Fluid dynamics in porous media with Sailfish

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Abstract
In this work we show the application of Sailfish to the study of fluid dynamics in porous media. Sailfish is an open-source software based on the lattice-Boltzmann method. This application of computational fluid dynamics is of particular interest to the oil and gas industry and the subject could be a starting point for an undergraduate or graduate student in physics or engineering. We built artificial samples of porous media with different porosities and used Sailfish to simulate the fluid flow through them in order to calculate their permeability and tortuosity. We also present a simple way to obtain the specific superficial area of porous media using Python libraries. To contextualise these concepts, we analyse the applicability of the Kozeny–Carman equation, which is a well-known permeability–porosity relation, to our artificial samples.

Keywords: fluid dynamics, computational physics, porous media, statistical physics

(Some figures may appear in colour only in the online journal)

1. Introduction
A porous medium is characterised by containing pores, i.e. void space, in its interior. These pores can be all connected, as in a sand pack, or not, as in Styrofoam. If the goal is to study...
the fluid flow in porous media, only those with connected pores must be considered. The understanding of fluid dynamic properties of porous media is particularly relevant to the oil and gas industry, since oil is found in underground porous rocks (reservoirs). It is crucial to estimate the permeability of a rock reservoir to hydrocarbons in order to assist decision-making and oil recovery strategies. Permeability can be measured experimentally or calculated as a function of other porous rock properties such as porosity, tortuosity and specific surface area (SSA). The most popular empirical relationship used to calculate the permeability from those quantities is the Kozeny–Carman equation \[ \frac{K}{f^2} \approx \frac{1}{C_d} \left( \frac{D}{L} \right)^2 \]

In this context, computational fluid dynamics (CFDs) plays an important role and the lattice Boltzmann method (LBM) has many advantages over other methods making it a good choice to address systems with complex geometries. LBM was first derived in 1988 by McNamara and Zanetti \[5\] and, since then, it has emerged as an alternative powerful method for solving CFD problems. It was very successful in simulating complex flows, such as fluids with immiscible components, interfacial problems and flows in complex geometries (e.g., in porous media). In recent years, LBM has been extended even to semiclassical \[6\] and relativistic fluids \[7\]. The advantage over other methods lies in the simplicity of its dynamics, easy handling of complex geometries and, especially, its flexibility for implementation in parallel computing. Sailfish \[8\] is an open-source LBM/CFD solver that comes with many examples ready to use. It has a simple Python interface, which is relatively simple to learn and is already optimised for graphics processing units (GPUs). Its advantages make it an appropriate choice for the study of flow in porous media, even for beginners in this subject.

Python as a programming language is often deemed unsuitable for high-end HPC applications for its relatively low performance when compared to compiled languages such as Fortran and C/C++. But with the advent of libraries like PyCUDA and PyOpenCL \[9\], one can offload the computationally intensive calculations to the GPU while keeping the user-friendly Python interface. Performance in LBM is usually measured in terms of lattice updates per second (LUPS). CPU-only LBM codes typically achieve \(10^7\) LUPS in desktop computers and \(10^8\) LUPS in HPC clusters \[10–13\]. GPU-enabled LBM codes, on the other hand, typically achieve \(10^9–10^{10}\) LUPS on a single GPU \[8, 12, 14\], for a fraction of the space and energy required by a cluster. This considerable gain in performance permits the concurrent computation and visualisation of results at a reasonable frame-rate for on-the-fly simulations. Although current laptop CPUs are still limited to 4 or 8 cores, it has become commonplace to find mobile GPUs with hundreds or thousands of cores, which represents a substantial increase in computing power without compromising portability. This enables the use of GPU-equipped portable computers for classroom live demonstrations of virtual CFD experiments.

