Graph neural networks for particle drag force predictions in dynamic flows

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NETL WORKSHOP 2024

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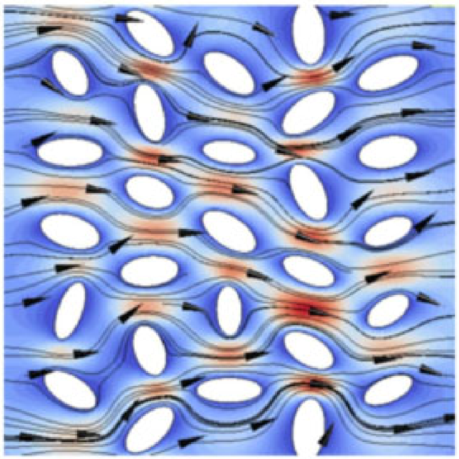
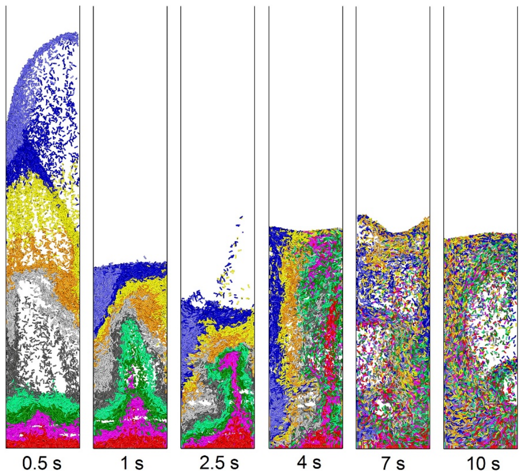
Introduction

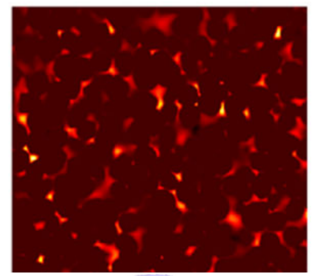


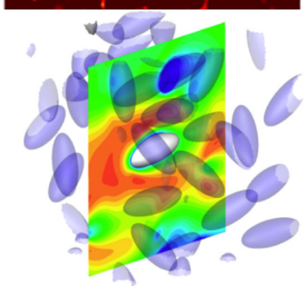
Flow through porous fibers[1]



Snapshots of rod like particles in a fluidized bed, adapted from CFD-DEM simulation of fluidization of rod-like particles in a fluidized bed [2]

Flow through porous solid[3]





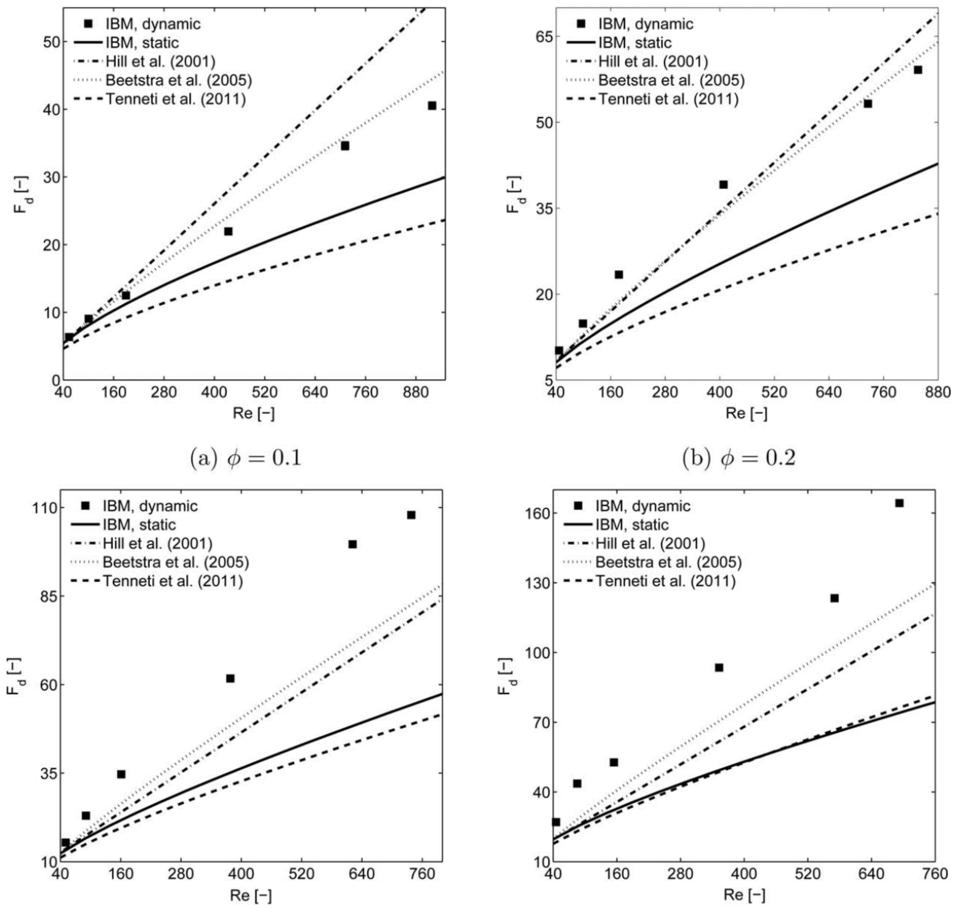
Flow through a random array of ellipsoidal particle[4]

- Flow across random arrangement of solid particles can be found in various applications.
- Studying them experimentally is challenging due to requirements of expensive experimental setups.
- Studying them numerically runs into the dilemma of accuracy vs computation expense.

