ML DRIVEN MODELS TO PREDICT THE DRAG COEFFICIENT OF A SPHERE TRANSLATING IN SHEAR-THINNING VISCOELASTIC FLUIDS

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2. Numerical Approach
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4. ML Validation | *Single sphere translating in viscoelastic Oldroyd-B fluid*
5. ML Validation | *Single sphere translating in viscoelastic Giesekus fluid*
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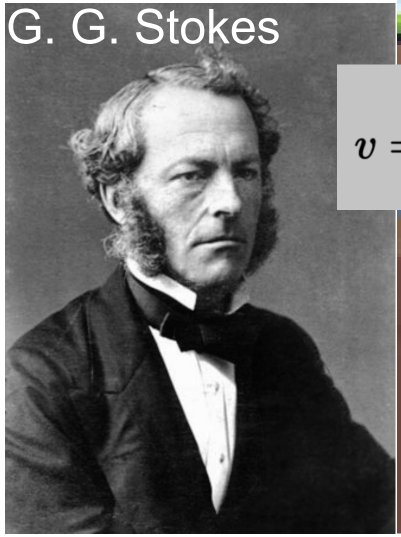
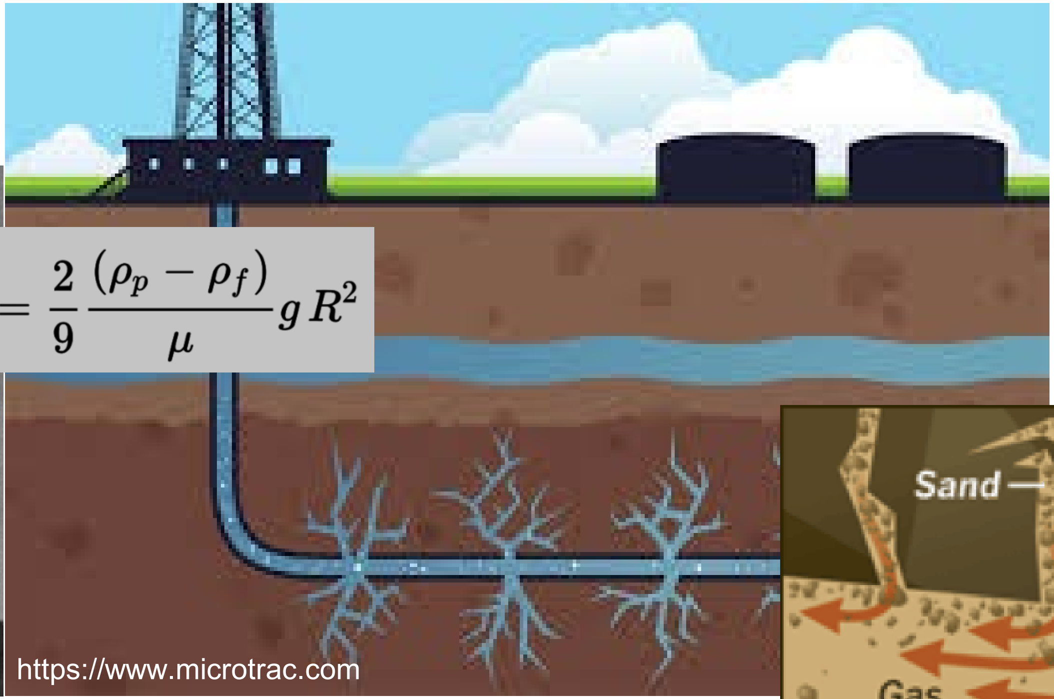
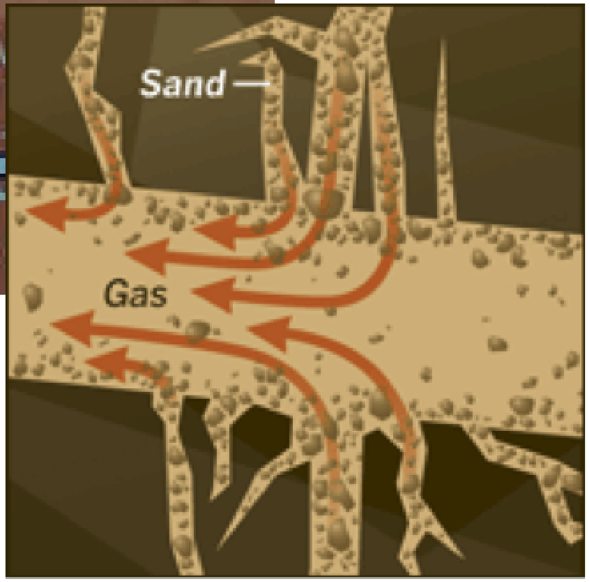
1. Introduction & Motivation



$$v = \frac{2}{9}\frac{(\rho_p - \rho_f)}{\mu} g\, R^2$$



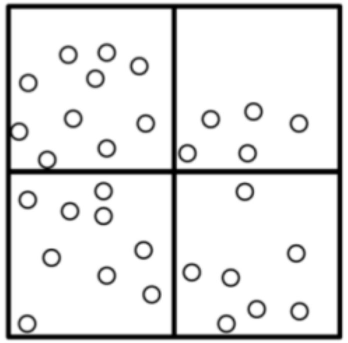


*A.C. Barbati, et al., "Complex fluids and hydraulic fracturing“, *Annual review of chemical and biomolecular engineering,* 7, 415, 2016.

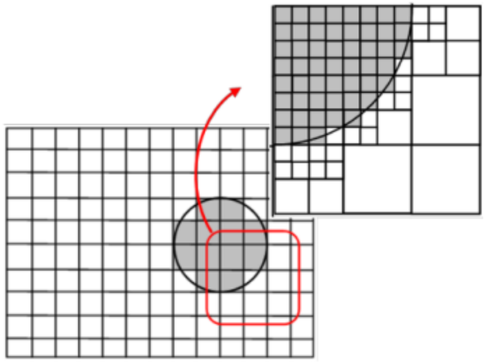
1. Introduction & Motivation

Fluid-particle interaction

Computational Fluid Dynamics (CFD) + **Discrete Element Method (DEM)**



- **unresolved CFD-DEM** ←
- **resolved CFD-DEM** →



- CFD-DEM
- coarse grained CFD-DEM
- MP-PIC

- Immersed Boundary Method
- Fictitious Domain Method

*C. Fernandes, et al., "Validation of the CFD-DPM solver DPMFoam in OpenFOAM through analytical, numerical and experimental comparisons", *Granular Matter*, 20, 64, 2018.

