Development and Evaluation of a General Drag Model for Gas-Solid Flows via Deep learning

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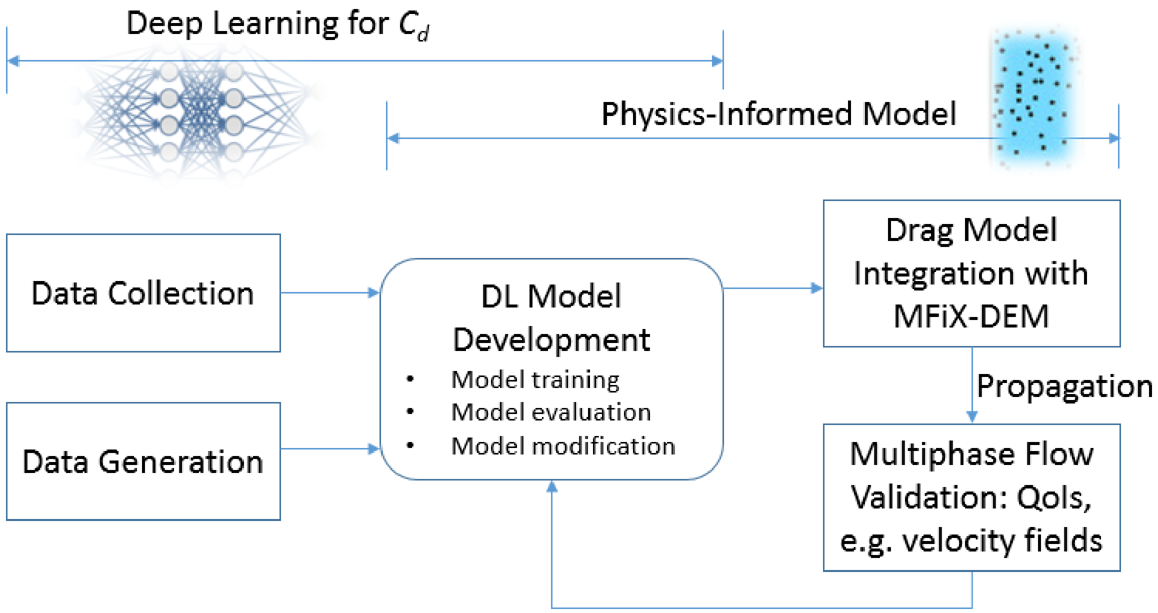
Agenda

- Project Objective
- Project Status
- Technical Progress
  - Background/Motivation for the Project
  - Data collection and Features identification
  - Gated DNN modeling
  - Integration with MFiX
  - Fluidized bed study
  - Volume fraction DNN
  - Fortran-PyTorch Library
  - Fluidized bed Simulations
  - Volume Fraction study for additional data
- Conclusions
- Path Forward

Project Objective

The overall objective of this project is to develop, test, and validate a general drag model for multiphase flows in assemblies of non-spherical particles by a physics-informed deep machine learning (PIDML) approach using artificial neural network (ANN).

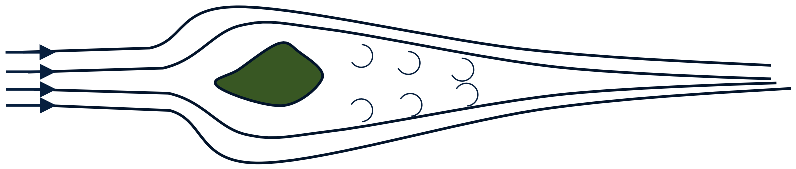


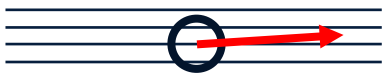
CFD Software

Project Status

Task Name	Assigned Resources	Year 1				Year 2				Year 3			
		Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4
Task 1.0 - Project Management and Planning	**PI**												
Task 2.0 - Data Collection and Generation	**Team**												
Subtask 2.1 Data Collection	Team												
Milestone A													
Subtask 2.2 Data Generation	Co-PI												
Milestone B													
Decision Point 1	Team												
Task 3.0 - ANN Model Development	**Co-PI**												
Subtask 3.1 ANN Model Training & Test	Co-PI												
Milestone C													
Subtask 3.2 ANN Algorithm Evaluation	Team												
Milestone D													
Decision Point 2	Team												
Task 4.0 - Drag Model Integration	**Team**												
Milestone E													
Decision Point 3	Team												
Task 5.0 - Multiphase Flow CFD Validation	**Team**												
Subtask 5.1 Multiphase Flow Validation	PI												
Milestone F													
Subtask 5.2 ANN Model Modification	Co-PI												
Milestone G													

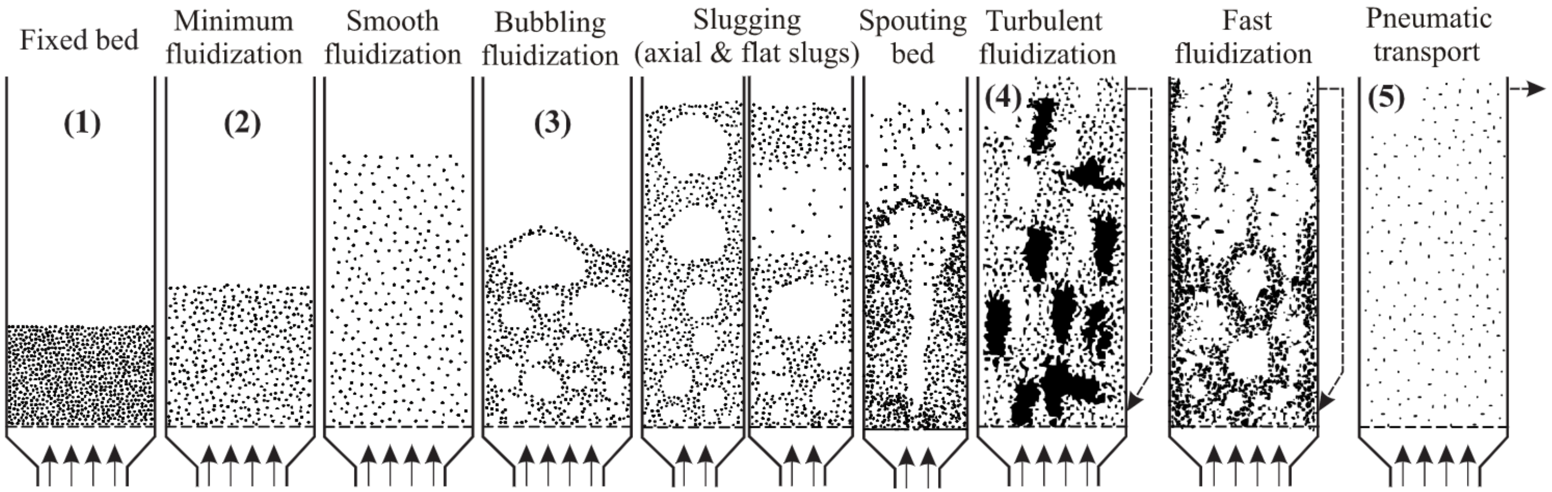
Motivation





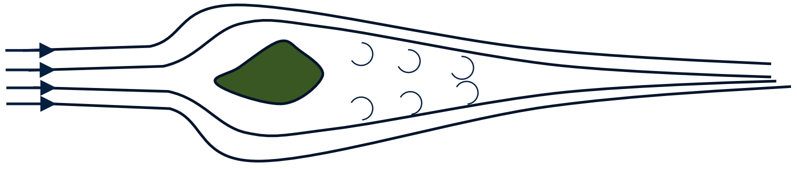
$$F = \frac{1}{2}\rho v^2 S C_D$$

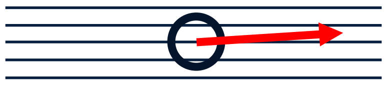
1. Energy industry
   - Gasifiers
   - Combustion
   - CO_2 capture
2. Food industry
3. Chemical process

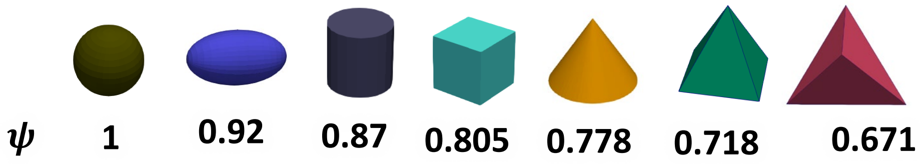


Alobaid, F., Almohammed, N., Farid, M.M., May, J., Rößger, P., Richter, A. and Epple, B., 2022. Progress in CFD simulations of fluidized beds for chemical and energy process engineering. *Progress in Energy and Combustion Science*, *91*, p.100930.