Aim

- Develop Deep Learning (DL) based models for accurate drag predictions, to deploy in less computationally expensive methods (such as CFD-DEM) for PRS/DNS level accuracy.
- **First attempt with DL for developing dynamic drag models.**
- Investigate the generalizability of said models across different parameters of the dataset.

Drag forces in stationary vs dynamics particle simulations



(a) $\phi = 0.1$ (b) $\phi = 0.2$

(c) $\phi = 0.3$ (d) $\phi = 0.4$

- State-of-the-art correlations/DL models are developed based on only fixed particle simulations.
- However, drag forces obtained from correlations developed from simulations of fixed particles show different statistics compared to drag forces obtained from dynamic particle simulations, as seen in the plots.
- The discrepancy between dynamic and stationary drag increases linearly with Reynolds number based on granular temperature.
- **Particle mobility effects are crucial for dynamic drag force predictions.**

TD0

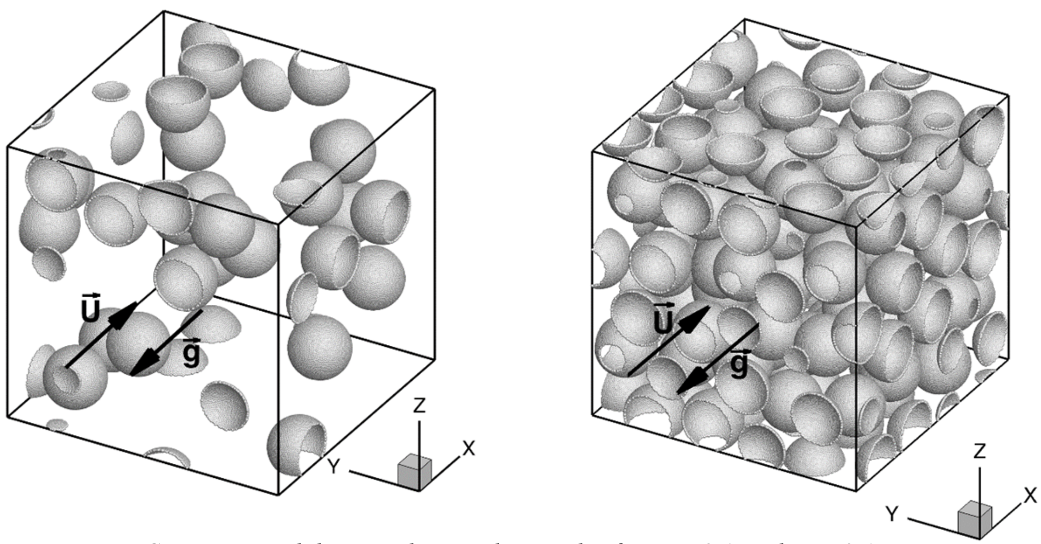
Y. Tang, E.A.J.F. Peters, J.A.M. Kuipers, Direct numerical simulations of dynamic gas-solid suspensions, AIChE J. 62 (2016) 1958–1969. https://doi.org/10.1002/AIC.15197.

Slide 4

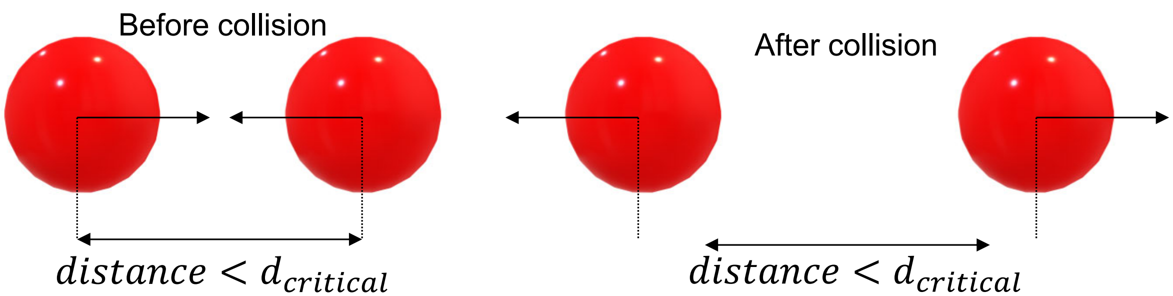
TD0 at what density ratio is this study done? BTW FYI these predictions of unsteady drag forces are high but for here it is OK to show.
Tafti, Danesh, 2024-08-12T12:47:18.553

RA0 0 the density ratio is 500
Raj, Neil Ashwin, 2024-08-12T13:03:25.860

Simulation setup and collision models



Computational domain along with particles for $\varphi = 0.1$ and $\varphi = 0.4$



- The computational domain is cubic with each side being $5d_p$, where d_p is the particle diameter. The flow is driven by a pressure gradient in the positive x-direction, and additionally, there is a gravitational force in the negative x-direction.

