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Particle transport and filtration in 2D and 3D porous media: coupling CFD and Deep Learning

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The study of particle transport in porous media is a research field of great interest as it is involved in a wide variety of applications [1]. The random nature of porous media systems makes it difficult to analytically correlate the impact and the synergy of the their geometrical parameters. Since these features make these systems a suitable candidate for machine learning (ML) approaches, in our work we employed neural networks for the realization of data-driven models. These techniques are able to grasp non-linear correlations between data and to account for a large number of input parameters. Moreover in the case of convolutional neural networks the entire system geometry can be used as input for the model, in this way it is possible to avoid the selection of the geometrical features [2-3].

In this work we coupled computational fluid dynamics (CFD) simulations with machine learning models. The results of a CFD simulations campaign are employed as a training set for the neural networks in order to obtain a computationally inexpensive data-driven surrogate model which is able to replace the CFD simulation, while keeping a good accuracy. The aim of the CFD investigation is the flow, transport, and filtration at the pore-scale, in this framework the first step is the creation of the geometries. We designed bi-dimensional [4] and three-dimensional [5] periodic packings of spheres via the open-source framework YADE DEM.

For each kind of geometry, hundreds of simulations are solved, each differing randomly in their geometrical parameters and input operating conditions. The CFD simulations are performed on the open-source code OpenFOAM. At first, the fluid flow is evaluated in the limit of small Reynolds numbers (<0.1), thus obtaining the medium permeability. Then the transport of dilute colloid particles is studied by solving the advection-diffusion equation, and the filtration rate is calculated [6].

Two kinds of models have been built: both for the prediction of the permeability of the porous media, and the filtration rate of the colloid through the grains. The first one is a simple fully-connected neural network whose input features are the geometric parameters and operating conditions. The second one is a convolutional neural network whose input is a porous medium geometry, in the form of a binary matrix. After the neural network training process, the end result is a surrogate black-box model capable of predicting the output values when given a new set of input features, or a new geometry; notably, the accuracy of this data-driven model is on-par or better than other analytical or empirical correlations.

This simple data-driven models can then be reliably used in place of expensive CFD simulations (or in general, all "first principles"methods), as one single call of the neural network has a computational cost which is orders of magnitude lower than the full CFD simulation: in our test problems, under a second versus several hours – with a total neural network training time of around four minutes, for the fully connected one, and of several hours, for the convolutional one.

Time Block Preference

Time Block A (09:00-12:00 CET)

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