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Multiscale modelling of permeability and effective dispersion coefficient in porous media: a deep learning approach

Thursday, 2 June 2022 14:15 (15 minutes)

The modelling of transport in porous media is of great interest in many fields of application in chemical and environmental engineering, such as packed bed chemical reactors, underground transport of contaminants or carbon capture and storage. Flow and transport in porous media are a multiscale phenomenon, in fact, both microscale and macroscale affect the transport properties of interest. We here focus on estimating the permeability and the effective dispersion coefficient of porous media.

In this work the flow and mass transport equations are solved numerically on both microscopic and macroscopic scales and are used to train and validate deep learning techniques. At the microscopic level the geometry of the porous medium is obtained by an in silico reconstruction or by the use of computer tomography, resulting in a domain for the solution of the relevant transport equations, most often the Navier-Stokes and advection-diffusion equations [1]. At the macroscale the porous media are not topologically detailed, and are instead described as permeability fields, which can be experimentally or mathematically reproduced. The Darcy equation can be solved at this scale, and homogenisation techniques can be exploited for the evaluation of the effective permeability and the effective dispersion coefficient in the porous media [2].

The computational cost of direct simulations together with the wide range of porous media structures impacting the permeability fields make the study of flow and transport in porous media a prime candidate for machine learning applications. The data-driven models trained can predict instantaneously new input data that could be useful in multiscale modelling or optimization problems. Neural networks can be trained on CFD data for the sake of obtaining data-driven models of highly non-linear problems, in particular, convolutional neural networks (CNN) can take as input image-like geometrical information and are employed for the prediction of integral descriptors and fields.

In this work CNN were used to predict the velocity in the main direction of flow, the effective permeability and the effective dispersion coefficient of porous media. Discontinuous permeability fields were produced in silico by using a spectral method [3], varying local permeabilities and correlation lengths. The mean velocity is calculated by the solution of the Darcy equation, the effective permeability and the effective dispersion coefficient were calculated by a homogenisation of the Darcy and the advection-diffusion equation by solving the cell problem with spectral decomposition. The input of the CNN are the permeability fields, and the prediction are quite accurate with average errors lower than 6%.

Convolutional neural networks can be employed for the prediction of integral values or entire fields, such as the detailed local flow field [4] or the concentration field of a chemical species. In the case of transport applications, it is necessary to provide the network with more information, i.e. both the geometrical description of the porous media and the diffusivity of the chemical species or the boundary conditions. The tuning of these kinds of multiple purpose architectures could lead this methodology to be effectively employed in a wide range of applications.

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Time Block Preference

Time Block B (14:00-17:00 CET)

Participation

Unsure

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