*C. Fernandes, et al., "Fully-resolved simulations of particle-laden viscoelastic fluids using an immersed boundary method", *Journal of Non-Newtonian Fluid Mechanics*, 266, 80, 2019.

2. Numerical Approach

Newtonian Fluid

$$\sum \mathbf{F} = \mathbf{F_a} + \mathbf{F_D} + \mathbf{F}_p + \mathbf{F}_{vol} + \mathbf{F}_{lift} + \mathbf{F}_{buoy} + \mathbf{F}_h,$$

$$\mathbf{F}_a = \frac{1}{2}\rho\frac{m_P}{\rho_P}\left(\frac{D\mathbf{U}}{Dt} - \frac{d\mathbf{U}_P}{dt}\right),$$

$$\mathbf{F}_D = m_p\frac{\mathbf{U}-\mathbf{U}_P}{\tau_P}, \qquad \tau_p = \frac{4}{3}\frac{\rho_p D_p}{\rho C_D|\mathbf{U}-\mathbf{U_p}|}$$

$$\mathbf{F}_p = -\frac{m_P}{\rho_P}\nabla p,$$

$$\mathbf{F}_{vol} = \frac{1}{2}\rho\frac{dV_P}{dt}(\mathbf{U}-\mathbf{U_p}),$$

$$\mathbf{F}_{lift} = C_L\rho\frac{m_P}{\rho_P}(\mathbf{U}-\mathbf{U_p})\times\omega,$$

$$\mathbf{F}_{buoy} = m_P\left(1-\frac{\rho}{\rho_P}\right)\mathbf{g},$$

$$\mathbf{F}_h = \frac{3}{2}D_P^2\sqrt{\pi\rho\mu}\int_0^t \frac{\frac{D\mathbf{U}}{Dt'} - \frac{d\mathbf{U_P}}{dt'}}{\sqrt{t-t'}}dt',$$

$$C_D = \begin{cases} \frac{24}{Re_p} & \text{if } \mathrm{Re}_p \le 0.1 \\ \frac{24}{Re_p}\left(1+\frac{1}{6}Re_p^{2/3}\right) & \text{if } 0.1 \le Re_p \le 1000 \\ 0.44 & \text{if } \mathrm{Re}_p > 1000 \end{cases}$$

* S. A. Faroughi, Theoretical Developments to Model Microstructural Effects on The Rheology of Complex Fluids, PhD Thesis, 2016.
* S. Subramaniam, Progress in Energy and Combustion Science, Elsevier, 2013.
* R. Hill, et al., "Moderate-Reynolds-numbers flows in ordered and random arrays of spheres", *Journal of Fluid Mechanics,* 448, 243, 2001.

Viscoelastic Fluid Oldroyd-B

Creeping flow conditions ($Re < 1$)

- $\phi \approx 0, \quad 0 < \zeta < 1, \quad 0 \le Wi \le 10$

$$\chi = \frac{C_D}{(24/Re)} = \begin{cases} 1 + \frac{\sum_{i=1}^{3}\left[Wi^{2i}\left(\sum_{m=1}^{3} a_{im}\zeta^{m-1}\right)\right]}{\sum_{j=1}^{3}\left[Wi^{2(j-1)}\left(\sum_{n=1}^{3} b_{jn}\zeta^{n-1}\right)\right]} & \text{if } Wi \le 1, \\ 1 + \frac{\sum_{k=1}^{3}\left[Wi^{2(k+1)}\left(\sum_{p=1}^{3} c_{kp}\zeta^{p-1}\right)\right]}{\sum_{s=1}^{3}\left[Wi^{2(s-1)}\left(\sum_{q=1}^{3} d_{sq}\zeta^{q-1}\right)\right]} & \text{if } Wi > 1. \end{cases}$$

- $0 < \phi < 0.2, \quad \zeta = 0.5, \quad 0 \le Wi \le 4$

$$\frac{\langle F\rangle(\phi, Wi)}{F^0(Wi)} = (1-\phi)^2(1 + 63.03\phi^{1.459})$$

* S. A. Faroughi, C. Fernandes, J. Miguel Nóbrega, and G. H. McKinley. A closure model for the drag coefficient of a sphere translating in a viscoelastic fluid. Journal of Non-Newtonian Fluid Mechanics, 277:104218, 2020.
* C. Fernandes, S.A. Faroughi, R. Ribeiro, A.I. Roriz, and G.H. McKinley. Finite volume simulations of the inertia-less steady translation of random arrays of spheres in viscoelastic fluid flows: application to hydraulic fracture processes. In preparation, 2021.

2. Numerical Approach

Continuity equation

$$\nabla \cdot (\rho \mathbf{u}) = 0$$

Momentum equation

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) + \nabla \cdot (p\mathbf{I}) - \nabla \cdot \boldsymbol{\tau} = 0$$

$$\boldsymbol{\tau} = \boldsymbol{\tau}_S + \boldsymbol{\tau}_P$$

Constitutive equations (shear-thinning Giesekus model)

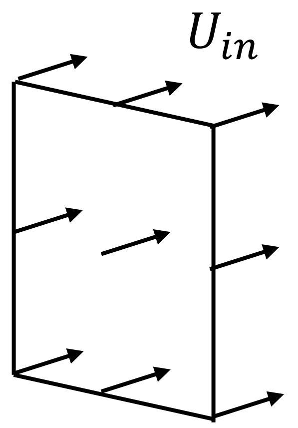
$$\boldsymbol{\tau}_S = \eta_S \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)$$

