Machine learning models for the prediction of the drag force exerted by a shear-thinning viscoelastic fluid in a sphere

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1. Introduction

Non-Newtonian fluid suspensions are widely used in several areas of our daily life, e.g., to produce bags, toys, car components, textiles, etc., and they are also commonly encountered in many advanced manufacturing and industrial operations, such as processing of battery slurries or hydraulic fracturing operations. However, an efficient numerical solver capable of simulating such processes is still missing in the scientific literature. For this purpose, a 3D CFD-DEM viscoelastic solver is developed in this work to handle particle-laden viscoelastic flows using a new approach, based on machine learning and deep learning models [1-3], to compute a particulate-phase drag model valid for a wide range of material parameters.

2. Governing equations

The basic equations governing transient, incompressible and isothermal laminar flows of viscoelastic fluids are the continuity, momentum and constitutive equations. The continuity and momentum equations read:

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

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

where ρ is the fluid density, $\mathbf{u}$ is the velocity vector, t is the time, p is the pressure, $\mathbf{I}$ is the identity tensor and $\boldsymbol{\tau}$ is the total extra-stress tensor, which is split into solvent $\boldsymbol{\tau}_S$ and polymeric $\boldsymbol{\tau}_P$ contributions, such that $\boldsymbol{\tau} = \boldsymbol{\tau}_S + \boldsymbol{\tau}_P$. Both stress terms are obtained by the following equations, which form the constitutive model,

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

$$\lambda\overset{\nabla}{\boldsymbol{\tau}}_P + \boldsymbol{\tau}_P + \alpha\lambda/\eta_P\,\boldsymbol{\tau}_P\cdot\boldsymbol{\tau}_P = \eta_P\,(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^{\boldsymbol{T}}),$$

where η_S and η_P are the solvent and polymeric viscosities, respectively, λ is the fluid relaxation time, α is the mobility parameter and $\overset{\nabla}{\boldsymbol{\tau}}_P$ indicates the upper-convective time derivative of the polymeric extra-stress tensor defined as

$$\overset{\nabla}{\boldsymbol{\tau}}_P \equiv \partial\boldsymbol{\tau}_P/\partial t + \mathbf{u}\cdot\nabla\boldsymbol{\tau}_P - \boldsymbol{\tau}_P\cdot\nabla\mathbf{u} - \nabla\mathbf{u}^{\mathrm{T}}\cdot\boldsymbol{\tau}_P.$$

For this model, a characteristic (polymeric) viscosity ratio can be defined by $\zeta = \eta_P/(\eta_S + \eta_P) = \eta_P/\eta_0$, known as retardation ratio, where η_0 is the total viscosity in the limit of vanishing shear rate.

3. Case studies

In order to develop an approximate model, based in ML predictions, for the drag coefficient of a spherical particle suspended in a shear-thinning viscoelastic fluid, we performed intensive DNS for the generation of datasets to be used for training the ML model.

3.1. Case Study 1: Validation of the machine learning models with the closure drag model for the viscoelastic Oldroyd-B fluid

The approximate closure model for the drag coefficient of a sphere translating in a viscoelastic fluid described by the quasi-linear Oldroyd-B model developed by Salah et al. (2019) [4] was employed to generate a dataset to train and test ML models.

In Fig. 1 we show the residuals plot for each one of the ML models employed in this work. The residuals, i.e., the prediction errors, are computed as the difference between the actual value and the predicted value by the ML model.

