prof. dr hab. inż. Jacek Pozorski
Institute of Fluid Flow Machinery
Polish Academy of Sciences (IMP PAN)
Fiszera 14, 80-231 Gdańsk
Tel.: 58 5225145, e-mail: jp@imp.gda.pl

Gdańsk, November 19, 2023

Opinion on the doctoral dissertation

"Applications of the lattice-Boltzmann method to solving advection-diffusion-reaction problems coupled with Navier-Stokes equations"

by Grzegorz Gruszczyński, MSc, Eng.

PhD advisor: Prof. Jacek Szumbarski; auxiliary supervisor: Dr. Łukasz Łaniewski-Wołłk, Warsaw University of Technology, Poland;

1. Actuality of the subject

Following well-established approaches in computational fluid dynamics (CFD), such as finite volume or finite element methods, for some 20+ years now, there has been an increased interest in the lattice-Boltzmann method (LBM) and its applications to the problems of fluid thermomechanics. This is due, among others, to the computational efficiency of the approach and the availability of HPC technologies. The LBM is an approach whose idea stems from statistical physics; therefore, due to its specific nature and mesoscopic roots, a variety of issues still need to be tackled, in particular for more accurate LBM formulations that are certainly worth a detailed scrutiny, also in the context of multiphysics problems. Therefore, the subject area remains of actuality, in terms of its practical as well as fundamental interest, and a PhD study devoted to it is well justified.

The motivation of the Candidate (and his Advisors) to undertake the present PhD work has been to improve the LBM formulation for solution of a generic advection-diffusion-reaction (ADR) equation, coupled to the Navier-Stokes (N-S) system in the weakly-compressible approach. The PhD subject is timely and the research problem has been correctly stated. The topic of the dissertation is evidently difficult and challenging in many ways. It requires an in-depth understanding of fluid mechanics and numerical methods. From the formal standpoint, the thesis can be assigned to the discipline of mechanical engineering, even though the emphasis is on further development of computational models and less so on the exemplification of practical flow cases solved using these models.

2. Methodology applied

The present PhD dissertation is of theoretical and numerical character. The Navier-Stokes (NS) and the continuity equations are solved together with an additional equation for a scalar variable, corresponding to the transport of energy, chemical species (reactants) or phase indicator. The LB-based computational model is further developed, including for the collision kernel aspects, the improved treatment of the source terms, and the formulation of boundary conditions. Then, some multi-physics phenomena are analysed in a geometrically simple setup, rather than focusing on complex-geometry "real-life" flow cases, which is perfectly correct at this stage of development.

Notwithstanding the emphasis on more fundamental issues, the study is illustrated by the LBM solution of a generic advection-diffusion-reaction equation and some practically-relevant computations of heat transfer and segregated multiphase flow.

3. Brief description of the contents

The main thrust of the PhD thesis are two original research papers published in *Computers & Mathematics with Applications* (2020, 2023) and another one that appeared in *International Journal of Heat and Mass Transfer* (2022). The Candidate has been the first and leading author in all three papers; this is explicitly stated in the Declaration of Authorship section (page iii). As the PhD findings have been reported in three multi-authored papers, I rely on the Candidate's honest declarations about his own contribution. It needs to be recalled that both CAMWA and IJHMT are renowned research journals in the subject area of mathematical modelling and computations in fluid thermomechanics.

