UNETs for flow field and drag force predictions in dispersed particle flows

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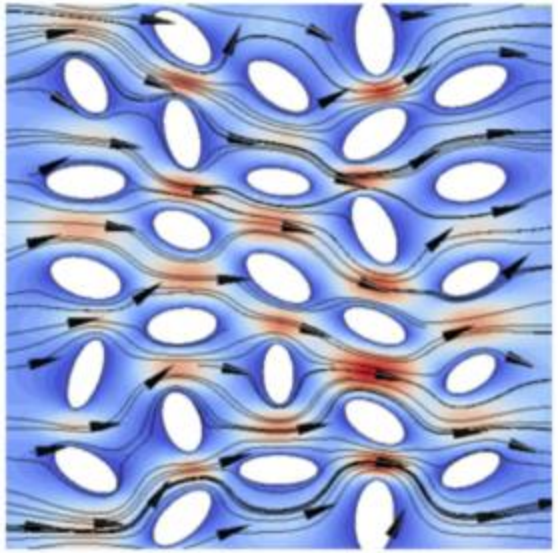
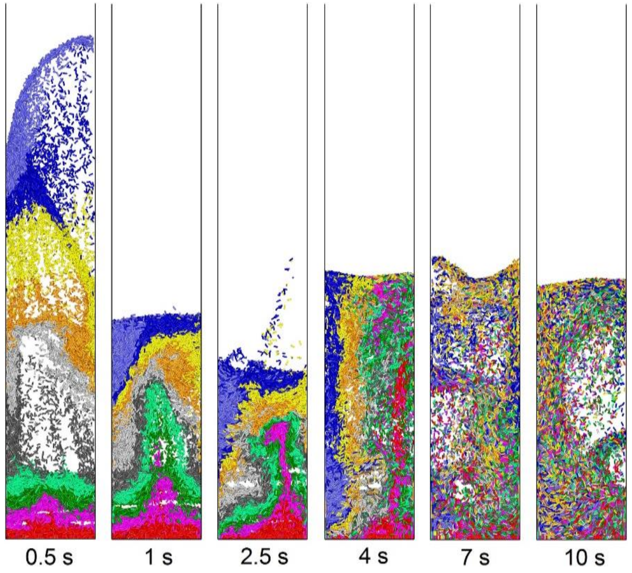
NETL WORKSHOP 2023

Introduction and Aim

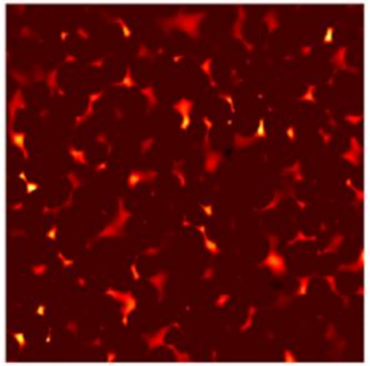


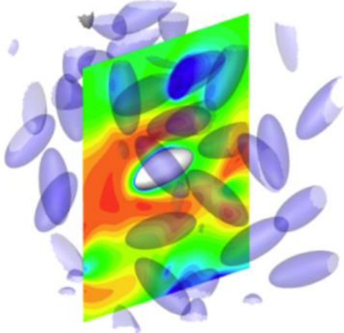
Flow through porous fibers



Snapshots of rod like particles in a fluidized bed, adapted from CFD-DEM simulation of fluidization of rod-like particles in a fluidized bed

