Communication with Referee1, 1st round:

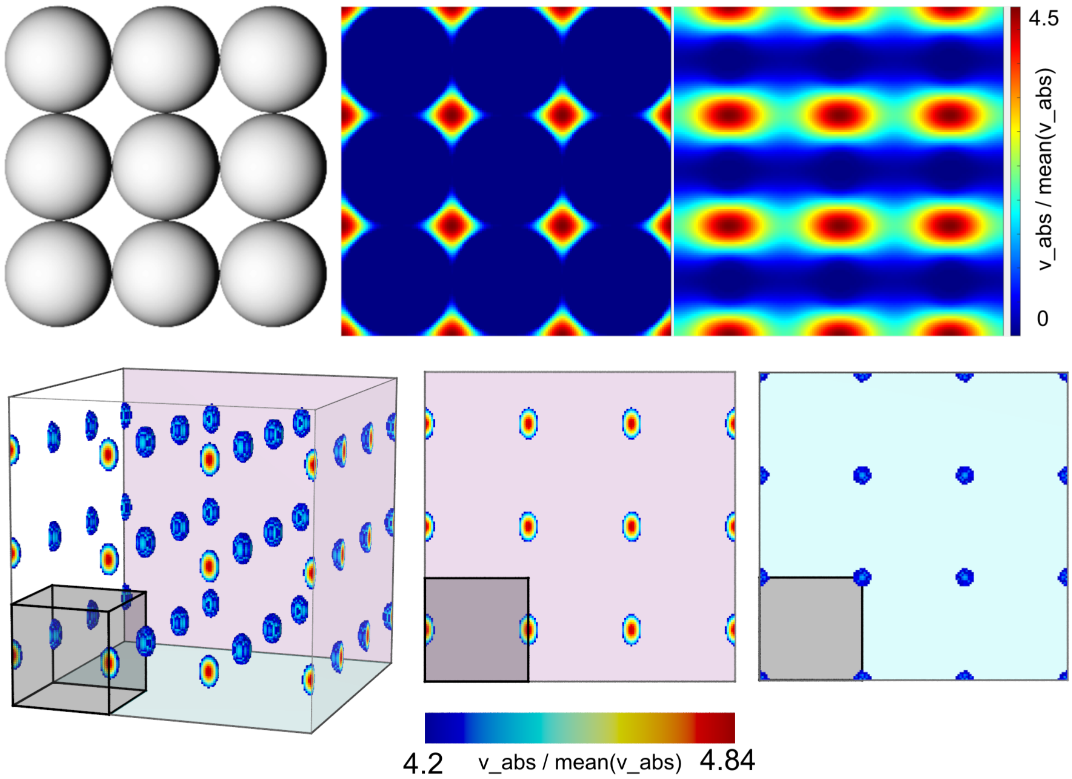
We appreciate the evaluation of our work by Referee1. With the arguments below we try to convince Referee1 that our study actually provides new insights and is worth publication in JFM. Motivated by the discussion below, we added Appendix Figures A2 and A3.

This paper demonstrates how to achieve high accuracy computation of the hydrodynamic permeability of sphere packings using lattice-Boltzmann simulations by suitable choice of a model parameter Lambda (termed a magic number). It is demonstrated that an optimal choice of this parameter (at least for creeping flow) varies approximately linearly with the microstructural geometry via a parameter Chi. The paper therefore demonstrates, by empirical means, optimization of lattice-Boltzmann simulations for low-Reynolds flows, e.g., via the linear regression in figure 4.