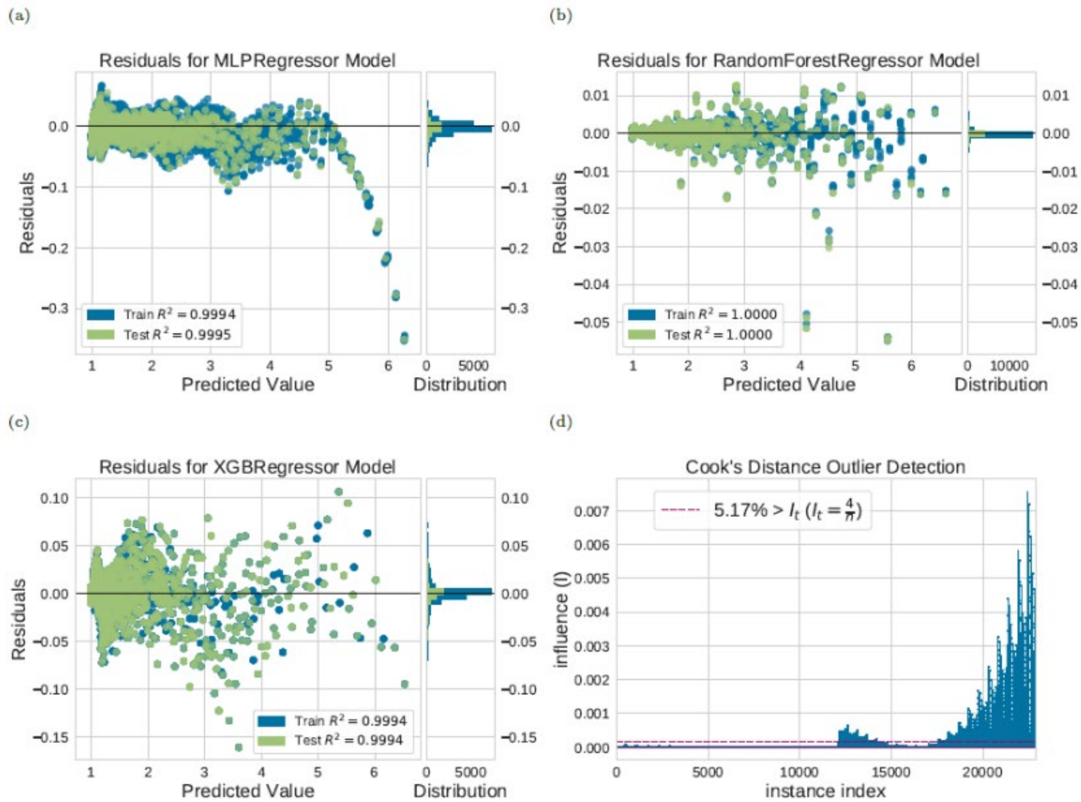

Figure 1. Residuals plot obtained when using the ML algorithms (a) Neural Network (b) Random Forrest and (c) XGBoost to predict the drag coefficient of a sphere suspended in the quasi-linear Oldroyd-B matrix-based viscoelastic fluid and (d) Cook's distance to evaluate data outliers.

3.2. *Case Study 2: Meta-model for the prediction of the drag coefficient correction of a sphere translating in the shear-thinning viscoelastic Giesekus fluid*

Direct numerical simulations were performed in this work to obtain the drag coefficient correction of a sphere translating in the shear-thinning viscoelastic Giesekus fluid under a wide range of dimensionless kinematic conditions, specifically $0 < \zeta < 1$, $0 < Re < 50$, $0 < Wi < 5$ and $0 < \alpha < 1$. A total of 2700 numerical simulations of the unbounded flow of the shear-thinning viscoelastic Giesekus fluid past a sphere were performed.

In Fig. 2 we show the residuals plot for each ML model, which presents the calculated difference between the actual value and the predicted value by the ML algorithm, i.e., the prediction error. Now it is for the Deep Neural Network model that the data points are more scattered around the horizontal axis, and for that reason the regression fit is better for this ML model, as shown in Fig. 2(a).

