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Keywords: diffusion, lattice Boltzmann method, BGK, heterogeneous media, stability, non-negativity, equilibrium distribution

Abstract. This paper shows the use of the Lattice Boltzmann Method for the simulation of the diffusion equation in heterogeneous media. The theoretical background of the method for both homogeneous and heterogeneous media is developed. A simple method of determination of the conditions of safe use of the LBM is proposed, accompanied by a practical example. The range of interest and condition of non-negativity of the equilibrium distributions are determined for a broad range of diffusive properties ratios.

Introduction

The Lattice Boltzmann Method (named LBM) is an explicit numerical method enabling in some cases, the large parallelisation of computationally intensive problems on graphical processing units. This method allows for the real-time determination of velocity, species or temperature distributions in porous media [1]. The attractiveness of the method lies in its relatively simple implementation and its fixed, regular grid, whatever be the geometry of interest. However, special attention is required regarding the stability of the method when heterogeneous media are considered with increasing relative thermal conductivity.

The Lattice Boltzmann Method for Diffusion

The LBM is a mesoscopic approach of the partial derivative equations problems. The evolution of a fluid or a solid is deducted from the consideration of a population of particles interacting with well-defined rules of collision. Unlike the well-known Navier-Stokes approach that uses the equations describing the macroscopic behaviour of a fluid and then discretizes them to the microscopic level, the LBM is an “ascendant” method, where the particles' agitation defined by the Maxwell-Boltzmann distribution of statistical mechanics allows for a consistent extrapolation towards the macroscopic behaviour. The link between micro and macroscopic scales is reached thanks to a Chapman-Enskog expansion [2].

Practically, the LBM consists in considering a population of particles streaming along given directions in the space systematically *on the points* of the grid. The particles' displacement is equal to unity in every direction, hence the time and space scales are strongly linked. At each time step, the particles' distributions stream orthogonally and diagonally to their neighboring nodes and exchange their energy by collision. Fig. 1 gives an example of distribution propagation for the D_2Q_9 model, where subscript “2” represents the dimension of space, “9” being the number of distributions streaming on the grid (8 possible space directions, plus the probability of staying on the same point).

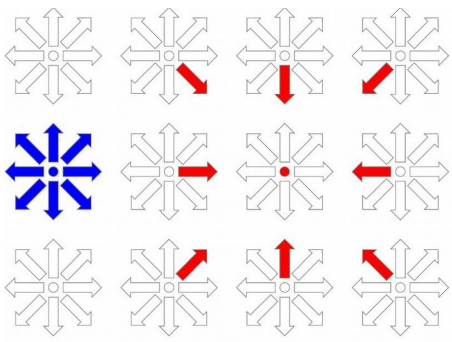

Figure 1**:** D2Q9 Scheme - Arrows representing the possible directions of propagation of the distributions

Boltzmann's equation ruling the particles' behaviour is given under following form, f begin the density of probability of the particles, c the speed of propagation and Ω the collision operator:

$$\frac{\partial f}{\partial t} + c\nabla f = \Omega(f). \tag{1}$$

After discretizing the space into D_2Q_9 as previously defined, with $0 \leq k \leq 8$ and $c_k = 1$ “lattice unit per time step in direction k” as the mesoscopic speed of the particle on the grid, one obtains:

$$\frac{\partial f_k}{\partial t} + c_k \frac{\partial f_k}{\partial dx} = \Omega_k. \tag{2}$$

In the Bhatnagar-Gross-Krook approach [3], the collision operator is approximated as a relaxation of the distribution function towards the equilibrium distribution:

$$\Omega_k = -\frac{1}{\tau}(f_k - f_k^{eq}). \tag{3}$$

The equilibrium distribution function f_k^{eq} of Eq. 3 is computed through the Taylor expansion of the Maxwell-Boltzmann distribution of a stationary perfect gas at the equilibrium, which simplifies for the diffusion process merely as Eq. 4:

$$f_k^{eq} = \omega_k \rho \frac{c_s^2}{c^2}. \tag{4}$$

The ρ factor in Eq. 4 is simply the sum of the f_k distributions at the point considered and represents the computed macroscopic, *e. g.* the concentration or temperature. The ω_k factor is a constant weighting relative to the propagation direction, such as $\sum(\omega_k) = 1$. Long displacements are less likely than short ones, hence the decreasing weightings of zero displacement, orthogonal displacement and diagonal displacement.