- The Immersed Boundary Method (IBM) is used to model the solid spheres, and all the simulations have been performed in the inhouse code GenIDLEST.

- The particle collisional forces are modeled using the soft sphere model, if two particles come closer than a critical distance of separation the particle forces are calculated and applied in the opposite directions for each of them.

Z. Cao, D.K. Tafti, Alternate method for resolving particle collisions in PRS of freely evolving particle suspensions using IBM, Int. J. Multiph. Flow 177 (2024) 104862. https://doi.org/10.1016/j.ijmultiphaseflow.2024.104862.

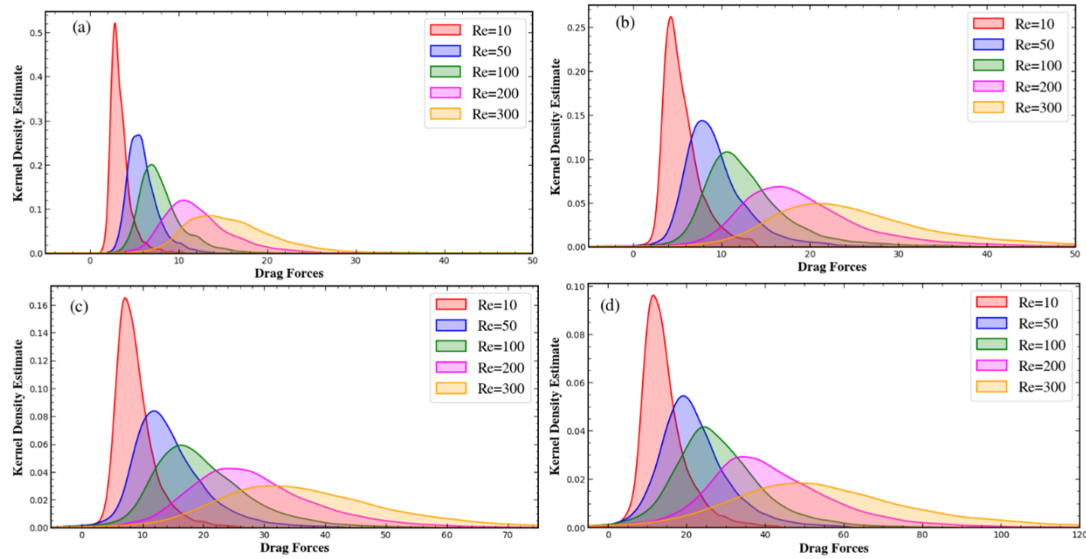
TD0 insert reference:
Cao Z, Tafti DK. “Alternate method for resolving particle collisions in PRS of freely evolving particle suspensions using IBM”. International Journal of Multiphase Flow. 2024 May 10:104862.
https://doi.org/10.1016/j.ijmultiphaseflow.2024.104862
Tafti, Danesh, 2024-08-12T12:58:46.906

n0 0 added
neilashwinraj, 2024-08-12T14:51:14.244

Dataset Description

Solid Fraction	Number of particles	Reynolds Numbers	Number of timeframes
0.1	*24*	*{10,50,100,200, 300}*	*2860*
0.2	*48*	*{10,50,100,200, 300}*	*3016*
0.3	*72*	*{10,50,100,200, 300}*	*3016*
0.4	*95*	*{10,50,100,200, 300}*	*1839*

Summary of different experiments



Kernel density estimates of the PRS drag forces for different Reynolds number for the different solid fractions (a)φ=0.1(b) φ=0.2 (c) φ=0.3 (d) φ=0.4

- The simulations used in this study consider particles of density ratio=2, and there are a total of 20 different experiments that form the dataset.
- An experiment is characterized by its solid fraction and Reynolds number, there 4 different solid fractions in this study, and for each of the 4 solid fractions there are 5 different mean Reynolds numbers.
- Drag force statistics show that along with an increase in the drag force with an increase in Reynolds number, there is also an increase in standard deviation. The same can be said about solid fractions.

