2020 UCR/HBCU Joint Kickoff Meeting

Development and Evaluation of a General Drag Model for Gas-Solid Flows via Physics-Informed Deep Machine Learning

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10/27/2020

FIU
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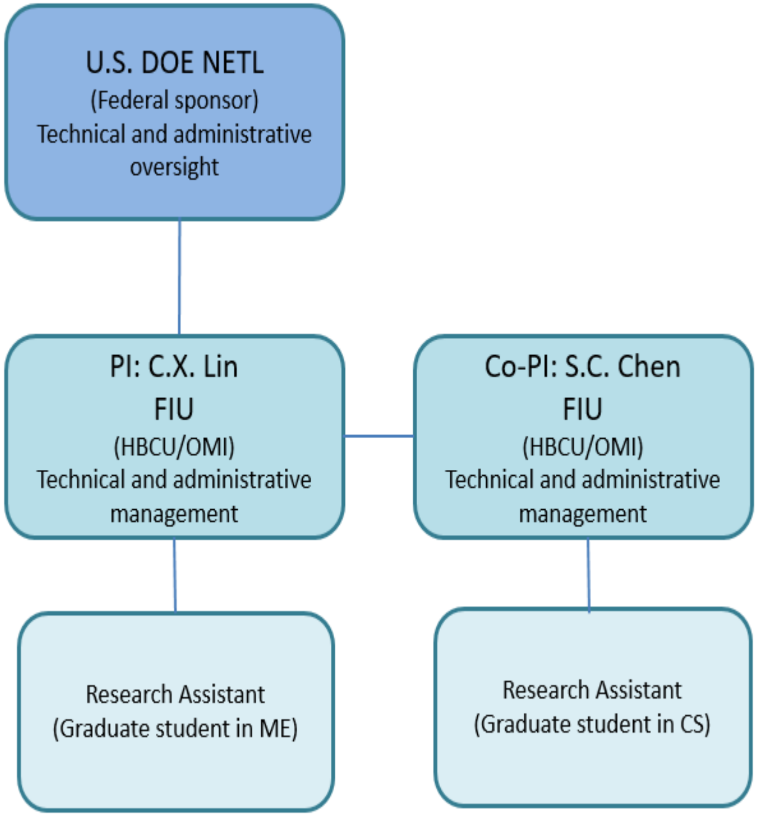
The Project Team

- PI: Dr. Cheng-Xian (Charlie) Lin, Associate Professor, Department of Mechanical and Materials Engineering, FIU
- Co-PI: Dr. Shu-Ching Chen, Professor and Associated Director, School of Computing and Information Sciences, FIU
- Two Ph.D. Students:
  - Maria E. Presa Reyes (Computer Science)
  - Beichao Hu, Pratik Mahyawansi (Mechanical Engineering)



Technical Background/Motivation for the Project

- Eulerian simulation of gas-solid multiphase flows requires accurate prediction of particle's drag coefficient C_D for momentum interface exchange in the drag model
- The C_D depends on both fluid flow and non-spherical particle's form related parameters, including Reynolds numbers (Re), solid volume fractions (ε_m), particle density ratios (ρ_r), Stokes numbers (St), sphericity (S), particle orientations (O_m) and particle aspect ratios (A_r).

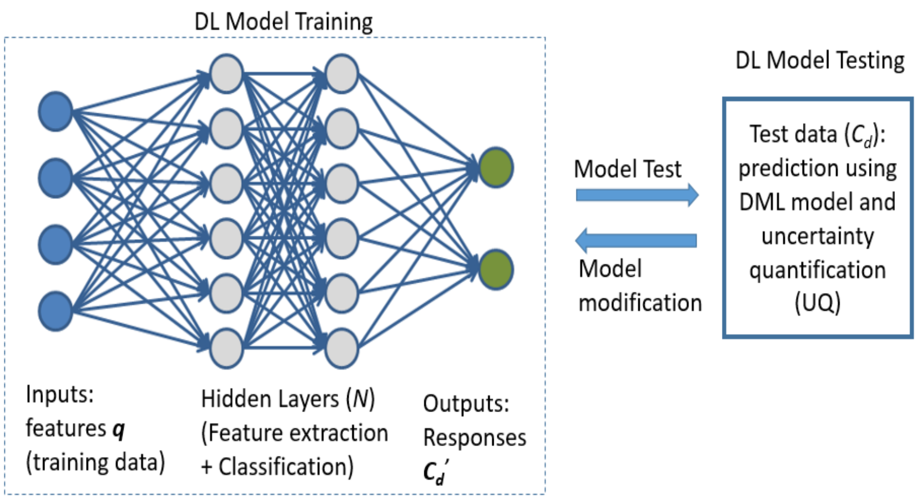
$$C_D = f(\mathrm{Re}, \varepsilon_m, \rho_r, \mathrm{St}, S, O_m, Ar)$$