Flow through porous solid



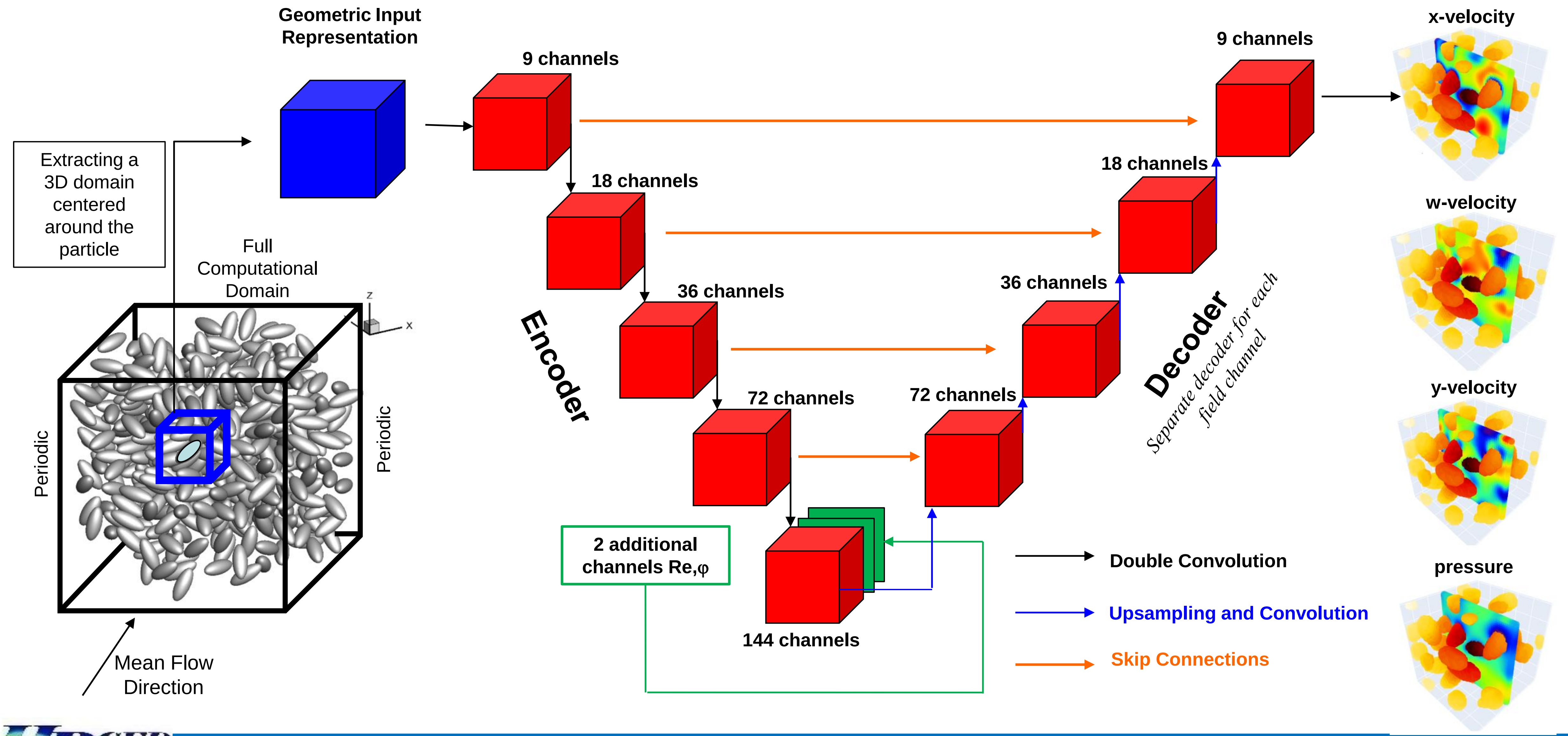


- Flow across random arrangement of solid particles can be found in various places.
- Can we develop surrogate models to get a quick estimate predict the flow field quantities.
- Can we use the predicted quantities for downstream tasks.

Aim

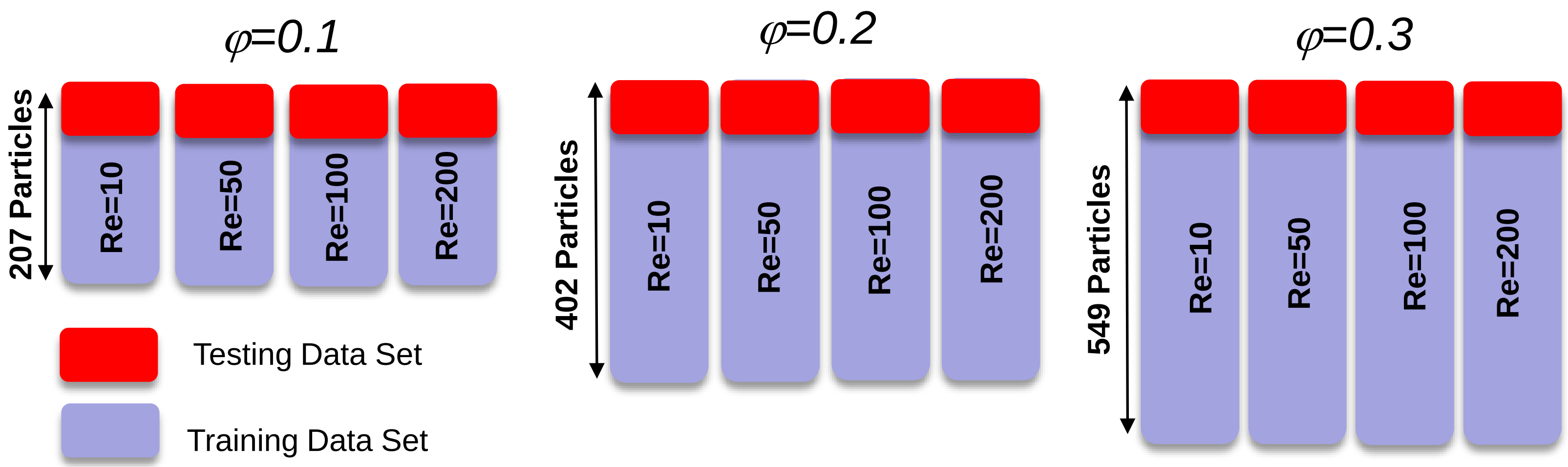
- Develop models to predict the x,y,z-directional velocity and pressure field surrounding prolate ellipsoidal particles using geometrical input representations.
- Studying the prediction capability of the trained models across different datasets
- Using predicted fields for downstream tasks such as drag force prediction

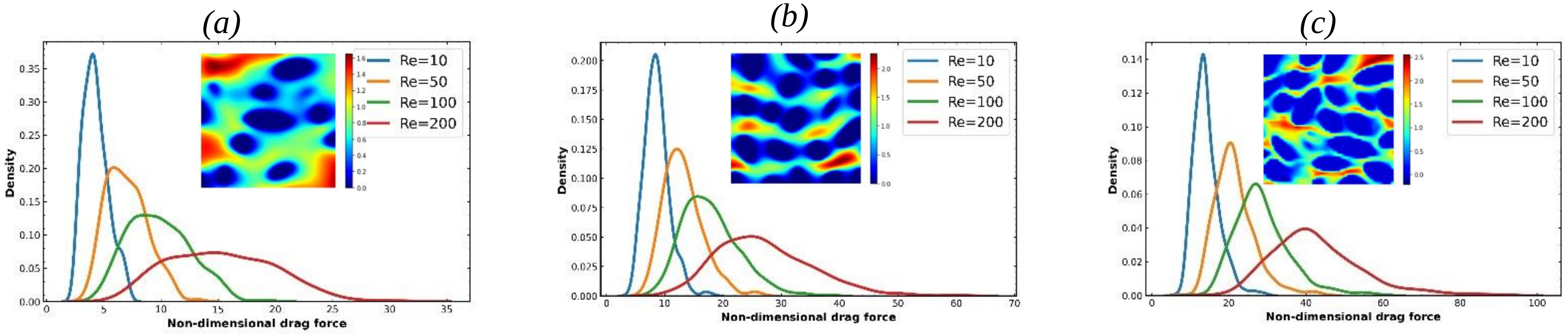
UNET Model


Geometric Input Representation
Extracting a 3D domain centered around the particle
Full Computational Domain
Periodic
Periodic
Mean Flow Direction
9 channels
18 channels
36 channels
72 channels
144 channels
72 channels
36 channels
18 channels
9 channels
Encoder
Decoder
Separate decoder for each field channel
2 additional channels Re,φ
Double Convolution
Upsampling and Convolution
Skip Connections
x-velocity
w-velocity
y-velocity
pressure