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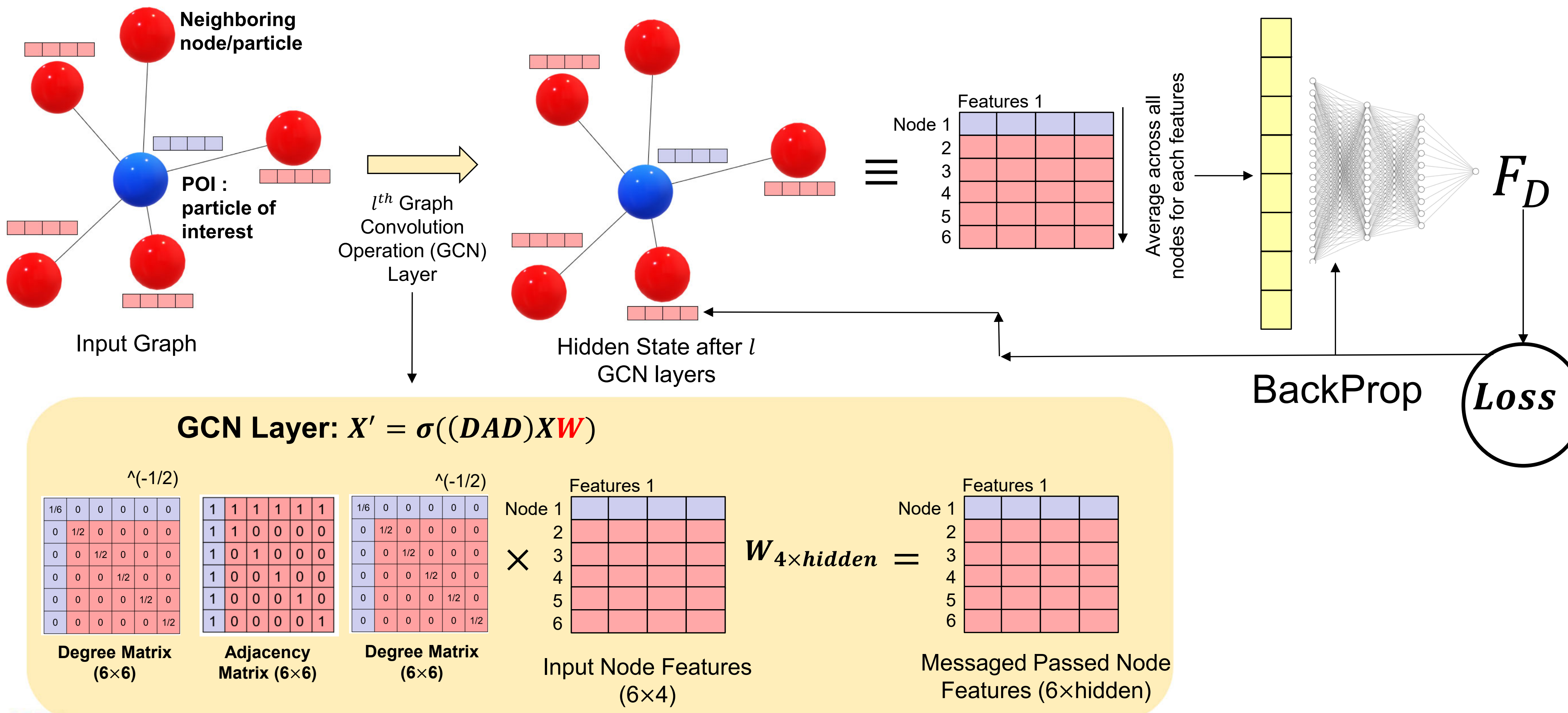
TD0 Frequency ?

Tafti, Danesh, 2024-08-12T12:59:35.642

Stationary model : Graph convolution



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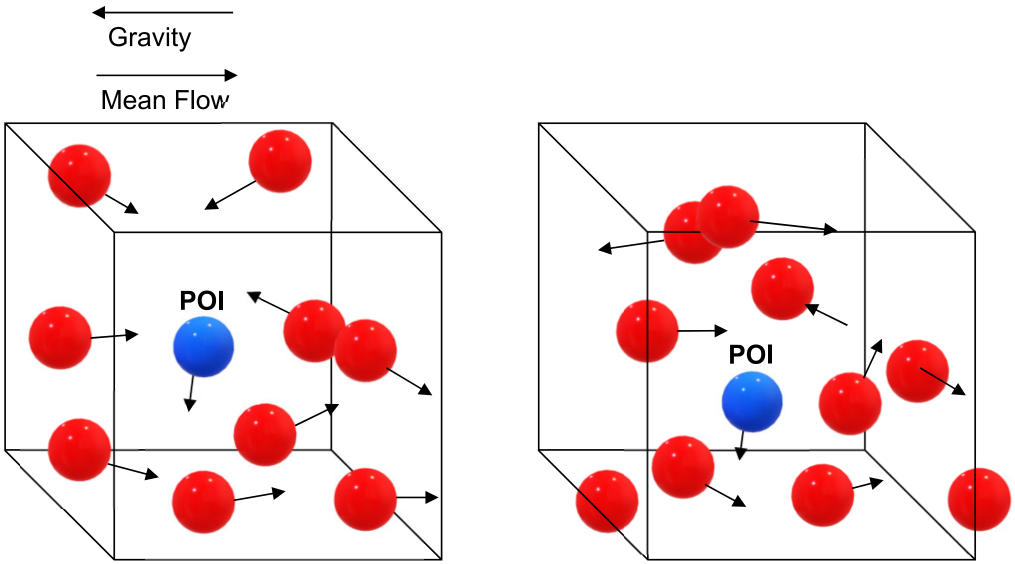
TD0 will have to explain to me - does not mean anything to me.
Tafti, Danesh, 2024-08-12T13:05:58.796

