DIGITAL-TWIN APPROACH TO PREDICT THE DRAG COEFFICIENT OF RANDOM ARRAYS OF SPHERES SUSPENDED IN GIESEKUS VISCOELASTIC FLUIDS

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Outline

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3. Direct Numerical Simulations
4. Random arrays of spherical particles translating in shear-thinning viscoelastic fluids
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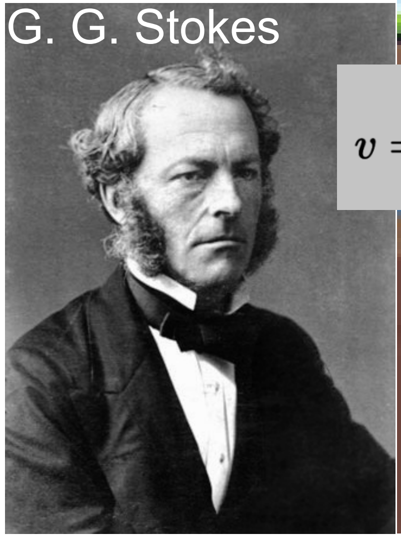
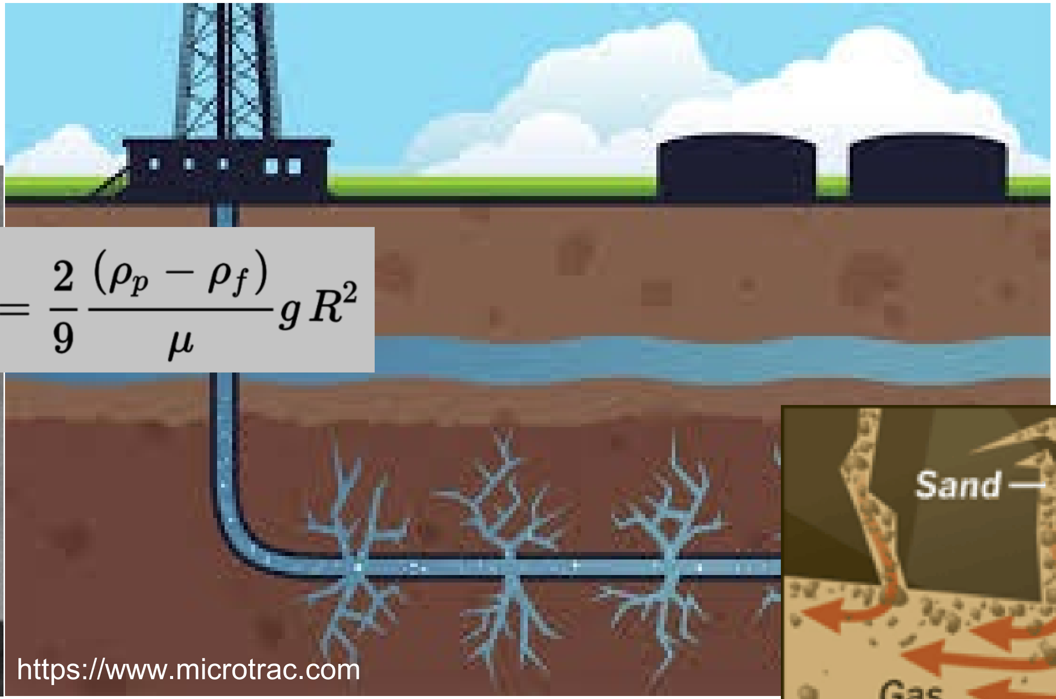
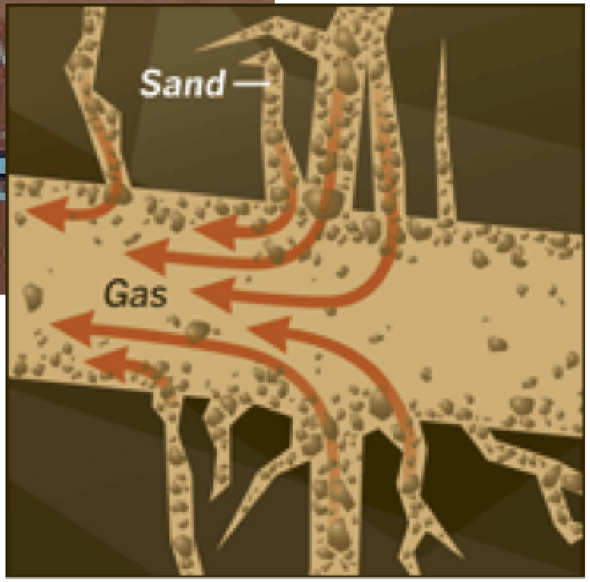
1. Introduction & Motivation