I will now briefly describe the contents of the PhD document. **Chapter 1** offers a general introduction to the problem under study. It is written both in English and in Polish and is fairly pleasant to read. The governing equations of fluid dynamics are recalled there together with the ADR-type equation in its variants suitable for the description of flows featuring heat transfer, for multiphase flows with interphasial surfaces (interfaces), and even for epidemic processes. The research hypotheses for the PhD thesis are then formulated. In **Chapter 2**, some fundamentals of LBM are recalled, followed by a more detailed presentation of the collision kernels (**Chapter 3**). A generic ADR equation is solved using LBM in **Chapter 4** (based on the CAMWA'23 paper). In **Chapter 5**, a set of ordinary differential equations (ODE) for a simplified description of epidemic dynamics are recalled; it is also argued that the ADR equations are suitable to tackle this problem in an improved way by including some spatial correlations as an extension of the ODE-based model. The energy equation in its several forms is recalled in **Chapter 6** that is followed by the presentation of possible ways to recover it from the LBM equations for population dynamics (**Chapter 7**). The formulation of boundary conditions in LBM is discussed in **Chapter 8**, in particular considering those of second-order accuracy. A problem of convective heat transfer is considered by solving the respective advection-diffusion (AD) equation translated to the LBM formalism together with the N-S equations (**Chapter 9**, based on the IJHMT'22 paper); this is preceded by the analysis of two benchmark problems (evolution of an initial scalar field in 2D and 3D) and a steady-state heat conduction. The LBM solution of the phase field method, formulated as another ADR-type equation, is addressed in **Chapters 10** and **11** (which is based on the recent publication CAMWA'23). Conclusions of the work (**Chapter 12**) are limited to a short list of original achievements, which is just too concise, and an indicative list of prospects for further study, which is appreciated.

As a whole, the dissertation of approximately 260 pages makes a demanding reading. The bibliography includes 270 entries which is quite exceptional for a PhD thesis. The cited literature covers the most important contributions to the subject, also some very recent ones.

4. Assessment of the original contributions

The doctoral dissertation reports on an ambitious and difficult research endeavour at the cross-roads of fluid dynamics and computational science, with a distinct flavour of applied mathematics. The subject of the thesis are applications of LBM. The overarching aim of the work has been to present some of these applications that involve the ADR-type equations.

In my opinion, the original contributions of the Candidate refer to:

1. A comprehensive study of the lattice Boltzmann approach for flow dynamics coupled to additional scalar variables, including in particular an implementation of the novel collision kernels formulated in terms of cumulants. Also, the LBM formulae for boundary conditions of 2nd order of accuracy were analysed and used, and a treatment of implicit source terms in the reaction-type equations to preserve 2nd order convergence of LBM was proposed, illustrated by the solution of benchmark problems;

2. A study of heat transfer problems that involve a disparity of length scales for the velocity and temperature fields (a high Prandtl number case). Here again, the cumulant formulation of the collision kernel was used (for both fields) and a steady forced convection problem was solved;

3. An application of LBM, with the so-called cascade kernel, for the phase field based modelling of multiphase flows, illustrated by a parametric 2D study of the Taylor bubble rise. It is worth noting that the CAMWA'20 paper, where these findings have been first published, has already been cited 24 times (as of October 2023).

4. As an addition, original but not situated directly in the mainstream of the thesis: an analysis of epidemic dynamics with proposals to account for spatial correlations, resulting in a model formulated in terms of the advection-diffusion-reaction equations, like in points 2-3 above.

4.1 Technical points, issues for discussion, remarks and questions

As a whole, the dissertation reports on extensive original findings. From the editorial viewpoint, the text is mostly written in good scientific English. My major reserve, however, is related to the very structure of the document. The PhD theses have traditionally been prepared as a standalone document reporting some original research results of the Candidate and the results are positioned with respect to the state-of-the-art preview. The present document was probably meant to have such a structure as well (but did not really succeed in this respect). Another variant, that in my opinion would better fit here, is the so-called "article thesis" based on published papers (here: the three mentioned already). It would consist of the Candidate's general guide (an extensive introduction, a description of the methodology, and the main results), followed by the original research papers and, possibly, Appendix section.

Quite a serious problem with the present structure, making the document not easy to follow, is that some well written and mature chapters (4, 9 and 11) are intertwined with others, sometimes very short, sketchy or written in a less clear way. In my view, a part of the material contained there could either have been integrated with other chapters, or shifted to appendix, or perhaps even not included in the PhD document which is already rich enough. Being more precise: Ch. 5 includes some very interesting (and timely) material on the modelling of epidemic processes. The SIR model is detailed there but the acronym is not immediately clear and the letter R that stands for Recovered (humans) is also ominously interpreted as Removed in the epidemic calculator in Fig. 5.1. Another minor problem is that some of the figures seem to have not been referred to in the text (Figs. 5.4 and 5.8) and some other (Figs. 5.9 and 5.10) are only very briefly commented. Although Ch. 5 is interesting and fresh, some one-paragraph subsections of it give an impression of draft notes waiting to be further expanded into a full-fledged research contribution. Ingenious ideas on how to encode some behavioral patterns, so to say, into a mathematical model in the form of the diffusion equation with a source term, Eq. 2.28, are very much appreciated. Also the correspondence with the *fil rouge* of the thesis, i.e. the applicability of the ADR-type partial differential equations to various processes or phenomena, is more than clear. However, the PhD dissertation is entitled "Applications of the LBM…" but the only mentions to LBM in Ch. 5 (pages 85 and 90) refer to possible future actions. As the bottom line: Chapter 5 seems to be an odd-man-out in the document and rather belongs elsewhere (**Question 1:** may I ask the Candidate to justify the contrary?). On the other hand, Ch. 3 provides some information on fairly difficult concepts, useful in the following, so it would perhaps be worth explaining them at more detail.