Stationary model : Data splitting and Training

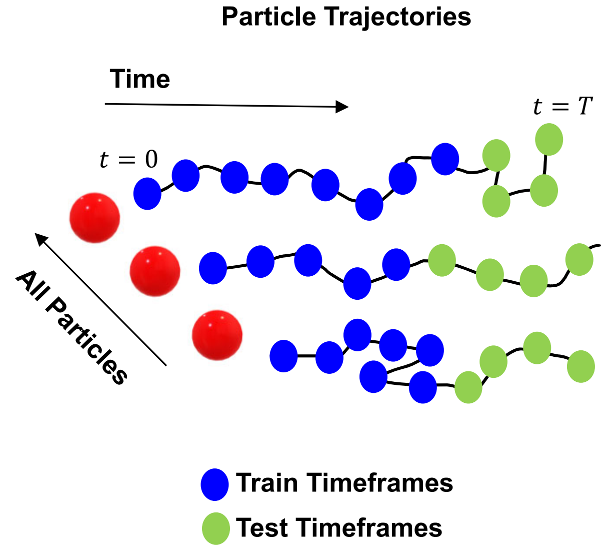


Datapoint 1; $\boldsymbol{t = 1}$ **Datapoint 2;** $\boldsymbol{t = 2}$

$$F_{D,pred} = f_\theta(Re_{local}, \vec{r}_{i,t=1})$$

$$F_{D,pred} = f_\theta(Re_{local}, \vec{r}_{i,t=2})$$

- Here f_θ is the trainable GCN model, Re and φ are the global parameters $\vec{r}_{i,t=1}$ and $\vec{r}_{i,t=2}$ are the position vectors of the n(here n=15) nearest neighbors at $t = 1$ and $t = 2$ respectively. TD0



- A single particle and its 15 nearest neighbors at a given time frame forms a single datapoint.
- For a particular experiment 80% of the time frames form the training dataset and remaining 20% form the testing dataset.

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TD0 i though RE was local
Tafti, Danesh, 2024-08-12T13:09:03.256

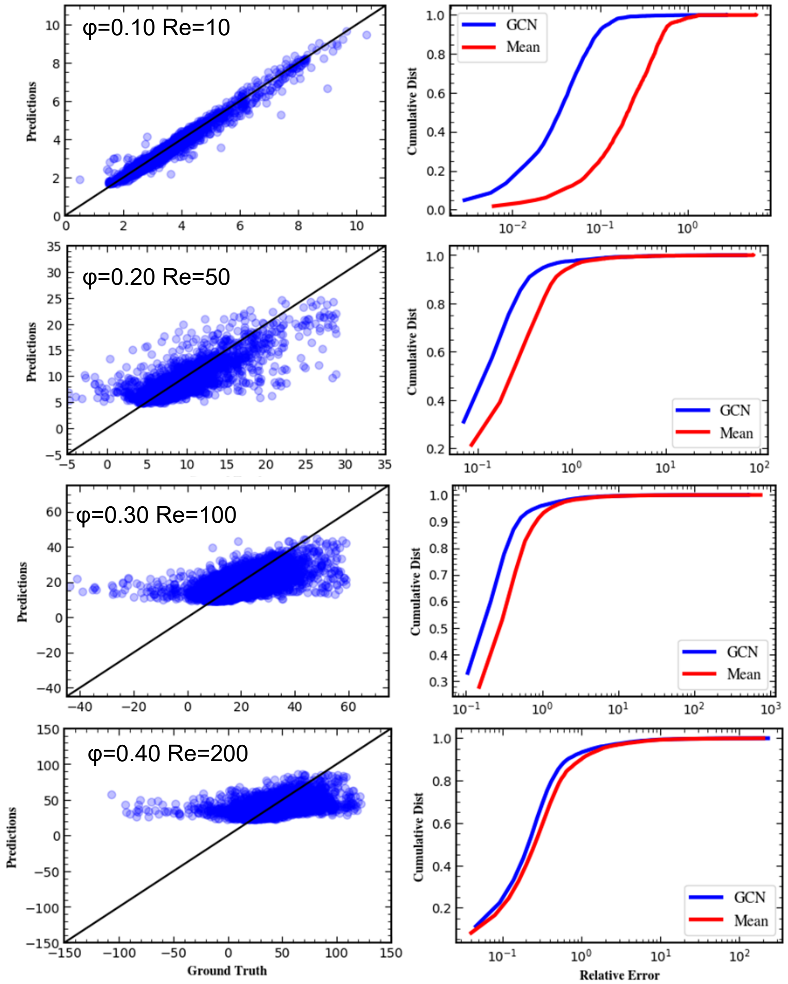
n0 0 corrected
neilashwinraj, 2024-08-12T14:30:37.782

Methods: Stationary

Stationary model : Predictions

φ/Reynolds number	10	50	100	200	300
φ=0.10	0.965	0.816	0.684	0.614	0.514
φ=0.20	0.810	0.571	0.532	0.417	0.484
φ=0.30	0.645	0.398	0.384	0.391	0.433
φ=0.40	0.632	0.274	0.249	0.203	0.245

- The performance deteriorates with an increase in Reynolds number and solid fraction.
- For all the experiments the GCN model performs better than the mean PRS drag force, and accuracy difference between the GCN and the mean drag reduces with an increase in Reynolds number and solid fraction.



