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Multi-scale high-performance fluid flow: Simulations through porous media

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ABSTRACT

Computational fluid dynamic (CFD) calculations on geometrically complex domains such as porous media require high geometric discretisation for accurately capturing the tested physical phenomena. Moreover, when considering a large area and analysing local effects, it is necessary to deploy a multi-scale approach that is both memory-intensive and time-consuming. Hence, this type of analysis must be conducted on a high-performance parallel computing infrastructure. In this paper, the coupling of two different scales based on the Navier–Stokes equations and Darcy's law is described followed by the generation of complex geometries, and their discretisation and numerical treatment. Subsequently, the necessary parallelisation techniques and a rather specific tool, which is capable of retrieving data from the supercomputing servers and visualising them during the computation runtime (i.e. in situ) are described. All advantages and possible drawbacks of this approach, together with the preliminary results and sensitivity analyses are discussed in detail.

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1. Introduction

For preventing catastrophic flooding scenarios that might occur under certain atmospheric conditions or for predicting the behaviour of fluid flows after they percolate into underground soil layers, researchers must either rely on historical measurements of an event and their statistical interpretation or attempt to recreate the natural conditions under which the event usually occurs and simulate the outcome and consequences beforehand. Owing to the recent advancement in the performance of modern supercomputers, highly detailed computational fluid dynamics (CFD) simulations are now possible. This allows engineers to study complex problems and obtain insight into the nature of different fluid flows. One typical application is the simulation of large and complex geometries, such as porous media, which are addressed in this paper. Such porous media can cover sufficiently large areas, often up to 1 km × 1 km. The classical approach toward solving this problem (e.g. [10,11]) entails the calculation of material properties such as local permeabilities based on measured transport quantities. Recently, several studies investigated the digital rock physics analyses (e.g. [12,13]). In this approach, only sieve curves or computer tomograms are taken from local soil samples and the flow properties are computed from these geometric data using Navier–Stokes simulations. Here, the advantage of a much simpler material testing process is coupled with the drawback of a dramatically increased computational effort, because the pore-level geometric scale must be taken into account. Using a grid of the complete computational domain uniformly refined up to the pore scale would result in a number of computational cells being too large by several orders for even the most advanced supercomputers. Hence, sophisticated approaches, such as multi-scale methods are inevitably necessary. In this paper, we present a multi-scale approach that allows users to compute data on different scales, ranging from a micro (pore) level (1 cm × 1 cm × 1 cm), to a coarse meso level (1 m × 1 m × 1 m) for evaluation of the results, up to the coarsest macro level (1 km × 1 km × 1 km). Such multi-scale approaches have already been investigated by numerous researchers, e.g. in [21–24,26–28,31,32,38,41,44,48]. Nevertheless, compared with previous approaches, our approach benefits from the inclusion of an interactive tool based on the hierarchical data structure applied. This tools allows users to retrieve computed data from the server on any scale and visualise them during the computation runtime [43].

With respect to the state of art, various models have been proposed to solve Navier–Stokes–Darcy coupling, some of which are

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based on finite element methods (see [31] and [14]), mixed finite element methods (see [45]), finite volume methods (see [39]) and methods of overlapping and matching grids to represent different problems in the same domain (see [41]). Although the majority of the research has been conducted on the basis of finite element theory, all of the above-mentioned methods strive to preserve a conservation of mass on all sub-grids, thus to exploit calculated data at all levels and any time sequence. Furthermore, owing to the complexity of the initial geometry as published in [50], the domain in the majority of the set-ups tested was discretised using an unstructured adaptively refined mesh.

A detailed comparison between structured, non-body-conforming grids and unstructured quadrilateral meshes percisely resolving the pore geometry is presented in [19]. Another line of research has been followed in the spirit of fictitious domain methods (e.g. [17,18]), where the (pore) domain of computation is immersed in a larger, fictitious domain, which covers both the solid and the pore phase. Although these methods have proven to be very powerful, avoiding the necessity of complex mesh generation, they cannot be easily extended to a strong, three-dimensional local mesh refinement, which is central to the approach presented in this paper.

We will present an approach based on a finite volume scheme with a hierarchical data structure, allowing a multi-grid-like solver (described in detail in Section 3.4) to be easily applied, accelerating the convergence and greatly reducing the total calculation time.

Although our approach does not resolve the pore geometry exactly in terms of the geometrically complex domain discretisation (e.g. densely packed spherical samples), our method efficiently produces an appropriate numerical domain, especially in single-point-touch cases between two inner solid objects. Moreover, numerical simulation is performed only inside the non-solid cells, dramatically reducing the amount of active computing cells within the domain as up to 50% of the total volume is set to be a solid material.