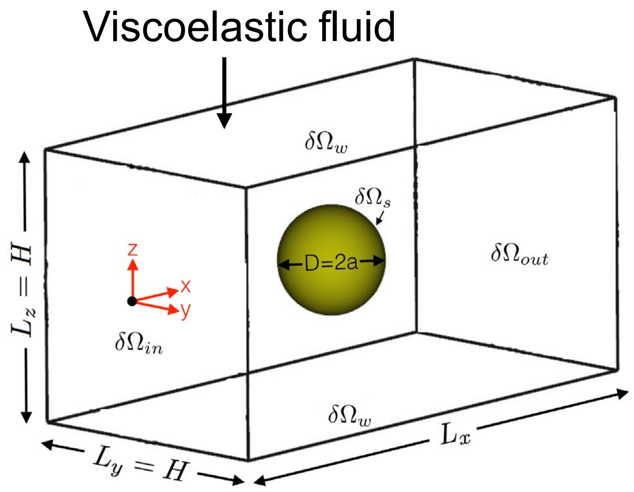
$$\lambda \overset{\nabla}{\boldsymbol{\tau}}_P + \boldsymbol{\tau}_P + \frac{\alpha \lambda}{\eta_P} \boldsymbol{\tau}_P \cdot \boldsymbol{\tau}_P = \eta_P \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)$$

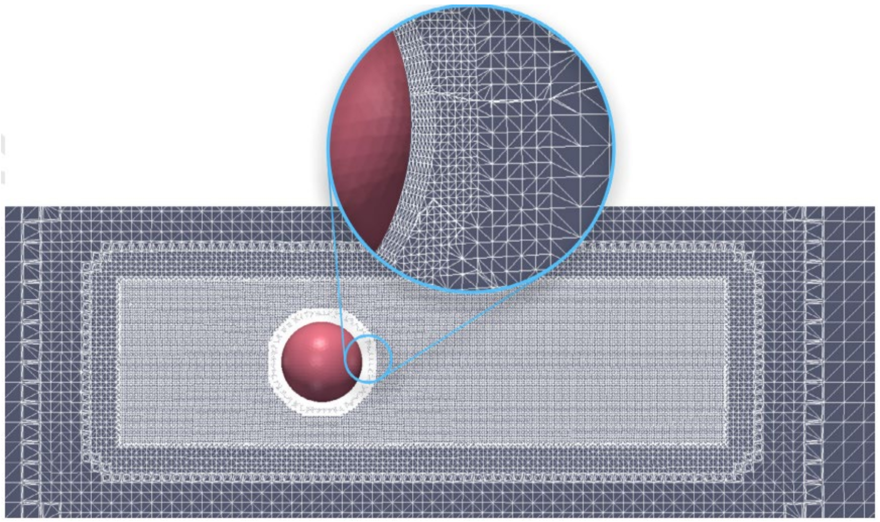
If $\alpha = 0$, then it is quasi-linear Oldroyd-B model

α is the mobility parameter, λ is the relaxation time, η_S and η_P are the solvent and polymeric viscosities, respectively.

3. Direct Numerical Simulations







Dimensionless numbers (input variables)

$$Re = 2Re_a = \frac{2a\rho U_{in}}{\eta_0}$$

$$Wi = \frac{\lambda U_{in}}{H}$$

$$\zeta = \frac{\eta_P}{(\eta_S + \eta_P)} = \frac{\eta_P}{\eta_0}$$

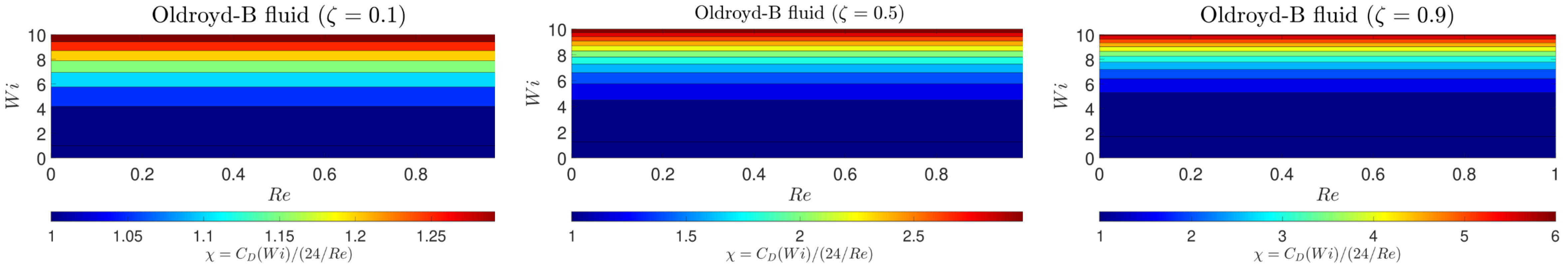
α is the mobility parameter

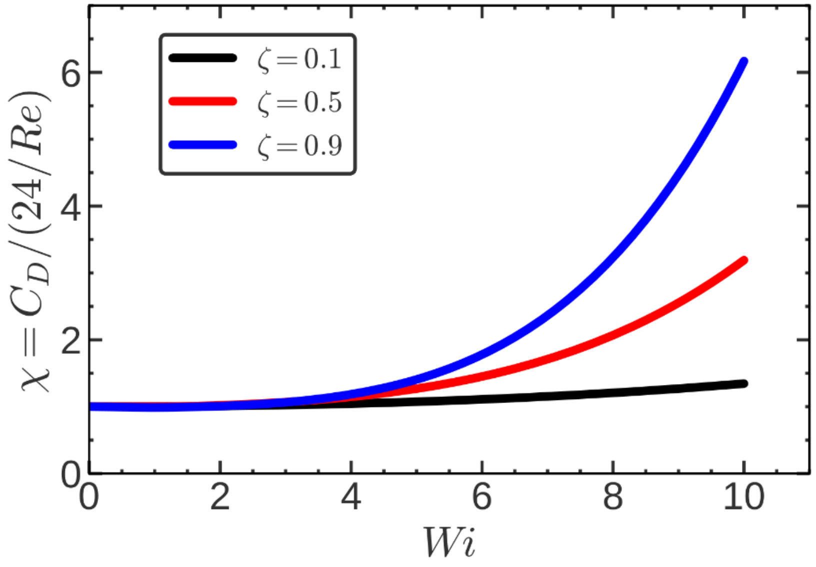
Drag coefficient correction (output variable)

$$\chi = \frac{C_D}{(24/Re)}$$

where $C_D = \frac{2}{\rho U^2 A} \int_{\delta\Omega_s} (\boldsymbol{\tau}_P + \boldsymbol{\tau}_S - p\boldsymbol{I}).\boldsymbol{n}.\boldsymbol{x} dS$