In this work we propose a simple and efficient way to study fluid dynamics in porous media by using Sailfish. We show how to calculate the most important fluid dynamics properties of porous media, in order to analyse the applicability of the Kozeny–Carman equation to samples of porous media we built artificially. These samples were generated by placing obstacles in random positions allowing them to overlap, which is more realistic than some other models in literature. For instance, many authors adopt a porous medium made of identical spheres placed in a regular lattice \[4, 15\] or used a two-dimensional porous media composed by identical squares placed in random positions \[16, 17\]. We also present an original and simple method to measure the SSA from a digital rock tomography based on Python image-processing libraries. All the content of this work was produced with open-source software.
This paper is organised as follows. In section 2 an introduction to Sailfish is presented. In section 3.1 the algorithm used to build artificial samples is explained. In section 3.2 we demonstrate how the permeability was calculated using the output from simulation. In section 3.3 we apply the Kozeny–Carman equation to our samples and calculate its Kozeny constant. In section 3.4 our method to calculate the SSA is presented and tested for a simple case and, in section 3.5, a simple way to calculate the tortuosity from the output data is shown. Finally, in section 4 a discussion about the results and our concluding remarks are provided.

2. Sailfish

This section contains a brief introduction to Sailfish [8], the software we used to simulate fluid flow in our artificially created porous media. We do not intend to provide a tutorial, for a very detailed one can be found at the developer’s website, where you can download and follow the instructions to start using it. Sailfish requires no actual installation step, since the code is written in an interpreted programming language: Python. The required packages are all enumerated in Sailfish’s website. A graphics card or GPU is also needed to run the calculations.

The main advantages of Sailfish are its ease of use and high performance. It comes with many strategic examples that can be run and easily adapted to the needs of the user. As all routines and examples are written in Python, they are easy to read and write—as compared to compiled languages like Fortran and C/C++—without compromising the computational performance, for all the time-consuming calculations run in the massively parallel GPU. Sailfish offers a high-level programming interface with several built-in functionalities, so that the user only needs to provide simple instructions like the boundary and initial conditions, physical parameters of the fluid and select the LBM relaxation dynamics. Programming general-purpose GPUs is usually a difficult task, but Sailfish hides this complexity away and makes all parallelization behind the scenes [8]. Simulations in Sailfish can be made interactive which, combined to its high performance, makes it a powerful tool to illustrate hydrodynamic principles in the classroom in real-time. While a simulation is running in visualisation mode, one can add new (solid) obstacles by freehand drawing them with a cursor.

The LBM [18], in which Sailfish is based, is a numerical method to solve the Boltzmann equation [19], that in its finite-difference form is

\[
\frac{f(x + \xi \Delta t, x + \frac{\xi}{m} \Delta t, t + \Delta t) - f(x, \xi, t)}{\Delta t} = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}},
\]

(1)

where \(x\) is the position, \(\xi\) is the microscopic velocity, \(t\) is the time, \(F\) is the external force and \(m\) is mass of the particles. Expanding (1) up to terms linear in \(\Delta t\), we obtain the Boltzmann equation in its continuous form, \(\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} \xi + \frac{\partial f}{\partial \xi} F = \left( \frac{\partial f}{\partial t} \right)_{\text{coll}}\). The above equation gives the time evolution of the distribution function, \(f(x, \xi, t)\), by knowing the collision operator, \(\left( \frac{\partial f}{\partial t} \right)_{\text{coll}}\), which includes all information about atomic aspects of scattering process of the particles in the gas. The Bhatnagar–Gross–Krook (BGK) collision term [20],

\[^3\text{Download Sailfish and see the tutorial at http://sailfish.us.edu.pl}\]
\[ \frac{\partial f}{\partial t} = \frac{f(x, \xi, t) - f^{eq}(x, \xi, t)}{\tau}. \]