Technical Background/Motivation for the Project

- Traditional methods to obtain drag coefficient models (empirical correlations), such as experimental measurement and numerical simulations, are not only expensive, but also limited in parameter numbers and ranges
- Assumption of spherical particle or use of a single sphericity parameter is common, but could cause unexpected errors.
- Recently, application of new techniques, such as Machine Learning (ML), in the development of drag coefficient model has received attentions from researchers. However, only two features (Re and S) were considered in the ML model.

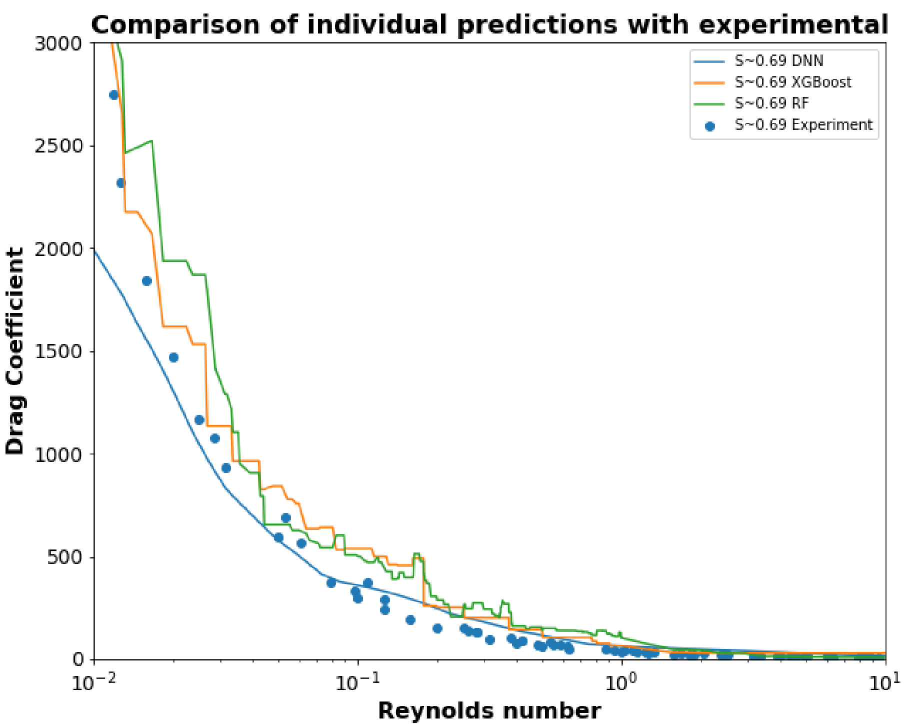
Technical Background/Motivation for the Project

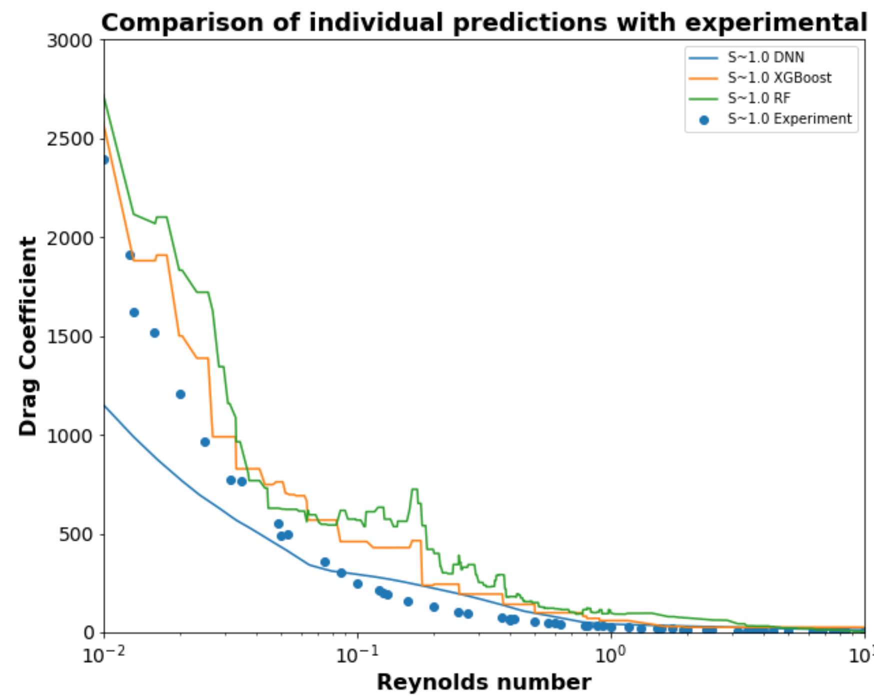
- On the other hand, deep learning (DL) emerges as a promising method in machine learning within the umbrella of multi-layer artificial neural network (ANN), and has proven to be more effective in many types of complex tasks as compared to traditional machine learning in many fields.
- Physics-informed deep learning could offer an alternate or better solution for developing a general drag model