Dynamic model: Graph Attention

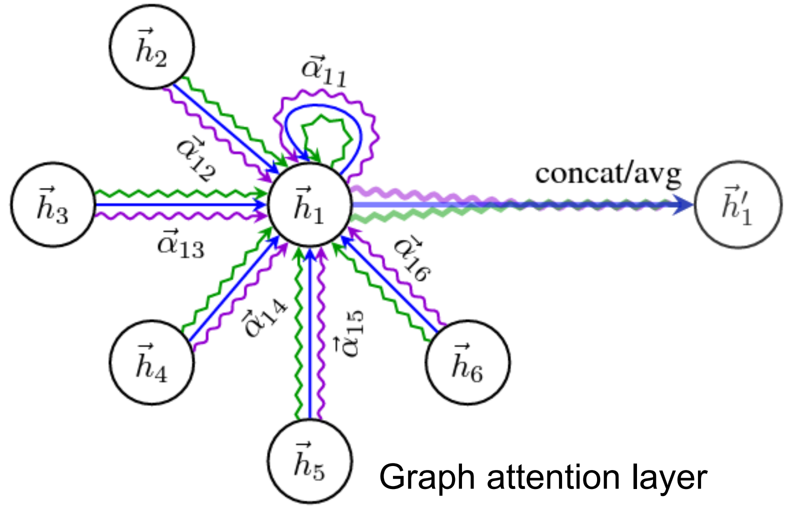
Graph convolution layer

$$\boldsymbol{x}_i^{(l)} = \sum_{j \in N(i) \cup \{i\}} \frac{1}{\sqrt{\deg(i)} \cdot \sqrt{\deg(j)}} \cdot \left(\boldsymbol{W}^T \cdot \boldsymbol{x}_j^{k-1}\right) + \boldsymbol{b}$$

Graph attention layer

$$\boldsymbol{x}_i^{(l)} = \sum_{j \in N(i) \cup \{i\}} \alpha_{i,j} \left(\boldsymbol{W}^T \cdot \boldsymbol{x}_j^{k-1}\right) + \boldsymbol{b}$$

$$\alpha_{i,j} = \frac{exp\left(\text{LeakyReLU}\left(\boldsymbol{a}^T\left[\boldsymbol{W}x_i || \boldsymbol{W}x_j\right]\right)\right)}{\sum_{k \in N(i)} exp\left(\text{LeakyReLU}\left(\boldsymbol{a}^T\left[\boldsymbol{W}x_i || \boldsymbol{W}x_k\right]\right)\right)}$$

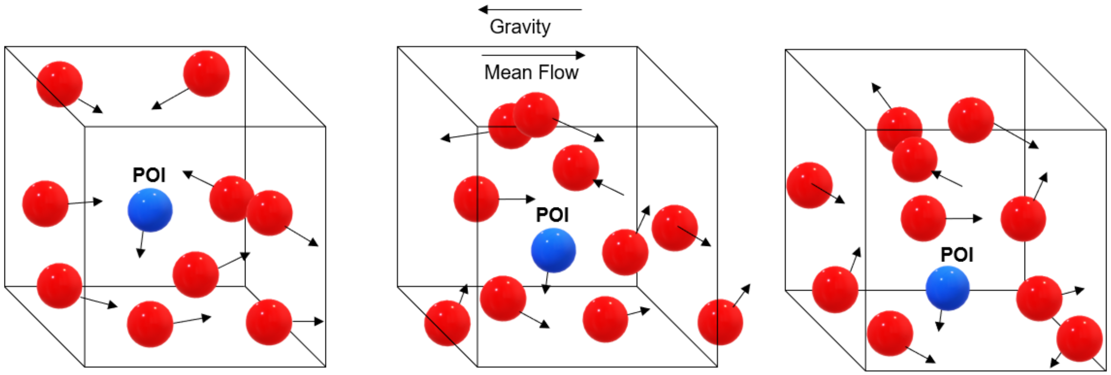


Graph attention layer

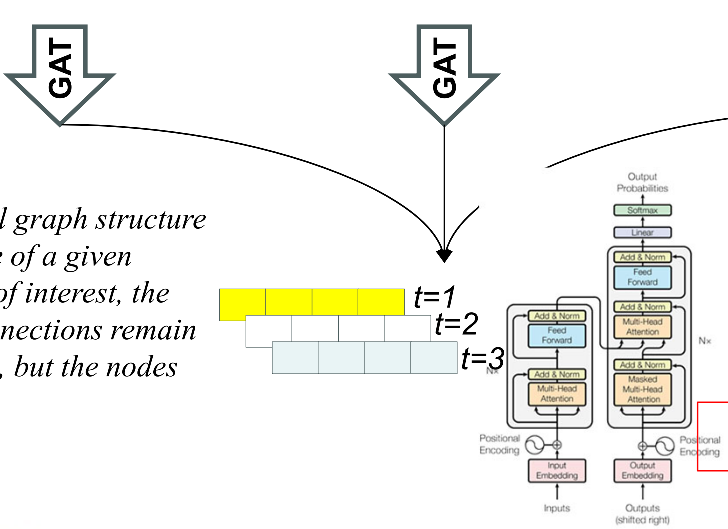
P. Veličković, A. Casanova, P. Liò, G. Cucurull, A. Romero, Y. Bengio, Graph attention networks, in: 6th Int. Conf. Learn. Represent. ICLR 2018 - Conf. Track Proc., International Conference on Learning Representations, ICLR, 2018. https://doi.org/10.1007/978-3-031-01587-8_7.

