Reply to Referee2

Text coloring: original Referee2 text, our non-manuscript comments, our in-manuscript text.

First of all, we appreciate a thorough study of our manuscript by referee2, initiating interesting discussion.

1 - Throughout the manuscript, authors should revise the citation style employed. In principle, the citations should be written inside parentheses. We adjusted the citation style accordingly.

2 - Section 1 includes a brief description on the discretization error. Here, it is provided a parenthesis featuring the following explanation: `` This discretization error should not be confused with the round-off error inherent to the floating-point arithmetic on digital computers.)''. In principle, there should be no risk of confusion between discretization error and round-off error. On the other hand, one admits the risk of confusion between the geometric discretization error (due to the real geometry meshing) and the governing equation discretization error (due to approximating the continuous PDE problem by some discrete representation). Perhaps, the explanation inside the parenthesis should focus on this last issue rather than the distinction between discretization and round-off error, which is trivial. We replaced the phrase "This discretization error should not be confused…" with the following: "In the context of flow simulations, the discretization error impacts both the geometry representation and the flow field, with the latter originating from the numerical solution of PDEs". Actually, this point is stated in our cover letter, and it is a good idea to have it in the main text.

3 - Section 1, in the last paragraph, it is mentioned ``magic number''. This terminology is repeated in Section 4. It is recommendable to replace the terminology ``magic number'' by a more insightful designation like the ``TRT free relaxation parameter'', for example. The terminology "magic number" was introduced by Irina Ginzburg and Dominique d'Humières in 2009 or earlier, who first identified and studied it. This terminology is already well-established in the field, and it appears that for us it is not a good idea to change it. From personal experience, S.K. recently attended one of the key conferences among the lattice Boltzmann community (ICMMES24, International Conference on Mesoscopic Methods in Engineering and Science) and the term "magic number" was routinely used by most of the participants. We cannot use "relaxation parameter" because Λ is the specific combination of the relaxation parameters, but not the relaxation parameter itself. This term also presents in the names of boundary conditions ("MCLI" – magic linear schemes, etc.) In other words, "magic number" appears to be too mature to rename it. Also, very recent study from LBM community:

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A MAGIC TWO-RELAXATION-TIME LATTICE BOLTZMANN ALGORITHM FOR MAGNETOHYDRODYNAMICS

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Abstract. The two-relaxation-time collision operator in discrete kinetic the-

4 - Section 3 describes the physical problem and how it is tackled numerically. For this latter, it is mentioned that the lattice Boltzmann method (LBM) is implemented following the setup of a previous work (Khirevich & Patzek 2018). For a clearer understanding of the reader, it is important to mention, already here, that the LBM running on the two-relaxation-time collision operator is used. Also, it is important to explicitly mention already here the boundary scheme employed. Only late in Section 4 it is mentioned that the standard bounce-back rule is used in this work, while a critical understanding of the results shown in Fig. 2 would require this information already. This is definitely a valid point and we extended the numerical approach description in the first paragraph of Section 3.

5 - Section 3, at the end, it is written the following sentence: `` NB, for the considered flow problem we are not aware of any numerical scheme constructed outside of a unit cell.'' However, by this brief statement, it is not clear what do the Authors mean by numerical scheme outside of the unit cell. Can the Authors elaborate a little bit more on this point or, at least, provide a citation where this procedure is explained? First, it appears that the thought behind this sentence can be formulated better. Thank you for noticing and asking. In a nutshell, in these sentences we highlight the basic fact about the employed schemes.

To solve Stokes problem, all numerical schemes we are aware of, such as LBM, finite difference, finite volume, finite element, are constructed using given lattice (or mesh) element such as voxel and its first-layer neighbors (in some less common cases the second-layer neighbors can also be used, but this greatly increases computation and communication demands). I.e., for the LBM streaming step:

$$f_i(\vec{x} + \vec{e}_i, t + \delta_t) = f_i^*(\vec{x}, t)$$

For the finite difference:

$$\frac{u_j^{n+1} - u_j^n}{k} = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}$$

The finite volume and element are similar. In all schemes above, the red color highlights the reference to the first-layer neighbor.

Let us mark voxels as “bulk” (or “fluid”) if they are not directly connected to a boundary node. Now, we need to add the solid boundary treatment to our scheme. This can be done using a) smooth (analytical) representation or b) stair-step representation. For a), higher-than-1st order boundary schemes can be constructed while for b) only 1st-order boundary scheme can be formulated, such as the bounce back. For b), the stair-step boundary will appear in the schemes above as a mesh element marked as “boundary” (or “solid”). After formulating the rule for updating “bulk” mesh element in the presence of “boundary” neighbor, we have the numerical scheme ready for computation.