Dataset and Splitting to Train and Validation

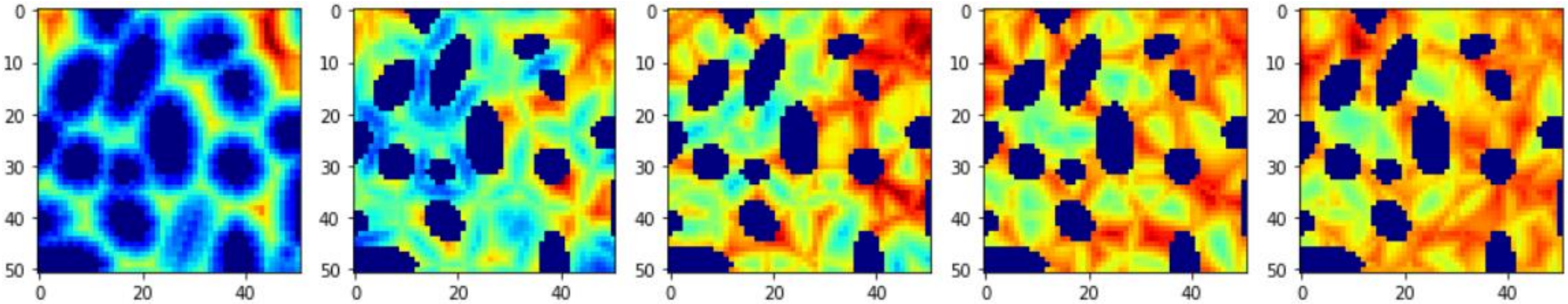
- The total dataset consists of 4632 particles , across three different solid fraction, each with 4 different Reynolds.
- For each solid fraction and Reynolds number we keep 40 particles in the validation dataset and the remaining in the train dataset.
- The drag forces obviously increase with increasing Re and solid fraction (φ); there is also an increase in variance with increasing Re.





Kernel density function of the PRS calculated drag forces for particles in (a) φ=0.1, (b) φ=0.2 and (c) φ=0.3 suspensions and inset image of an example datapoint