- The concept of the "attention mechanism" in deep learning refers to weighing the different embeddings or latent space representations within a deep learning architecture.
- For the problem of drag predictions using the nearest neighbors, this would mean that the GNN can now in the course of training can assign higher importance to the nearby nodes as they will influence the drag forces more than the far away nodes, something which is not explicitly performed by a conventional GCN layer.

Dynamic model: Combining Graph Attention with Transformers



Datapoint 1;$t = 1$ Datapoint 1;$t = 2$ Datapoint 1;$t = 3$



Temporal graph structure sequence of a given particle of interest, the edge connections remain the same, but the nodes will vary

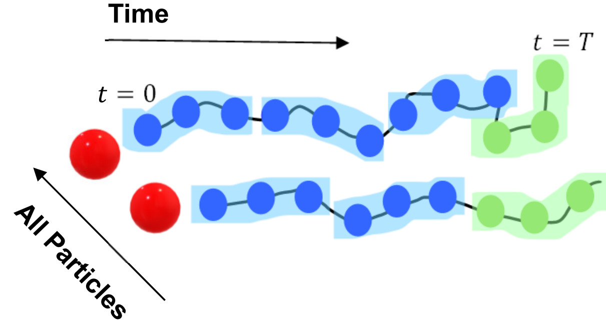
Many to one mapping

$$F_{d,poi} \; at \; t = 3$$

Seq to Seq mapping

$$F_{d,poi} \; at \; t = 1, 2, 3$$

Particle Trajectories



Train Timeframes
Test Timeframes

- A temporal sequence of a particle and the location of its 15 nearest neighbors constitutes a single data point.
- Two different training regimes are explored one, where the trajectory sequence is mapped to the drag at the final time step and another where it's mapped to a sequence of drag forces

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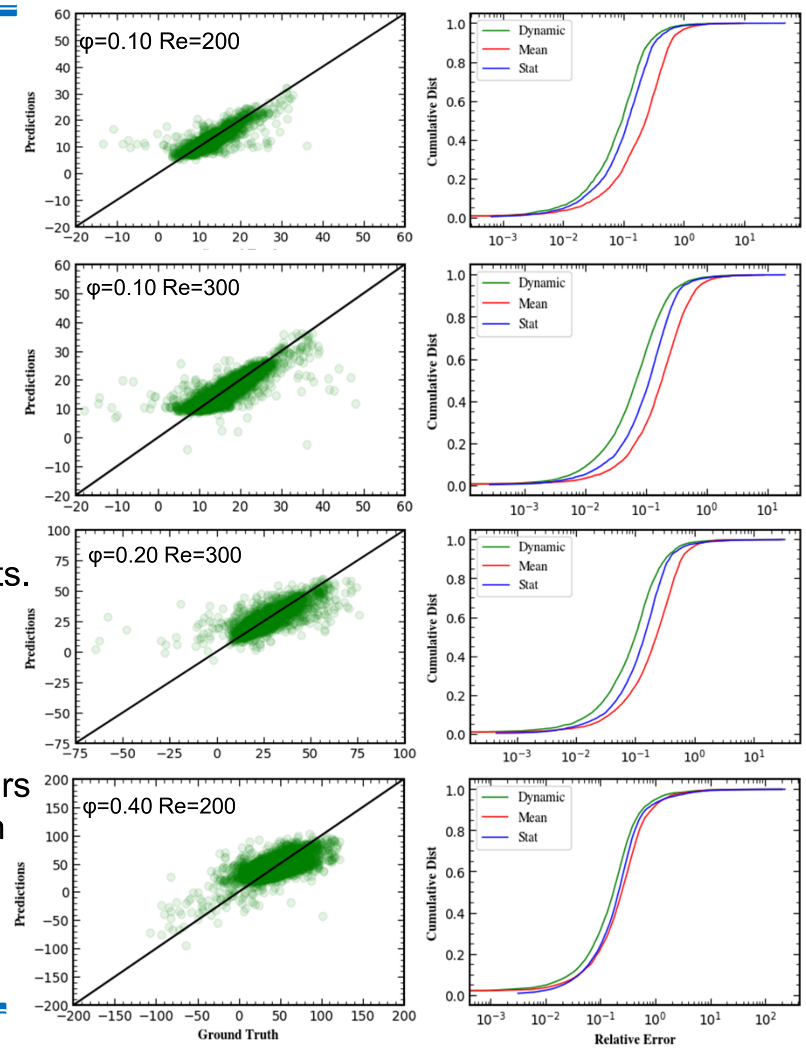
TD0 explain what transformer is in simple language when presenting