A Deep Learning Neural Network (DNN) with *N* Hidden Layers

Preliminary Results

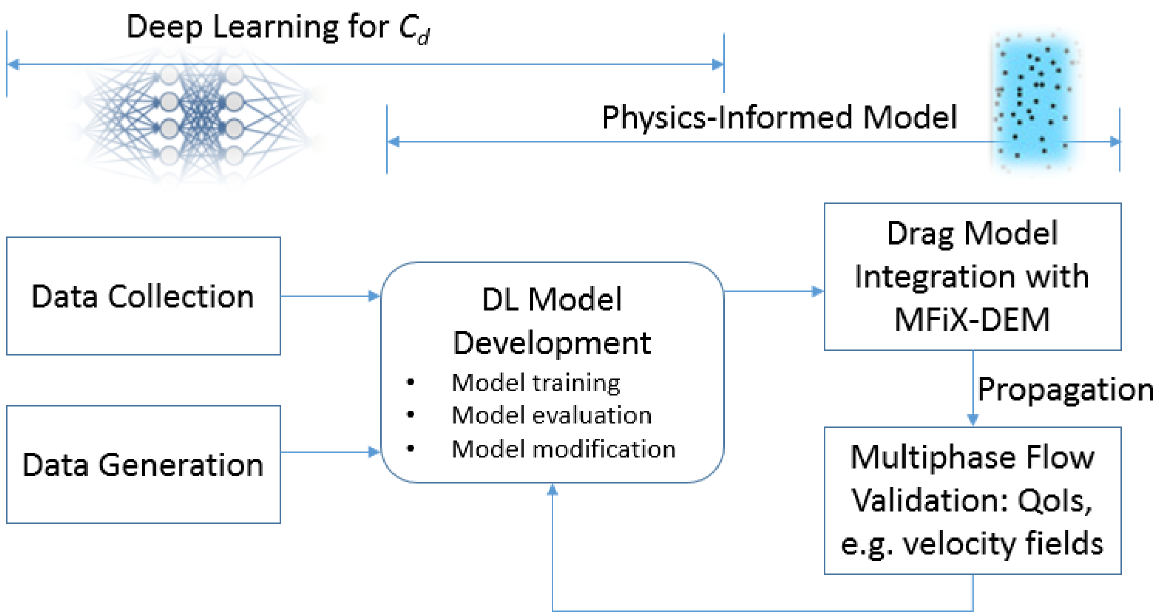




Comparison of Individual NN Predictions with Experimental Data for Particles with Sphericity (S) of 0.69 (left) and 1.0 (right). Baseline setup.

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).