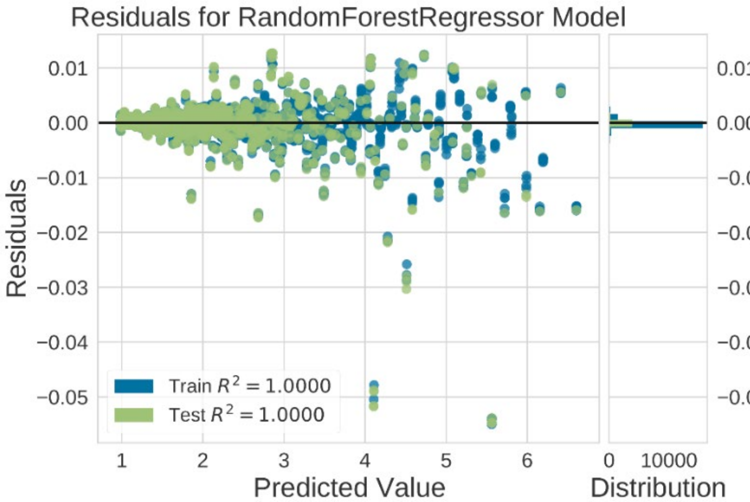
4. ML Validation | *Single sphere suspended in viscoelastic Oldroyd-B fluid*

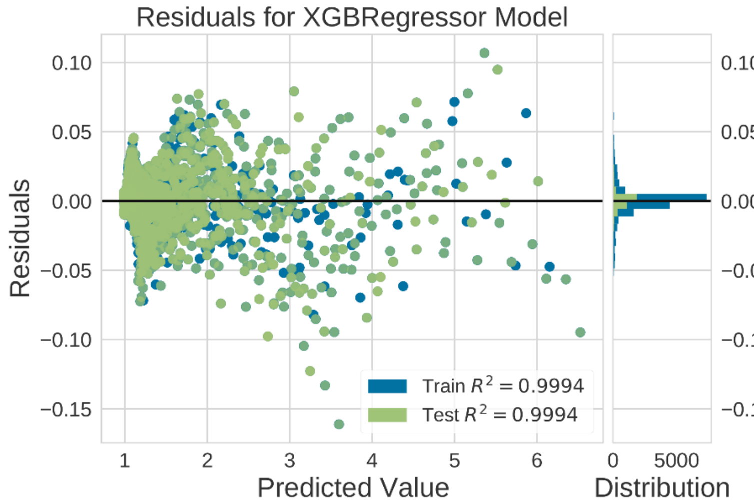


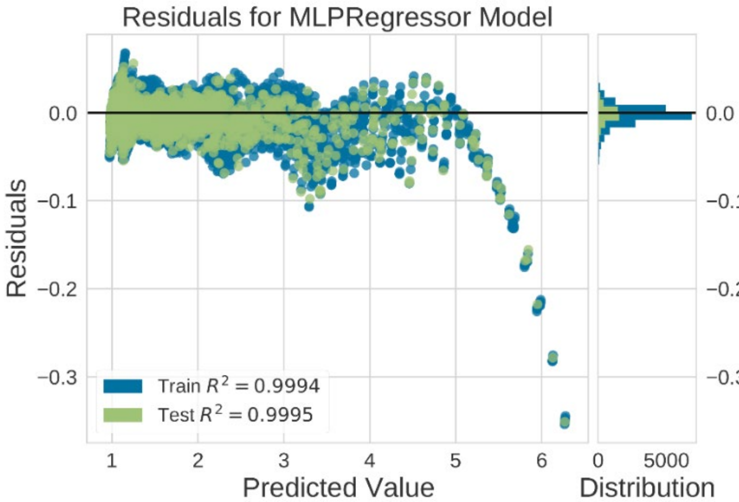


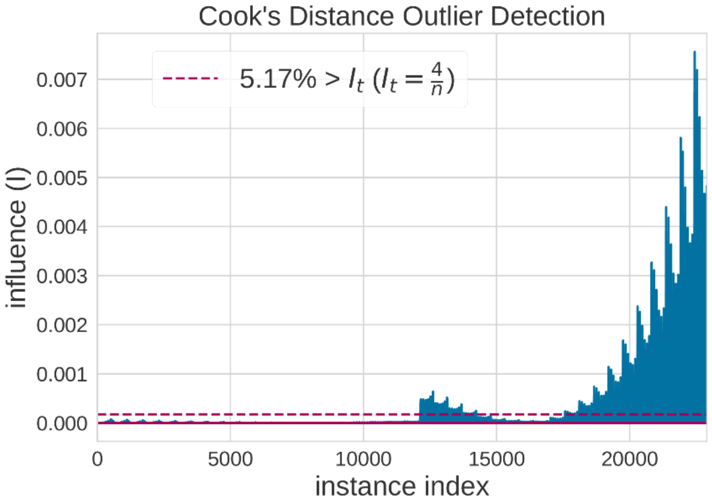
- Total of 23040 input values generated by the closure model developed by Faroughi et al. (2020).
- The range of the input data used varied within Reynolds number 0 < *Re* ≤ 1, Weissenberg number 0 ≤ *Wi* ≤ 10, retardation ratio 0 < ζ < 1.
- The increase of the retardation ratio leads to a drag correction coefficient increase.