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



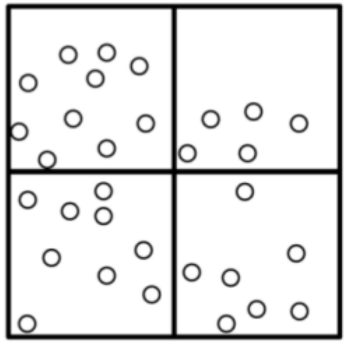


*A.C. Barbati, et al., "Complex fluids and hydraulic fracturing“, *Annual review of chemical and biomolecular engineering,* 7, 415, 2016.

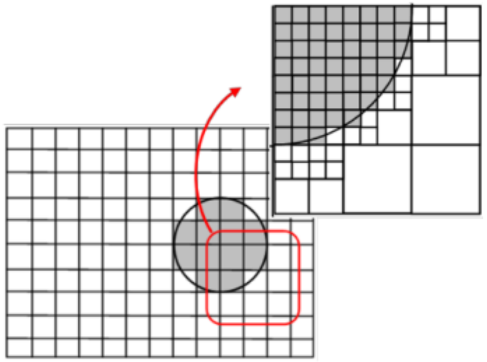
1. Introduction & Motivation

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 ($Re < 1$)

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

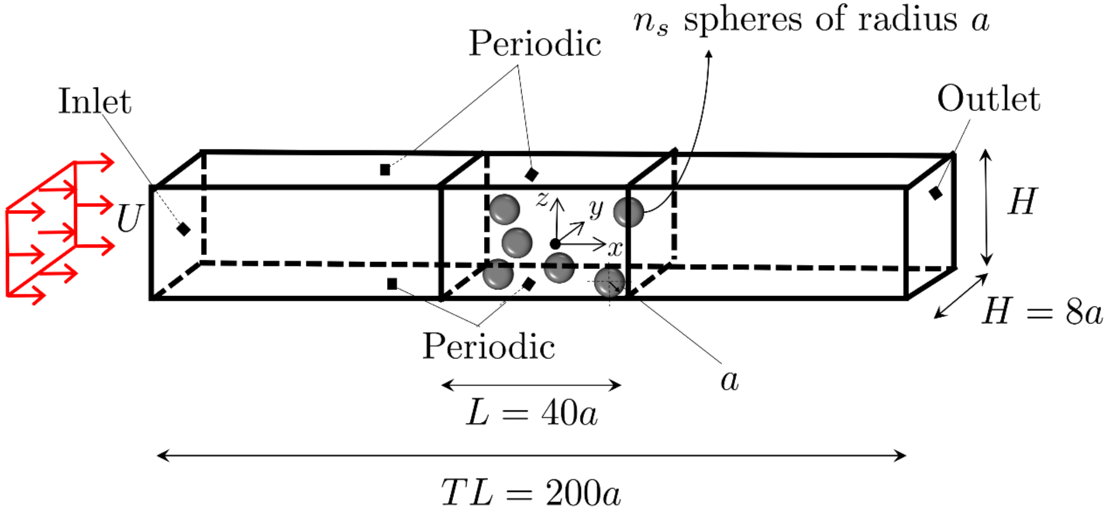
$$\chi = \frac{C_D}{(24/Re)} = \begin{cases} 1 + \frac{\sum_{i=1}^{3}\left[Wi^{2i}\left(\sum_{m=1}^{3} a_{im}\zeta^{m-1}\right)\right]}{\sum_{j=1}^{3}\left[Wi^{2(j-1)}\left(\sum_{n=1}^{3} b_{jn}\zeta^{n-1}\right)\right]} & \text{if } Wi \le 1, \\ 1 + \frac{\sum_{k=1}^{3}\left[Wi^{2(k+1)}\left(\sum_{p=1}^{3}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

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

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

* 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.