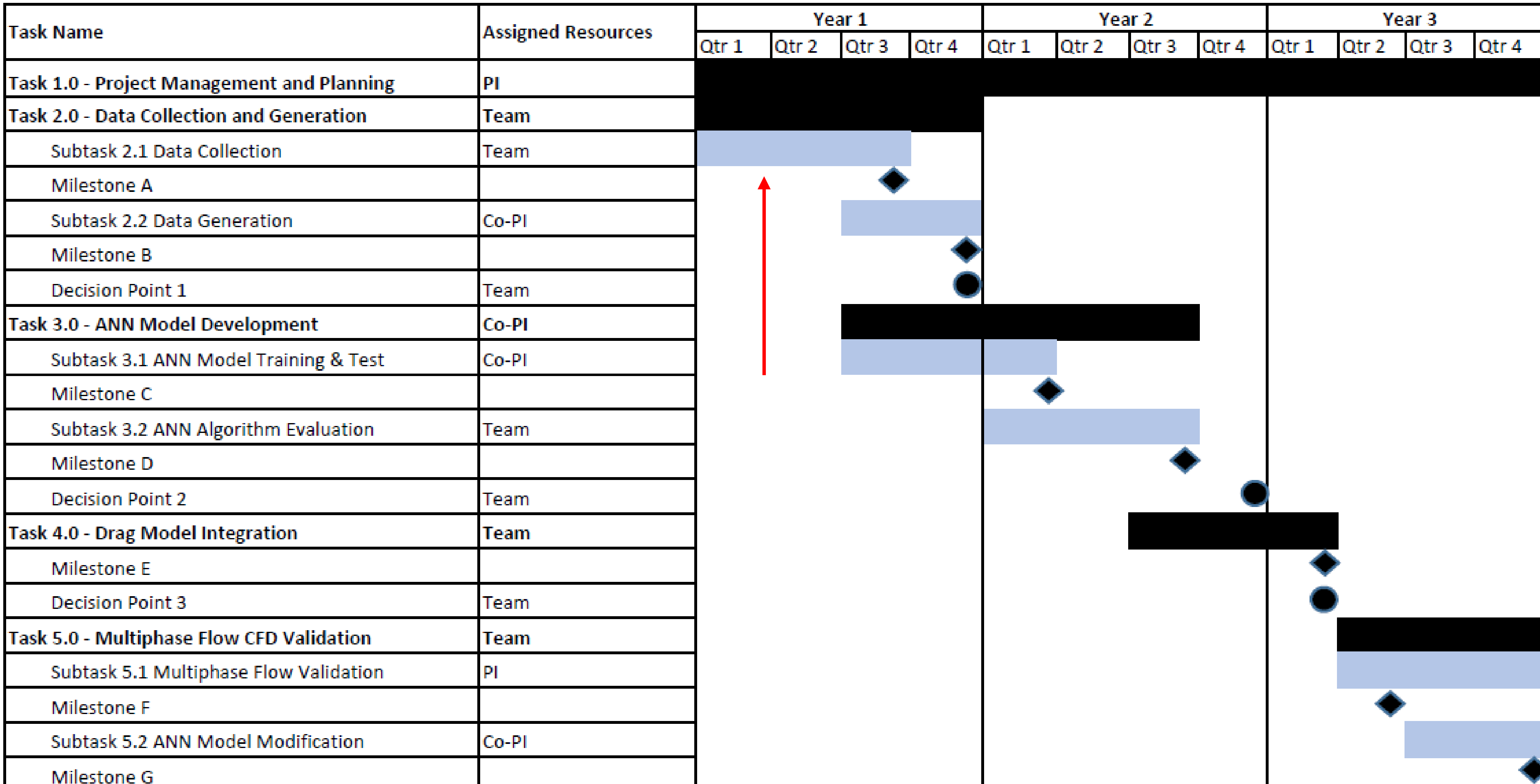


Relevancy and Significance to Fossil Energy

- Gas-solid multiphase flows are important phenomena that can be found in many fossil energy technologies such as sorbent-based CO_2 capture, coal/biomass gasification, fluidized bed combustion, chemical looping and others.
- The deep learning based general drag model, once validated and implemented in a CFD code, such as MFIX, can be used toward the design of more efficient fossil energy technologies within wide ranges of parameters.

Schedule as Related to SOPO Tasks

Project Timeline (Gantt Chart)