4. ML Validation | *Single sphere suspended in viscoelastic Oldroyd-B fluid*









- The data set is divided into training and testing subsets to compare with the predicted data, in percentage 80/20.
- For each ML model, the following hyperparameters were tuned:

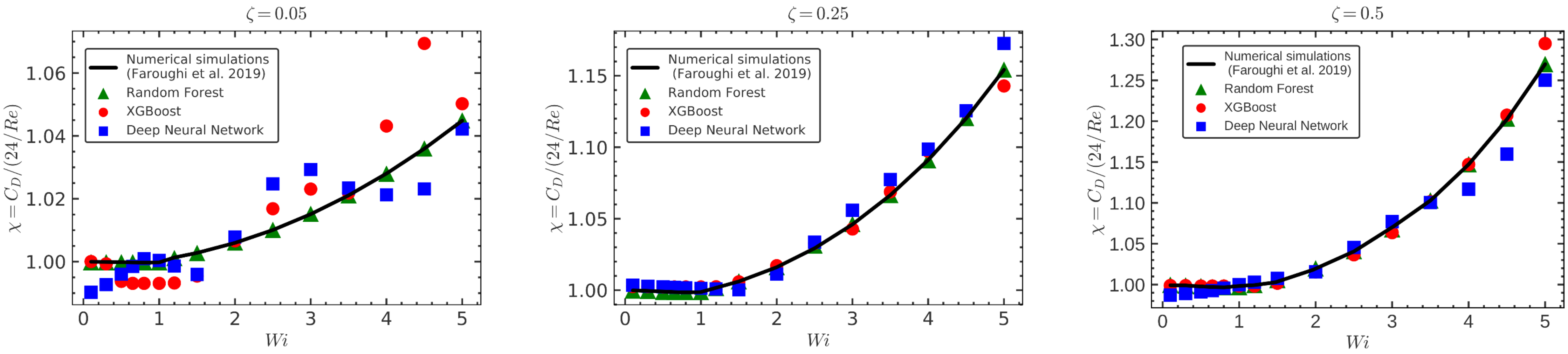
Random Forest: n_iter = 50, cv = 3, verbose=2, random_state=42, n_jobs = -1, max_depth= 100, min_samples_leaf: 2, min_samples_split: 5, n_estimators=800 (RandomizedSearchCV).

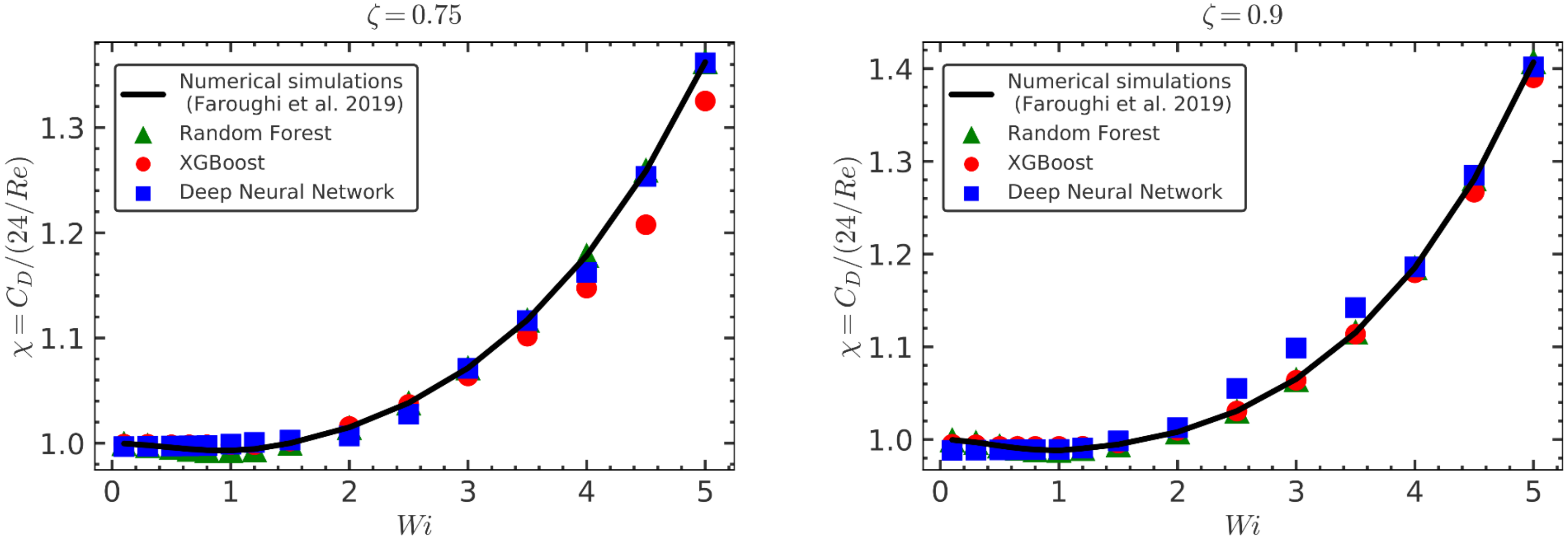
XGBoost: objective="reg:gamma“, random_state=42.

Neural Network: hidden_layer_sizes=(50,40,30), max_iter=8000, random_state=42.

- The best R^2 is obtained for the Random Forest model.
- The main distribution of the residual error is around zero for all the ML algorithms employed.
- The Cook's distance plot shows that about 5% of the data can be considered outliers.