is the simplest and most commonly used in LBM. It assumes that the non-equilibrium function \( f(x, \xi, t) \) tends to the equilibrium function \( f^{eq}(x, \xi, t) \) with a characteristic time \( \tau \), called ‘relaxation time’. To illustrate this, note that when the external force is zero the integration of Boltzmann–BGK equation in its continuous form becomes \( f = f^{eq} + (f^{\text{init}} - f^{eq})e^{-t/\tau} \), where \( f^{\text{init}} \) is the distribution function at \( t = 0 \). Despite its simplicity, the BGK collision term leads to the correct equations of mass and momentum conservation (Navier–Stokes equations) \([18]\). As a consequence of using a single relaxation time, the macroscopic moments, i.e., density and velocity, change at the same rate. The choice of relaxation time in the simulation has an impact on fluid flow, since the kinematic viscosity depends on \( \tau \) \([18]\). In LBM the position and velocity spaces are discretized \([21]\) as illustrated in figure 1. The time step \( \Delta t \), used in (1), is the time for a particle move from its site to the first neighbour site and this time step with the lattice parameter \( (a) \) form a system of unities called lattice units \([18]\), which can be converted for any other system of units.

3. Fluid flow in porous media

The most relevant quantities related to fluid dynamics in porous media are porosity, tortuosity, surface area and permeability. In this section we define these concepts and relate them using the Kozeny–Carman equation.

We start with the porosity, that is defined as the fraction \( \phi = \frac{V_{\text{pores}}}{V_{\text{total}}} \) of the total volume that is occupied by connected pores. Media with non-connected pores, as in Styrofoam, do not allow flow, and therefore, need not be considered for our purposes. In case the medium has both connected and non-connected pores, the volume occupied by the latter must be disregarded.

Tortuosity \([22, 23]\) is a geometrical figure-of-merit that indicates how much the fluid flow streamlines deviate from straight paths. It is defined as the ratio between the total length along the streamline and its effective length (the length of the straight line connecting final and initial positions), as depicted in figure 2. Note that \( \tau \gg 1 \). If the streamline is given by a function \( f(x) \), as exemplified in figure 2, the tortuosity can be calculated as
The internal area of obstacles in contact with the fluid greatly influences the fluid dynamics. Ultimately, the SSA (or ‘surface-to-volume ratio’) is responsible for the strength of surface interaction effects. This figure-of-merit is defined as $s = A_{\text{obs}} / V_{\text{obs}}$, where $A_{\text{obs}}$ is the surface area of obstacles and $V_{\text{obs}}$ is their total volume.

In general, permeability is the quantity of greatest interest in the study of flow through porous media. It quantifies how easily a specific fluid passes through the media, i.e., the inverse of a ‘flow resistance’. In its simplest formulation, it depends only on the geometry of the medium and the viscosity of the fluid, $\mu$, and can be calculated using Darcy’s law [24, 25],

$$k = \frac{C}{3} \left( \frac{d}{\phi} \right)^2, \quad (4)$$

where $\frac{d}{\phi}$ is the pressure gradient along direction $x^i$ and $\langle u^i \rangle$ is the average velocity of the fluid in the direction $x^i$. Note that, in general, permeability is a $3 \times 3$ tensor, but in practical cases we are usually interested only in the diagonal components $\kappa_{xx}, \kappa_{yy}, \kappa_{zz}$. The SI unit for permeability is $m^2$, however, the ‘darcy’ ($1 \text{ darcy} = 10^{-12} \text{ m}^2$) is the most used.

The four concepts presented previously are related by the Kozeny–Carman equation

$$\kappa = \frac{1}{C \phi^2 (1 - \phi)^2}, \quad (4)$$

where $C$ is an empirical and dimensionless constant, known as Kozeny’s constant, that depends only on the geometry of the media. In this model, the porous medium is assumed to be equivalent to a conduit, in which the pore space is reproduced by an array of cylindrical channels. The fluid flow inside these channels is described by the Hagen–Poiseuille equation [25]. Consider, for instance, a medium composed of identical spheres with diameter $d$, equally distributed in a bed packed [26]. In this case, the SSA is $s = A_{\text{sphere}} / V_{\text{sphere}} = 6 / d$. So (4) becomes

$$\kappa = \frac{d^2}{36C} \frac{\phi^3}{(1 - \phi)^2}. \quad (5)$$
Note that the dimensionality is entirely contained within $a^2$, which agrees with the fact that the dimension of $\kappa$ is length-squared. The Kozeny–Carman is not the only existing permeability-porosity relationship [3], but it works fairly well for granular beds as in our case.