Milestones, as Related to SOPO Tasks

Milestone	Task/ Subtask	Milestone Title and Description	Planned Completion Date	Verification Method
A	Subtask 2.1	drag data collected – drag coefficient data in open literature are collected	End of 3rd quarter, Year 1 04/30/2021	Spreadsheet with collected data on drag coefficients
B	Subtask 2.2	Drag data generated – additional drag data for identified parameters are synthesized	End of 4th quarter, Year 1 07/31/2021	Spreadsheet with drag coefficient data for identified parameters
C	Subtask 3.1	Deep neural network trained – At least one deep neural network (DNN) is trained using the obtained drag data	End of 1st quarter, Year 2 10/31/2021	Drag data predicted by deep neural network in graphs or tables
D	Subtask 3.2	Best neural network identified– A deep neural network model of the best performance is identified	End of 3rd quarter, Year 2 04/30/2022	Comparison of predicted results between the best DNN with other models
E	Task 4.0	Drag model implemented in CFD – The DNN model is implemented in CFD code MFiX	End of 1st quarter, Year 3 10/31/2022	Demonstration of MFiX source code linked to the developed drag model
F	Subtask 5.1	CFD validation – Comparison between the predicted flow fields using the DNN based drag model and available experimental results	End of 2nd quarter, Year 3 01/31/2023	Comparative results on Vs and Ps by both DNN and experiments for selected flow problems
G	Subtask 5.2	Drag model finalized	End of 4th quarter, Year 3 07/31/2023	DNN model training performance data and CFD validation results in graphs and tables

Project Risks and Risk Management Plan

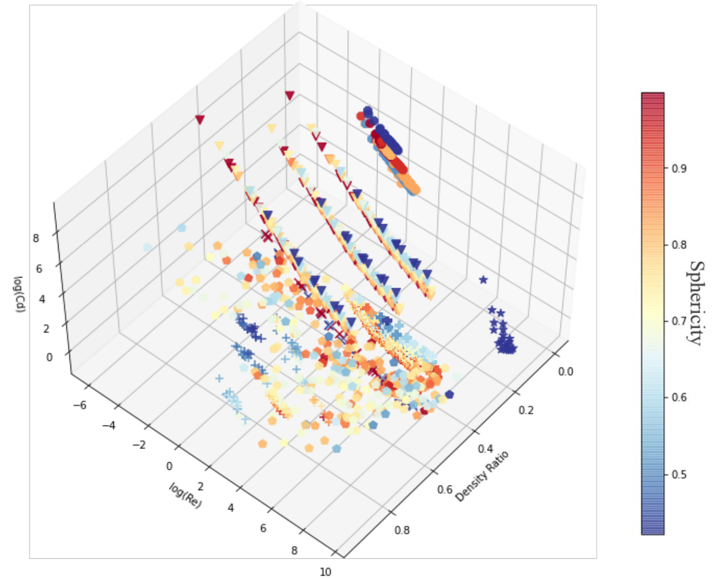
Perceived Risk	Risk Rating			Mitigation/Response Strategy
	Probability	Impact	Overall	
	(Low, Med, High)			
Technical/Scope Risks:				
Lack of drag data	low	medium	low	Data synthesis

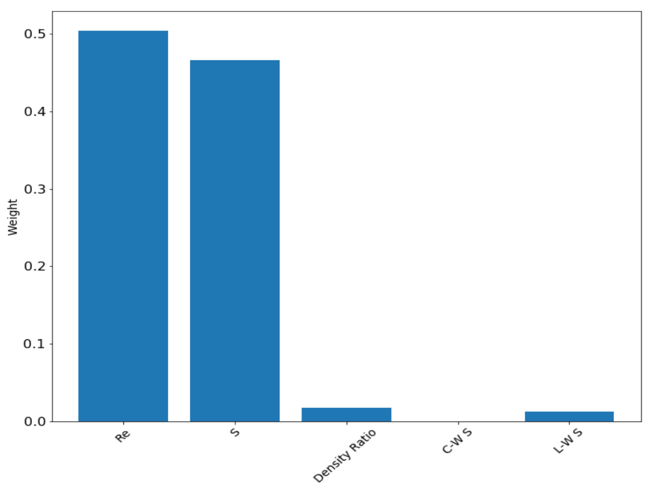
Current Project Status

- Task 1 Project Management and Planning
  - Subtask 1.1 Project Management Plan: updated 07/22/2020
  - Subtask 1.2 Data Management Plan (DMP): submitted before award
- **Task 2 Obtain and Generate Drag Data: ongoing**
- **Task 3 Develop ANN Model: ongoing**
- Task 4 Drag Model Integration
- Task 5 Multiphase Flow CFD Validation