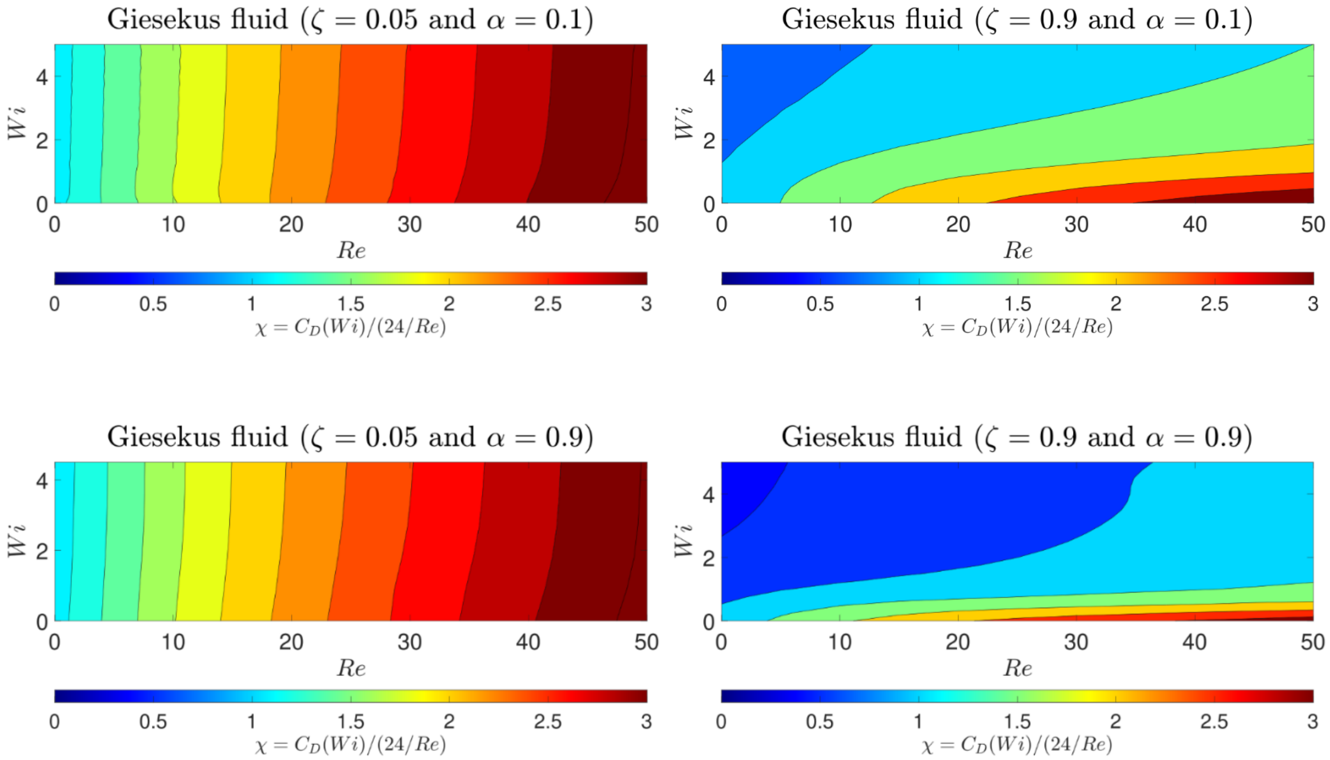
4. ML Validation | *Single sphere suspended in viscoelastic Oldroyd-B fluid*

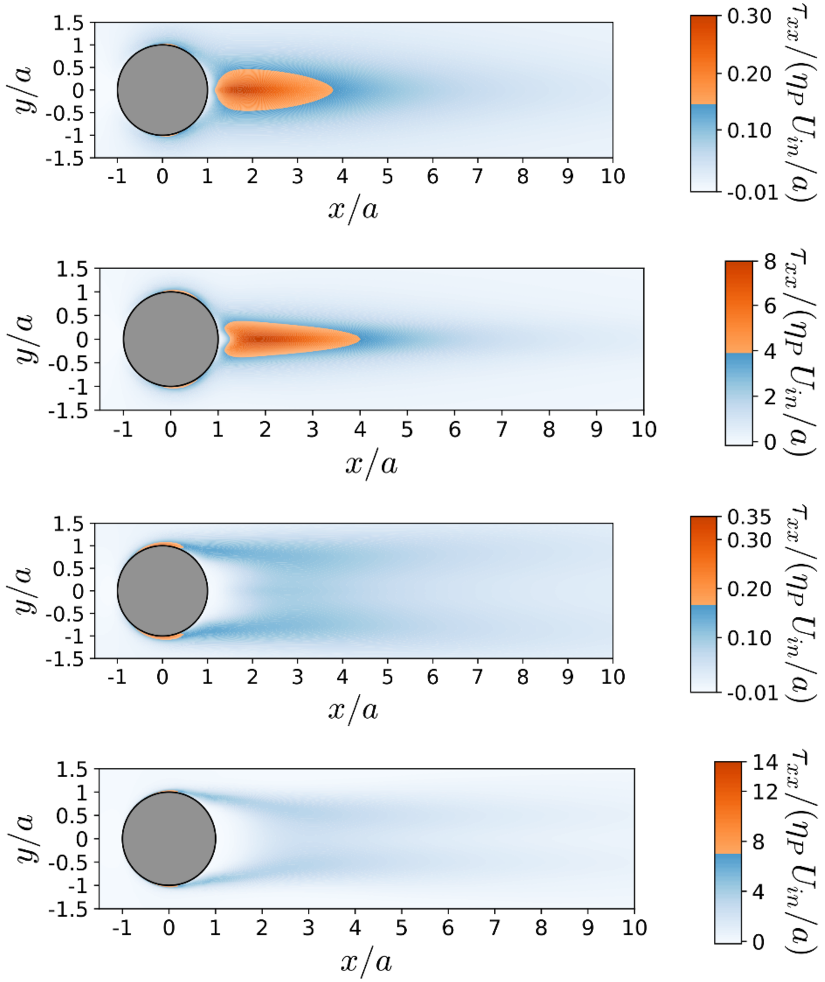




- Validation of the ML model predictions by comparing against numerical simulation results (using blind data).
- It can be confirmed that the best predictive model is the RF, because the predictions overlap the results obtained in the numerical simulations.