The hierarchical data structure behind the Navier–Stokes–Darcy coupling model enables a more detailed exploration of the fluid flow field through porous media. A contribution to the study of porous media flows can be found in [14–16], in which the steady-state formulation of Darcy's law was coupled to the Navier–Stokes model and the obtained results were compared to the output of a direct numerical simulation (DNS). The DN simulation was based on a finite element discretisation, and the verification of the numerical routines is conducted on the basis of the grid study as well as the sensitivity analysis of the porosity and permeability values with respect to the domain size.

This paper is based upon Perović et al. [1] and further addresses such aspects as:

- improvement of the geometry generation algorithm, which is now capable of creating various testing geometry sets in a large span, some of which are presented in this paper,
- further research on the grid complexity and efficiency of adaptive mesh refinement for the Navier–Stokes fluid solver,
- sensitivity analyses with respect to both hydraulic and physical parameters on different scales and
- comparison between numerically simulated and experimentally obtained results as part of code validation process, with respect to the treatment of geometrically complex domains within fluid flow simulations.

The remainder of this paper is as follows: In Section 2, a detailed description of the integrated models based on different scales as well as their coupling and application to the previously generated geometry domain is presented. Furthermore, the geometry generation process is described in detail. The implemented data structure, its benefits and its limitations are discussed in Section 3 together with the numerical treatment and algorithms applied en route from the partial differential equations to the final solution. Within the same section, a measured result for the communication time, necessary for data exchange between neighbouring cells as well as the speedup curves obtained on the 155,000-core supercomputer SuperMUC installed at the Leibniz Supercomputing Centre in Garching are depicted. Finally, in Section 4 the application set-up used for testing purposes is presented and explained, followed by the obtained results and a sensitivity analysis with respect to the porosity value of the domain tested.

2. Physical and geometrical modelling

This chapter presents the basic mathematical representations of two distinct models, followed by a description of the coupling procedure. Because there are numerous definitions of the presented laws, depending on the conditions under which the equations are applied, only the implemented formulations are described here. The scientific notation used throughout this article refers to the standard used in e.g. [10,29,30].

2.1. Macro level: Darcy's law

Darcy's experimentally derived hydraulic law is usually used to describe the fluid flow on a macroscopic scale. Referring to its experimental setting and the theoretical description given in [10,11,49], the macroscopic Darcy flux is obtained by volume-averaging, as depicted in general form in Eq. (1), where ψ stands for an arbitrary transport quantity and the notation $\langle\cdot\rangle$ is used to express an averaged entity:

$$\langle\psi_i\rangle = \frac{1}{V_0}\int \psi_i dV. \tag{1}$$

The control volume V_0 includes both the solid and the fluid phase (V_s and V_f, respectively), yielding the difference between the superficial velocity $\langle U_i\rangle$ (the Darcy flux) and the intrinsic averaged velocity $\langle u_i\rangle$ in [m/s]. In the case of $\langle u_i\rangle$, a solid phase V_s is assumed to be zero, thus yielding the control volume $V_0 = V_f$. As the volumetric ratio of the fluid phase V_f to the total control volume V_0 is constant and defined by the porosity value $\epsilon = \frac{V_f}{V_0}$ [-], the relationship between the superficial $\langle U_i\rangle$ and intrinsic averaged velocity $\langle u_i\rangle$ in the case of a single-phase flow is given by:

$$\langle U_i\rangle = \epsilon\langle u_i\rangle. \tag{2}$$

On the basis of (1) and (2), the steady–state form of Darcy's law is given by

$$\langle U_i\rangle = -\frac{k}{\mu}\cdot\nabla\langle pe_i\rangle, \tag{3}$$

where $i \in \{x, y, z\}$ denotes the three Cartesian coordinate directions, in which the Darcy flux $\langle U\rangle$ in [m/s] is computed, μ is the dynamic viscosity [kg/(m · s)] and e_i [-] is the unit vector in direction i. The permeability tensor k [m^2] represents the ability of the porous medium to conduct the fluid flow.

On the basis of these three correlations, we apply a volume-averaging technique on the velocity and pressure fields calculated on the micro-scale, yielding the discrete values of the permeability k (see Fig. 1) on the macroscopic level. However, to ensure that the obtained values conform to the concept of porous media as continua on the macro-scale, a kriging interpolation method (also called Kolmogorov Wiener prediction) should be applied (see [5,6]). This method provides the best linear unbiased estimation of the interpolated values at the unobserved spatial points of the domain based on available previously calculated discrete (permeability) values. This method, widely used in the field of spatial analyses, yiels a continuous estimated field of an analysed parameter on which basis various further computations and analyses can be

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