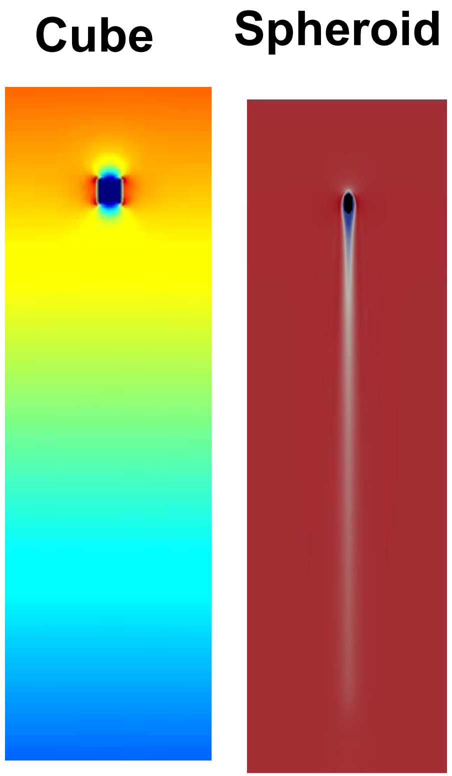
Motivation

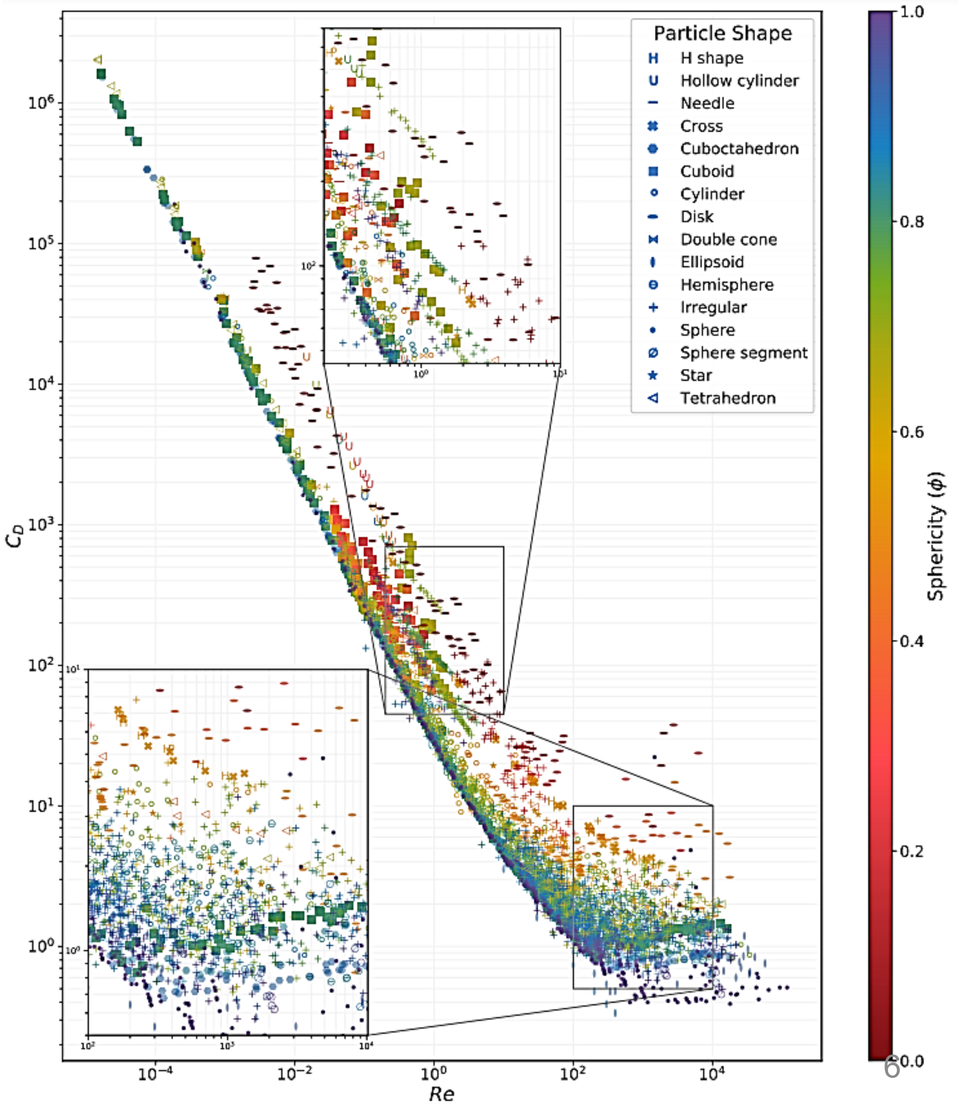






- The drag coefficient primarily depends on
  - Shape
  - Reynold number
- The variations are highly non-linear
- Single correlation cannot cover all the particles
- Requires more sophisticated modelling such as Neural network





Current State-of-the-Art

RMSE

Haider & Levenspiel (1989)

$$C_D = \frac{24}{Re}(1 + 8.1716\exp(-4.0655\psi) * Re^{0.0964+0.5565\psi} + 73.69 * Re * \frac{\exp(-5.0748\,\psi)}{Re + 5.378\exp(6.2122\,\psi)}$$

37

Yow et al. (2005)

$$C_D = \frac{a_1}{Re} + \frac{b_1}{\sqrt{Re}} + c1$$

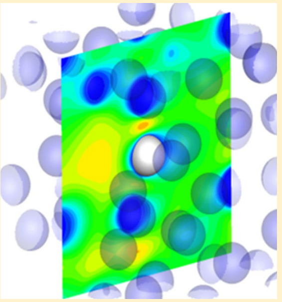
200

Hölzer & Sommerfeld (2008)

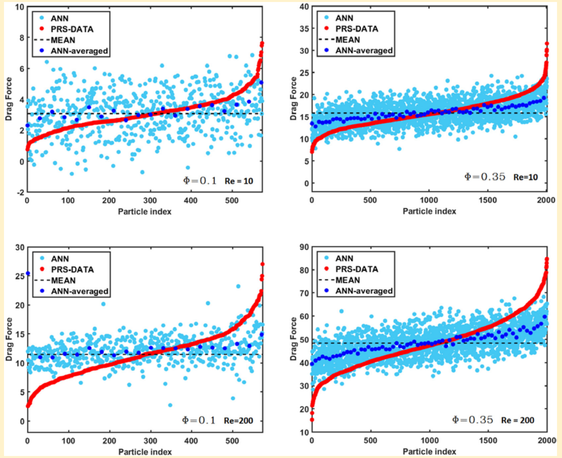
$$C_D = \frac{8}{Re}\frac{1}{\sqrt{\psi_{||}}} + \frac{16}{Re}\frac{1}{\sqrt{\psi}} + \frac{3}{\sqrt{Re}}\frac{1}{\psi^{3/4}} + 0.421^{0.4(-\log\psi)^{0.2}}\frac{1}{\psi_{\perp}}$$

55

He & Tafti (2019)

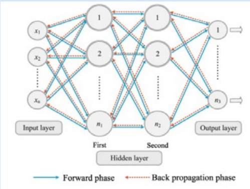


Nearest Particles' location

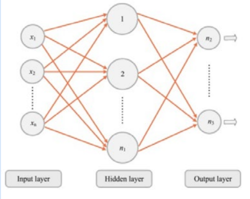


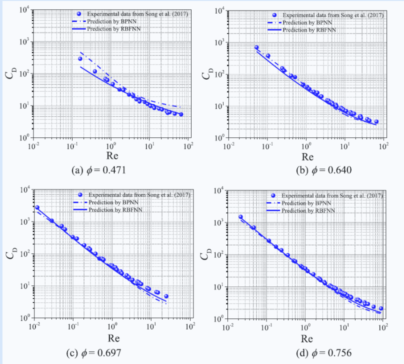
Yan et al. (2019)

BPNN



RBFNN



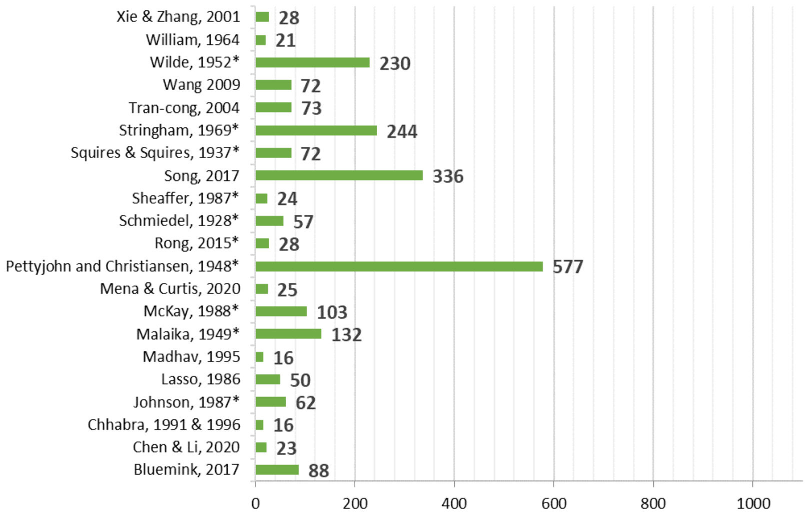


$$\lg C_D = A_0 + A_1 \lg \mathrm{Re} + A_2(\lg \mathrm{Re})^2 + A_3(\lg \mathrm{Re})^3 + A_4(\lg \mathrm{Re})^4$$

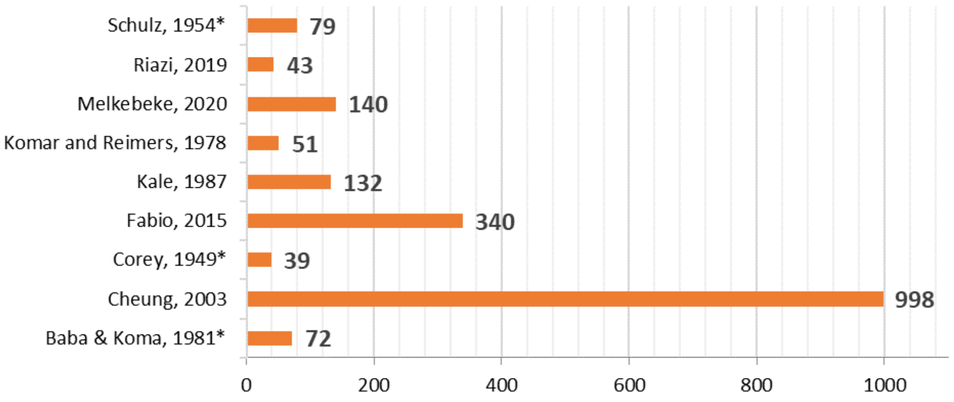
Existing drag models have large errors and narrow range of applications