As you see, the formulation of the numerical scheme(s) above is done at the level of a single mesh element plus its direct neighbors. This is the scale below a single-unit cell (for example, of regular packings we used), while we demonstrate that the superstructures significantly exceed the scale of a single unit cell. These superstructures control flow in low-resolution simulations, not the pores of the original non-discretized geometry. This means that any numerical scheme constructed on a single-voxel scale cannot capture the flow features originating from the superstructures.

We added the following text: "the numerical schemes such as lattice Boltzmann and finite difference rely on the information from a given voxel plus its direct neighbors, which is below the unit cell scale."

6 - Section 4, it is written the following sentence: `` A free parameter known as the "magic number", $\Lambda$, controls the discretization error in lattice Boltzmann simulations d'Humieres & Ginzburg (2009).'' should be revised. First, the $\Lambda$ should be renamed using a more insightful designation, rather than ``magic number. Second, how it is written, the sentence itself is misleading. The Λ parameter controls the SPATIAL discretization error in TWO-RELAXATION-TIME LB simulations. Like shown in a previous work by Khirevich and Ginzburg (2015), other LB collision operators lead to different relaxation parameters as coefficients of the numerical errors. Only TRT is controlled by Λ alone. Thank you for pointing this out. We modified and extended 2nd paragraph of Section 4, making our statements correct.

7 - Section 4, it is written the following sentence: `` Then Λ is a specific combination of the LBM collision rates d'Humieres & Ginzburg (2009).''. Once again, this sentence is oversimplified and may be misleading, as the reference to the two-relaxation-time collision scheme is never given in the manuscript. The reference to TRT LBM presents in the originally submitted manuscript:

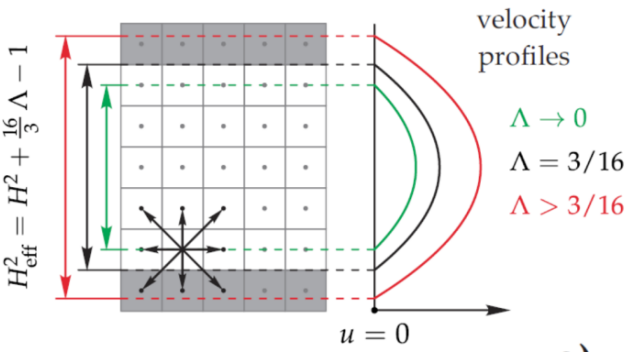
GINZBURG, I., VERHAEGHE, F. & D'HUMIERES, D. 2008 Two-relaxation-time Lattice Boltzmann scheme: About parametrization, velocity, pressure and mixed boundary conditions. *Communications in Computational Physics* **3** (2), 427–478.

Nevertheless, we have re-checked it, as this reference must be cited.

It would be worthwhile mentioning in this section that the minimal collision operator that separates the viscosity determination from the discretization error is the TRT scheme and that Λ is the combination of the two relaxation rates provided by this scheme. We extended 2nd paragraph of Section 4 in this regard.

8 - Section 4, it is written the following sentence ``ii) the magnitude of the discretization error or its contributions''. What does this discretization error refer to? If Λ controls the location of the no-slip velocity BC, it will logically also determine the discretization of the solid geometry. So, this point ii) to be different from point i) does it refer to the magnitude of the discretization in bulk? That is, in the description of the Stokes fluid part? It appears that the original "In this context" sentence was misleading. We changed the original text to the following: "Λ can be seen as the parameter controlling i) the location of the zero-flow boundary (and the corresponding pore ``width'') between solid and fluid voxels (Khirevich2015), or ii) the magnitude of the discretization error or its contributions (see Figure 3 in Khirevich & Patzek (2018); also eq. (15) in Rohde et al. (2003), where parameter τ can be interpreted as the one impacting the discretization error)."

There are different views on how Λ impacts the final flow field. Point i) is the geometrical interpretation for the location of zero-velocity boundary or effective channel width:



Here it is important to understand that variation of Λ does not change the geometry (in reply to original comment "it will logically also determine the discretization of the solid geometry."), it just changes flow-field solution in the presence of a given geometry. That is, a voxelized representation can be exact, while a variation of Λ can introduce error of an arbitrary magnitude to the flow field for this exact geometry. But the opposite is also true: for the incorrect, highly-voxelized geometry Λ can reduce the error in some features of the flow field (such as the average flow rate or related permeability).