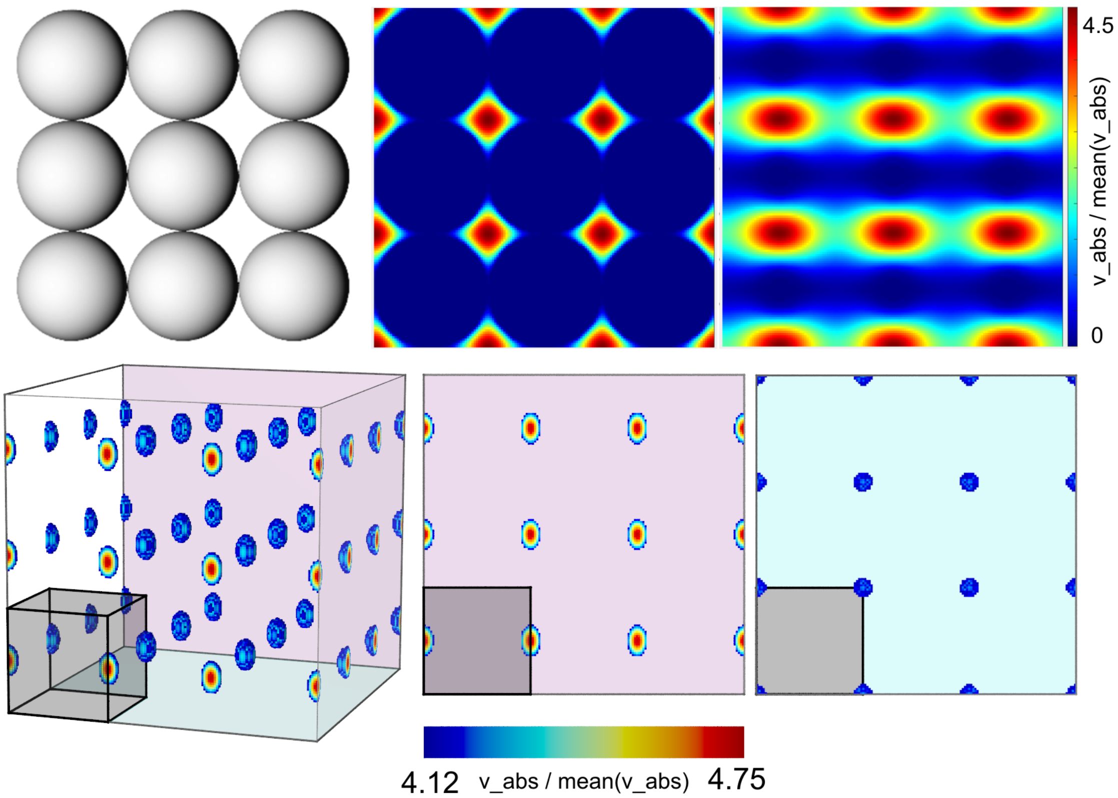
We would like to highlight that the main point of our paper is the existence of discrete superstructures in low-resolution images (Figures 1 and 3). Also, we introduce the concept of the null point, P0, where inaccurate, low-resolution flow field provides accurate permeability thanks to superstructures. We demonstrate that the discrete superstructures are an inherent property of the low-resolution flow fields obtained from a numerical PDE solution. The superstructures visible in regular geometries, and do exist in irregular geometries (although they are not visible). Parameter $\chi$ is the next step, which could also do not exist at all (i.e., curves in Figure 4b should not necessarily coincide). But the demonstrated similarity for $\chi$ in Figure 4b does not cancel the existence of the superstructures, which we report for the first time to our knowledge.

Some very broad claims are made, but it was not clear to me how this work (in a very specific context) is to be translated to other computational methods and applications, such as finite elements or finite volume.

1) In regard of the finite difference (FD) method. Let us perform flow simulations in a simple cubic (SC) geometry of touching spheres replicated 3 times in all Cartesian directions (i.e., U = 3). Initially, we use the high resolution of 50 voxels per sphere diameter and employ the finite difference scheme using this FDMSS solver, doi: 10.1016/j.cageo.2018.01.005. The lattice dimensions are $151^3$ voxels. Below we show analytical geometry, slices of the full flow field of absolute velocities (top row), top 1% of voxels with the largest absolute velocities (bottom row). In the left panel of bottom row the flow direction is vertical.