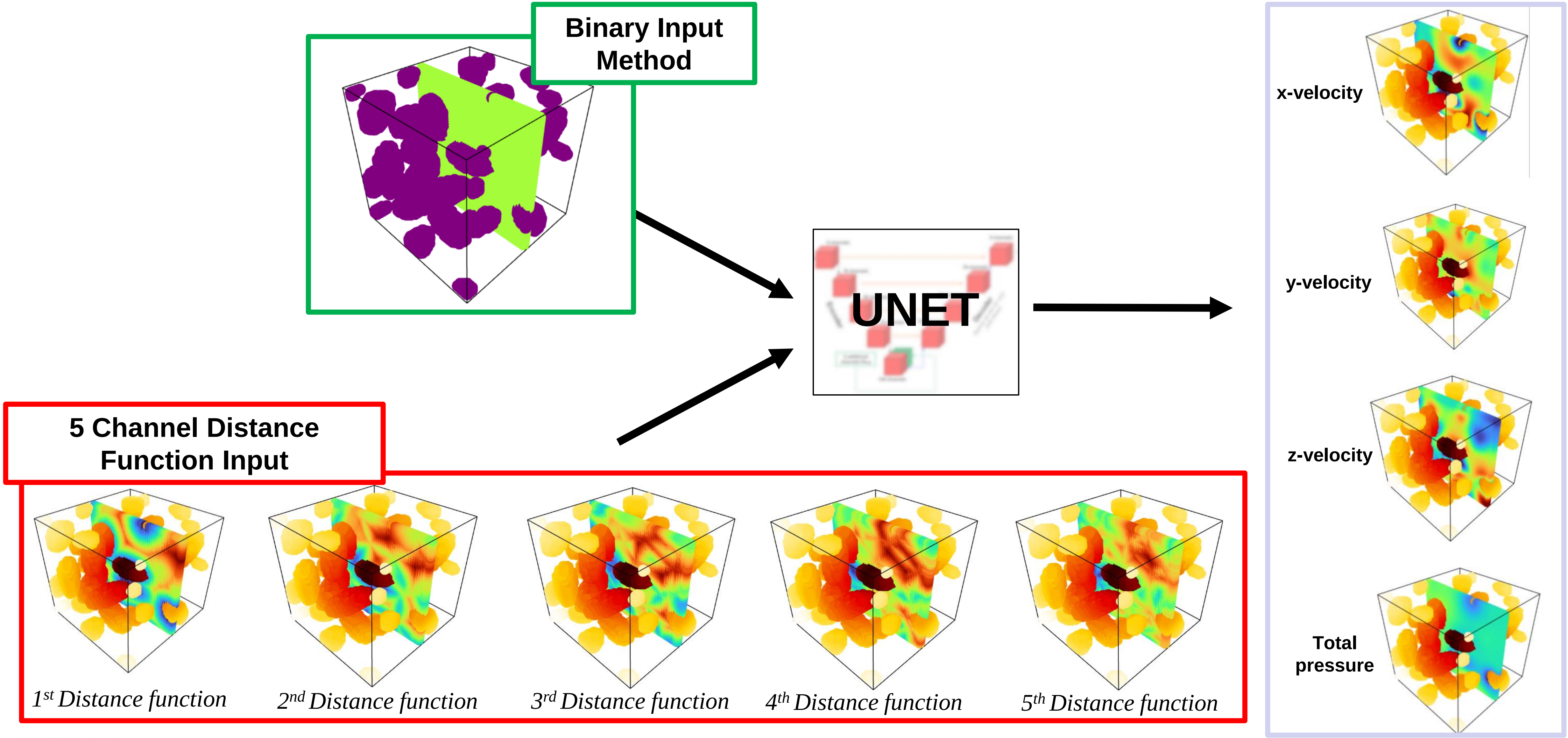
UNET Recap : Inputs to the UNET model



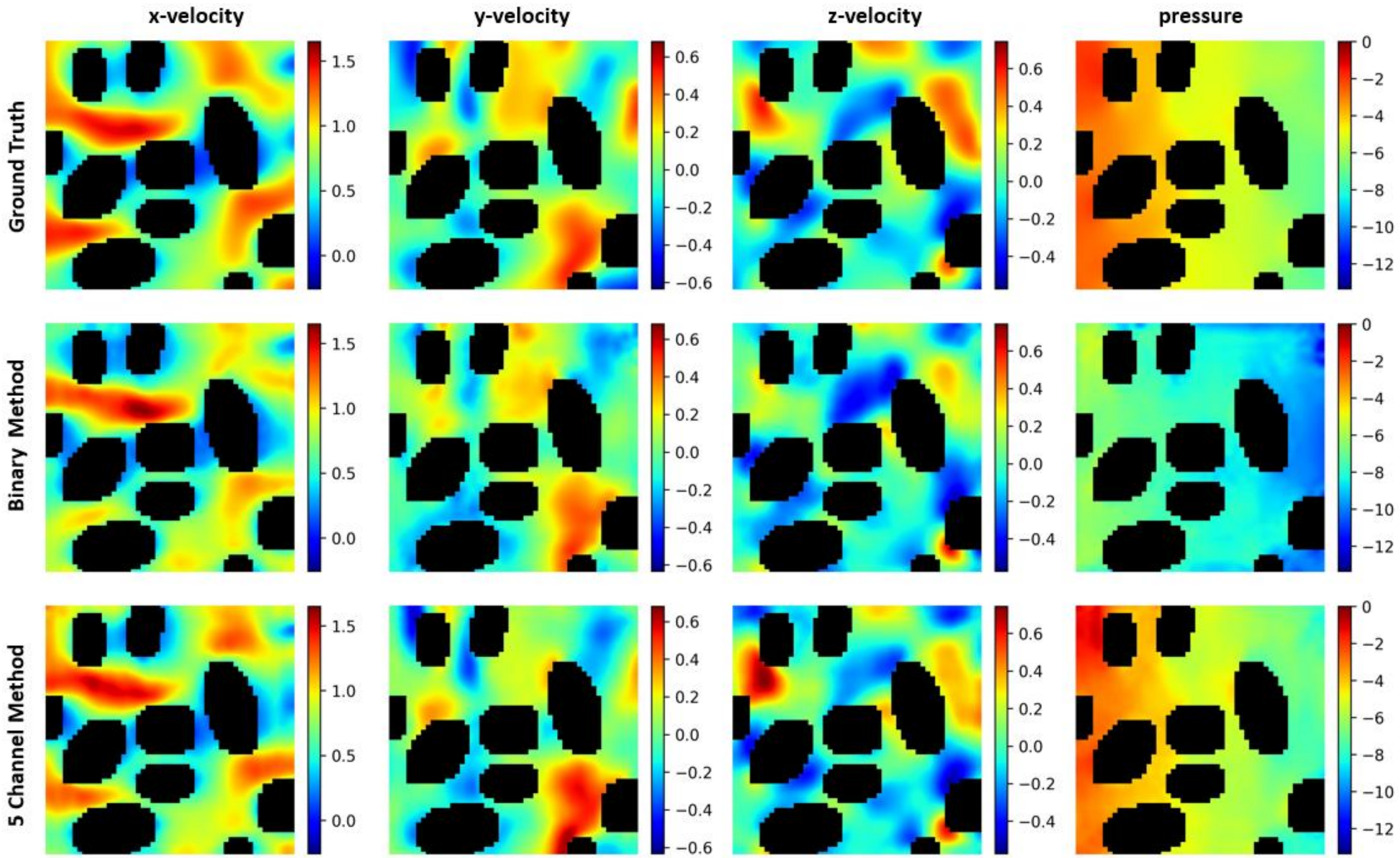
1^{st} Distance function | 2^{nd} Distance function | 3^{rd} Distance function | 4^{th} Distance function | 5^{th} Distance function

- The inputs to the network are the distance function if the computation domain.
- The images shown are one slice of the 3D image which originally of size 51*51*51
- The value of the 1^{st} distance function is zero at the solid pixel and at the fluid pixel the value is the value of the closest surface on the nearest particle from that fluid pixel.
- The value of the 2^{nd} distance function is zero at the solid pixel and at the fluid pixel the value is the value of the closest surface on the second nearest particle from that fluid pixel.

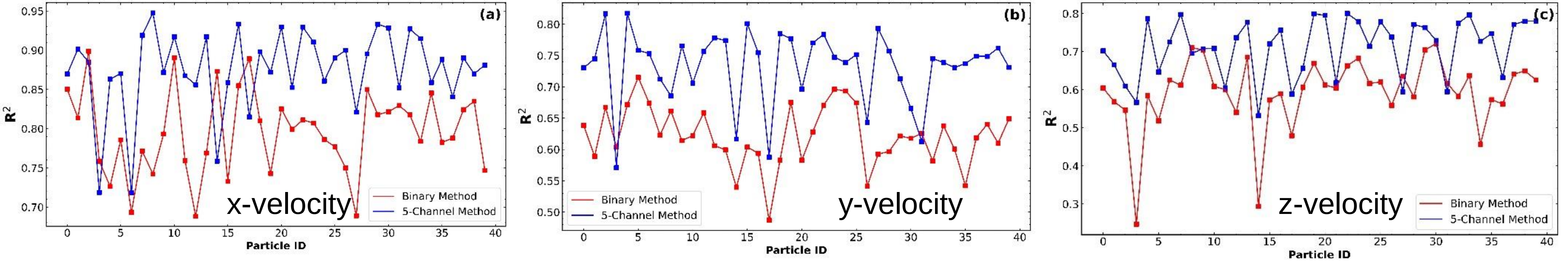
Models based on different input representations