5. ML Validation | *Single sphere suspended in viscoelastic Giesekus fluid*

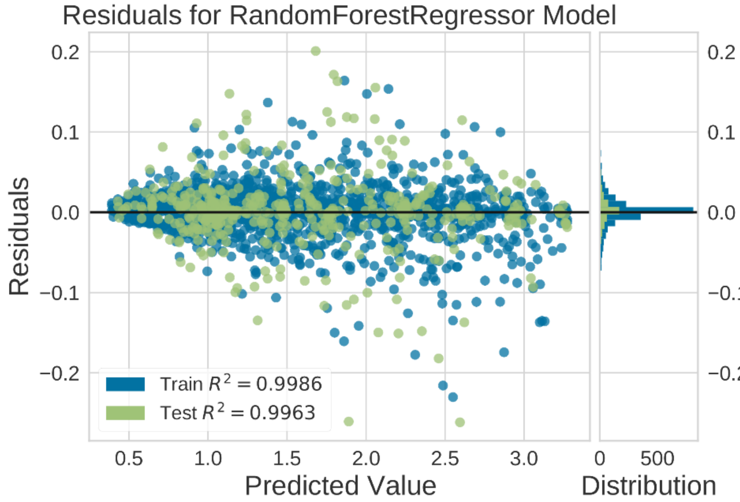


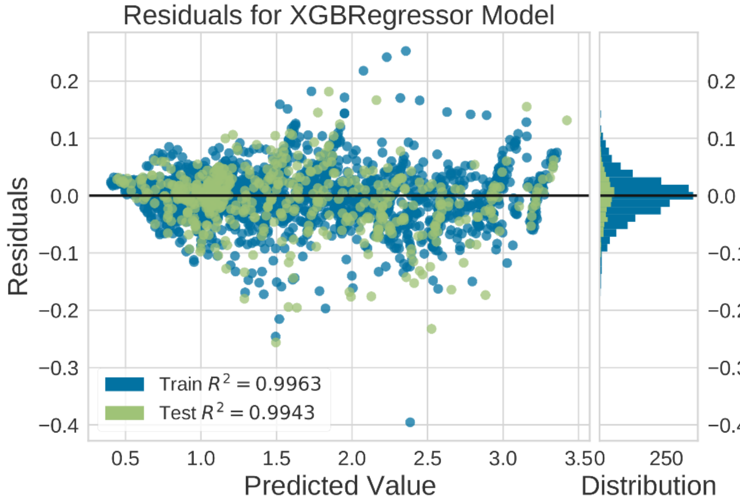


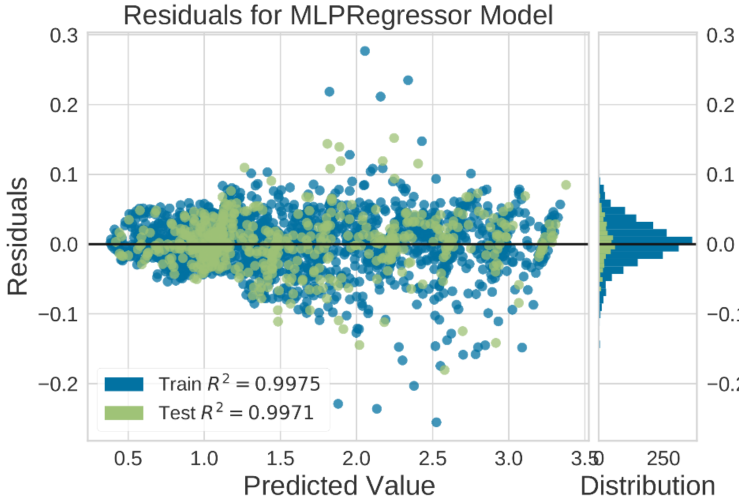
- A total of approximately 3000 DNS.
- Reynolds number $0 < Re \leq 50$, Weissenberg number $0 \leq Wi \leq 5$, retardation ratio $0 < \zeta < 1$, and the shear-thinning mobility parameter $0 < \alpha < 1$.

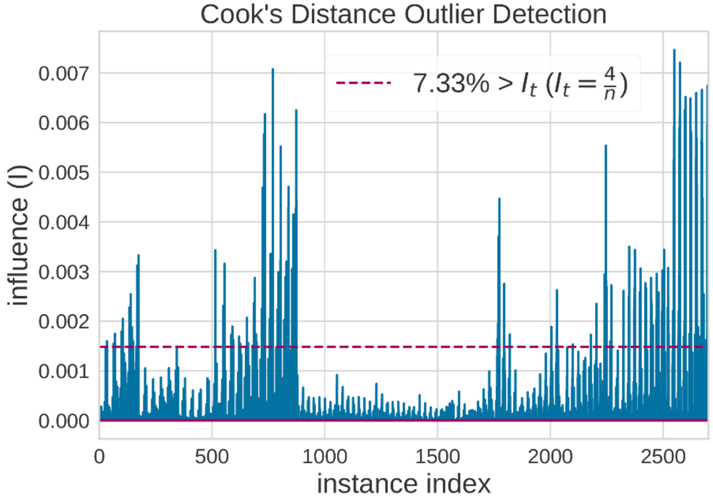
- Drag decreases with Wi at $Re << 1$.
- Drag increases with Re (even at $Wi \approx 0$).
- Weaker drag increase with Re when $Wi \neq 0$.