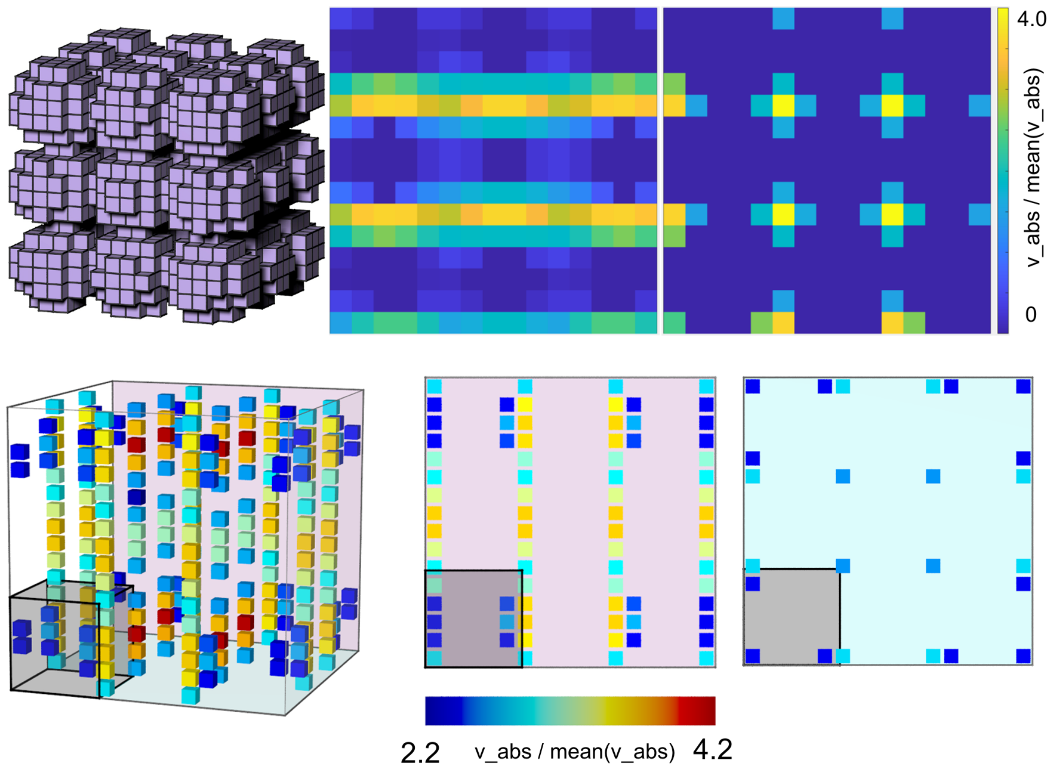



Now, the same geometry (SC with U = 3, $151^3$ voxels) but with the lattice Boltzmann method:

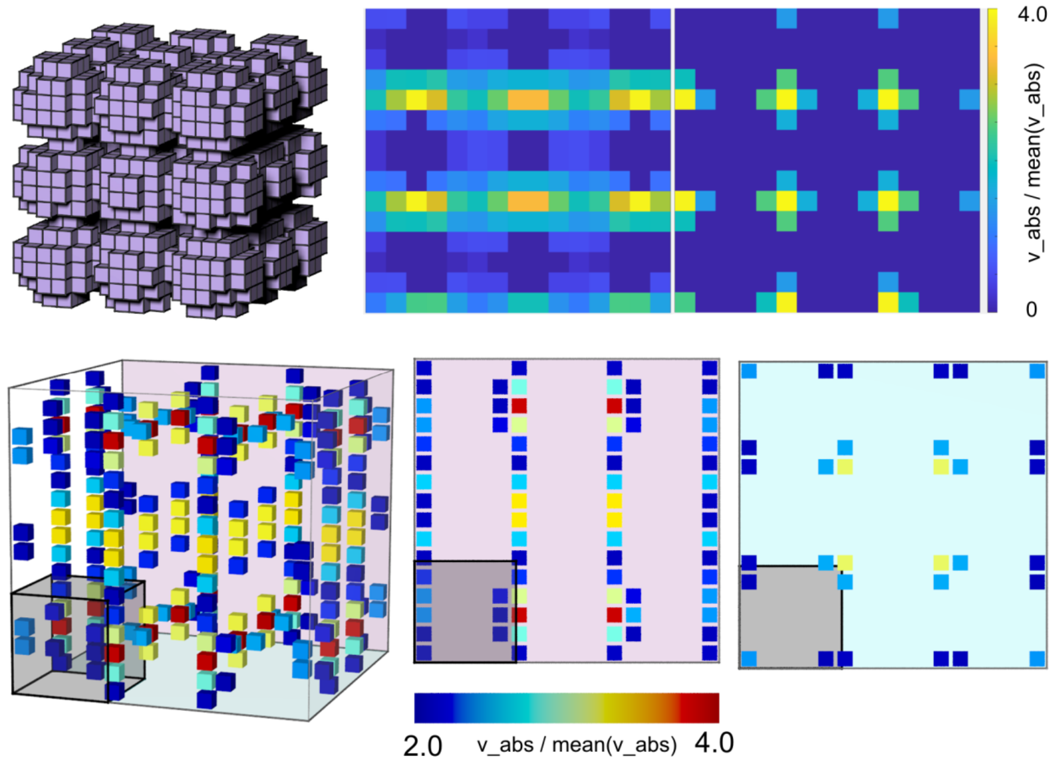



In the two figures above, the flow field is almost identical. Flow is faster in larger openings. I.e., nothing is unexpected or new here, and the finite difference toghether with the lattice Boltzmann show identical results.