### 3.1. Artificial porous media

In this section we describe the algorithm we developed to build artificial samples. An object-oriented implementation example for such algorithm, written in Python, is available as a supplementary material. Our intention was to produce a more realistic porous medium than the usual bed packed, but with more controllable parameters than the real samples digitised from rock tomography. In this way, we can, for instance, relate the geometry of the obstacles to permeability.

The input parameters for the algorithm are: the length of obstacles, the length of the sample and the target porosity. The obstacle’s shape is determined by the equation of a spheroid with radii $r_x, r_y, r_z$ centred at $(x_c, y_c, z_c)$. The samples are rectangular parallelepipeds, for which three lengths $L_x, L_y, L_z$ are required as inputs. The last input is the target porosity $(\phi_t)$, that is the desired porosity for the sample within a tolerance $\varepsilon$.

Given these input parameters, the algorithm builds a sample by placing obstacles in random positions, one at a time. After creating an obstacle, the algorithm checks if the target porosity has been reached. If not, another obstacle is added. The algorithm stops when $|\phi - \phi_t| \leq \varepsilon$, as depicted in figure 3.

For our simulations, we used samples with $208^3$ nodes, spherical obstacles with diameters between $d = 12$ and $d = 30$ and porosities in the range $0.2 \leq \phi \leq 0.4$. The number of nodes ($\sim 9 \times 10^9$) was limited by the available GPU memory. In figure 4, we show some slices of artificial samples generated by our algorithm side-by-side with slices of real digitized rock tomography samples for comparison. The agreement is good for highly homogeneous rocks such as sand packs and most sandstones, but our algorithm may not be as suitable for more inhomogeneous rocks such as carbonates and shales, for they exhibit porosity at multiple scales. These artificial samples have the same obstacle diameter ($d = 20$) but different porosities: 0.2, 0.3 and 0.4. Since the spheres are allowed to overlap, they form more complex structures that are very close to those observed in real porous media. This leads to more realistic simulations of fluid flow.

### 3.2. Permeability

The two main methods for inducing fluid flow in a porous medium using Sailfish are: by setting a pressure difference across the sample or a body force acting on every fluid node. Although the pressure method is closer to what is done in experiments, we observed that the steady-state flow is reached much faster with the force method. This happens because all points of the fluid feel the driving force at the same time when using the force method, instead of by propagation of shock waves as in the pressure method. In order to detect when the steady-state is achieved in our simulations, we calculate $||u_{\text{new}}| - |u_{\text{old}}||/|u_{\text{new}}|$ at every time
step for every point of the fluid and, when the maximum value of this quantity is less than a given threshold, the simulation stops. We found \(5 \times 10^{-7}\) to be sufficient for our purposes.

The permeability is calculated using Darcy’s law but, as it assumes a pressure gradient instead of a body force, we modify it using the relation \(\frac{dP}{dx} = \frac{F_j}{A_j}\), where \(F_j\) is the body force along direction \(x_j\) and \(A_j\) is the cross-sectional area of the fluid at the boundary where the pressure is applied. The cross-sectional area of the fluid is \(\phi\) times the total area. Therefore, given a force density \(\mathbf{f} = f_i \mathbf{i}\), Darcy’s law becomes

\[
\kappa = \frac{\mu \langle u_i \rangle \phi}{f_i},
\]

which is the equation used to calculate permeability.