Tafti, Danesh, 2024-08-12T13:20:13.733

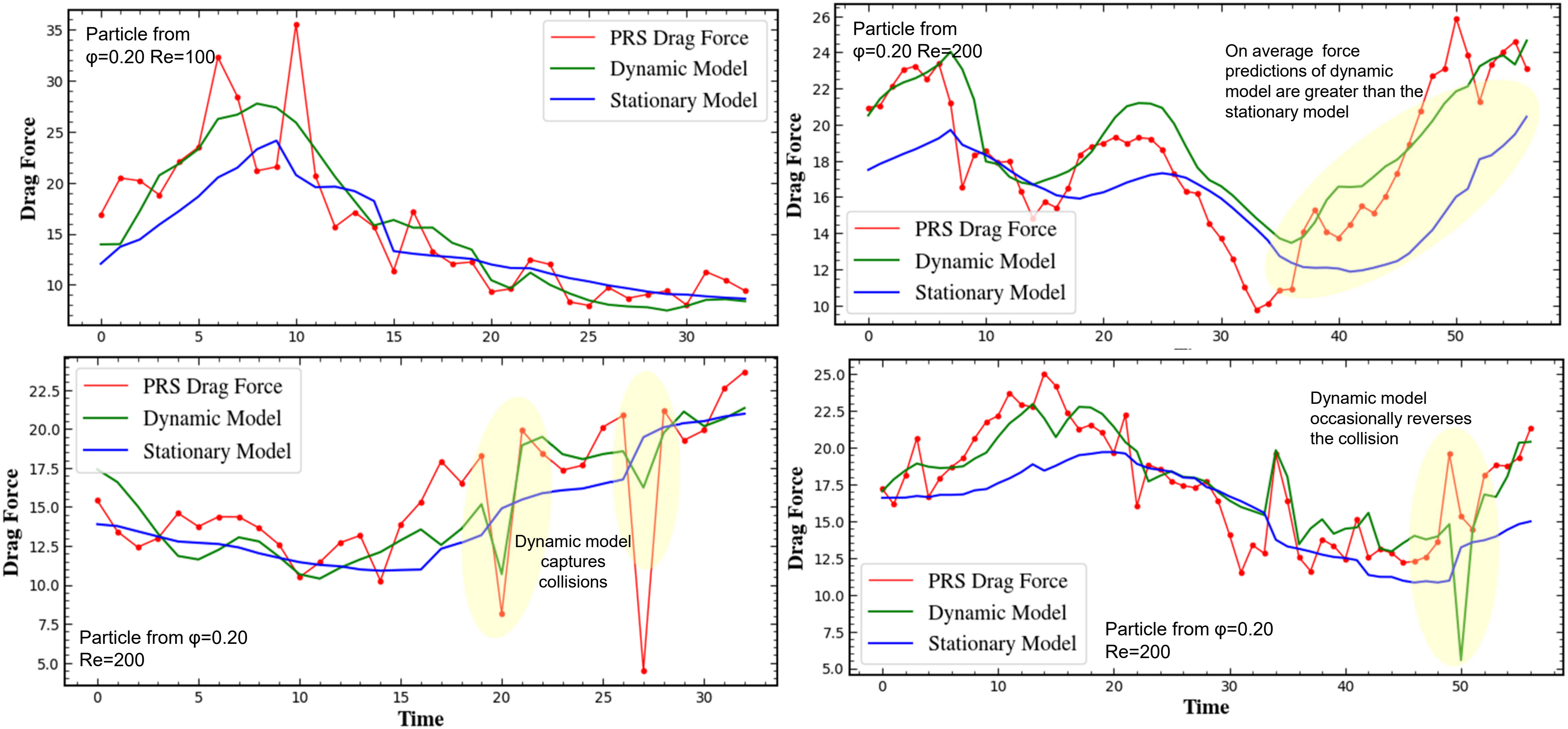
Dynamic model: Predictions

	Stationary					Dynamic				
φ/Reynolds number	10	50	100	200	300	10	50	100	200	300
φ=0.10	0.965	0.816	0.684	0.614	0.514	0.931	0.82	0.705	0.680	0.675
φ=0.20	0.810	0.5706	0.532	0.417	0.484	0.857	0.579	0.659	0.561	0.604
φ=0.30	0.645	0.398	0.384	0.391	0.433	0.764	0.573	0.553	0.514	0.493
φ=0.40	0.632	0.274	0.249	0.203	0.245	0.697	0.475	0.477	0.486	0.415



- The dynamic model outperforms the stationary model across all the experiments.
- The model sees the same trend pf performance deterioration with increasing Reynolds numbers and solid fraction.
- The improvement in performance is more prominent at higher Reynolds numbers and solid fractions, essentially meaning that a lower Reynolds and solid fraction the flow field the difference between the dynamic and static flow fields is not significantly different.

Dynamic model: Predictions on Single Particles



Conclusions and Further Work

- Graph neural networks-based models were assessed in their ability to model drag forces in dense suspensions of spherical particles across different solid fractions and Reynolds numbers.
- The dynamic model outperformed the stationary model across all dataset, thus including trajectory history is crucial in developing accurate drag models.
- The sequence-to-sequence based training outperforms the many to one mapping model.

Future Work:
- Introducing hierarchical learning framework by using hypergraph convolutions
- Incorporating physical constraints on the training datasets, such as rotational equivariance and invariance.

1. 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.
2. 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.
3. 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.
4. He, L. and Tafti, D., 2018. Variation of drag, lift and torque in a suspension of ellipsoidal particles. *Powder Technology*, *335*, pp.409-426.

Thank You

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