Now, let us repeat the same simulation (SC geometry with U = 3) but at low resolution, and the lattice dimensions not evenly divisible by 3 such as $16^3$ voxels. Here, the resolution is about 5.3 voxels per sphere diameter. First is the finite difference method:




And the lattice Boltzmann method for the $16^3$ lattice:




Note that the superstructures differ *locally* for FD and LBM simulations because FD has 6-voxel connectivity while LBM has 18-voxel connectivity.

Bottom rows of two figures above show flow patterns that are not a simple replication of the unit cell marked in gray: the patterns significantly exceed the unit cell. These patterns we call "superstructures" and they make the *qualitative* difference between the $16^3$ and $151^3$ boxes. The superstructures originate from geometry, not from the difference scheme (either FD or LBM). Therefore, FD and LBM methods produce similar qualitative results.

Finite difference method relies on the finite difference coefficients (w.wiki/_raia), which originate from the Taylor expansion up to desired order. These coefficients are analogous to the LBM parameter Λ, and definitely they can be varied to change the discretization error (and the convergence rate, of course). How exactly? This is the topic to be addressed separately. In the FDMSS solver (doi: 10.1016/j.cageo.2018.01.005) they appear while discretizing 2$^{nd}$ derivatives up to the 2$^{nd}$ and 4$^{th}$ order (table below is a snapshot from w.wiki/_raia):

Laplace operator:

$$\Delta v_x = \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \quad \text{(B.12)}$$

The velocity derivative along the x axis will be similar for all voxels independent of the local calculation geometry:
$\frac{\partial^2 v_x}{\partial x^2} \approx \frac{v_x(x_0-\delta x)-2v_x(x_0)+v_x(x_0+\delta x)}{2(\delta x)^2}$ for a 2nd order accuracy and
$\frac{\partial^2 v_x}{\partial x^2} \approx \frac{-v_x(x_0-2\delta x)+16v_x(x_0-\delta x)-30v_x(x_0)+16v_x(x_0+\delta x)-v_x(x_0+2\delta x)}{12(\delta x)^2}$
for a 4th order accuracy. Derivatives along directions

| Derivative | Accuracy | −3 | −2 | −1 | 0 | 1 | 2 | 3 |
|---|---|---|---|---|---|---|---|---|
| 2 | 2 | | | 1 | −2 | 1 | | |
| | 4 | | −1/12 | 4/3 | −5/2 | 4/3 | −1/12 | |
| | 6 | 1/90 | −3/20 | 3/2 | −49/18 | 3/2 | −3/20 | 1/90 |

2) In regard of other methods and applications.

a. Finding accurate permeability of porous media for low-resolution geometries means that *integral* information (permeability) about the geometry features (i.e., complex pore space) was recovered from the unresolved geometry.
Now, let us switch from a complex geometry such as porous media to a simpler one (say, open pipe flow), and increase Reynolds number. Here we may start analyzing moving flow features (say, flow vortices) mapped onto a coarse discrete regular mesh. The discrete superstructures still will be there if the discretization resolution is low relative to the feature (vortex) size. And they may help extracting integral measures describing the flow. How exactly? This is the separate topic to be addressed.

b. Discrete superstructures originate from the features of analytical object and its mapping onto a uniform discrete mesh. In this definition, there is no dimensionality, i.e., if we perform the analysis similar to Figure 1 but in one-dimensional space, we again will end up with some large-scale patterns exceeding one unit cell. When this one-dimensional space is time, the proposed approach can be extended in this direction.

c. Let us describe our work in the following way: "*We simulated flow in voxelized geometry using the lattice Boltzmann method and obtained accurate simulation results for permeability, which is the quantity of practical interest*." Alternative and more abstract formulation of our work: "*We found the solutions of PDE (Stokes) using 2$^{nd}$ order difference scheme (such as the lattice Boltzmann method, doi: 10.1002/num.1018 ) with 1$^{st}$ order boundary condition, and obtained accurate solutions for experimentally accessible integral quantity.*" According to the second formulation, it is highly unlikely that our findings will be limited only to flow. The findings originate from the combination of PDEs, uniform mesh, difference scheme with its convergence rate, and an integral quantity. These are very broad terms covering many application areas. The actual applicability and limitations of the approach presented in our work is a separate topic to be addressed.