Data collection and Features identification (Task 2)

Regular-shaped Particles (Total: 2277)



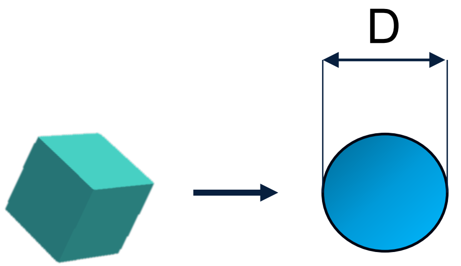
Irregular-shaped Particles (Total: 1894)



1. Reynold number (Re)
2. Sphericity (ψ)
3. Fixed Crosswise Sphericity ($\psi_\perp$)
4. Fixed Lengthwise Sphericity ($\psi_\parallel$)
5. Aspect ratio (AR)

$$\psi = \frac{\pi D^2}{Surface\ area\ of\ the\ particle\ (A_s)}$$

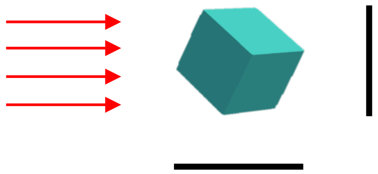
$$AR = \frac{Longest\ side}{Smallest\ side}$$



Volume Equivalent Sphere

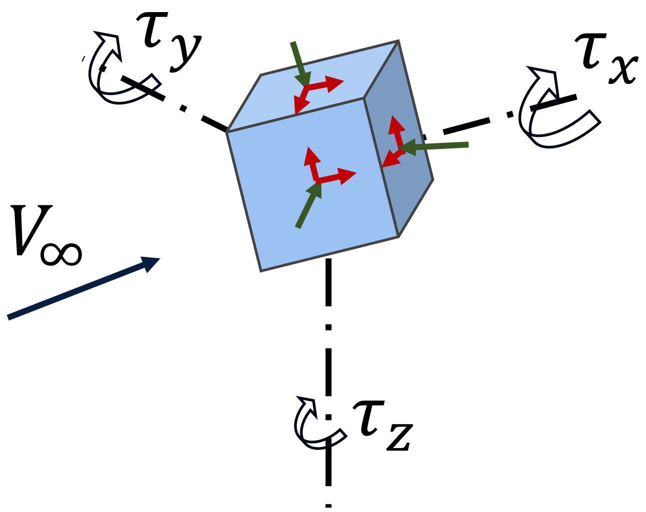
$$\psi_\perp = \frac{0.25\pi D^2}{Projected\ area\ \ perpendicul\ to\ the\ flow}$$

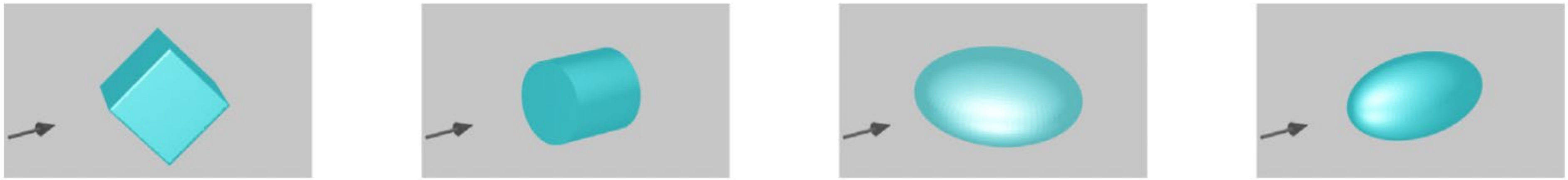
$$\psi_\parallel = \frac{0.25\pi D^2}{0.5A_s - Mean\ longitudinal\ projected\ area}$$



Projected Area

Settling Orientation Study

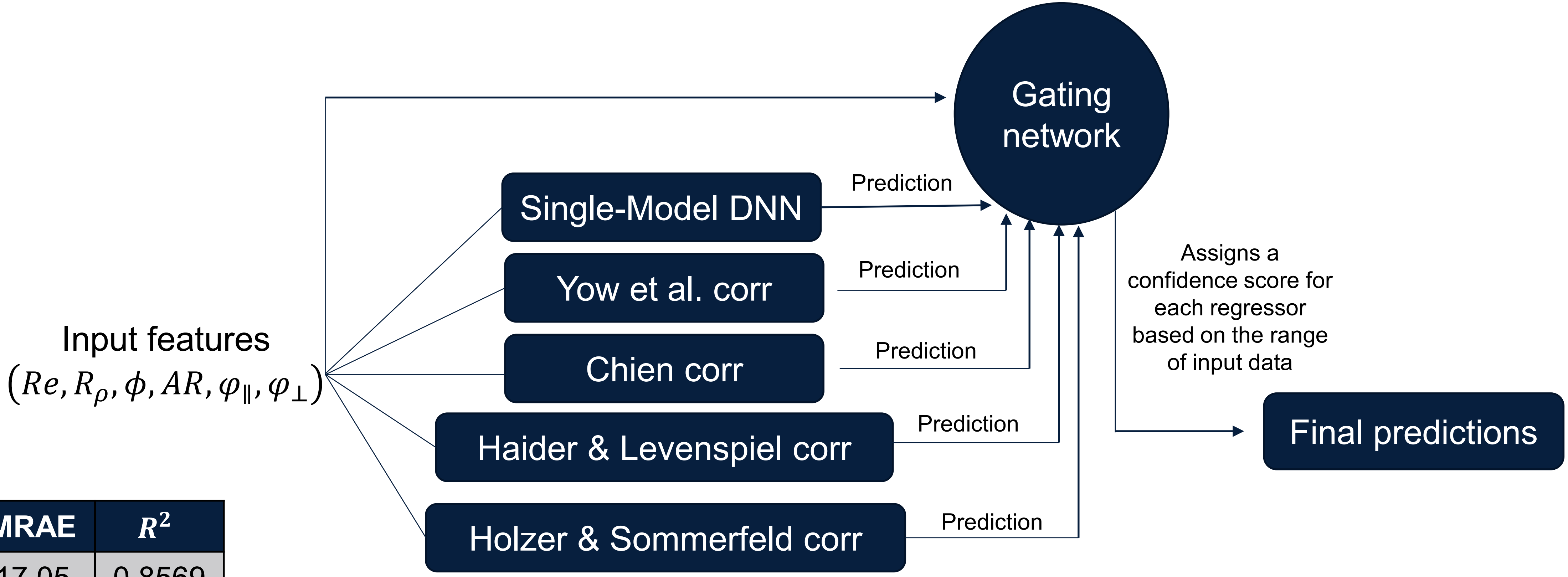




Final torque on the body is zero or oscillate with a fixed amplitude and frequency

Drag Coefficient Correlation-aided Deep Neural Network (DCC-DNN) (Task 3)

Mixture of Experts (MoE) Architecture



RMSE	MRAE	R^2
25.98	17.05	0.8569

Presa-Reyes, M., Mahyawansi, P., Hu, B., McDaniel, D. and Chen, S.C., 2024. DCC-DNN: A deep neural network model to predict the drag coefficients of spherical and non-spherical particles aided by empirical correlations. *Powder Technology*, *435*, p.119388.

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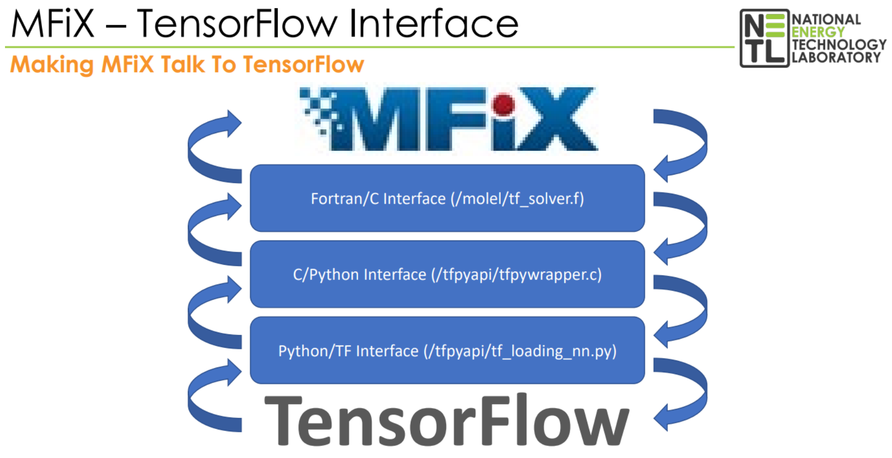
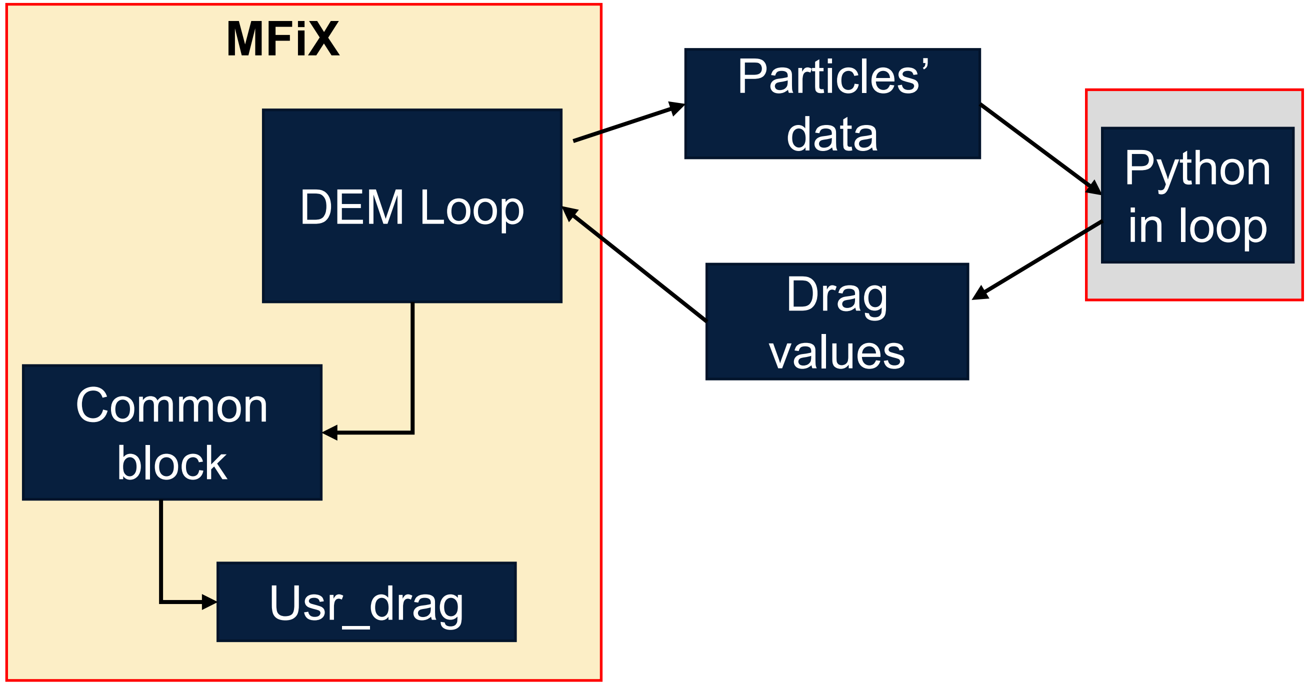
Makeshift Integration with CFD (MFiX)