Current Project Status

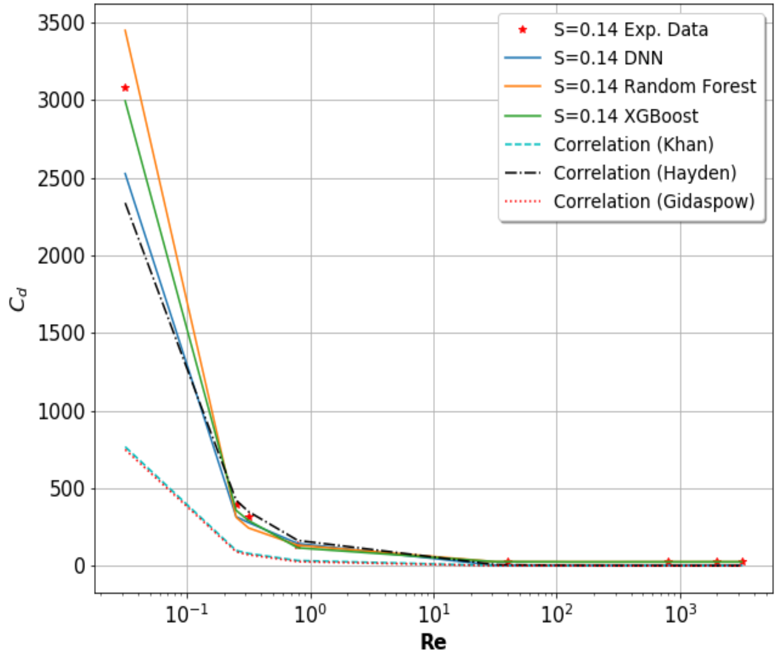
- Data Collected So Far
  - Digitalized several more papers/reports (> 2K data points)
  - Created a combined spreadsheet with data of drag coefficients at identified features
  - Performed preliminary data analysis of feature importance and feature correlation