d. Finite volume (FV), finite elements (FE), and difference methods originate from the same principle: discretization of continuous PDEs. The difference between these approaches is in their subsequent formulations. We do not have sufficient expertise to discuss FV or FE methods in greater detail, but it is highly likely they have the adjustable coefficients similar to FD, *probably* entering FV scheme while choosing the reconstruction approach. For example, see the discussion about controlling the order or convergence of FV:
https://scicomp.stackexchange.com/questions/40234/what-determines-the-order-of-a-finite-volume-scheme

And here we need to mention the key aspect of our work: the uniform mesh. This mesh is a must for discrete superstructures to appear. If the mesh follows the features of geometry (i.e., pores) or features of the flow field, discrete superstructures will disappear — at least according to our current understanding.

While the approach appears to furnish the hydrodynamic permeability, albeit at zero Reynolds number, with economy, other important features of the flows, such as the velocity fluctuations (variance and correlation), appear to be greatly obscured. The authors did not address any of these.

The superstructures may differ significantly even for similar discretization resolutions (Figure 1). Studying their geometrical and flow properties, including variance and correlation, is a further development from this study.

Overall, I feel the broad conclusions drawn are overreaching, with too few new physical insights of fluid mechanics.

In addition to our explanations above about FD method and possible extensions, we would like to highlight the point that we use similarity in the error in permeability (Figure 2) to demonstrate the existence of superstructures in random geometries (including experimental samples). I.e., here we use fluid dynamics to demonstrate new geometrical property (existence of superstructures). We are not aware about any other geometrical analysis capable of doing this task. In this regard, we provide new view on fluid dynamics simulations.

Communication with Referee1, 2nd round:

Reply to Referee1:

I have carefully considered the authors’ response to my review. In their rebuttal, they highlight the paper as about the ``existence of discrete superstructures in low-resolution images’’, so I am still struggling to see concrete insights into the physics of fluid flow.

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The authors imply very broad consequences, but these remain speculative, the authors repeatedly claiming that such topics will be addressed elsewhere, e.g.,

> ``And they may help extracting integral measures describing the flow. How exactly? This is the separate topic to be addressed.’’;
>
> ``The actual applicability and limitations of the approach presented in our work is a separate topic to be addressed.’’;
>
> ``How exactly? This is the topic to be addressed separately.’’;
>
> ``Studying their geometrical and flow properties, including variance and correlation, is a further development from this study.''

These sentences refer to the *possible*, *long-term* extensions of our study, and they were motivated by the original questions by Referee1. Please do not mix them with concrete results already presented in our work (superstructures, P0 concept, selection of free «magic» parameter, the match with experimental data in Fig. 5). Moreover, we added the example using different scheme (finite difference method) to support our claim on possible extensions, which was not directly related to our work. In the next Referee1 reply, this information (i.e., how presented knowledge can be translated to, for example, finite difference scheme) is ignored.

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It is my opinion that the work may be much better appreciated in the literature on odes and image analysis.

From the JFM main page, the scope of the journal:

Access: Subscribed, Past subscription, Archive Contains open access

**ISSN:** 0022-1120 (Print), 1469-7645 (Online)
**Editor:** Professor C. P. Caulfield *Dept of Applied Mathematics and Theoretical Physics | Centre for Mathematical Science | Wilberforce Road | Cambridge CB3 0WA | UK*
Editorial board

*Journal of Fluid Mechanics* is the leading international journal in the field and is essential reading for all those concerned with developments in fluid mechanics. It publishes authoritative articles covering theoretical, computational and experimental investigations of all aspects of the mechanics of fluids. Each issue contains papers on the fundamental aspects of fluid mechanics and its applications to other fields such as aeronautics, astrophysics, biology, chemical and mechanical engineering, hydraulics, materials, meteorology, oceanography, geology, acoustics and combustion.

Our study explains the methodology of obtaining the all-important integral macroscopic permeability of complex porous media. We demonstrate that the computed flow field and the resulting physical quantity of permeability are inherently coupled with discrete superstructures.

Discrete superstructures we report can be seen as an artifact of imaging or meshing procedures (of geometry ***and*** flow field). The imaging or meshing procedures are identical in a nutshell, as we explain in the introduction. Meshing is an inherent, unavoidable property of most computational approaches which approximate the physics of fluid flow. We need to remember, however, that the approximate physics is contaminated by the model artifacts, and if we need this "physics" (whatever it means), we *have to* deal with numerical artifacts.