Setting out $\omega = \Delta t/\tau$ and writing the Boltzmann equation with its discrete form, one obtains the explicit equation of the space-time evolution of the f_k functions:

$$f_k(x + \Delta x, t + \Delta t) = f_k(x, t) - \omega(f_k(x, t) - f_k^{eq}(x, t)). \tag{5}$$

For stability reasons of the LBM, the ω factor has to remain strictly between 0 and 2. In the case the case of two-dimensional diffusion in a single given medium, the relationship between ω and the “LBM diffusivity” d is as follows:

$$d = c_s^2(\frac{1}{\omega} - \frac{1}{2}). \tag{6}$$

In Eq. 6, $c_s = 1/\sqrt{3}$ is a parameter called the sound speed in the LBM space-time, but is actually only a scaling factor in the case of diffusion [3, 4].

In order to make a LBM simulation with a given number of time steps t_{LBM} and a mesh size N with the evolution t_{real} of a real domain L, one has to make their Fourier numbers correspond:

$$F_o = \frac{d_{LBM} t_{LBM}}{N^2} = \frac{d_{real} t_{real}}{L^2}. \tag{7}$$

Changing the “LBM diffusivity” or refining the mesh will hence affect the number of time steps to be computed. For more details about the LBM and its boundary conditions, please refer to [2].

Regarding the simulation of diffusion in two materials a and b, the best practice is to define a relaxation factor for one of them and then determine the value of the other one depending on the ratio of real diffusivities, as developed hereinafter:

$$\omega_a = \text{cst}. \tag{8}$$

$$d_a^{LBM} = c_s^2(\frac{1}{\omega_a} - \frac{1}{2}). \tag{9}$$

$$d_b^{LBM} = d_a^{LBM} \times \frac{d_b^{real}}{d_a^{real}}. \tag{10}$$

$$\omega_b = (c_s^2 d_b^{LBM} + \frac{1}{2})^{-1}. \tag{11}$$

The major interest of the LBM is its simple numerical implementation even for complex morphologies, the controlled change of the relaxation factor ω depending on the type of media considered on the regular grid allowing for a correct representation of the physics, without having to change the mesh at the interface.

As we have seen, two parameters ω_a and ω_b have to be controlled in order ensure a consistent result, which will be detailed in following section.

Numerical Stability, Non-negativity and range of use for heterogeneous media

Another aspect of this study is the behaviour of the LBM-BGK algorithm depending on the variation of the relaxation factor ω, which affects the precision, computational cost and stability of the method.

As mentioned in the previous section, the relaxation factor depends on the LBM-diffusivity for a chosen problem. It also affects the computational cost, i. e. the number of iterations required to reach a given real time and the precision of the method [5]. Taking the explicit Finite Differences Method (FDM) as a reference for comparison, one can see on Fig. 2 the evolution of the error ratio between LBM and FDM, as well as the time steps ratio. The horizontal dotted line is the unity ratio for both methods' time steps and gives a measure of the time steps ratio required for the LBM compared to the *explicit* FDM. From Fig. 2, one can conclude that the relaxation factor shall be small enough to be competitive versus classical methods, ideally below the unity ratio, yet big enough to allow for a sufficient precision of the method.