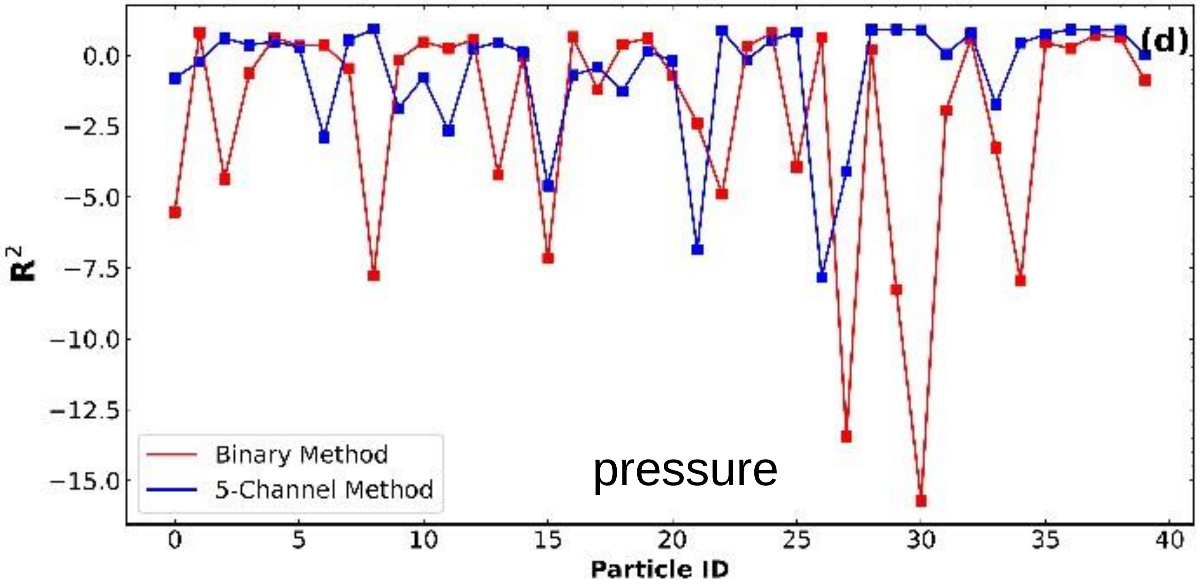


Qualitative Predictions of the two methods (Re=10;φ=0.1)



Quantitative Predictions of the 2 method (Re=10;φ=0.1)





Method	Mean R^2 for x-velocity	Mean R^2 for y-velocity	Mean R^2 for z-velocity	Mean R^2 for pressure
Binary Input Method	0.796	0.621	0.593	-2.13
5 Channel Methods	0.876	0.733	0.711	-0.579

$$\boldsymbol{R^2} = \frac{\sum_{n=1}^{n=n_{fp}} (\boldsymbol{\Phi}_{i,j} - \boldsymbol{\Phi}'_{i,j})^2}{\sum_{n=1}^{n=n_{fp}} (\boldsymbol{\Phi}_{i,j} - \bar{\boldsymbol{\Phi}})^2}$$

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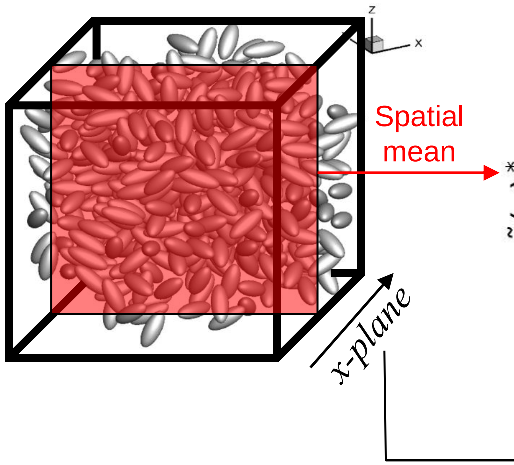
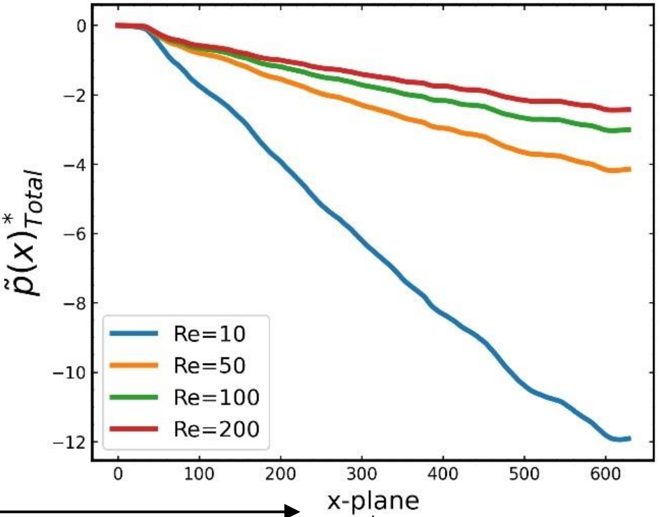
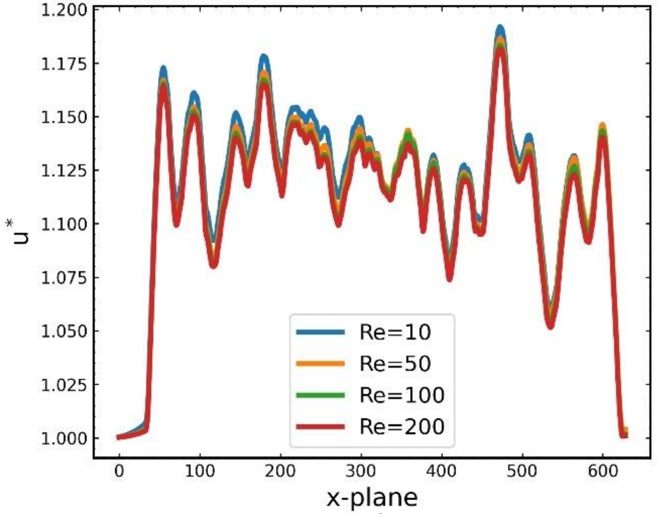
Total Pressure and Fluctuating Pressure