For example, the classical JFM studies we cite (Fig. 1 in Hill, Koch, Ladd, 2001; Figs. 2-4 in Hoef, Beetstra, Kuipers, 2005) address the finite-size effects or perform resolution studies. Obviously, meshing can introduce errors in the simulated physical quantities with the magnitude exceeding the quantity itself. In our study, we use fluid mechanics and visualize this fundamental problem (and feature at the same time) of meshing: it can transform the original geometry into the discrete superstructures. When this happens, any physics simulated using such meshes needs to be considered from a different perspective, which we provide. In such coarse simulations, fluid no longer "flows" trough the unresolved pores, but through the much larger-scale superstructures. The question then is how to make sure that this approximate flow field still renders a correct value of the physical quantity of interest, here permeability. Our paper answers this question in detail.

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(citation repeated) It is my opinion that the work may be much better appreciated in the literature on odes and image analysis.

(We believe that "odes" stands for ODEs, ordinary differential equations, but we deal with the Stokes partial differential equation(s), PDEs). We do not develop a computational method or boundary condition(s) to solve PDEs. We use the existing, established, popular computational method and demonstrate i) its fundamental limitations, and ii) how one can use this method to recover the physics of flow at accuracy levels previously considered to be impossible, see Fig. 5A,B. More accurate simulations result in better understanding of flow physics. We have provided an insight into computational meshes from the point of an image analysis to put our study into a broader multi-disciplinary perspective.

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As it stands, I believe the study is too speculative, providing inadequate physical insights on fluid mechanics.

We kindly ask to be more specific, i.e. what *exactly* is too speculative in our work?

The irony behind our study is that the simulated flow physics becomes "inadequate" in terms of the current understanding after the original geometry conducting flow is transformed into the superstructures with the resolution decrease. This transformation is i) unavoidable, and ii) is smooth (there is no abrupt change in permeability error vs. resolution curve) meaning that it starts to poison the flow physics gradually with the resolution decrease.

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Motivated by the discussion above, we added the following text to highlight the connection of our results with the physics of flow:

Introduction, 2nd paragraph, we added: "As a result, this discretization error contaminates the physics of flow simulations."

Introduction, last paragraph (added is underlined text): Here, we analyze and aim to minimize the discretization error in simulations of flow through a porous sample, <u>providing the new physical insights into flow simulations.</u>

Conclusion, 2nd paragraph (added is underlined text): However, we show that flow simulations on these highly-voxelated images can accurately reproduce the experimental permeability <u>(i.e., the flow physics)</u> because of the existence of superstructures, which retain information about the pore space over scales significantly exceeding a single pore dimension or representative volume of a porous sample. <- In our view this insight alone is worthy of propagating through the scientific community interested in improving models of fluid flow in complex, insufficiently-resolved geometries.

Communication with Referee1, 3rd round, reject, and the red text below therefore was not seen by Referee1 during submission process.

Reviewer(s)' Comments to Author:

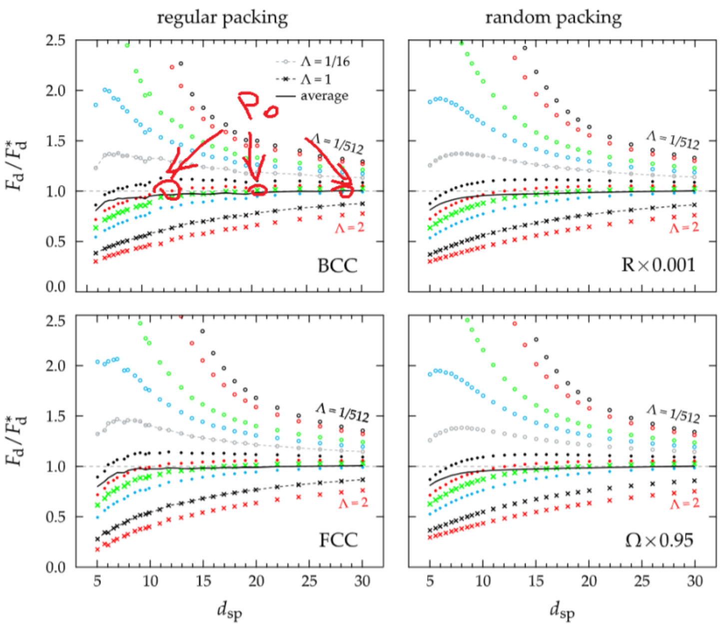
Referee: 1

Comments to the Author

I have examined the revised manuscript at some length.