1. MFiX is written on Fortran
2. Neural network model is written on Python



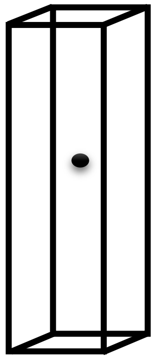


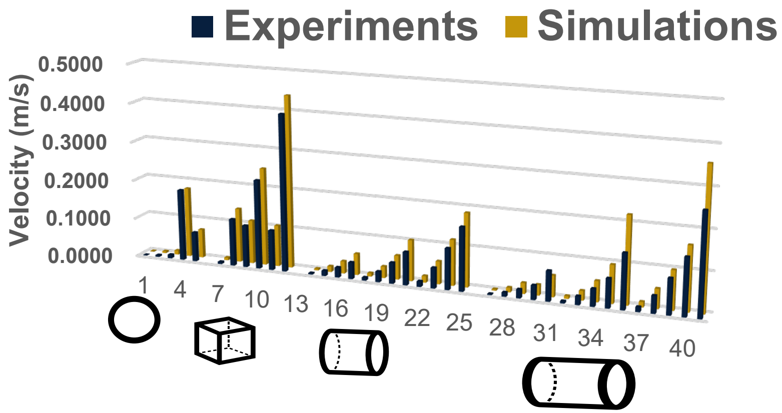
- **~11000 particles cost approximately 5 seconds to complete the DEM loop.**
- File writing takes place only once
- CFD of lab scale setup is practical
- Large scale can be time consuming

https://www.netl.doe.gov/sites/default/files/2020-11/UCR_HBCU_OMI/Dirk%20VanEssendelft%20Presentation-2020UCRHBCU_Kickoff_MFIXAI_Overview.pdf

Fluidized bed Simulation

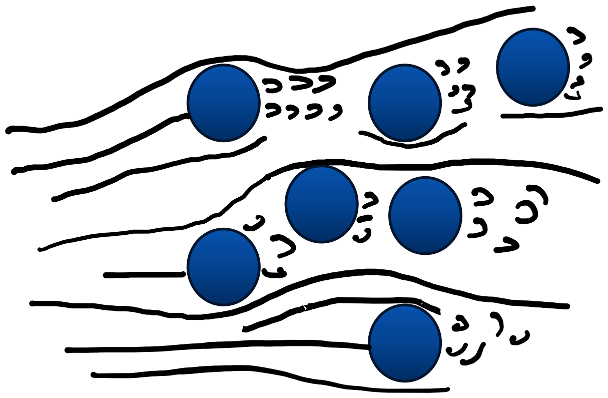
Single Particle settling



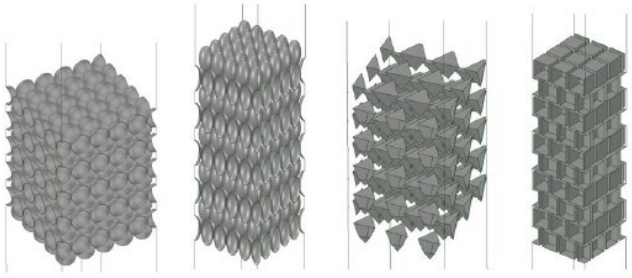


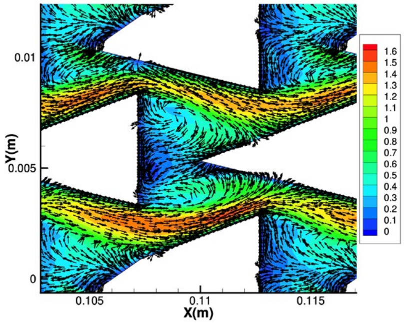
Assemblies of Particles

Fluidized Bed Exp

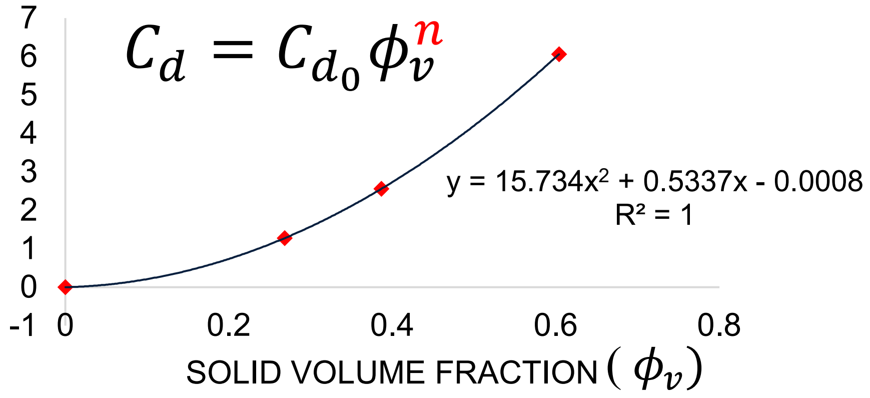


PR-DNS





Volume fraction correlation



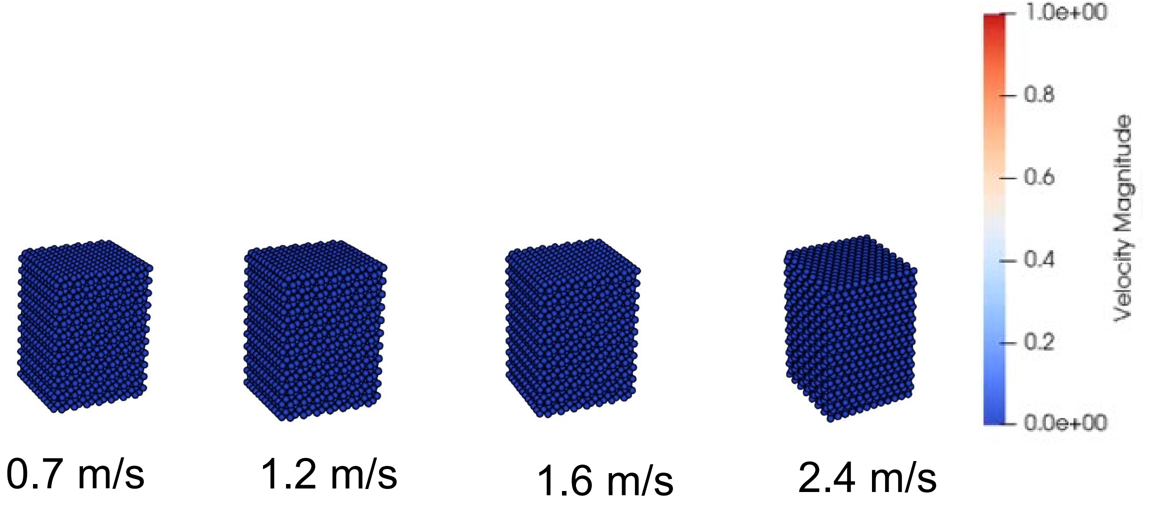
Mahyawansi, P. and Lin, C.X., 2021, August. An Investigation of the Effects of Volume Fraction on Drag Coefficient of Non-Spherical Particles Using PR-DNS. In *Fluids Engineering Division Summer Meeting* (Vol. 85284, p. V001T02A024). American Society of Mechanical Engineers.