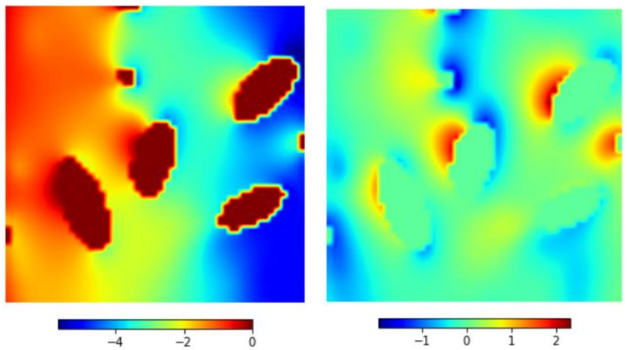
Y-z plane



Mean plane-wise p^* in the streamwise direction for different Reynolds numbers



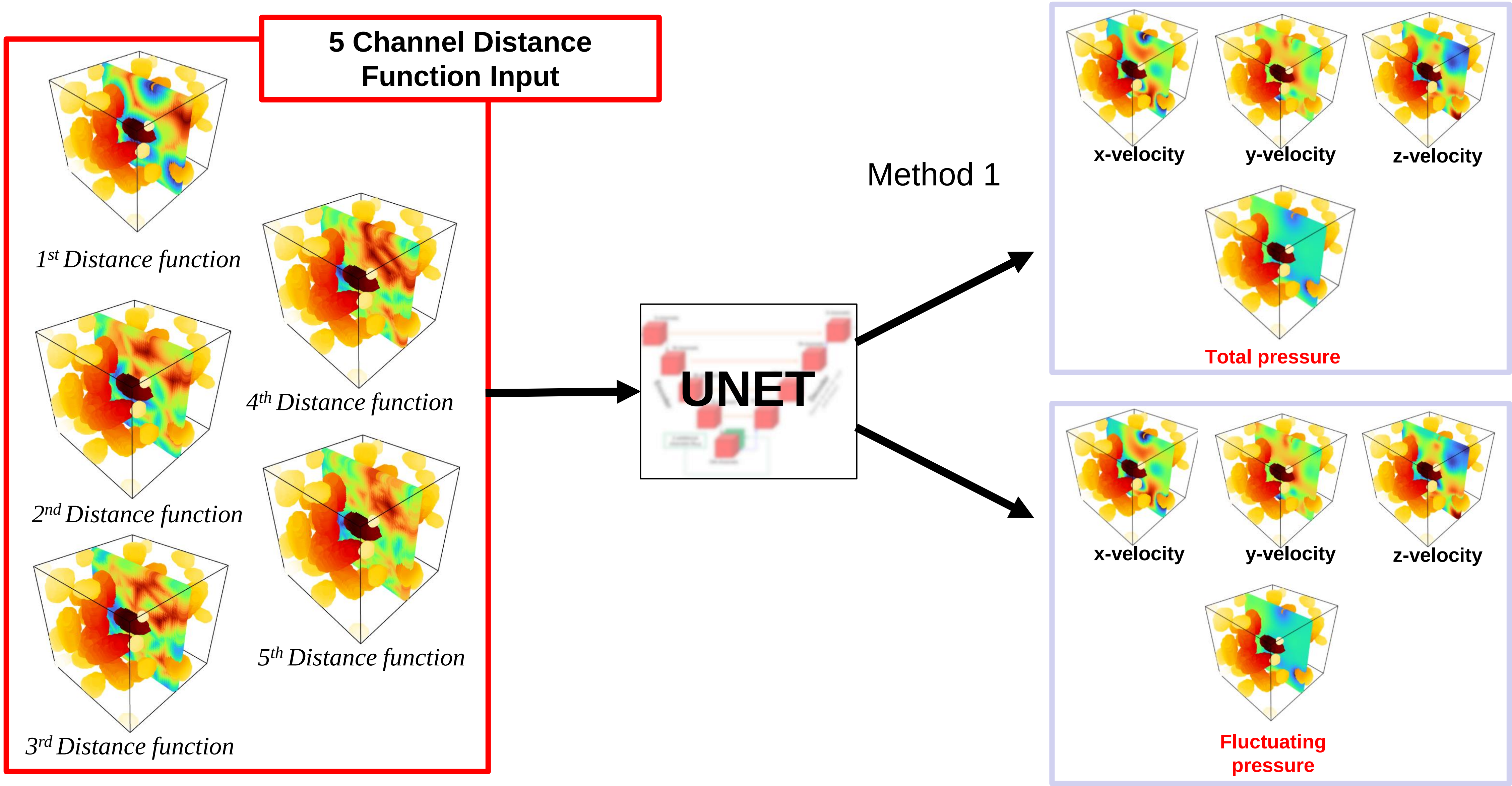
Mean plane wise u^*in the streamwise direction for flow fields at different Reynolds numbers



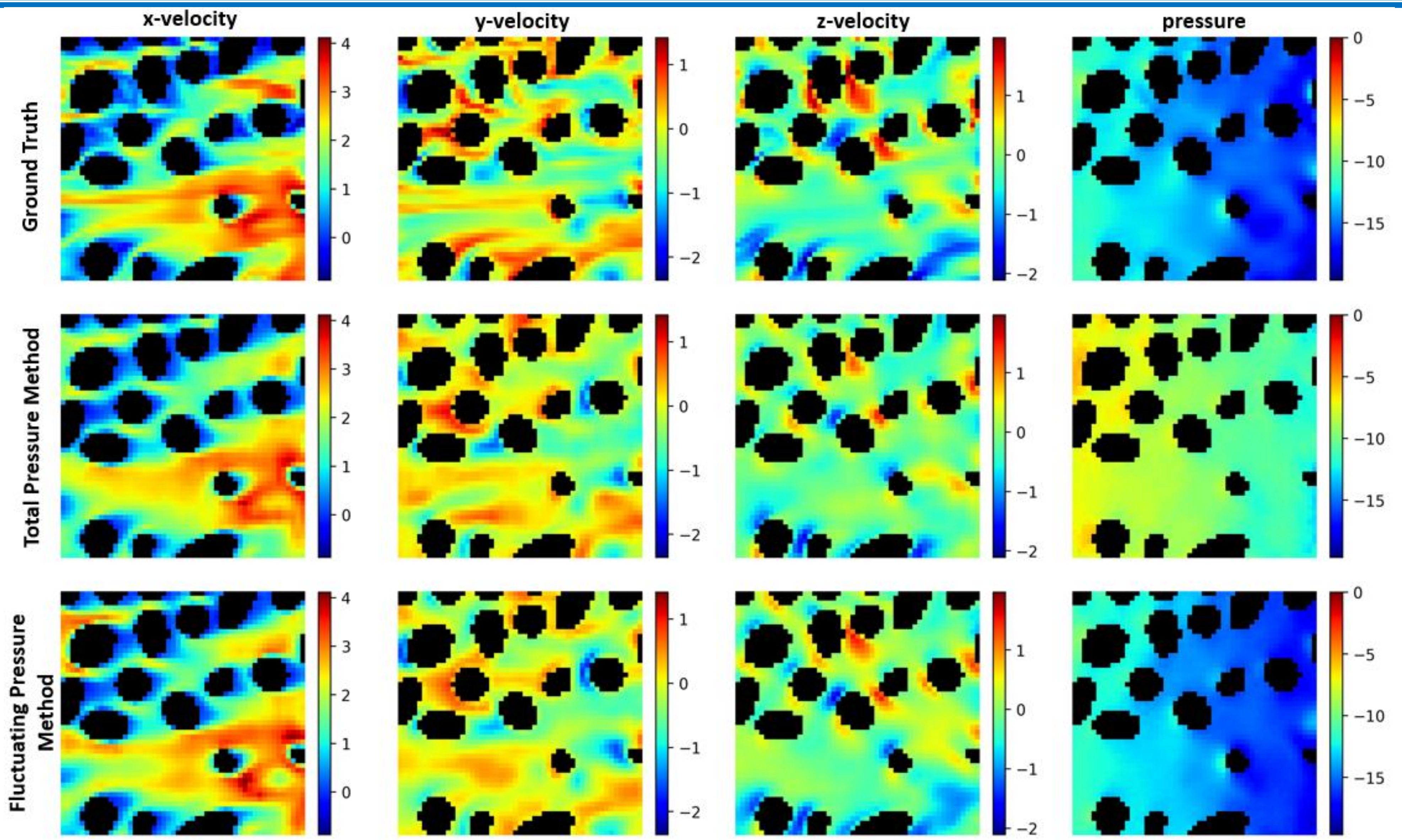
Total and fluctuating pressure for the same particle