5. ML Validation | *Single sphere suspended in viscoelastic Giesekus fluid*







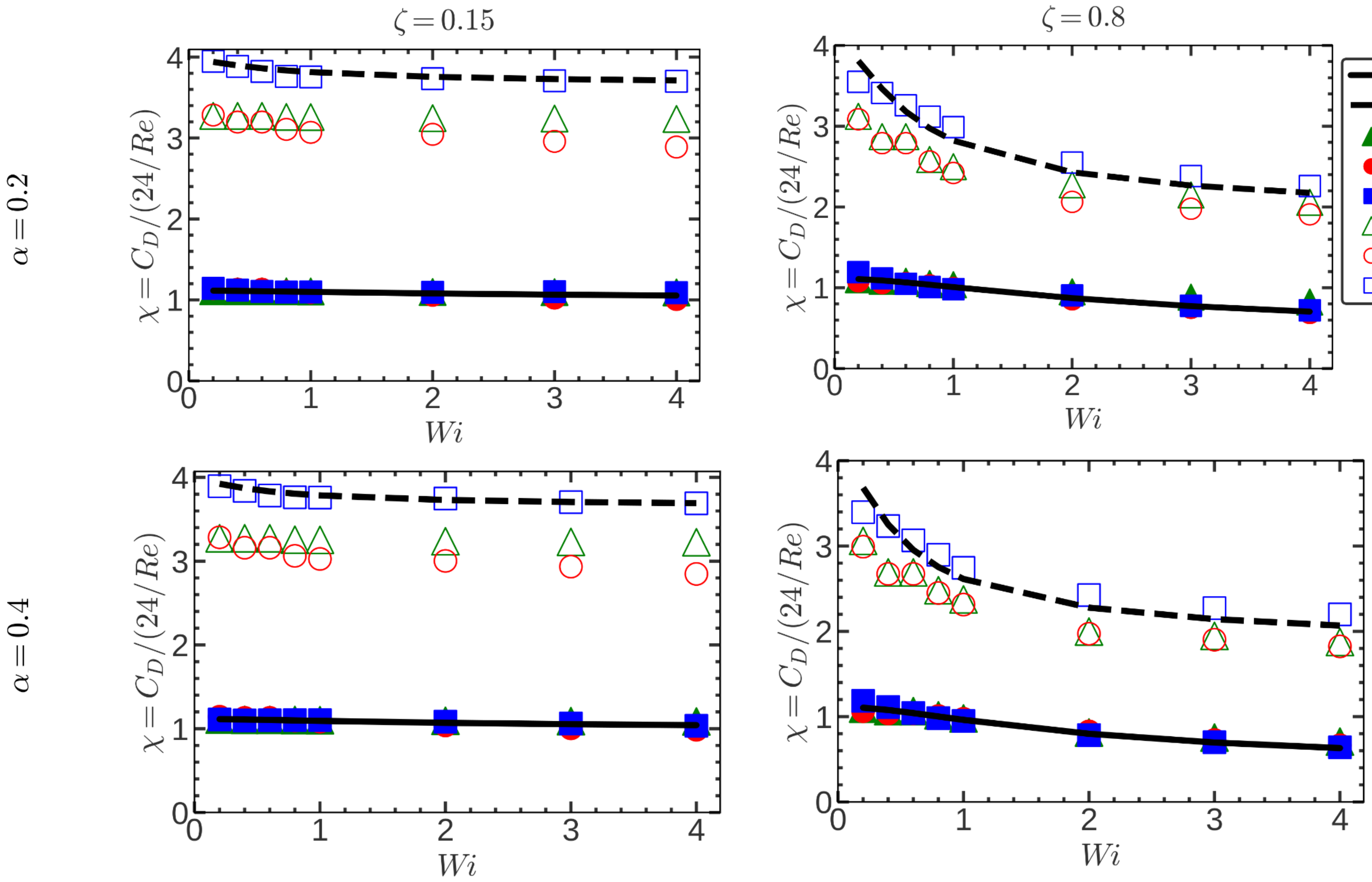


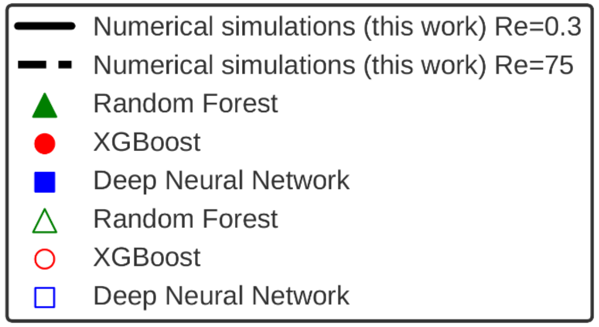
- The data set is divided into training and testing subsets to compare with the predicted data, in percentage 80/20.
- For each ML model, the following hyperparameters were tune:

Random Forest: Random_state=42, n_iter = 50, cv = 3, verbose=2, n_jobs = -1, max_depth: 100, min_samples_leaf= 2, min_samples_split= 5, n_estimators=800 (RandomizedSearchCV).
XGBoost: Objective:"reg::gamma", Random_state=42.
Neural Network: hidden_layer_sizes=(50,50,55,25), max_iter=8000, Random_state=42.

- The best R^2 considering train and test data sets is obtained for the Deep Neural Network model with a value of 0.9971.
- The main distribution of the residual error is around zero for all the ML algorithms employed.
- The Cook's distance plot shows that about 7% of the data can be considered outliers.

5. ML Validation | *Single sphere suspended in viscoelastic Giesekus fluid*





- Validation of the ML model predictions by comparing against numerical simulation results (blind data).
- It can be confirmed that the best predictive model is the DNN, because the predictions overlap the results obtained in the numerical simulations.

6. Conclusions

- ✓ The dataset to train and test the ML models for Oldroyd-B fluid was constituted from a total of 23 040 input values generated from a closure drag law found in the scientific literature, where the kinematic input variables varied within Reynolds $0 < Re \leq 1$, Weissenberg $0 \leq Wi \leq 10$ and polymeric retardation ratio $0 < \zeta < 1$.

- ✓ The dataset to train and test the ML models for Giesekus fluid was constituted from a total of 2 700 input values generated from direct numerical simulations, where the kinematic input variables varied within Reynolds $0 < Re \leq 50$, Weissenberg $0 \leq Wi \leq 5$, polymeric retardation ratio $0 < \zeta < 1$ and shear-thinning mobility parameter $0 < \alpha < 1$.

- ✓ The ML model with the best R-squared for the Oldroyd-B fluid was the Random Forest, and for the Giesekus fluid was the Deep Neural Network.

- ✓ This work would increase our ability to facilitate the coupling across scales, e.g. in a multiphase algorithm based in the momentum transfer approach constituted by a discrete particle method with a viscoelastic continuum phase.

- ✓ The key concept towards this direction is the creation of a statistically large database that could be incorporated from a powerful machine learning framework. In summary, simulations and ML techniques can coexist with the purpose of accelerating numerous engineering applications.

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  - **Gompute HPC** Cloud Platform (URL: https://www.gompute.com);
  - **Minho Advanced Computing Center** (MACC) within the project number CPCA/A2/6052/2020 (URL: https:// macc.fccn.pt).
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Thank you for your attention!