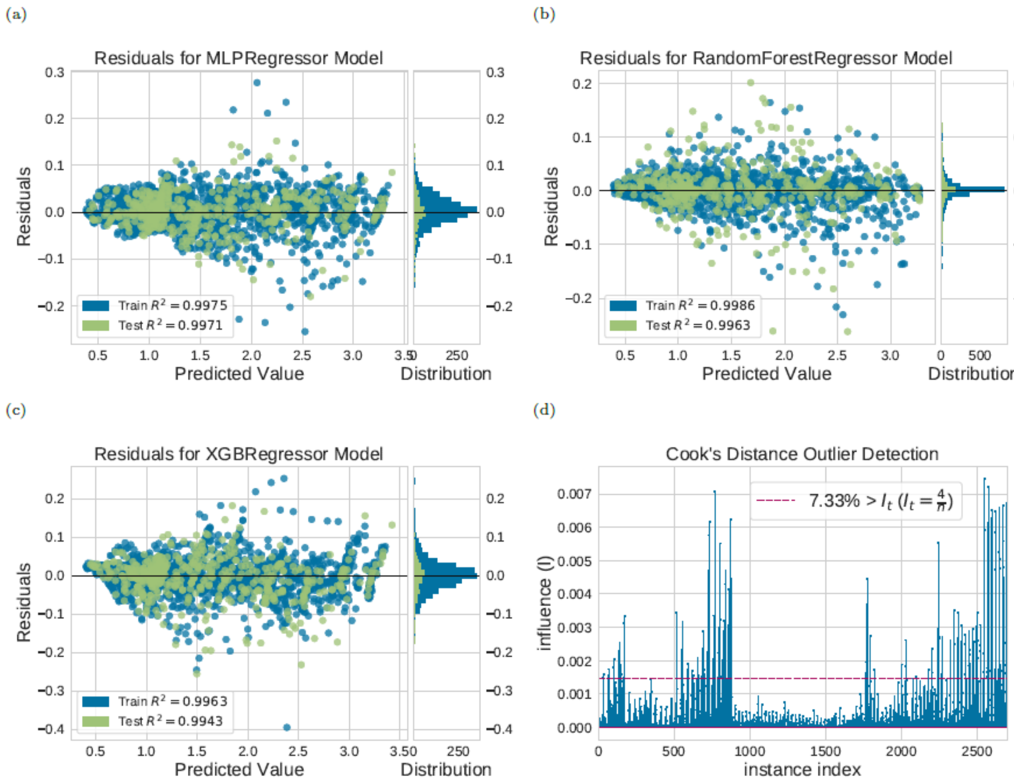

Figure 2. Residuals plot obtained when using the ML algorithms (a) Neural Network (b) Random Forrest and (c) XGBoost to predict the drag coefficient of a sphere suspended in the shear-thinning Giesekus matrix-based viscoelastic fluid and (d) Cook's distance to evaluate data outliers.

4. Conclusions

A total of approximately 3000 DNS were performed and the results obtained enable the development and validation of deep learning models which relate the input data (specifically Re, De, ζ and α) to the output (response) variable, here the dimensionless drag coefficient on the particle. A number of different learning algorithms are considered, including the Random Forest, Gradient Extreme Boosting and Deep Neural Network. These physics-based data-driven model can then be integrated into a 3D CFD-DEM viscoelastic solver to enable simulations of particle laden viscoelastic suspensions in more complex flow fields.

Acknowledgments: This work is funded by FEDER funds through the COMPETE 2020 Programme and National Funds through FCT (Portuguese Foundation for Science and Technology) under the projects UID-B/05256/2020, UID-P/05256/2020, APROVA-Aprendizagem PROfunda na modelação de escoamentos com fluidos de matriz Viscoelástica Aditivados com partículas (POCI-01-0145-FEDER-016665) and HPC-EUROPA3 (INFRAIA-2016-1-730897). The authors would like to acknowledge the Minho University cluster under the project NORTE-07-0162-FEDER-000086 (URL: http://search6.di.uminho.pt), the Minho Advanced Computing Center (MACC) (URL: https://macc.fccn.pt), the Texas Advanced Computing Center (TACC) at The University of Texas at Austin (URL: http://www.tacc.utexas.edu), the

Gompute HPC Cloud Platform (URL: https://www.gompute.com) and Consorzio Interuniversitario dell'Italia Nord Est per il Calcolo Automatico (CINECA) for providing HPC resources that have contributed to the research results reported within this paper.

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