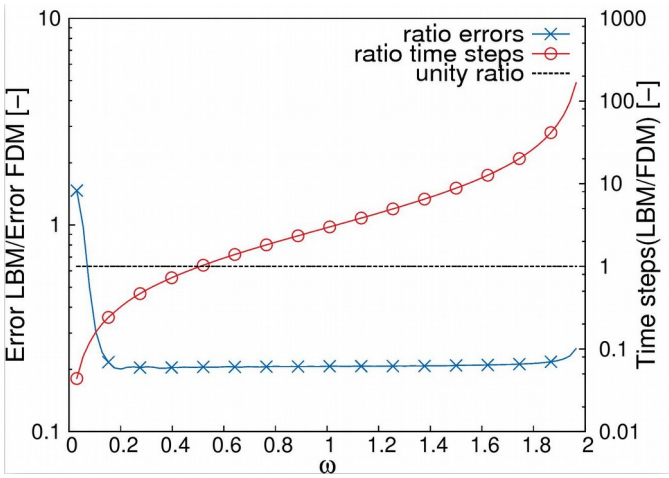

Figure 2: Comparison of the LBM versus the finite-differences method for the diffusion problem

The experience shows that for heterogeneous media with a diffusivity ratio reaching several orders of magnitude, some perturbations might appear at the interfaces between the phases. A first method of control of these instabilities is to ensure the non-negativity of the equilibrium distributions, as well as staying within the range of stability of the numerical scheme.

Non-negativity analysis for the D_2Q_9 lattice arrangement and heterogeneous diffusion.

The non-negativity analysis is a simple way of checking that the solution obtained have a physical meaning, i.e. a positive value of probability. It consists in verifying the positivity of the equilibrium distributions [4], which is very straightforward and leads to following set of equations:

$$1 \leq k \leq 4 : f_k^{eq} = \frac{1}{3} F_o \tag{12}$$

$$5 \leq k \leq 8 : f_k^{eq} = \frac{1}{12} F_o \tag{13}$$

$$f_0^{eq} = 1 - \frac{5}{3} F_o \tag{14}$$

The resulting positivity condition from Eq. 6, Eq. 7 and Eq. 14 is hence:

$$\omega > \frac{10}{23} \tag{15}$$

Range of use for heterogeneous materials.

Eq. (8-11) show the relationship dependency of the relaxation factors with the diffusivity ratio, as presented on Fig. 3. On this figure, one can read the dependency between both relaxation factors with the diffusivity ratio as a parameter, with diffusivities presenting a difference of several orders of magnitude. As the considered ratios can be inverted, the problem obviously shows a symmetry with respect to the first bisector. The LBM-BGK simulation of the diffusion process in heterogeneous media hence requires a control of the relaxation factors ensuring the positivity of the equilibrium distribution functions for given properties.

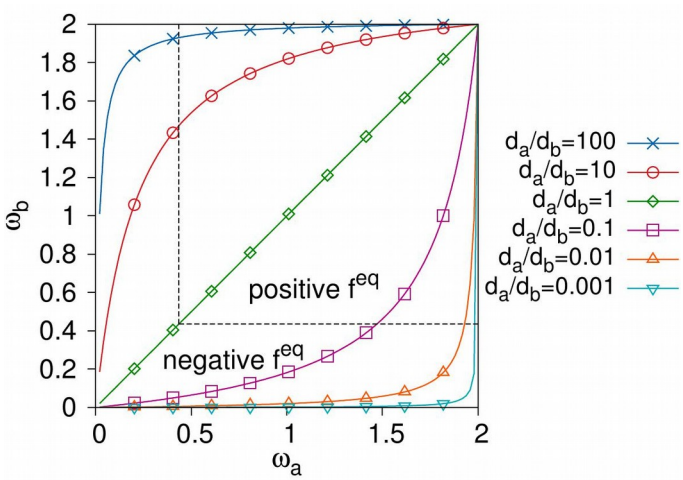

Figure 3: Influence of the diffusivity ratio on the relaxation factors and non-negativity zone

Application to a diffusion problem

The theoretical aspects of the method being set, the validation of the model will be developed in next section, followed by an application to diffusion in hydrated cement paste. The apparent diffusivity of the materials considered was calculated by integration of the normal flux to the surfaces as in [6].