Fluidized bed Simulation

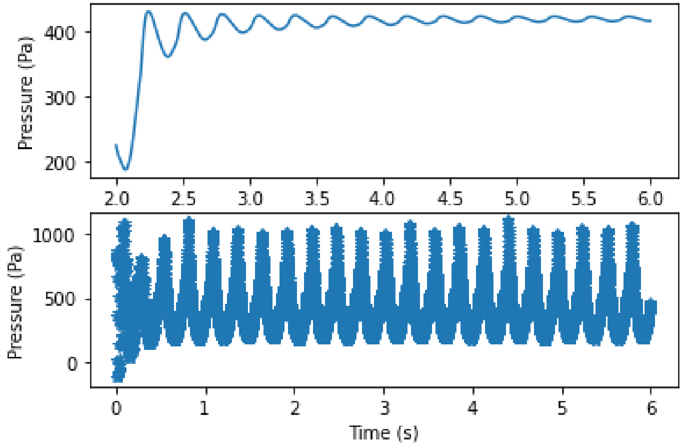
Vollmari's Fluidized bed Experiments

Shape	Sphere	Sphere	Ideal Cylinder	Cube	Cube
d_e–class [mm]	7	5	7	5	7
Size [mm]	7.2	5	6.1 6.2	4.2 4.3 4.5	5.2 6.3 6.3
ϕ [–]	1.00	1.00	0.87	0.81	0.80
ρ_p [kg/m³]	772.5	823.0	708.5	639.7	746.9
L_{fb} [mm] / $\bar{\varepsilon}$ [–]	95 0.40	88 0.40	98 0.36	98 0.37	103 0.43
Shape	Elongated Cylinder	Elongated Cuboid	Elongated Cuboid	Plate	Elongated Plate
d_e–class [mm]	7	5	7	5	5
Size [mm]	3.9 14.0	3.0 3.0 7.1	4.2 4.2 11.4	2.0 4.9 6.0	2.0 4.0 8.0
ϕ [–]	0.75	0.75	0.73	0.71	0.69
ρ_p [kg/m³]	764.4	745.6	639.7	754.1	756.6
L_{fb} [mm] / $\bar{\varepsilon}$ [–]	103 0.44	103 0.42	115 0.40	102 0.43	108 0.46
Shape	Elongated Cuboid	Plate	Elongated Plate		
d_e–class [mm]	5	7	7		
Size [mm]	2.0 3.0 11.0	2.2 9.0 9.8	2.0 6.0 14.9		
ϕ [–]	0.64	0.63	0.58		
ρ_p [kg/m³]	728.1	672.8	721.7		
L_{fb} [mm] / $\bar{\varepsilon}$ [–]	117 0.48	121 0.46	124 0.51		

MFiX Simulations

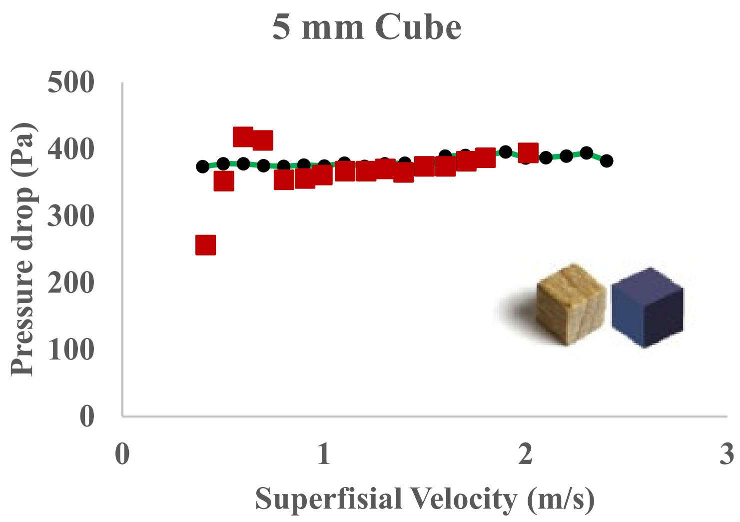


Pressure drop history

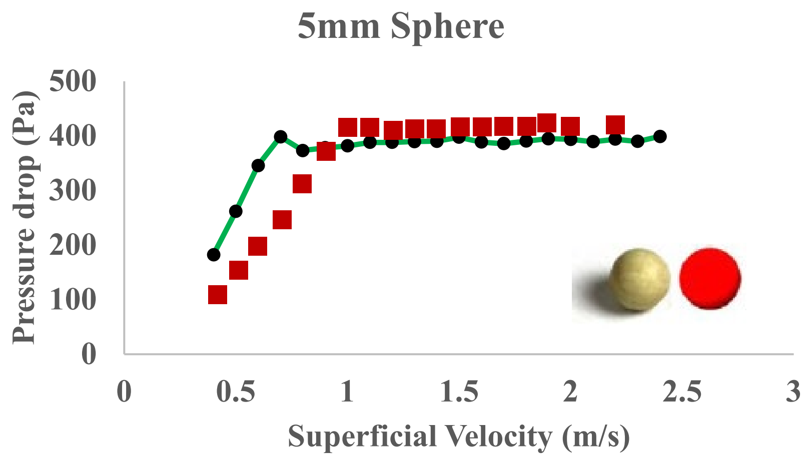


Vollmari, K., Jasevičius, R. and Kruggel-Emden, H., 2016. Experimental and numerical study of fluidization and pressure drop of spherical and non-spherical particles in a model scale fluidized bed. *Powder Technology*, *291*, pp.506-521.

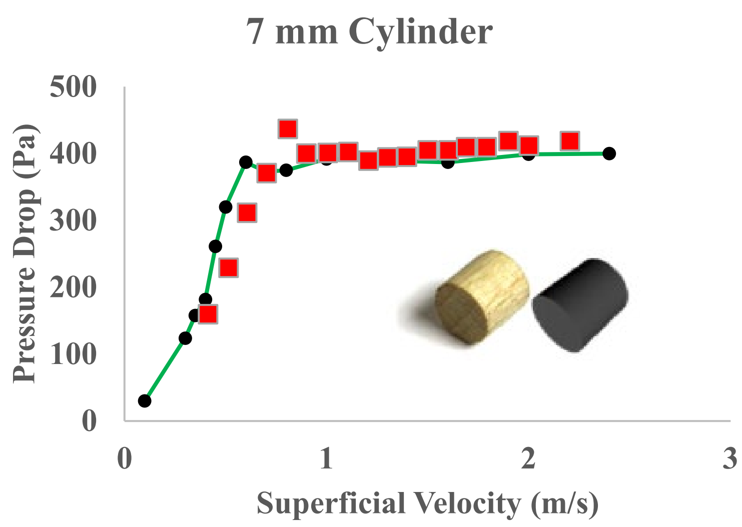
Results



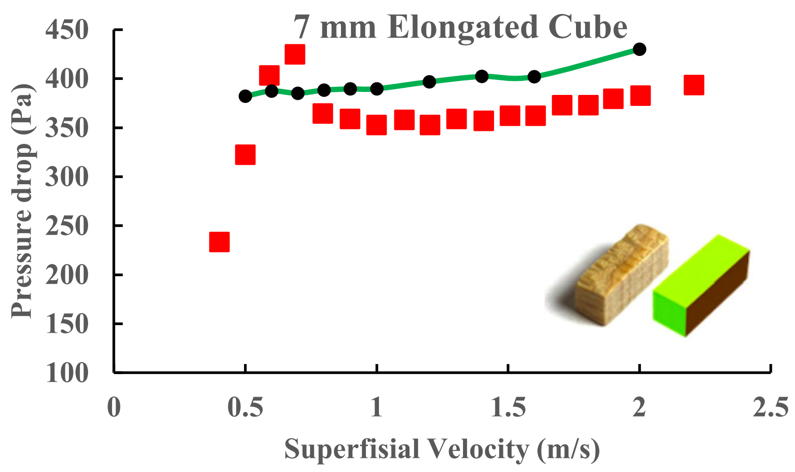
5 mm Cube
Pressure drop (Pa)
500
400
300
200
100
0
0
1
2
3
Superfisial Velocity (m/s)



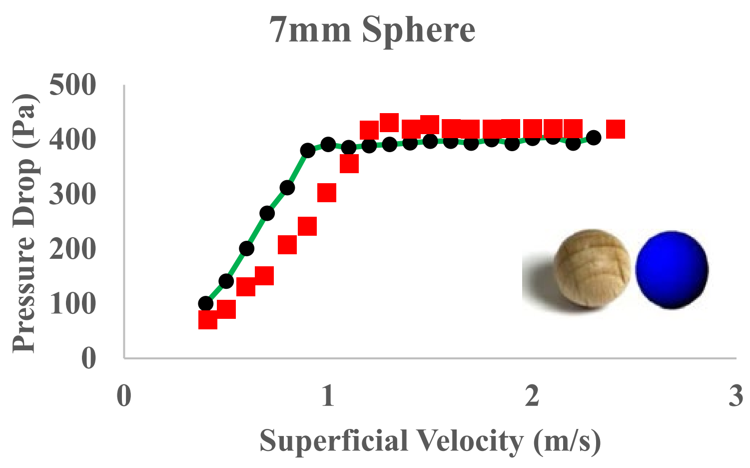
5mm Sphere
Pressure drop (Pa)
500
400
300
200
100
0
0
0.5
1
1.5
2
2.5
3
Superficial Velocity (m/s)



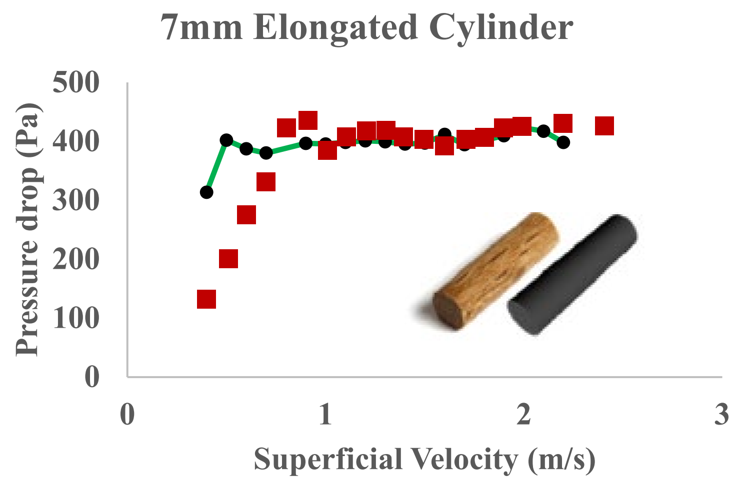
7 mm Cylinder
Pressure Drop (Pa)
500
400
300
200
100
0
0
1
2
3
Superficial Velocity (m/s)



