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# Reviewer's report of doctoral thesis

**Candidate:** Dawid Strzelczyk

**Thesis:** Study of fluid transport phenomena using meshless Lattice Boltzmann Method

## Overview

The thesis explores advancements in computational fluid dynamics, focusing on the Meshless Lattice Boltzmann Method (MLBM) as an alternative to traditional Lattice Boltzmann Method (LBM). After introducing the significance of transport phenomena and numerical methods for solving the Boltzmann and Navier-Stokes equations, it outlines MLBM methodology and its potential to overcome limitations of LBM. Through convergence analysis and validation against benchmark problems, including porous medium flows, the thesis investigates the applicability of MLBM mainly in low-Reynolds flow regimes.

Four peer-reviewed articles, of which the candidate is first author on three and second author on one, constitute the main body of the thesis. As listed in the thesis, the main contributions of the work include: implementation and analysis of MLBM, applicability of MLBM to porous media flows, investigation of diffusive tortuosity in porous media and exploration of the use of convolutional neural networks (CNN), use of the Reynolds number enhancement procedure in MLBM, and investigation of the $\tau = 1$ approach for both LBM and MLBM. The value of the author's results lies in the complexity of the work, which combines state-of-the-art ideas and methods. Therefore, it is not surprising that all stated objectives of the thesis were fully achieved in all intermediate steps.

The thesis is well structured, easy to read, and I encountered only a minimum of errors and typos. By the way, in the very first paragraph of Chapter 2, it was unfortunately Mr. Boltzmann who suffered one of these few typos. From the overall graphic design of the figures, tables and equations, it is clear that the author has taken great care in the preparation of the thesis.

## Questions

During the defense, the candidate should answer the following questions during the discussion.

1. Section 3.1.10 quite briefly summarizes the use of LBM to train CNN for predicting diffusion in porous media and the work is published in [2], i.e., in one of the four papers (co-)authored by the candidate. Since this approach is just marginally described in Chapter 3 (among "Methods") and not in a separate, dedicated chapter, what was candidate's contribution to [2]?

2. What is the precision of the floating-point arithmetic used to produce Figure 4.6 (and other results in the thesis)? Can the convergence halt phenomenon discussed in Section 4.4 be related to floating-point precision?

3. It is not entirely clear to me how the methods LBM and MLBM used in the thesis were implemented (or maybe I overlooked it somewhere?). I understood from page 7, that the MLBM was implemented using the Medusa C++ library, however, there is no information about LBM. In the thesis, the candidate should have commented on / declared authorship of the code and

results as in Chapter 5 on page 67 in the case of MNS (ACM) results. Did the candidate implement both MLBM and LBM or did he use some in-house code or some available software? This is particularly important for the results presented in Chapters 4 and 6, where LBM results are used as references.

4. In Figure 6.5, the computational performance of MLBM vs. LBM is illustrated on a single-threaded CPU run. However, LBM is particularly efficient in parallel implementations (especially on GPUs) due to communication with neighboring lattice sites only. I like the analysis of computational complexity in Section 3.3.3 and the comment that "the interpolation during the streaming step introduces the overhead to the computational complexity of MLBM and MLBM1", which I believe can dramatically turn the tables in LBM's favor. Since parallel implementation of the methods was not one of the goals of the thesis, can the candidate at least comment on the aspects of implementing MLBM in parallel (on CPUs / GPUs)?

5. The major headaches with LBM always start with the boundary conditions, and I fear that MLBM will be no exception. In Chapter 6.2, the inflow and outflow boundary conditions used are not consistent with the Navier-Stokes equations because one cannot fix the same pressure on both ends of the domain. Although the results for the velocity in Figure 6.3 look reasonable, the pressure should be shown as well and the choice of these inflow and outflow equilibrium boundary conditions should be explained. Does the MLBM approach allows for similar boundary condition strategies as discused, for instance, in our recently published paper `https://doi.org/10.1016/j.camwa.2024.08.009` ?

6. The choice of the TRT relaxation times (frequencies) appears out of the blue. Why $\omega^+ = 1/0.53$ and $\omega^- = 0.500625$ are used in Section 6.2? Why Eq. (6.8) is used? A sensitivity analysis with respect to these two parameters should be given using benchmark problems from Chapter 4.

## Further Comments and Remarks

In the following list, I have summarized some additional comments and remarks that may be discussed during the defense (if time permits).

1. In general, the continuity equation given by Eq. (2.2) contains a source/sink term and its absence in Eq. (2.2) should be at least meantioned in the thesis. Obviously, no matter is produced or lost in the problems considered throughout the thesis, so this is just a minor comment, however, consideration of a non-zero source/sink term in Eq. (2.2) might have some non-trivial consequences for Section 2.3, where the continuity equation is recovered from BTE (2.33).

2. In Chapter 2, I lack physical units for the quantities defined therein, although I understand that these have little importance in the rest of the thesis. The use of physical units and dimensional analysis would reveal that $g_\alpha$ is actually the acceleration [m s$^{-2}$] and not the body force density [kg m$^{-2}$ s$^{-2}$].

3. Concerning Eq. (2.19), a more general approach to obtain a fully explicit scheme is to substitute $\hat{f} := f - \frac{\delta_t}{2} S$. This approach is useful because it directly allows other collision operators than BGK (SRT) in Chapter 3 (c.f. Section 3.1.8).

4. The benchmark problems selected in Chapter 4 are well selected, but they are only for 2D flows. It would be good to use at least one benchmark problem in 3D such as, for instance, the one we used in `https://doi.org/10.1016/j.camwa.2018.10.045`.

5. Choice $\omega^+ = \omega^- = 1$ in Section 5.2 means, that the collision operator is just SRT.

6. Below Eq. (5.12), the candidate states that "*Further refinement, however, was prohibited by the limited computational resources*", however, the computational resources used to obtain these results are not described in the thesis. The same remark holds for Figure 5.14.

Formal comments:

1. Some reordering of definitions should be done in the thesis:
   (a) The abbreviation "BTE" is used for the first time on page 21, but its definition is given on page 22.
   (b) Surprisingly, apart from the abstract, the same is true for "LBM", which is used in Chapters 1 and 2 but not defined until Chapter 3.
   (c) Definition of the BGK collision by Eq. (2.45) should be perhaps given earlier after Eq. (2.33) and not in the midst of Chapman-Enskog's sorcery.
2. Comments on equations:
   (a) In Eq. (3.2), $f^0$ lacks a factor of $\frac{1}{2}$ in the argument of the exponential. Moreover, the arguments of $f^0$ are not just $\mathbf{v}$ but also $\rho$, $T$, and $\boldsymbol{V}$.
   (b) There is a bracket missing in Eq. (3.5).
   (c) In Eq. (3.10), there should be $\omega(\boldsymbol{v}_k)$ in the denominator.
   (d) Page 38: is there an equation missing after "takes the following form"?
   (e) Should there be an absolute value in the denominator of Eq. (4.4)?
   (f) Reference for Eq. (5.11) is missing.

## Reviewer's Verdict

During his work, the candidate proved his ability to master difficult problems of interdisciplinary character. The submitted thesis is of high quality and represents major scientific contributions which is endorsed by a number of peer-reviewed papers. The dissertation fulfills all the requirements for a doctoral thesis, consists of original solutions to scientific problems, and demonstrates the candidate's general theoretical knowledge in the given field as well as the ability to conduct independent scientific work. Therefore, I recommend to the Doctoral Thesis Committee that the candidate be awarded the degree of Doctor of Philosophy and that the thesis deserves a distinction.

Praha, November 26, 2024

**Radek Fučík**