Validation of the model with an analytical solution. Mori & Tanaka's [7] analytical approach of homogenisation allowed to verify the aptitude of the code for the apparent diffusivity of the material with inclusions. Spherical, regular inclusions were put in the matrix (see Fig. 4) and the apparent diffusivity was

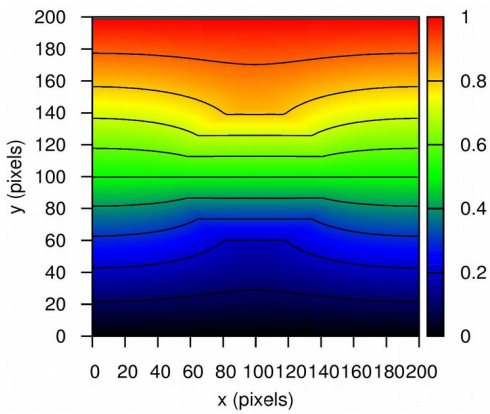

Figure 4: Isovalues of concentration for the test case $f_v = 0,15$

computed for different volumic fractions of inclusion f_v and different diffusivity ratios d_a/d_b, resulting in a good accordance with Mori & Tanaka's method as presented on Fig. 5.

Diffusion in hydrating cement paste. In order to get a realistic description of the fresh cement paste, we used the level-set morphology reconstruction technique. The resulting morphology is shown on Fig. 6, for more information, see the very complete references [8, 9].

The hydrating cement paste is composed of water-saturated porosity, hydrated cement and anhydrous cement, the latter being considered as impermeable to diffusion. The volumic fractions and respective diffusivities are summarised in Table. 1

The apparent diffusivity obtained by this method is $2,13.10^{-11}[m^2/s]$, which is coherent with the order of magnitude of cement paste diffusivity at early ages.

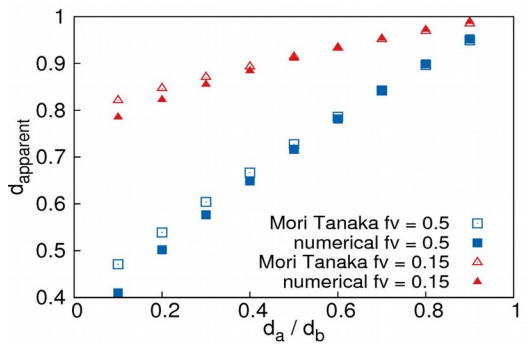

Figure 5: Benchmark of the code versus Mori-Tanaka's analytical approach

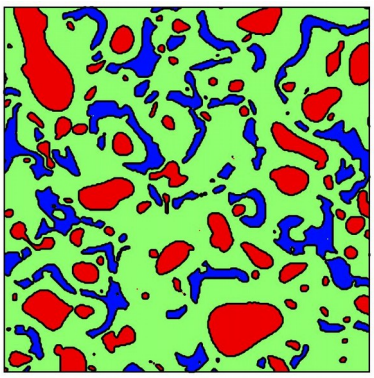

Figure 6: Morphology - Red: anhydrous cement, Blue: water, Green: hydrated cement

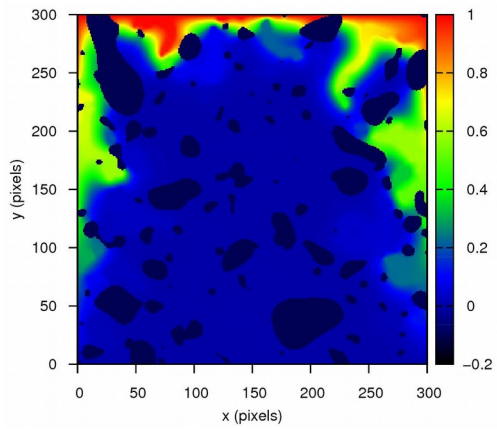

Figure 7: Diffusion into the reconstructed morphology

Phase	**Volumic fraction [%]**	**Diffusivity [m²/s]**
Water	12,1	$2.10^{-}9$
Hydrated cement	68,6	$2.10^{-}12$
Anhydrous cement	19,3	0

Table 1: Properties of the hydrating cement paste considered

Conclusion

The theoretical background of the LBM for homogeneous and heterogeneous media have been developed in the frame of this work and a zone of safe usage of the method was proposed for a broad variety of diffusivity ratios. The LBM code was validated with Mori and Tanaka's analytical method of calculation of heterogeneous media apparent properties. An application to cementitious material is proposed.

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