7 mm Elongated Cube
Pressure drop (Pa)
450
400
350
300
250
200
150
100
0
0.5
1
1.5
2
2.5
Superfisial Velocity (m/s)

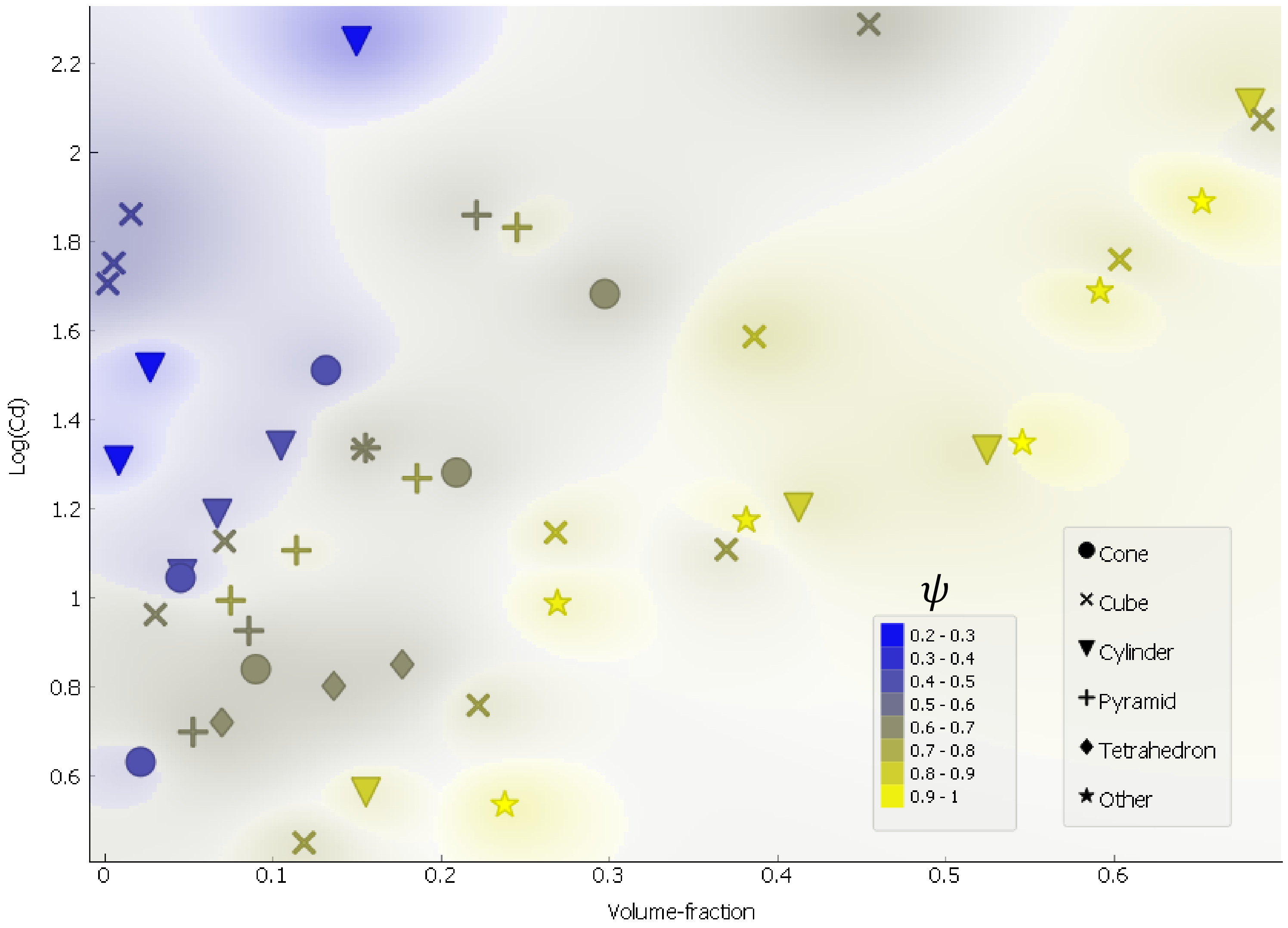


7mm Sphere
Pressure Drop (Pa)
500
400
300
200
100
0
0
1
2
3
Superficial Velocity (m/s)



7mm Elongated Cylinder
Pressure drop (Pa)
500
400
300
200
100
0
0
1
2
3
Superficial Velocity (m/s)

Effect of Volume Fractions on Drag for Re = 500



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Modelling Volume Fraction Using Neural Network

$Re, AR, \psi, R_\rho, \psi_\perp, \psi_{||}$

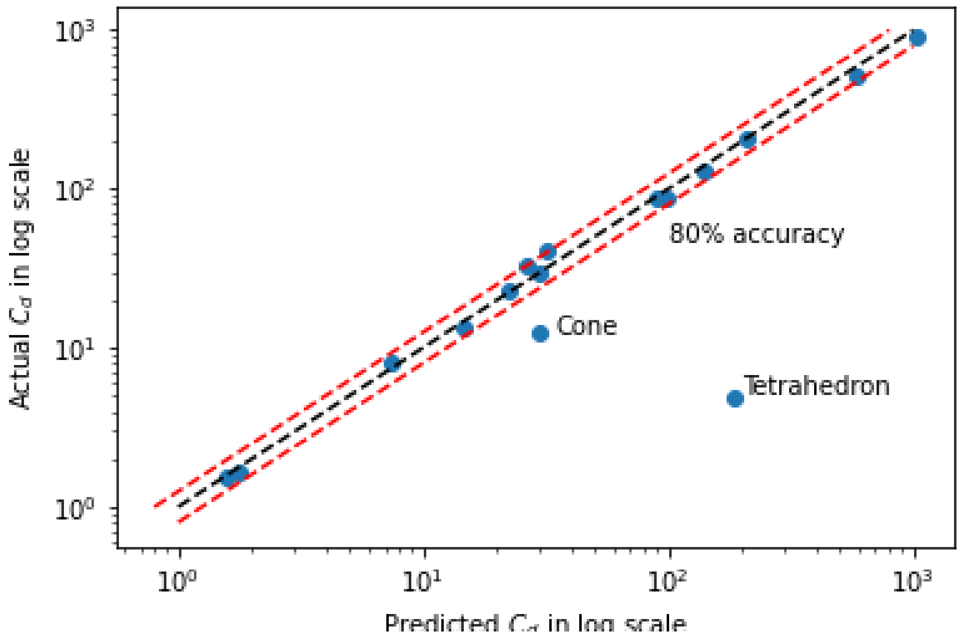
Deep Neural Network 1 (Mixture-of-Experts)