Whereas the authors claim to have discovered `discrete superstructures', these are already evident in figure 5 of Khirevich et al. (Journal of Computational Physics 281 (2015) 708–742). The authors also claim novelty of a `null point', but these are also evident in figure 15 of Khirevich et al. (2015) on low-resolution discretization (vanishing for high resolution discretization).

This statement is not true. Below is the figure 15, but where is null point highlighted, indicated, or discussed? This is *exactly* what we say in the current manuscript ("…P0 is present but not discussed in other studies…")



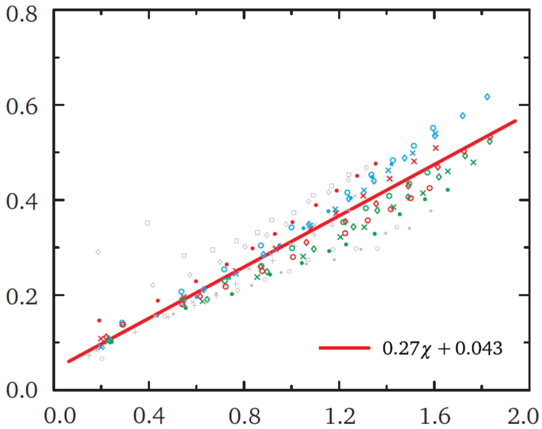

Khirevich et al. (2015):``Our analysis suggests that there always exists at least one Λ value which provides the exact solution, but its value depends on the discretization resolution, except for the straight and diagonal channels.''

Please do not mix things up. Null point, P0, is the situation when the error contributions self-cancel, and it is not limited to Λ/LBM. And yes, P0 depends on Λ. And the impact of Λ on the error *contributions* for permeability of complex geometry (i.e., porous media) was demonstrated in Khirevich 2018 phys fluids (i.e., 3 years after j comp phys 2015 paper).

Moreover, ``A special attention was given to the discretization procedure resulting in dramatic reduction of the scatter of the drag force (or permeability) simulated in the regular packings at low grid resolutions (Fig. 6). The low drag force scatter allowed us to examine its dependency on Λ and to demonstrate the similarity between the drag force coefficients of random and regular packings obtained on the coarse grids.''

Thus, much of what is presented in the JFM submission seems to be present in the earlier work by Khirevich et al. (2015). The present work references permeability, which is equivalent to the drag force in Khirevich et al. (2015), and the ``Λ value which provides the exact solution'' from Khirevich et al. (2015) is surely an identification of the ``null point'' in the language of the present work.

Yes, in 2015 paper figure 5b shows that “strange” discretization artifact and fig 6 shows similarity in errors. And these two figures are 10 years old already. Has Referee1 taken any effort to find at least one case of using this knowledge? Without the context presented in the rejected (thank to Referee1) paper, these are just fun figures. It is the same as showing the figure below without axes and legend (i.e., without the context), what is the practical value of it then?




There are still some aspects of the results presented in the present work that are not adequately transparent. Whereas figure 2 demonstrates a notable effect of U (domain size) on the permeability, similarly to figure 6 of Khirevich et al. (2015), the values of U for the results in figure 4 are not reported, so it is not clear how the ``discrete superstructures'' identified in figures 1 and 2 manifest in figure 4. It seems that the ordered arrays in figure 4 might have large values of U, but this is not stated. If U is small, then there should be effects of small U.

First of all, why do not ask this in the revision request instead of rejection? Answering the question, U = 3 there, or can be 4, 5,… — does not matter. The only important thing is that it is not U = 1, which would be just way scattered because a superstructure has no space to exist.

From Khirevich et al. (2015), it would seem that fluctuations in the permeability may be interpreted in terms of spurious fluctuations in the apparent porosity. Whereas such fluctuations were highlighted in Khirevich et al. (2015), the present work does not explicitly address the discrete porosity fluctuations, which are presumably damped with increasing U (for ordered arrays at low resolution, since this averages over more positions of the spheres on the discrete lattice), again not explicitly addressed in the present work. So, it's not clear what is new, neither is it surprising that small changes in analytical porosity for periodic structures at low resolution will manifest in abrupt changes in permeability.