Point ii) is about the magnitude of the total discretization error in permeability, which includes the error in geometry, flow field (bulk scheme error + boundary condition), and integration:

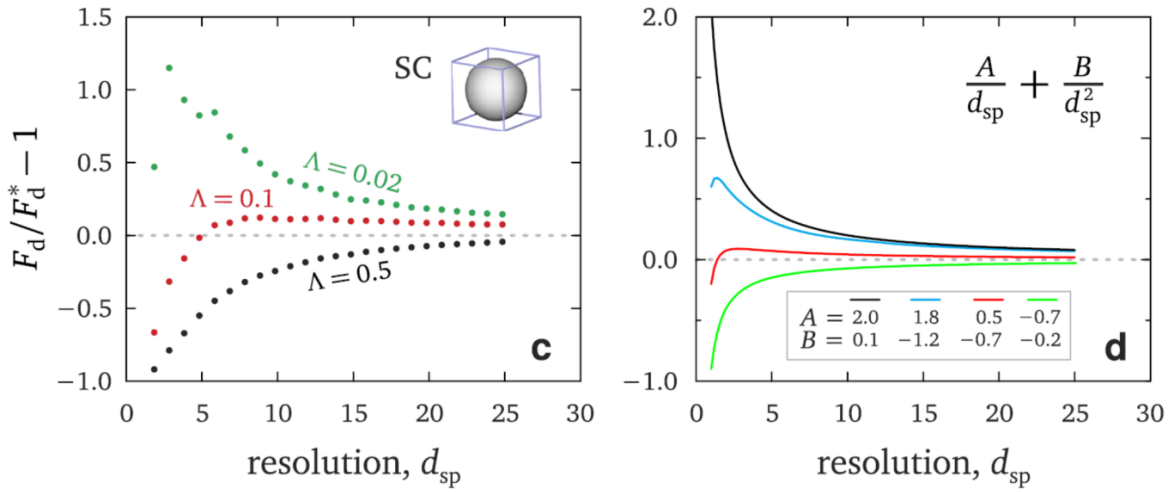


Figure above is from our previous study (doi:10.1063/1.5042229) and it shows a) error in permeability in SC geometry for Λ values, and b) just a function of two free parameters, y = A/x + B/x^2, where linear term mimics the error contribution due to 1st order boundary condition and quadratic term mimics the error contribution due to 2nd order bulk scheme + integration. Variation of the parameters A and B in right panel produces curves similar to the left panel. It is important to note that, for complex geometries, we are not aware of analysis of these contributions separately, but still we can control all of them simultaneously via Λ. This is what we actually do in the current study.

9 - Section 4, starts a sentence with ``I.e.'', which is odd. Please replace it by ``That is,'' or something alike. Corrected.

10 - Section 5, the Null point P0 approach. It is fair to explicitly mentioned that the use of this P0 optimal point has been studied in [1] Khirevich et al. (2015), but also previously studied in other works, such as: [2] Ginzburg, F. Verhaeghe, D. d'Humières, Study of simple hydrodynamic solutions with the two-relaxation-times lattice Boltzmann scheme, Commun. Comput. Phys. 3 (2008) 519–581. [3] G. Silva, I. Ginzburg, The permeability and quality of velocity field in a square array of solid and permeable cylindrical obstacles with the TRT–LBM and FEM Brinkman schemes, C. R., Méc. 343 (2015) 545–558. Sorry, but we disagree with this comment. The concept of P0 is new and it is introduced in this study. The key idea behind P0 is motivated by superstructures, and this idea is to accept a locally-inaccurate flow field (highly-voxelized geometries) and to extract the accurate integral (as opposed to local) quantities such as the average flow rate/permeability. At P0, local errors can be large, but they cancel out in the integral quantity. This is diametrically opposite to the strategy taken in [1], [2], [3], where authors aim to get the locally-accurate flow field to obtain the accurate integral quantities (this approach works, no doubts here). The direction of avoiding the locally-inaccurate flow fields is stated explicitly in a recent (2020, 10.1098/rsta.2019.0404) study by Dr. I. Ginzburg and co-authors:

1. Introduction

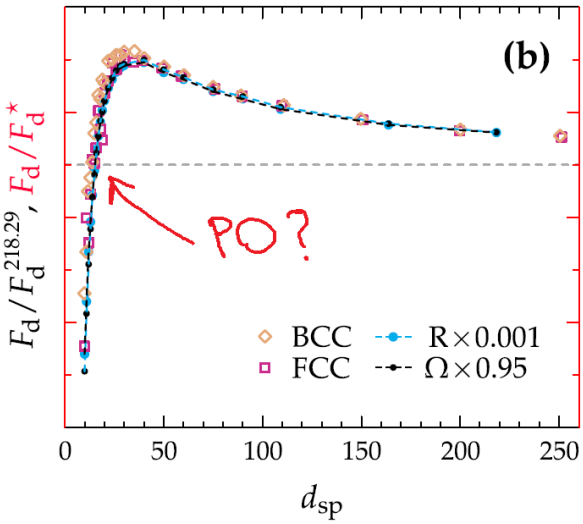
The computational fluid dynamics (CFD) modelling of flows in porous media is relevant in a wide range of applications [1]; from the groundwater movement in aquifers to smaller-scale systems associated with transport in soils. In all cases, the simulation accuracy gets strongly determined by the discretization of the bounding geometry [2]. While the lattice Boltzmann method (LBM) displays numerous advantages as a CFD tool, see [3,4], it formulates on an uniform Cartesian mesh, by default. Therefore, the task of prescribing boundary conditions over arbitrarily shaped surfaces requires particular care in order to avoid the inaccurate staircase discretization. This task is further complicated by the fact that LBM's working variables correspond to mesoscopic

If we discuss in more detail the aforementioned references [1-3], then study [2] addresses the errors in local (pore-scale) flow field, and states the need for the locally-accurate flow fields (obtainable with the locally-accurate boundary conditions), which is not in P0 direction:

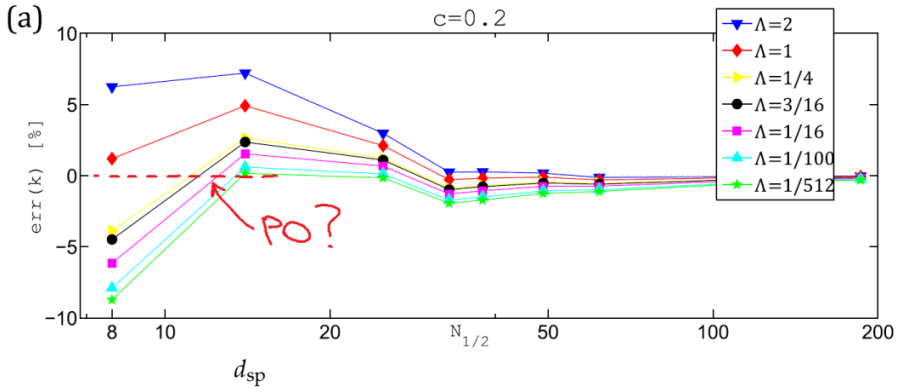
5 Concluding remarks

We have presented several multi-reflection algorithms for velocity and pressure boundary conditions and for their mixed combination. Numerical computations validate the Chapman-Enskog and the dimensional analysis [16], based on exact population solutions, in simple problems with an analytical solution. They show that highly accurate boundary schemes are needed in corners and for small resolutions, typically for flow through soil pores. A very similar performance can be achieved with the Dirichlet velocity and mixed schemes when they are based on the multi-reflection components which are equivalent in accuracy. Whereas an effective accuracy of "linear" schemes depends

For the case of [1], P0 could be highlighted and discussed in Figure 9 (or similarly in Figures 10, 15):



In the case of study [3], which deals with the case of partially-permeable solid phase (Brinkman equation), P0 could be discussed in Figure 2a (and panel (b) similarly):



11 - This latter in the context of both Stokes- and Brinkman-flow simulations in porous media arrays. Please see our discussion for the comment 10, although here additional Brinkman-flow physics is involved, which is beyond scope of our study.

12 - Section 5, the construction of the dimensionless parameter χ presented in Eq. (5.1) is it based on any specific work? In other words, for reference, it is not clear how this ``discretization measure'' has been considered (if ever considered) in past studies? This measure was derived for the first time in this work, as per our knowledge. However, while working on the revision of the manuscript, we found, that (5.1) (now (5.2)) is very similar to the definition of hydraulic radius found in, for example, Whitaker (1972). Therefore, we added this information to the manuscript and described our strategy to identify χ.

13 - Section 6 shows that with the proposed $\Lambda^\star$ correlation it is possible to reach highly accurate permeability solutions at significantly low number of voxels per sphere diameter (i.e. low-resolution). However,

at the beginning of the manuscript, the problem was introduced, not only as one of accuracy, but as a trade-off between the accuracy and the computational overhead. So, the information that is still lacking at the end of this section is a relation between these two parameters. Namely, how does it cost to obtain a solution for a given resolution and how much was saved with the approach proposed in this work? We added a paragraph with discussion about computational efforts and CT time savings at the end of section 6.

11-Nov-24, message from editors:

Referee: 2

Comments to the Author

The authors have successfully addressed the Reviewer's original comments. Therefore, the revised version of the manuscript can be considered suitable for publication.