Since permeability, porosity and viscosity are not velocity-dependent, we expect the applied force \(f_i\) and the mean velocity \(\langle u_i \rangle\) to be proportional to each other in the steady state. We tested this by taking an artificial sample with porosity \(\phi = 0.3\), obstacles with diameters \(d = 16\) nodes and using it as input for fluid flow simulations with different driving forces. The fluid had viscosity \(\mu = 0.01\) in lattice units. The result is shown in figure 5. We fit the data points with the function \(\nu_i = \alpha f_i\), obtaining the proportionality constant \(\alpha = (26.67 \pm 0.02)\) in lattice units. Using (6), we can determine the permeability of the sample to be \(\kappa = (8.001 \pm 0.006) \times 10^{-2}\) in lattice units.

### 3.3. The Kozeny–Carman equation

We calculated the permeability using (6) and estimated the Kozeny’s constant of the artificial porous media samples created using the method described in section 3.1. In order to
determine the individual contributions from porosity and obstacle dimension to the permeability, we built 210 samples with 2083 nodes: 10 obstacle diameters \(d\) and 21 porosities \(f\), for each diameter. The fluid viscosity was 0.01 and the external force, \(f_r = 10^{-5}\). The results are shown in figure 6(a). One sees that permeability increases with porosity for a given obstacle diameter. Analogously, for a given porosity, permeability also increases with obstacle diameter. Next, we investigate the suitability of the Kozeny–Carman equation to describe our data.

Equation (5) tells us that permeability is proportional to \(d^2\) or, in other words, that there is a scale-law involving obstacle dimensions and permeability. In order to turn permeability into a scale-free non-dimensional quantity, we calculate \(\kappa/d^2\), and confirm that all points fall (despite fluctuations) within the same curve (see figure 6(b)). We fit the function
to the data points, with \( C \) (Kozeny’s constant) as the free parameter. Its value was determined to be \( C = 3.18 \pm 0.02 \). As the fit uncertainty represents less than 1% of the main value, we consider (7) to be in good agreement with our simulated data points.

For simplicity, some approximations were made while fitting (7) to the data points. The obstacle diameter \( d \) is taken as the theoretical diameter but the effective one might be slightly different due to the ‘digital’ nature of the spheres, i.e., being composed of cubic pixels (see figure 7(b)). Also, we used the SSA of non-overlapping spheres, \( s = 6/d \), although we allow the spheres to overlap. In the next sections we present an analysis of the impact of such approximations.

Despite those simplifications, the value we obtained for Kozeny’s constant is consistent with previously published values in the literature [28]. For instance, \( C = 5 \) for a bed packed of non-overlapping spheres [3] and, typically, between 2.2 and 8.9 for a fibrous media [29].
3.4. Specific superficial area

With the increasing popularization of digital rock physics [30, 31], some recent works proposed new techniques to calculate the SSA [27, 32], but they are still quite complex and indirect. Measuring the SSA of porous rocks experimentally is a hard task [33] but it is important to understand the rock’s properties [34]. We propose a methodology to calculate the SSA using widely available Python libraries for image-processing. The advantage of our method is that it provides a visual interpretation of what is being calculated, making it simple enough to be understood and applied by beginners.

To calculate the SSA of a digital rock sample, we use the binary_erosion method of the SciPy library\(^4\). This operation erodes the image by removing a layer of pixels at the rock/pore boundary. When the eroded image is subtracted from the original, what remains are the pixels at the surface, which allows us to calculate the SSA using its basic definition. A Python implementation example is provided in the supplementary material section.

The first application of this method is a simple problem with analytical solution that consists in calculating the SSA of a single sphere for different radii. In figure 7(a), we see the results for radii ranging from 5 to 70 compared to the analytical solution, \( s = 3/R \). We see that the data follows the same behaviour of the analytical curve, but with a small discrepancy that decreases as the radius increases. For instance, the relative difference between measured and analytical SSA for \( R = 5 \) is 28\% and for \( R = 70 \) it decreases to 18\%. This difference is due to a limitation in the spatial resolution that all digital images are subjected to. In figure 7(b) we see three slices of spheres with different radii. The sphere with \( R = 5 \) is far from a spheroidal shape, while that with \( R = 70 \) is much closer. The better the spatial resolution, the more accurate is the proposed methodology. However, since the available GPU memory is limited, we cannot use arbitrarily large sample sizes to achieve higher resolutions.