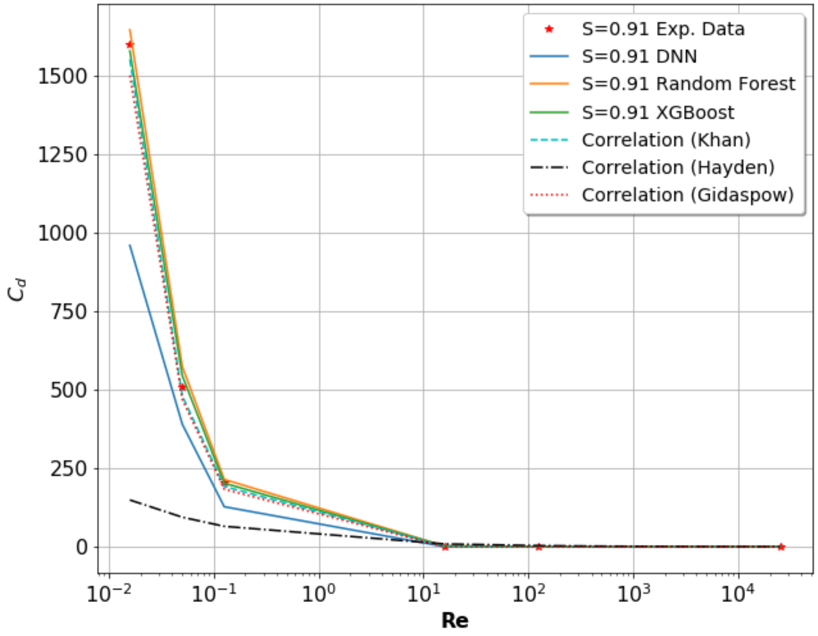


Current Project Status

- Performed Additional Preliminary ML/DL Training and Testing



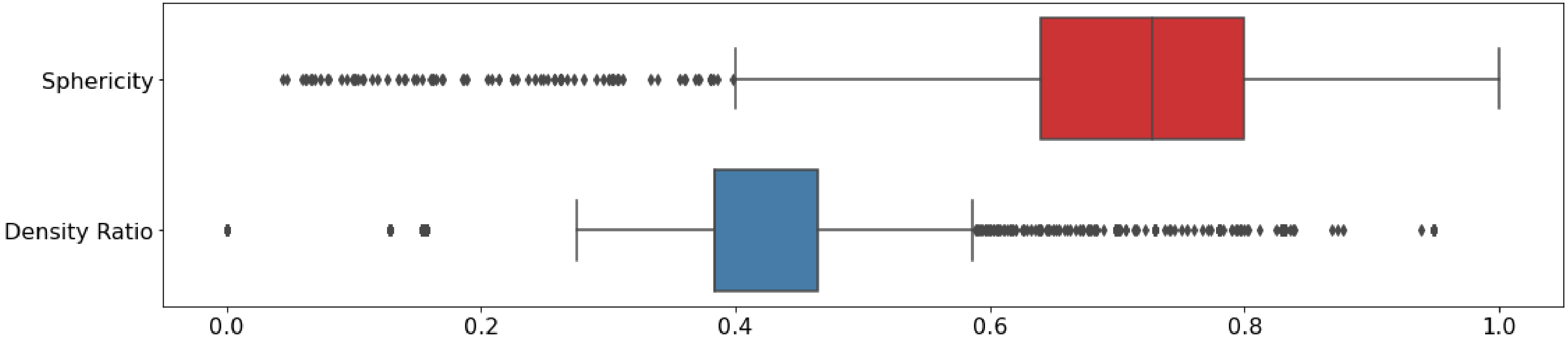
Predicted C_D for S=0.14

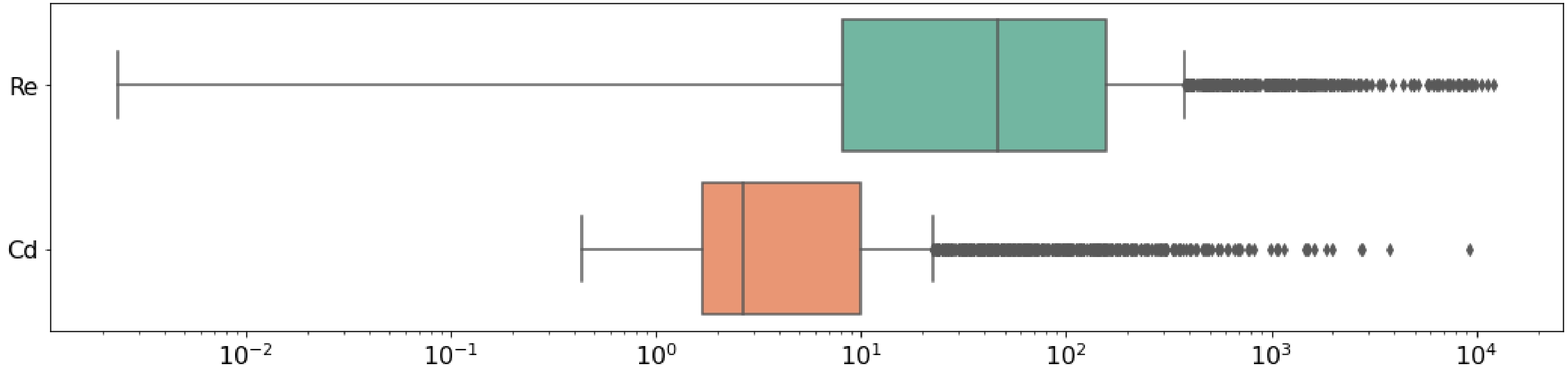


Predicted C_D for S=0.9.

Current Project Status

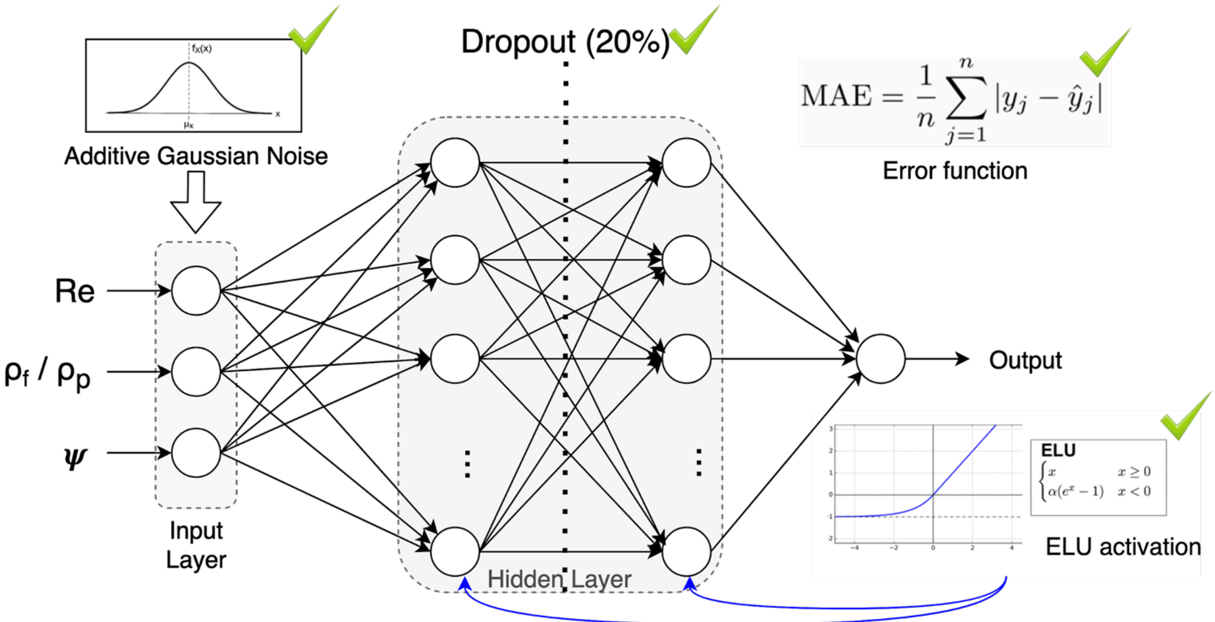
- Addressing the Skewed Data (Outliers) Issue with More Datasets Being Added