- There is an inherent difference between the pressure and velocity field , the pressure field has a gradient in the x-direction. This is because the x direction boundary conditions are a velocity inlet and outlet (set to 1 at both), which in turn develops a pressure gradient.
- Thus, it will be tougher to train the model on this “total pressure field” as there is dependence on x-location and there is a large range of values across different Reynold numbers and solid fractions.
- We therefore decided to train the model with the fluctuating pressure field. The fluctuating pressure field is calculated by planar mean pressure from the total pressure as, $\boldsymbol{p^*_{Fluc}(x,y,z) = p^*_{Total}(x,y,z) - \tilde{p}^*_{total}(x)}$

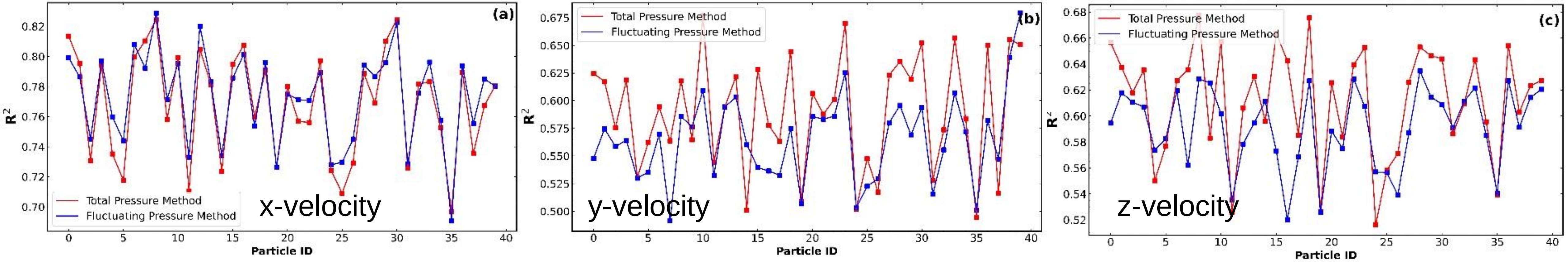
Models based on different pressure representations

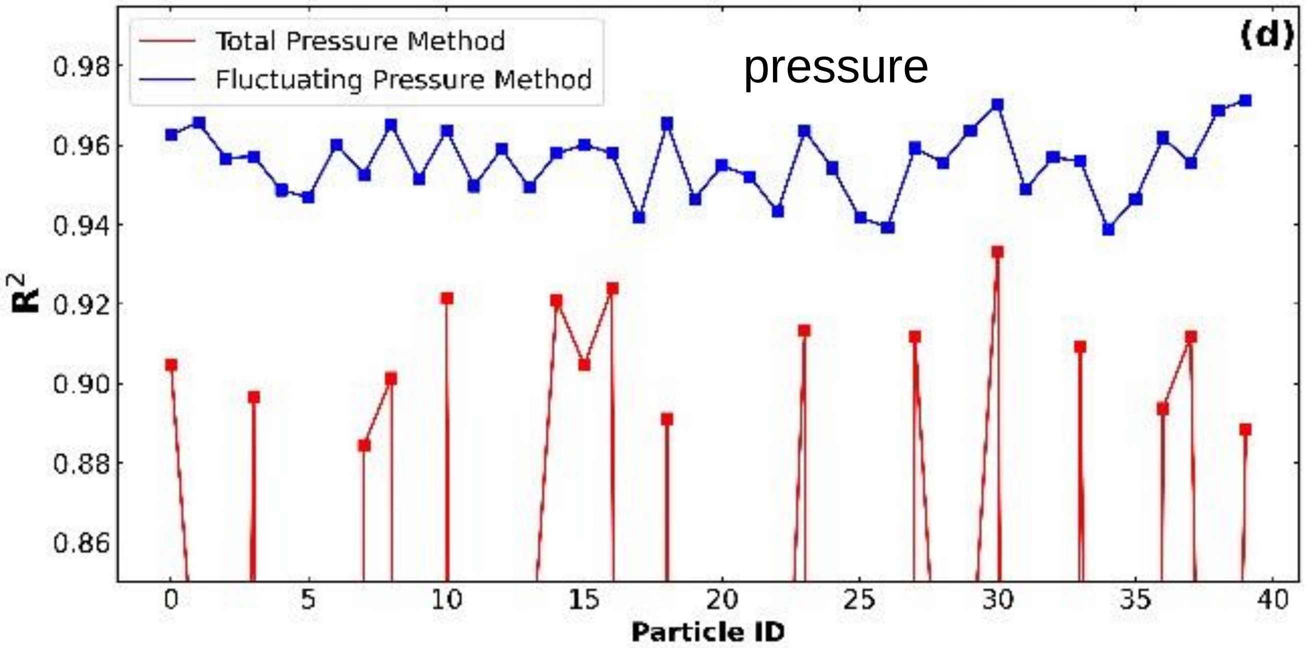


Qualitative Predictions of the two methods (Re=200;φ=0.3)