C_{d0} of a single particle

$C_{d0}, \phi_v, Re \; and \; \psi$

Deep Neural Network 2

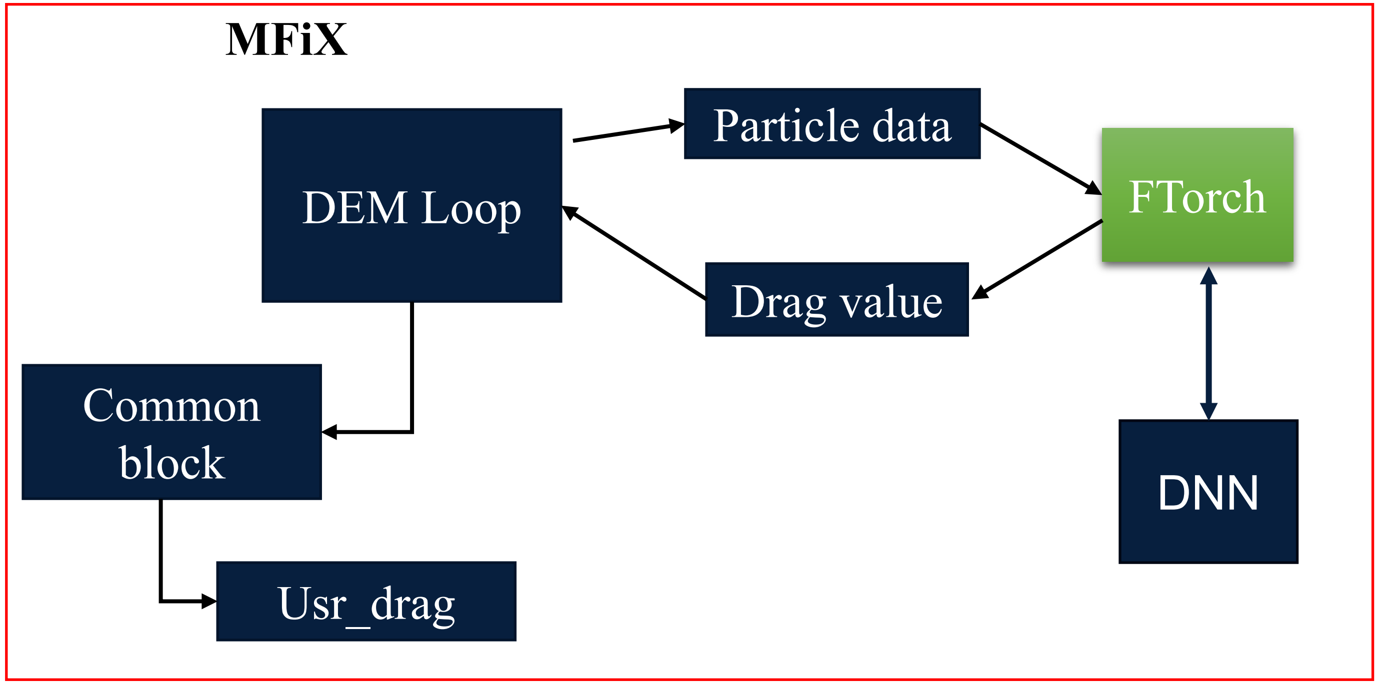
C_d for group of particles



Predicted vs. Actual scatter plot

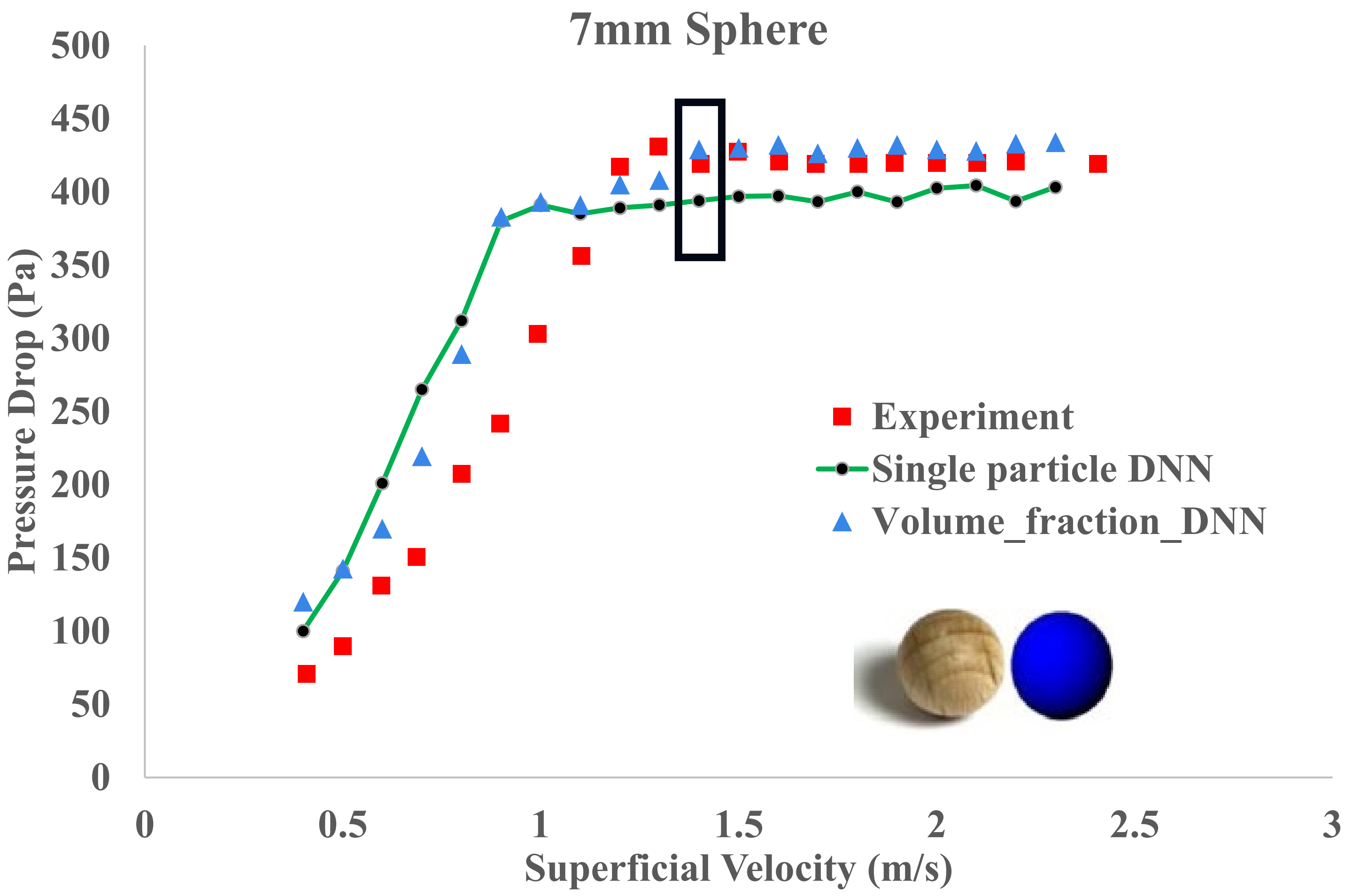
Final Integration with MFiX (Task 4)

- Fortran PyTorch Lib (Ftorch) is developed by Cambridge ICCS (Institute of computing and climate science)
- We compiled this library for MFiX and developed it.
- The complex DNN model is transferred using the tracing command.

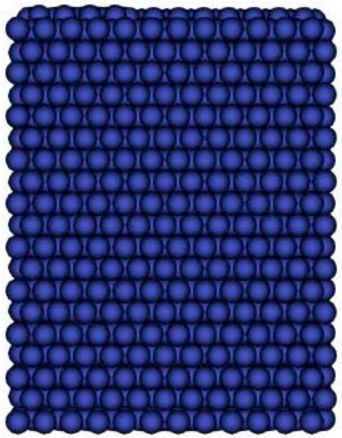


Methods	Simulation time
MFiX-Python file sharing method for each particle.	~30 days
MFiX-Python file sharing method for all particle together.	~1 day
MFiX-FTorch	< 2 hour

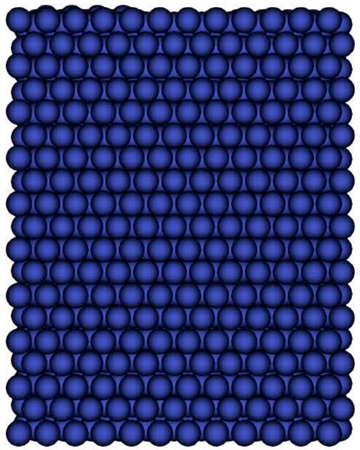
Result (Task 5)



For inlet velocity 1.4 m/s



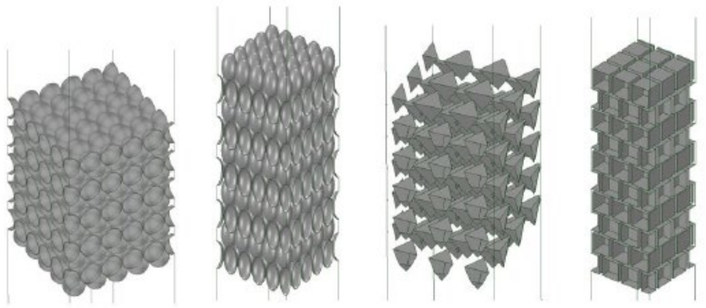
Volume Fraction

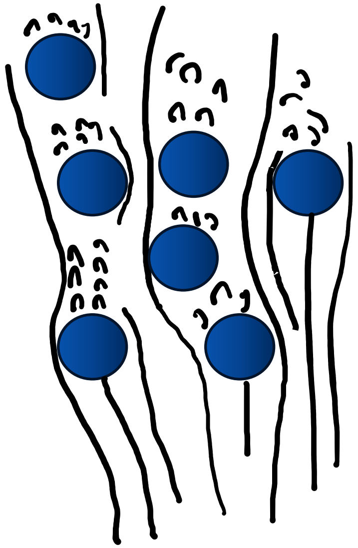


Single particle

Volume Fraction study for Additional data

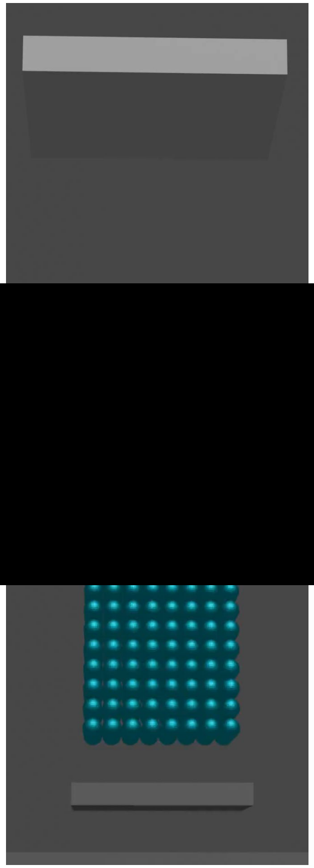
Physics Simulations → Fluidized particle arrangement → STL to CAD → Extract Volume fractions → Mesh → CFD Simulations → Extract Drag Force





Volume Fraction study for Additional data

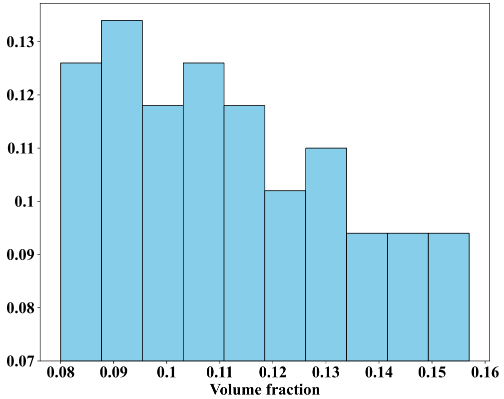
Physics Simulation



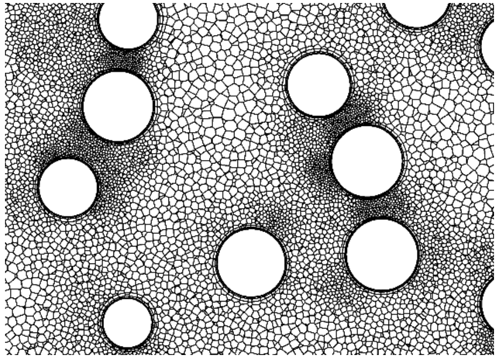
CAD

[redacted]

