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Optimum configuration for accurate simulations of chaotic porous media with Lattice Boltzmann Methods considering boundary conditions, lattice spacing and domain size

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ABSTRACT

Simulations of the flow field through chaotic porous media are powerful numerical challenges of special interest in science and technology. The simulations are usually done over representative samples which summarise the properties of the material. Several factors affect the accuracy of the results. Firstly the spatial resolution has to be fine enough to be able to capture the smallest geometrical details. Secondly the domain size has to be large enough to contain the large characteristic scale of the porous media. And finally the effects induced by the boundary conditions have to be diluted when more realistic options are not available. This is the case when the geometry is obtained by tomography and the periodic boundary conditions cannot be applied to delimit the sample because its geometry is not periodic. Impermeable boundary conditions are usually chosen to enclose the domain, forcing mass conservation. As a result, the flow field is over-restricted and the total pressure drop can be over-estimated. In this paper a new strategy is presented to optimise the computational resources consumption keeping the restrictions imposed by the accuracy criteria. The effects of the domain size, discretisation thickness and boundary condition disturbances are studied in detail. The study starts with the procedural generation of chaotic porous walls which mimics acicular mullite filters. An advantage of this process is the possibility to create periodic geometries. Periodicity permits the application of advanced techniques such as cyclic cross-correlations between the phase field and the velocity component fields without aliasing. From cross-correlation operations the large characteristic scale is obtained. The result is a lower threshold for the domain size. In second place a mesh independent study is done to find the upper threshold for the lattice spacing. The Minkowski–Bouligand fractal dimension of the fluid–solid interface corroborates the results. It has been demonstrated how the fractal dimension is a good candidate to replace the mesh independent study with lower computational cost for this type of problems. The last step is to compare the results obtained for a periodic geometry applying periodicity and symmetry as boundary conditions. Considering the periodic case as reference the resultant error is analysed. The explanation of the analysis includes how the intensity of the error changes in space and the limitations of symmetric boundary conditions.

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1. Introduction

Direct simulations of chaotic porous media have widely varying applications in several fields such as biological flows, material science, geology or engineering. Solving these simulations was not feasible short time ago. Modelling the material by their macroscopic properties was the unique option. Nowadays the increasing computational power allows direct simulations of internal flow through chaotic porous media. Nevertheless the entire domain can usually not be calculated at once. In such cases what is simulated is just a sample, a representative portion with the same properties than the total. It is the aim of this paper to explain how the simulation of this sample has to be conducted.

Every simulation in space is limited by two scales. The upper scale or integral scale is defined as the size of the phenomena to be analysed. The lower scale or micro-scale is required to reproduce the smallest details accurately. The large scale fixes the domain size. The small one is an upper-threshold for the discretisation of the simulation. More details require higher resolutions. When these two scales differ, the simulation of the whole domain is unfeasible. Therefore a simplification is needed.

One way for simplifying is the replacement of the whole domain by a sample. It can be done when the physical phenomena are uniform. Then the upper scale, which fixes the size of the domain, can be reduced to the size of the sample. This technique is widely extended to simulate porous media at micro-scale level. After the simulation the macroscopic properties can be obtained as a post-processing task by integration. The integral values have to cover enough material to be representative, avoiding anomalies and damping statistical noise. This type of simulations are becoming common with the increase of computational power and the development of 3D tomography. Moreno-Atanasio et al. summarise in their review [1] a large set of techniques where tomography and Computational Fluid Dynamics (CFD) are used together. The information returned by tomography can be either direct 3D imaging to be immediately used or descriptive parameters to construct computer-generated geometry. As it is mentioned in their paper, the most common method for determining the fluid flow and transport properties is the Lattice Boltzmann Method (LBM). These simulations are usually applied to study rocks, filters or simply beds of particles. One of the pioneering papers in this matter is written by Coles et al. [2]. They obtain the geometry directly from a 3D tomography and solve the fluid field afterwards. Other example, also cited in the review of Moreno-Atanasio et al., is the article of Sukop et al. [3]. They validate the LBM results of multiphase fluid in porous media at micro-scale level with the data obtained by tomography. Jia and Williams [4] use a similar technique to simulate dissolution. The solid phase is computer-generated and characterised by a sample gained by tomography. The flow field is calculated afterwards. All these measurements and simulations can be used to characterise filters. This is in fact what Yamamoto's team does. They investigate the filtering process of Diesel particulate filters (DPF) calculating on a sample measured by tomography [5–8]. A similar technique is followed by Stewart's team. They simulate the deposition process of a Diesel filter made of acicular mullite to understand the influence of the micro-structure topology [9]. The alternative to the measured sample is its procedural generation. This option is very interesting when the parameters which describe the geometry of the porous media have to be studied separately. This is a topic the Fraunhofer institute is working on. They developed a software specialised in procedural generation of micro-structures and, in addition, they have the capability to simulate the flow field through it afterwards. The work developed by Shi et al. [10] and Calo et al. [11] about porous membranes are good examples of this procedure.

The second option for simplifying is to model the lower scales. One of the most famous macroscopic models of porous media is Darcy's law. It describes the relationship between the pressure gradient and the flow rate. In fact, the simulation of porous media at micro-scale can be used to calculate the permeability tensor which resumes the properties of the material at macro-scale level. Stewart, Ward and Rector relate the micro-structure with the macro-characterisation of the material [12]. The permeability results can be used afterwards for simulations where the porous size is much smaller than the discretisation, so the material appears to be continuous. However, as it can be seen in this paper, the calculation including the lower scale is feasible, these types of simplifications are not applied here. This means that the details of the chaotic structure have to be captured by the discretisation. High resolution is a new requirement.

From a mathematical point of view, high resolution is a synonym of large number of degrees of freedom in the system. Of course, the resources needed for a simulation scale at best linearly with the number of unknowns, memory consumption, computational time and scalability become restrictions. The prime design objective of the waLBerla software framework is High Performance Computing (HPC) capabilities. Its suitability for HPC-demanding tasks was demonstrated in the work presented by Godenschwager et al. [13]. This software focuses on the Lattice Boltzmann Method (LBM) as the numerical solver. LBM shows some advantages with respect to the conventional Computational Fluid Dynamics (CFD) tools such as the Finite Volume Method (FVM), especially for very large mainly parallel simulations. First of all, the formulation of LBM is explicit. No matrix inversion has to be done for each time step. It saves time reducing the number of operations and the communication between processes. Because of the high locality of the method high scalability can be achieved. Secondly LBM works with distributions for each point instead of using physical variables such as density, pressure or velocity. All of them are calculated during the post-processing step. As a consequence, the pressure correction loop (a requirement for convergence in classical CFD tools) is not needed, saving again iterations. The disadvantageous counterparts are the memory consumption, which is usually larger with respect to conventional CFD tools, and its mandatory time dependence. Nevertheless, the most important advantage for the simulation of porous media is the set of boundary conditions. Coherent meshes are not required. The boundary conditions can be immersed into the cell instead of being one of the cell faces, so meshing the topology is much easier than using classical techniques.

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