3. Direct Numerical Simulations



$$Re_D = 2Re_a = \frac{2a\rho U}{\eta_0} \leq 50$$

$$Wi = \frac{\lambda_1 U_{in}}{a} \leq 4$$

$$\beta = \frac{\eta_S}{\eta_S + \eta_P} = \frac{\eta_S}{\eta_0} < 1$$

$$\alpha \leq 0.5$$

$$0 \leq \phi \leq 0.2$$

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

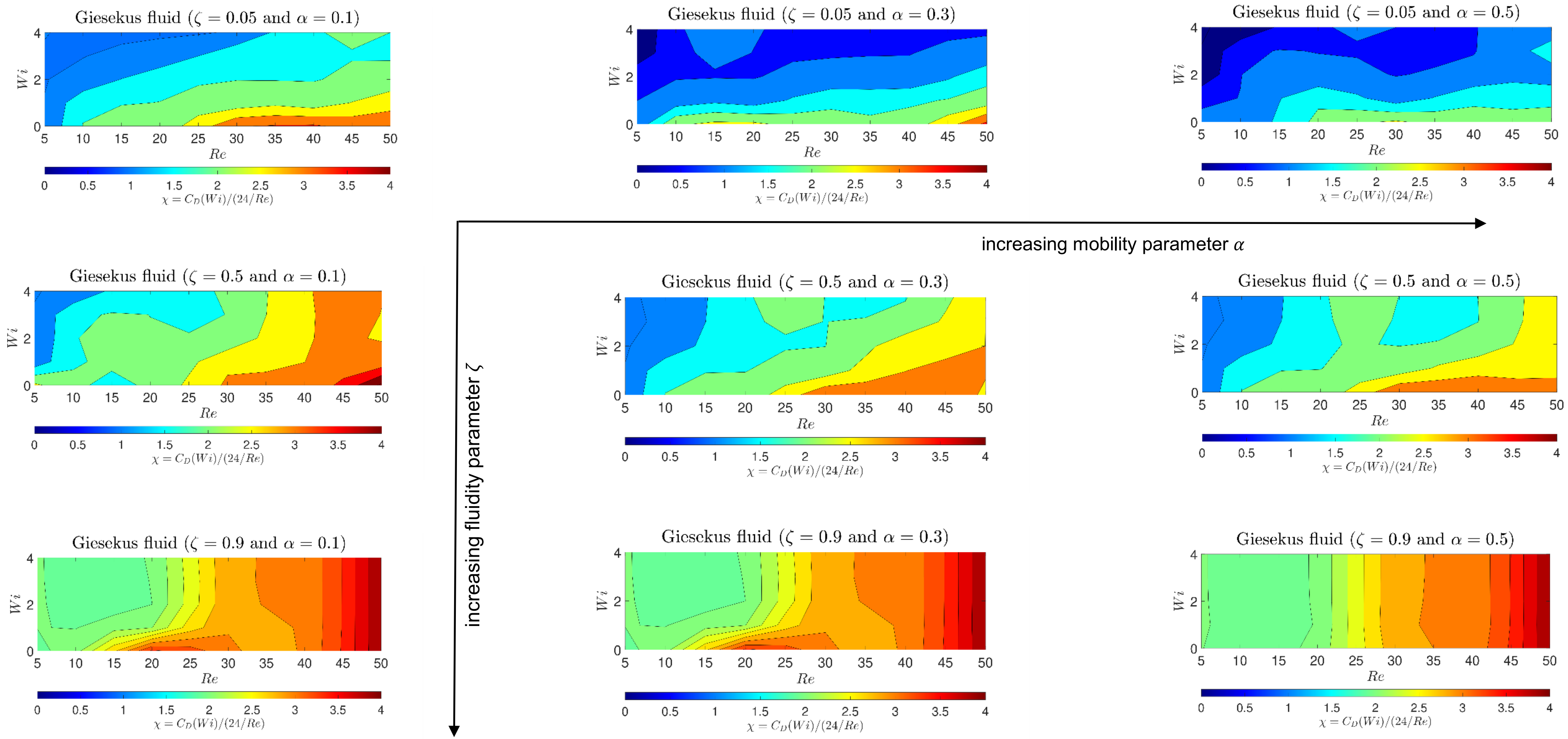
where,

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

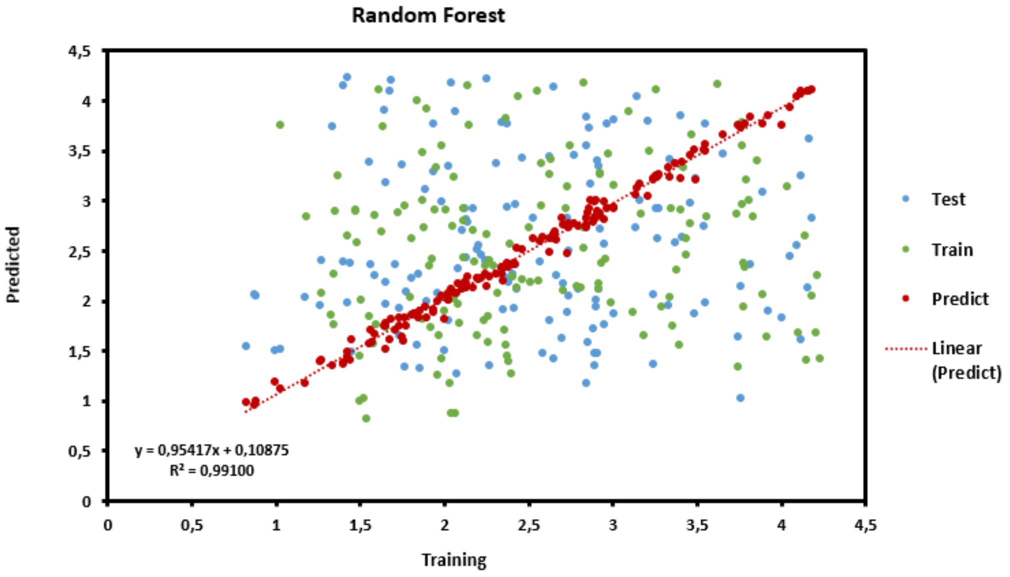
A total of approximately 8000 Direct Numerical Simulations

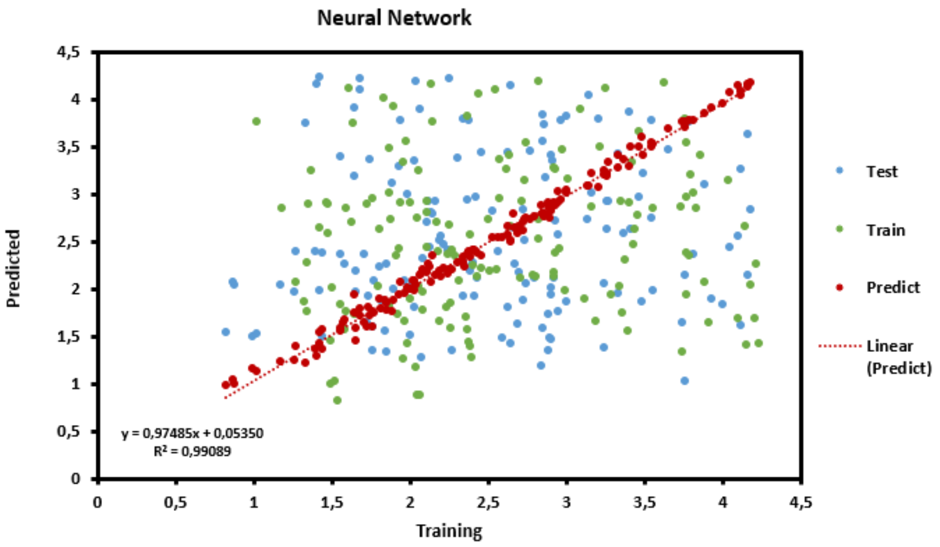
4. Random arrays of spherical particles translating in shear-thinning viscoelastic fluids