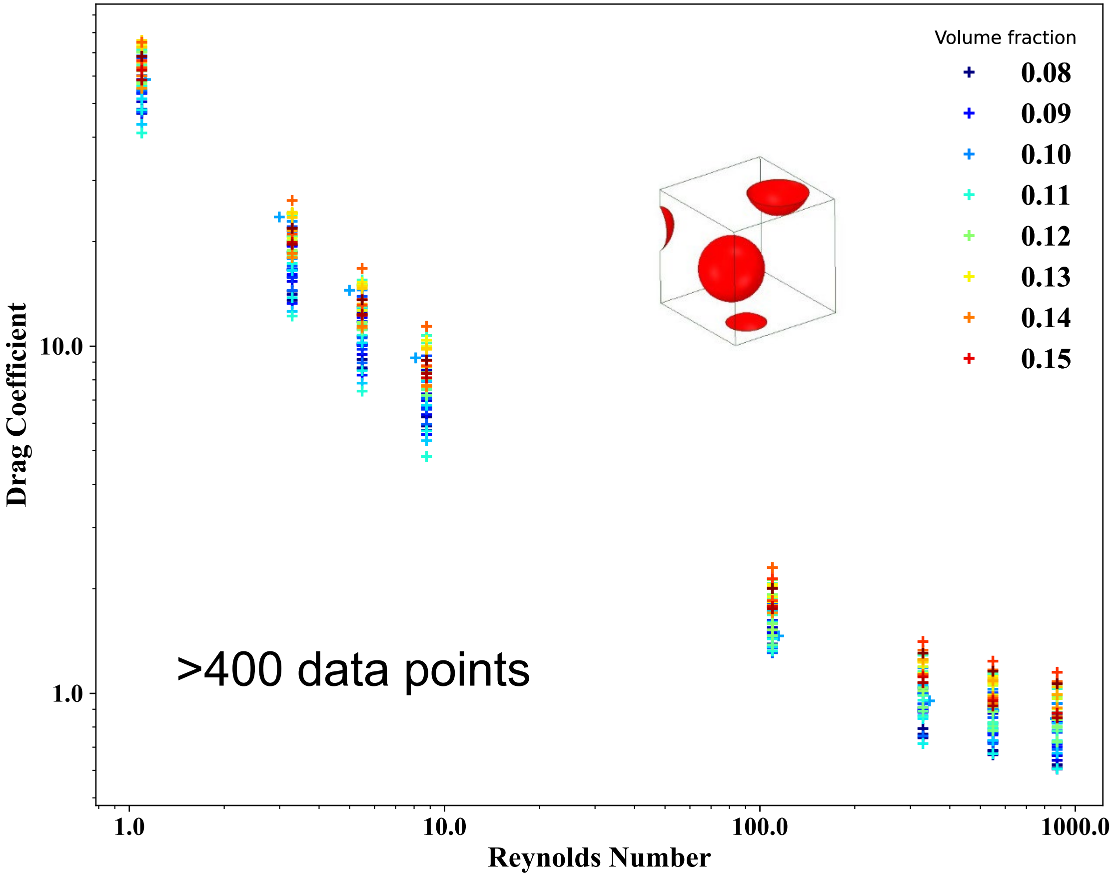
Histogram



Mesh



Drag Coefficient

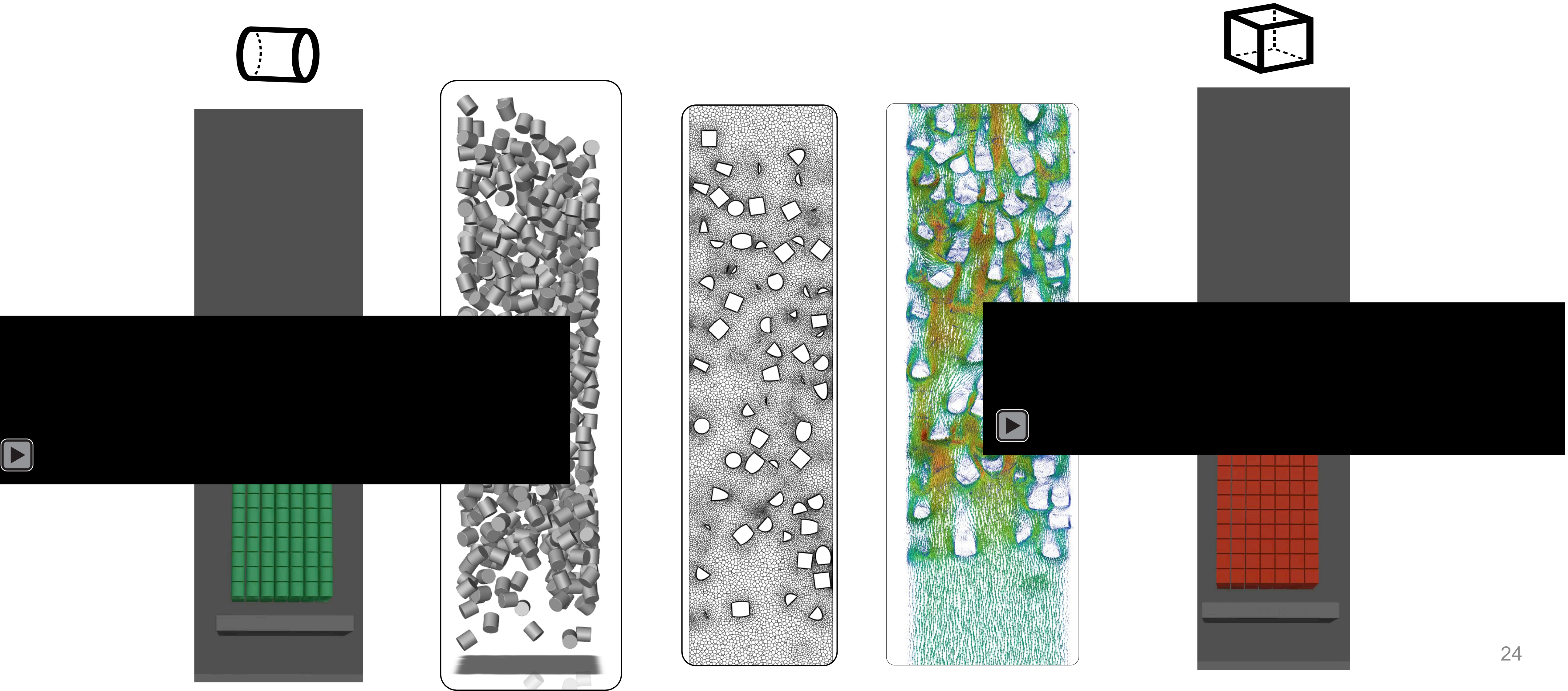


Blender Development Team. (2023). Blender (Version 3.6) [Computer software]. https:*//www.blender.org*

Conclusions

- Drag force on non-spherical particles depends on shape factor and Reynold number.
- Gated DNN model gives better predictions compared to previous correlations.
- DNN-assisted fluidized bed simulations shows excellent predictions in terms of pressure drop.
- The solid volume fraction effect are now accounted in the second level of DNN model.
- The volume fraction DNN have improved the prediction performance.
- Additional data for volume fraction is generated using PR-DNS of realistic arrangements of particles
- Physics simulations are effective in mimicking fluidized arrangement of particles.

Future Study



Acknowledgement

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Appendix

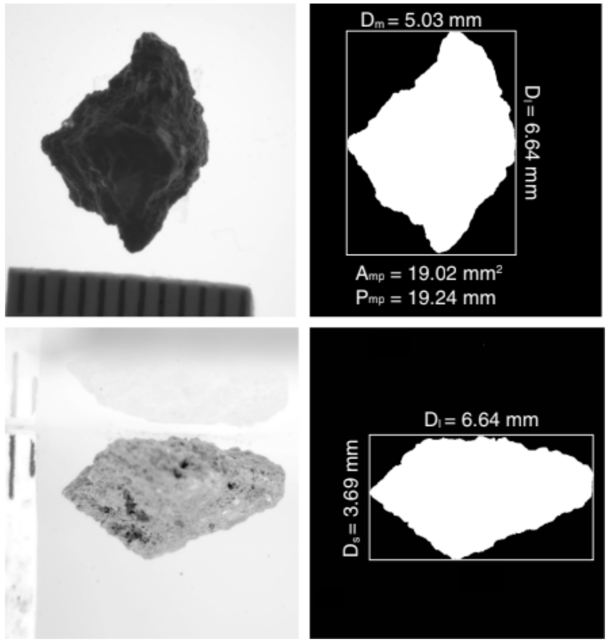
Regular vs. Irregular Shaped Particles

Regular shaped particles:

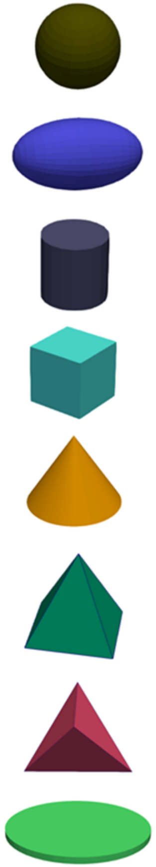
- A particle of geometric parameters such as volume and surface area that can be mathematically determined

Irregular shaped particles:

- An arbitrary random particle whose geometric parameters cannot be precisely calculated



Irregular-shaped Particles[1]



Particle Shape	Sphericity
Sphere	1
Spheroid	0.92
Cylinder	0.87
Cube	0.805
Cone	0.778
Pyramid	0.718
Tetrahedron	0.671
Disk	≈ 0.213

Regular-shaped Particles

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