

Referee #1 (Comments to Both Author and Editor):

The paper tries to analyse the transport in a porous structure through improving the capturing of "superstructures" in low-resolution images of porous media. The manuscript is heavily dependent to the authors' previous published works, and it makes following the provided analysis quite difficult, even for someone in the field. It is difficult to understand the flow of discussions accordingly.

Our work is based on i) "magic number" (not our result), ii) reference permeability values (Tables I and II) obtained from extrapolation (our results <https://doi.org/10.1063/1.5042229> but can be obtained in many different ways), iii) the fact that discretization error have several possibly self-cancelling contributions (can be observed in earlier studies such as eq. (15) in 10.1103/PhysRevE.67.066703 or in our work <https://doi.org/10.1063/1.5042229>). Probably, our work will require some time to be understood, but we hope it worth it because we are not aware of any other approach to obtain accurate permeability values for highly-voxelated images (Fig. 5A,B). Our of three points above, the second can be the most specific and based on our previous work. Therefore, we add the following text to add more clarification for point ii) at the end of first paragraph in Section III: "Both SC and irregular geometries have their own  $\sim 0.1\%$ -accurate reference permeability values  $k_{ref}$  obtained using extrapolation, see Tables I and II for the complete list of values. *These reference values can be obtained in different ways, for example pushing resolutions to prohibitive levels such as  $\sim 10^3$ – $10^4$  voxels/sphere diameter, replacing bounce back with higher-order boundary conditions and using moderate resolutions of  $\sim 10^2$ , or using any non-LBM numerical scheme which will provide resolution-free permeability values based on the solution of Stokes equation for the geometry of interest.*"

I also have a critical issue with the provided "magic number" concept. It is assumed, without any theoretical discussions and purely based on limited "results", that there is a magical point in which various errors cancel out each other and a significantly improved prediction becomes "always" possible. This needs a detailed mathematical/physical investigation to see whether such a "magical phenomenon" is possible and what limitations and restraints should be considered.

Here are several points.

1. "Magic number" parameter is a feature of the lattice Boltzman method, and it was introduced by D. d'Humières, I. Ginzburg and co-authors; the terminology itself is not ours. This parameter is derived from the rigorous theoretical analysis of the lattice Boltzmann numerical scheme: <https://doi.org/10.1016/j.camwa.2009.02.008> This parameter a) is free and b) controls the spatial discretization errors up to machine accuracy ( $\sim 10^{-15}$  for double precision), and in our work we only suggest how to choose it. Direct analogue of the magic number in classical schemes such as finite difference is the finite difference coefficients <https://w.wiki/BTKT> and their variation will change the discretization error, flow velocity, and resulting permeability. We hope that these clarifications highlight the theoretical origin of the magic number or finite difference coefficients.
2. In our work, we just analyze the behavior of the discretization error in computer simulations. And we operate with simple (and robust) facts which are of theoretical origin too. Our main points are: error changes with resolution, error originates from the method's error contribution away from boundaries with the convergence rate of  $-2$  and from the boundary condition with the convergence rate of  $-1$ . These points are theoretically

demonstrated, for example, in 10.1103/PhysRevE.67.066703 for 2D geometry and simplified LBM implementation. Further, we observe that for some resolutions and geometries the mentioned error contributions can self-cancel, and simply exploit this fact.

3. We do not state that the presented approach will work always and in any porous geometry. We simply provided the results for the packed beds of analytical, computer-generated, and laboratory origin. And found some... similarities there. This work can be seen as the demonstration of potential for the presented point of view on flow simulations in porous media, and can go way beyond flow simulations.

It is also difficult for me to accept that there is a magical way to improve the analysis of a low-resolution image, specifically for an irregular porous structure, simply because a low-resolution image means low-level of data about the structure.

If somebody showed to me the results from Fig. 5A-C (~1% permeability error for 4voxels/diameter resolution) a few years ago, I would reply exactly in the same manner as Referee1: this is not possible because there is insufficient information about pores at such low resolution. But this is the main point of the manuscript: on the level of each pore the information is lost, but at low resolutions the \_simulated\_ flow occurs through the superstructures which a) differ from the original pore-space geometry, and b) have significantly larger size compared to the original pores (i.e., looking at individual pore is not the right route to take). That is why not resolved geometry still can provide accurate average flow rate (or permeability) values, which is an integral quantity collecting information over many pores. This point is stated, for example, in 2<sup>nd</sup> paragraph in conclusion (“Currently, performing accurate simulations...”).

We hope that our clarifications will help in understanding our work and consider it suitable for publication.

Referee #2 (Comments to Both Author and Editor):

The paper presents a significant advancement in the understanding of flow through porous media using low-resolution images. But it still needs improvement for publication. Revisions should be made for these points :

1. at the introduction, a brief superstructure concept could be included to enhance reader comprehension.

