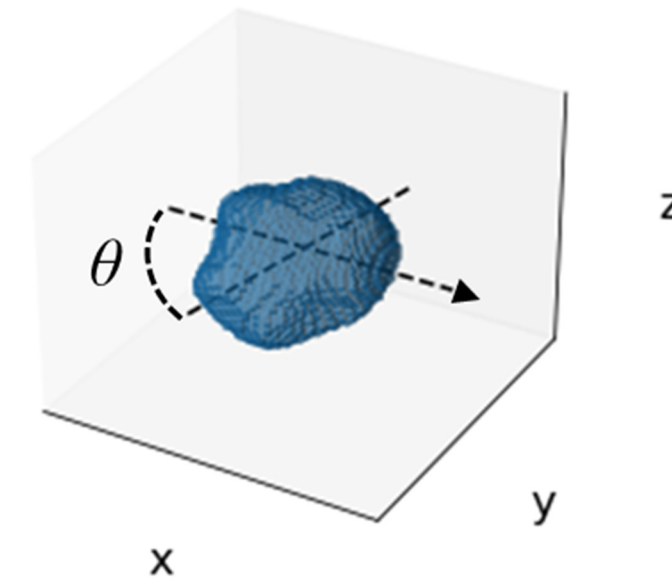
- 3 particles ( $d = 0, 0.25, 0.5$ )
- More accurate prediction on the lifting force and torque coefficients.

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

$$C_l = \left( \frac{b_1}{Re^{b_2}} + \frac{b_3}{Re^{b_4}} \right) \sin^{b_5+b_6 Re^{b_7}}(\theta) \cos^{b_8+b_9 Re^{b_{10}}}(\theta) \quad (3)$$

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

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





## Market Benefits/Assessment

MFiX only provides the drag force model for spherical particles

Industrial CFD application requires the comprehensive interaction force model

## Technology-to-Market Path

This project will provide the interaction force model including lifting force and torque which can be implemented in MFiX

Data for the higher Re regime will be collected

Multi-particle system will be studied to predict the interactive force for the dilute and dense system.





- This study provide the interaction force model for the non-spherical particle which is practical in industry.
- In MFiX-DEM, the NN based force can be implemented to obtain the interaction forces.
- Wider range of  $Re$  will be studied and the neighboring effect will be included in the future work for the multi-particle system.



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