After this simple, but revealing, example we calculated the SSA for our porous media samples. Figure 8(a) shows the surface of the obstacles, that is, the outermost layer isolated using the erosion operation. We clearly see the contour of the overlapped spheres and some partially filled circles, due to the finite resolution issue. In figure 8(b) we show the SSA obtained as a result of our method for 21 samples with \( d = 20 \) and different porosities. The SSA clearly depends on porosity, which was not considered in our previous calculation of the Kozeny’s constant. This dependence occurs due to obstacles being able to overlap \([16]\), which changes their shape to non-spherical. If the spheres were isolated from each other, as in a close-packed structure, the SSA would be \( s = 3/R \) as for a single sphere.

3.5. Tortuosity

In general, it is difficult to calculate tortuosity using its basic definition, (2), for one would have to know exactly the central streamline. However, if one has the velocity field, there is an easier way to perform this calculation. It has been shown [17] that (2) is equivalent to

\[
\tau = \frac{\langle |\mathbf{u}| \rangle}{\langle u^j \rangle},
\]

where \( |\mathbf{u}| \) is the magnitude of local velocity, \( u^j \) is the component of local velocity along the direction of flow \( x^j \) and \( \langle \cdot \rangle \) represents the average over the entire system volume. This method has been extensively tested [35] and its results agree with theoretical predictions. For instance, for the trivial case of flow in a straight channel, \( |\mathbf{u}| = u^j \) for every point in the fluid, which

\(^4\) See http://scipy-lectures.org/advanced/image_processing/
gives $\tau = 1$. This is the same result predicted by (2) since all streamlines are straight in this case [35]. If the streamlines in a particular flow are not straight, $|u| \geq u^l$ for each point and $\tau > 1$ as in (2).

The tortuosity was calculated using the aforementioned method for samples with $d = 20$, as in figure 9. We found a linear relationship between $\tau$ and $\phi$ in this range of porosities,
despite all the noise, similar to previous reports in the literature [16, 17]. We adjusted a linear function to the data points and obtained $\tau(\phi) = 1.79 - 1.08\phi$.

4. Conclusion

This present article had two goals: (i) constructing an algorithm to build artificial porous media samples and (ii) presenting how the main properties of porous media are calculated using the output from LBM simulations. The first goal was addressed in section 3.1. Identical spheroidal obstacles were placed in random positions (allowing overlap), creating structures similar to those observed in real rock samples, as exemplified in section 3.1.

To achieve the second goal, we developed the following analysis. In section 3.2 we calculated the permeability of a particular sample using Darcy’s law and verified that the drift velocity is linear to the external force. In section 3.3 we investigated whether the Kozeny–Carman equation applies to the permeability-porosity relationship of our samples, obtaining a good agreement as seen in figure 6(b). Although we allowed obstacles to overlap in our artificial samples, destroying their otherwise spherical shape, figure 6(a) shows that permeability still depends on the obstacle diameter, which allowed us to use a scale-law leading to figure 6(b). In section 3.4, we developed our technique for calculating the SSA in digital samples, tested it on a single sphere for different radii and obtained good agreement to the analytic solution for big radii. In section 3.5 we presented a simple method to calculate tortuosity from the velocity field of the fluid.

Sailfish is a powerful LBM solver with many features that are out of the scope of this work. More complex flows can be simulated in porous media using Sailfish, such as multiphase [36] and turbulent flows [37]. One can also use Sailfish and the techniques described here to perform fluid dynamics studies inside fractures, which is another interesting subject for the oil and gas industry. The relationship between SSA and porosity in porous media is yet another interesting subject for future works [16].

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