This is a valid point but, again, why do not ask this in the revision request instead of rejection? And there is a sentence for this in 2025 manuscript: “…For regular geometries and low discretization resolutions, we maintain the discrete porosity of each geometry close to its analytical value with minor adjustments of the sphere radii during discretization, if there is a noticeable difference between analytical and discrete porosities…” And this point was not even discussed further because it is trivial and impact of the porosity was eliminated at the very beginning of this study.

As I tried to articulate in the previous review, I find the broader claims to be too speculative. The authors have focussed on the magic number for a specific lattice-Boltzmann algorithm, essentially furnishing an interpretation of their previous studies on how the magic number affects drag or permeability for Stokes flows in densely packed ordered and random arrays of spheres.

"…essentially furnishing an interpretation…" – very nice )

Whereas the authors have included in the appendix results for finite-difference computations, this appears to identify geometrical artifacts due to the discretization of ordered arrays, not how to prescribe the finite-difference analogue of the lattice-Boltzmann magic number, which would have supported some of the broader claims.

$$\frac{\partial^2 v_x}{\partial x^2} \approx \frac{1 v_x(x_0 - \delta x) - 2 v_x(x_0) + 1 v_x(x_0 + \delta x)}{2(\delta x)^2}$$

Change in difference coefficients (say, 1.1 instead of 1 and −1.9 instead of −2) -> change in the converged velocity vectors -> change in the average velocity or permeability. L – logic? And if one would like to know exact values of these FD coefficients, we will need to perform detailed analysis similar to the rejected paper. But it is a separate study easily worth one or more paper(s).

In terms of the practical results presented in figure 5, I feel the authors have glossed over how the discretization imparts fluctuations in the apparent void fraction. To this, I feel the more detailed results available in Khirevich et al. are just as insightful, but still ambiguous as to the values of U.

Apparent void fraction (or discrete porosity) is 0.1%-or-better accurate in random geometries (i.e., used in Fig. 5) relative to the prescribed analytical value. It is straightforward to obtain very accurate discrete porosity for random geometries, and such a question can raise only the person with very little experience in that area.

Another factor that has not been addressed among the claims of computational efficiency, is the number of lattice-Boltzmann time steps for the relaxation to steady state (although it is implicitly addressed by the O(resolution^5) inference). Presumably this is affected by Chi and thus Lambda, but I could not identify the actual values of these parameters for results presented in figure 5, neither could I identify the discrete porosities (assuming the the porosity is the analytical porosity).

And again, we are ready to discuss it, but why not to ask this in the manuscript review? The number of LBM iterations is secondary in this manuscript (all presented results are converged, i.e. the number of iterations is "sufficient"). And convergence is almost exclusively determined by resolution: 3 powers come from the number of lattice nodes and 2 powers come from the number of iterations to reach steady state. Λ little/almost no impact on convergence time (as well as \chi, which defines Λ), viscosity only matters.

The topic of Stokes-flow permeability via lattice-Boltzmann algorithms has been addressed in considerable detail in other literatures, including 9 references to the author's works on this problem (some of which are data). I still feel the present work is more appropriate to readerships focussed on the computational methods and discretization.

And now person with very little background in Stokes flows in complex geometries (which can be seen from terminology used and questions asked) judge this study in all seriousness. And the editor supports it. Good job, what can I say.

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Here, either Referee1 does not understand what he/she is doing, or understands and does it intentionally in terms of connecting 2015 paper to the rejected study. Lack of experience in that particular area does not stop Referee1 from judging and, intentionally or unintentionally, manipulating with the context (of 2015 paper) in order to support the initial assumption “to reject, no matter what”.  Here, I see the problem that the person with such approach in principle cannot find anything new (if doing science nowadays still implies that) because “new” means something different from the existing knowledge and initial assumptions, and discovering new means *changing the initial assumption* based on observations, which is exactly the opposite to Referee1’s approach.

Handling editor could (and actually was asked to) step in here, but it seems that there is no sufficient author names/institutions weight to do that. And the situation is double funny because several years ago during another JFM submission, different handling editor actually stepped in but in the opposite direction: after few months of review, two-out-of-two referees independently accepted the manuscript submission, but the handling editor “after consulting with some friends” rejected it afterwards claiming that there is nothing new. And of course, own JFM articles of this editor contain exclusively new… content because the opposite cannot happen by design :D