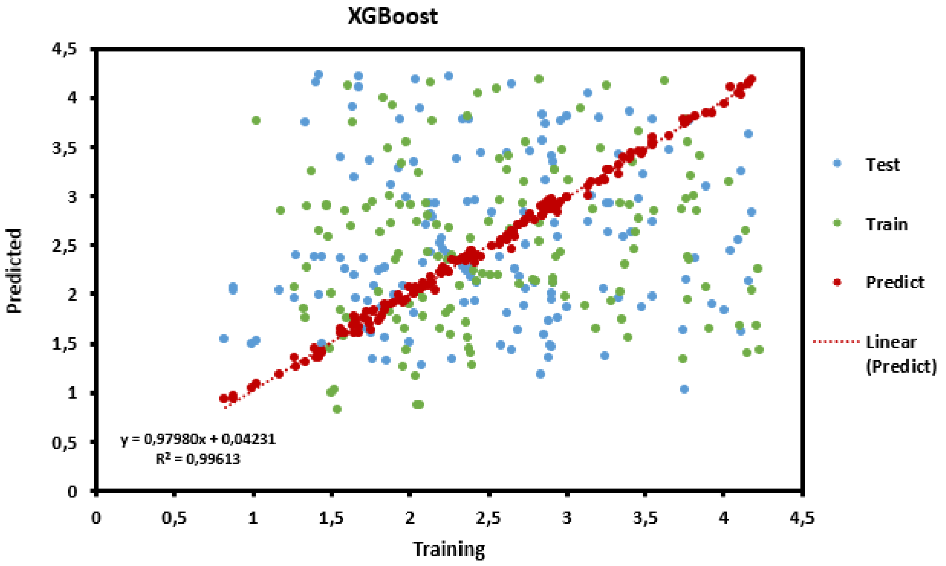
$\phi = 0.04$



4. Random arrays of spherical particles translating in shear-thinning viscoelastic fluids







To evaluate the performance of the ML models, we present these indicators in the following table:

$$R^2 = \frac{\sum_{i=1}^{n}(y_i - y_i^*)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i^*)^2} \;,\; RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - y_i^*)^2} \;,\; MAPE = \frac{1}{n}\sum_{i=1}^{n}\frac{|y_i^* - y_i|}{y_i} * 100\%$$

where y_i^* are the observed values, $\bar{y}_i^*$ is the mean of the observed values and y_i are the predicted values.

	Neural Network	XGBoost Model	Random Forest
RMSE	0.0786	0.0525	0.0823
$\boldsymbol{R^2}$	0.9908	0.9961	0.9910
MAPE	3.0875	1.9935	2.9586

5. Conclusions

- Direct numerical simulations (DNS) of **random arrays of spherical particles** immersed in **shear-thinning viscoelastic** liquids were performed using a finite-volume method.

- The ML models applied to predict the drag force of monodisperse spherical particles translating in shear-thinning viscoelastic fluids, described by the Giesekus model had good performance results. The model that best suits our case study is the XGBoost model with the highest value of R^2 (0.9961) and the lowest RMSE (0.0525).

- ML models can be a valuable predictive tool. Numerical simulations combined with ML techniques can coexist (e.g. Eulerian-Lagrangian viscoelastic solver where the drag coefficient C_D $(Re, Wi, \zeta,\alpha,\phi)$ is given by a ML model) for the development of new promising possibilities in computational science and engineering problems.

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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!