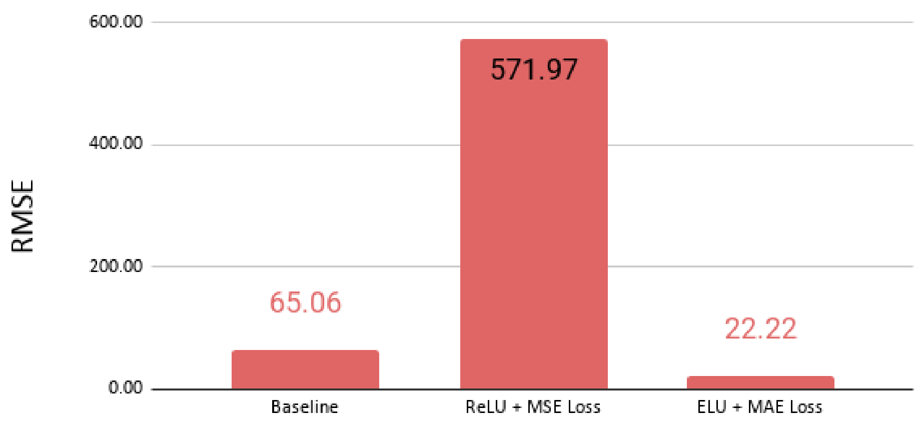
Current Project Status

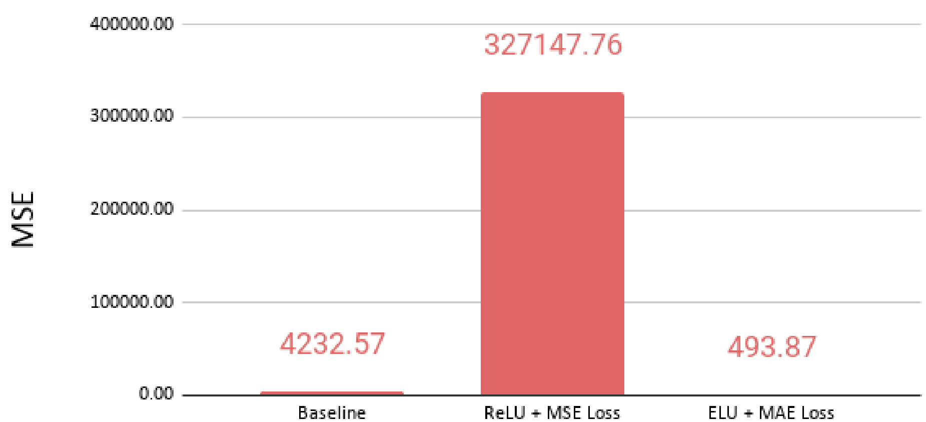
- Refining/Adjusting the DNN algorithm through model regularization and generalization
  - Noise Augmentation
  - Dropout Layer
  - Mean Absolute Error (MAE) Loss Function
  - Exponential Linear Unit (ELU) Activation



Current Project Status

- Performance Summary with Current Datasets





ReLU: Rectified Linear Units activation function

Baseline: less data and less skewed

Thank You !