Solid Earth Discuss.,
https://doi.org/10.5194/se-2019-84-AC1, 2019

Interactive comment on “Pore-scale permeability prediction for Newtonian and non-Newtonian fluids” *by* Philipp Eichheimer et al.

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Received and published: 21 August 2019

We thank Kirill Gerke for his review. His useful comments helped us to improve our manuscript.

Please find below a point by point response to the comments (comments of the reviewer in black and our response in blue) and the revised version in the supplement.

Sincerely, on behalf of the authors Philipp Eichheimer

1. I guess as the code is the part of the LaMEM now, it should be open source, isn't it? If so, please, provide a link to the repository somewhere at the relevant part of the paper.

   A link to the open-source repository as well as the revision number, which has been used to reproduce the results of this work, has been added. (Page 18, line 4)

2. Within your abstract and introduction you mention that non-Newtonian code is necessary for nano-fluids and some related problems. I would suggest a couple of sentences to explain this a bit, because technically you provide a solution for micro-scale. I would also guess that magma flow is a potential object of simulations with your code.

   We rewrote the section in the introduction to provide more information on nanofluids and magma flow. (Page 2, line 20-27)

3. Equation 5 is a technically valid for any flow direction, not sure why do you talk about z-direction here. I would suggest re-writing it for the general case, especially considering that later on in Eq.6 you do you generalized form to compute permeability.

   This is correct, but the version of LaMEM, used in this study, only computes a volume average z-velocity. This velocity is then used to compute permeability in z-direction using eq.(6). We therefore decided to leave eq.(5) and (6) as is.

4. Something went wrong with Eq.12-13 (probably while converting to pdf?). Please, fix these.

   We changed the equations to make sure they are displayed properly. (Page 8, line 1-4)

5. Could not completely catch the meaning of all elements on Fig.3. You have black

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lines with attached numbers of 3 and 0.25 (the latter is partially covered by the tube flow figure inset). Please, consider fixing this.

The black lines show local slopes of the curve. In order to clarify this issue we added this information into the figure captions and moved the inset of figure 3.

6. I found a disagreement between Eq.18 and Fig.4 - in the text you assign R3=4, R4=8, while the pipe #3 is larger on the figure, plus you report that #3 contributed more to the flow. Seems like you interchanged #3 and #4 at some point.

   Sorry for this mistake, we changed the the values on page 9 line 17 to fit the inset in figure 4.

7. Fig.5 - you have quite slow (blue) flow lines at the same positions as higher (yellow- red) flow lines at the same locations along the flow direction. I find this to be somewhat strange, considering that the flow should be symmetrical around the spheres under periodic boundary conditions (you should use them, otherwise you can't compare against analytical solutions for drag forces).

   We changed the figure as the rendered streamlines were not representative and thus the figure was perhaps confusing. Figure 5 now shows computed streamlines of the velocity around the spheres. This should make it easy to understand and highlight the flow structure.

   Concerning the boundary conditions we use free-slip at the side boundaries of the domain and no-slip at the internal solid-fluid interface. In the case of simple cubic systems the velocities at the boundary are symmetric and therefore the effect of boundaries on the result should be negligible. We added an additional sentence in Methods section to clarify the employed boundary conditions. (Page 5, line 15-16)

8. Not 100 % sure here, but i do not think that Eq.19 was derived by Bear, as analytical solutions for spheres (not only SC, but BCC and FC packings) comes

from preceding papers, e.g.: Sangani, A.S., Acrivos, A., 1982. Slow flow through a periodic array of spheres. Int. J. Multiph. Flow 8, 343–360. doi:10.1016/0301-9322(82)90047-7.

We added the reference of Sangani and Acrivos (1982) as they describe the flow through a periodic array of spheres for simple cubic packing. However, the exact expression used in our manuscript is not explicitly stated in Sangani & Acrivos, but rather in Bear (1988), which is why we kept both references.

9. Fig.8 and the text related to this figure. First, how did you produce those different resolution figures? From the results i would guess you simply "magnified" each voxel 2 times to consist of 4 voxel for each magnification step. Please, describe your methodology. Because i would expect somewhat different behavoir if you would scale your samples while conserving its spatial statistics: Karsanina, M. V., & Gerke, K. M. (2018). Hierarchical Optimization: Fast and Robust Multi-scale Stochastic Reconstructions with Rescaled Correlation Functions. Physical Review Letters, 121(26), 265501. Now, you mention that LBM also converges from above and cite some papers with such behaviour. I guess these papers used single-relaxation LBM. Technically, LBM can converge from below, above, and from below and above at the same time. To improve this section of the text i recommend reading and citing the following papers: Khirevich, S., Ginzburg, I., & Tallarek, U. (2015). Coarse-and fine-grid numerical behavior of MRT/TRT lattice-Boltzmann schemes in regular and random sphere packings. Journal of Computational Physics, 281, 708-742. Khirevich, S., & Patzek, T. W. (2018). Behavior of numerical error in pore-scale lattice Boltzmann simulations with simple bounce-back rule: Analysis and highly accurate extrapolation. Physics of Fluids, 30(9), 093604. Zakirov, T., & Galeev, A. (2019). Absolute permeability calculations in micro- computed tomography models of sandstones by Navier-Stokes and lattice Boltzmann equations. International Journal of Heat and Mass Transfer, 129, 415-426.

Thank you for your suggestions. We added a description on how we increased the numerical resolution on page 14 line 13-15. We do not apply any interpolation or stochastic reconstructions to conserve spacial statistics as suggested in the mentioned paper in your comment, but rather used a "magnification" where voxels are subdivided into a certain amount of subvoxels without modifying their phase.

Concerning the convergence from above and below, we added the suggested references and discussed this issue in the corresponding section as well as in the discussion. For the given sample, it is not clear how the method used in Andrä et al. (2013) performs as they only provide results for a single resolution.

10. I would recommend to present a very brief comparison against existing FDM codes, for example FDMSS. I would expect that your code is more accurate, yet takes much longer time to converge and more computationally heavy in terms of CPU and RAM.

    It is hard to compare timings of our simulations to other FDM as we used different numerical settings depending on the size of the setup, meaning that the number of cores was varied between simulations with different resolutions (simulations were also partly run on a different cluster). The different computation times are therefore not really comparable. We added an example of the employed number of cores, RAM and timing for one specific simulation (Page 17, line 29-33). Your expectations were quite right, as LaMEM requires more computational resources and also takes more time to converge as e.g. FDMSS., yet LaMEM is therefore more general as it can compute non-Newtonian fluid rheologies.