We were considering this option while preparing the manuscript, but it appears that showing a single picture will require additional textual explanations, which then again will be repeated in the text later. Nevertheless, we added the following text at the end of the introduction: “apply fractional discretization and visualize superstructures, *which can be visible when regular sphere packings are mapped onto the discrete mesh at low resolutions*,...”

2. Also, magic number and null point should be clearly defined in the introduction to familiarize the terms

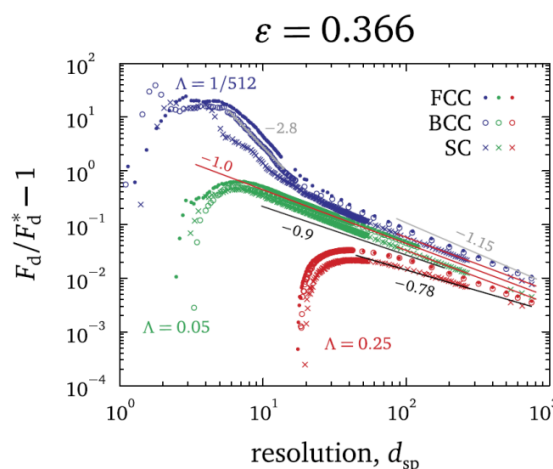
Thank you, valid point. We added the following text at the end of the introduction: “the free adjustable parameter of the *lattice Boltzmann* flow solver, *which controls the discretization errors* (“magic number”),” and “the existence of the “null point”, *where low-resolution flow field provides accurate permeability value due to self-cancellation of the discretization error contributions*,...”

3. In Figure 1, could you explain more about how to get the discretization, as I see it, the analytical and discrete are different.

We added the following text to the caption of Fig. 1 to provide more details and simplify reader’s understanding: “For SC geometry,  $L/U=5/1 = 5$  in the left column while  $L/U=11/5$  and  $L/U=16/3$  in the middle and right columns, resulting in the simulation domain sizes of  $5^3$ ,  $11^3$ , and  $16^3$ , respectively.”

4. In Figure 2, did you also simulate the irregular packing? How about FCC and BCC?

Yes, permeability of irregular packing was obtained from pore-scale simulations (as well as for all geometries in this study), and to clarify this point further, we add the following text to the Fig. 2 caption: “...The reference permeability values (i.e., the gray dashed line) are different for SC and irregular packings, and are provided in Tables I and II...” We did not provide FCC and BCC in Fig. 2 to avoid overloading it with information (which we are prone to quite often). But BCC/FCC similarity can be seen in Fig. 4 or in our previous studies, for example in Fig. 4 from <https://doi.org/10.1063/1.5042229> :

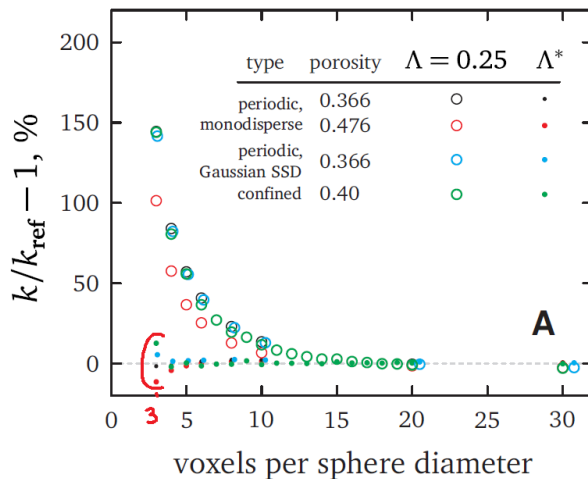


5. In Figure 3, why include U=4 and U=5? please explain why not include U=1 in this figure.

This just happened over the course of revisions of this manuscript. Original version contained U = 2 and U = 4, and one of referee’s concern was that we may be trying to hide something while not showing U = 3 :) We therefore extended Fig. 3 to two figures to cover U = 2,3,4,5, and placed one into the appendix to keep the panels large enough for comfort studying our work. The main goal of showing different U’s is to demonstrate the diversity the superstructures can take for regular geometries at similar discretization resolution of ~5 voxels per sphere diameter. It gives an idea that simple geometrical analysis of superstructures highly unlikely will provide meaningful insights. We did not show U = 1 because of the following key point: for U = 1, the size of the flow field skeleton (highlighting the superstructure) cannot exceed one unit cell by definition. I.e., here we have just a flow field structure within underlying geometrical structure, and there is not enough space to construct any superstructure. We added the following text in Fig. 3 caption to clarify this point: “We do not show  $U=1$  geometries because the flow field dimensions are limited to a single unit cell.”

6. what are the minimum voxels per sphere diameter you suggest based on your result?

As can be seen from the panel 5A, at the resolution of 3 voxels/diameter there is some deviation between different geometries, while 4 seems to be suitable:



This moment is subject to additional investigation, we will try to improve it in our following studies if any.