Quantitative Predictions of the two methods





Method	Mean R^2 for x-velocity	Mean R^2 for y-velocity	Mean R^2 for z-velocity	Mean R^2 for pressure
5 Channel Methods with p^*_{total} supervision	0.768	0.590	0.613	-0.01
5 Channel Methods with p^*_{fluc} supervision	0.773	0.565	0.591	0.955

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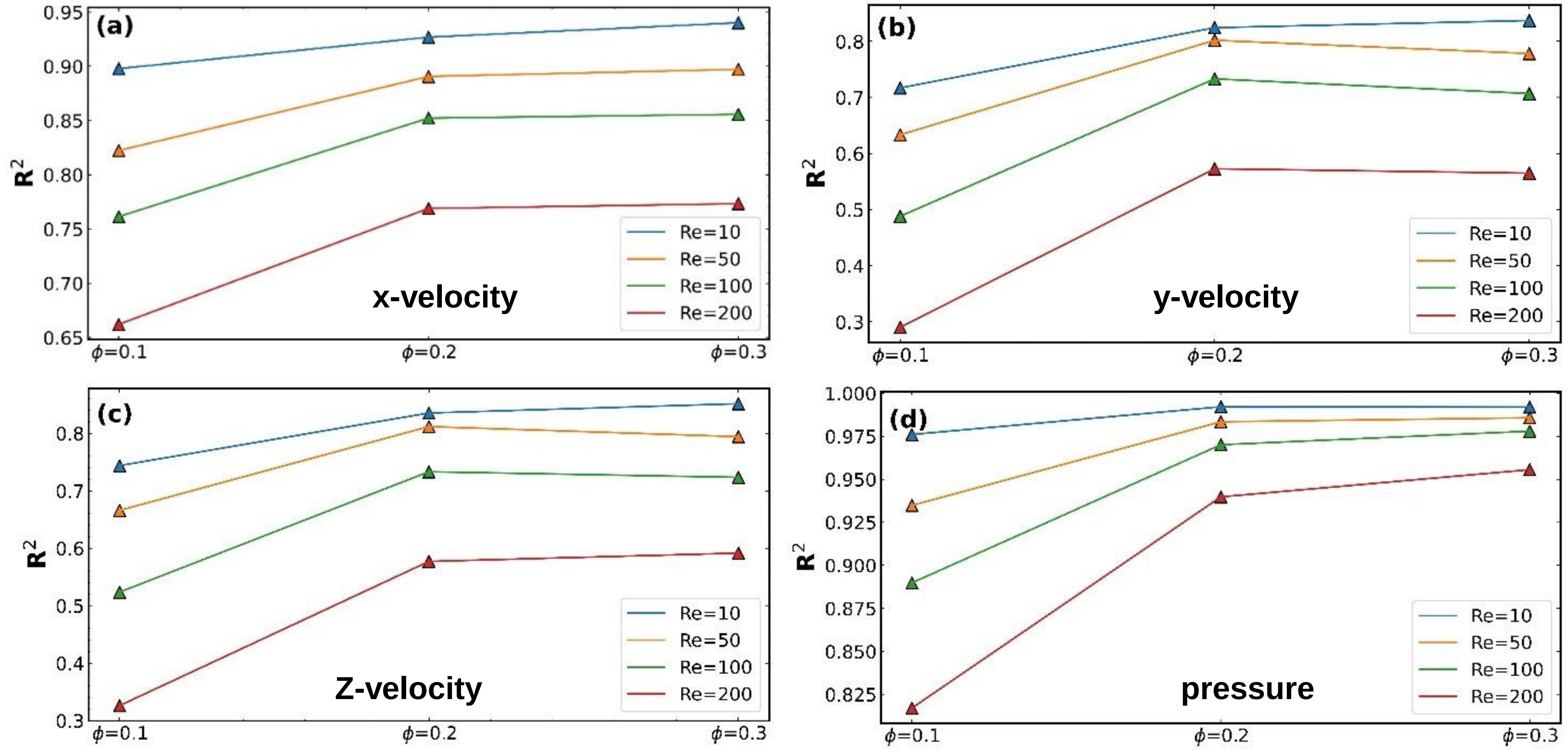
Performance on different datasets



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Conclusions

- A Unet model was trained to predict the velocity and pressure field surrounding particles in a randomly dispersed suspensions of different Reynolds numbers and solid fractions.

- The trained models were analyzed on unseen particles from different Reynolds number and solid fractions and the errors were studied.

- **Errors in the predicted fields increase with an increase in Reynolds numbers and decrease with an increase in solid fraction**

References:

- *Shirzadi, M., Fukasawa, T., Fukui, K. and Ishigami, T., 2023. Application of deep learning neural networks for the analysis of fluid-particle dynamics in fibrous filters. Chemical Engineering Journal, 455, p.140775.*
- *Ma, H., Xu, L. and Zhao, Y., 2017. CFD-DEM simulation of fluidization of rod-like particles in a fluidized bed. Powder technology, 314, pp.355-366.*
- *He, L. and Tafti, D., 2018. Variation of drag, lift and torque in a suspension of ellipsoidal particles. Powder Technology, 335, pp.409-426.*
- *Santos, J.E., Xu, D., Jo, H., Landry, C.J., Prodanović, M. and Pyrcz, M.J., 2020. PoreFlow-Net: A 3D convolutional neural network to predict fluid flow through porous media. Advances in Water Resources, 138, p.103539.*