Concerning chapter 2: the Candidate's effort to introduce the LBM is appreciated, the more so that the proposed treatment of the implicit source term seems to be novel and important. However, for the sake of better clarity, another explanation effort would be welcome. For example, the appearance of the sampling space variable $\boldsymbol{\xi}$ along with $\mathbf{u}$ is not common. [BTW (unless I missed something): is variable $\mathbf{u}$ in Eq. 2.1 correct?]. Then: it would be good to name χ in Eq. 2.7; what is m below Eq. 2.15? the meaning of ψ used in p. 17 becomes more clear only in p. 35, etc. Also Figure 2.1(b) may be misleading as it is meant to refer to the mesoscopic scale in the spirit of Boltzmann equation but the LBM lattice is plotted there. The same remark pertains to the text in the bottom of page 14 where the upscaling should not necessarily be explained in terms of discretized distributions and velocities, in particular given the formulae that follow (Eqs. 2.1 through 2.5). Then, it has not been quite clear for me whether, for the implicit source term *Q(φ)* in Eq. 2.22, the introduction of a shifted distribution does indeed remove the implicitness, the more so that the iterative process suggested in page 23 seems to indicate the contrary (?). It is appreciated that the 2^{nd} order of accuracy is achieved but the scheme stays implicit, right? Finally, the presentation of the LBM features in Fig. 2.5 in terms of advantages only, and no drawbacks, is simply unfair w.r.t. other CFD approaches; see also the remark below about the results of Sec. 9.3.4.

Chapter 6 is very short and contains a rather standard material on the energy conservation equation and various forms of it, mostly known from basic fluid mechanics courses. In my opinion, if there is a need to recall (some of) these equations in the PhD document, then they may rather be shifted to Appendix.

Chapter 7 (of a bit imprecise title) touches one of the difficulties of LBM: how to design ingredients of the approach (evolution equations, weights, equilibrium distributions) so that a given macroscopic balance equation is recovered from the mesoscopic simulations? Here again, the material is interesting but demanding to read and it would be welcome to present it with more care, in more detail and to better structure the contents, in particular the description of the five ways. Also, it is not clear whether the contents of this chapter are relevant for other parts of the PhD document or rather refer to some plans for future developments, such as conjugate heat transfer modelling.

As already stated above, a proper formulation of boundary conditions (Ch. 8), consistent with the approximation order of the discrete LB schemes in the bulk of the flow is a necessary condition to achieve a desired accuracy overall. In Eq. 8.5, there is a remark on proper boundary conditions in LBM, mentioning the LBM solution of turbulent boundary layer. As a more general curiosity (**Question 2**): how can the BC for a TBL look like? What are the achievements of LBM in predicting turbulent flows and how are (or how can be) turbulence models implemented in LBM?

The original findings of chapter 9 are very much appreciated, including the use of a collision operator based on cumulants, both for the fluid velocity and temperature fields. It may be noticed, however, that the benchmark cases considered in Secs. 9.3.1 to 9.3.3 do not involve the high Prandtl numbers (there are none, in fact). In Sec. 9.3.4, an extensive parametric study of flow past a heated cylinder at varying Pr is reported together with the resulting Nusselt numbers. The results are less precise than those resulting from a finite element solver (on a single mesh?) and seem to converge only slowly for higher Pr. Two remarks are in order here. First, the comparison in terms of Nu reported in Tab. 9.4 is unfair for the LBM, since a body-fitted and non-uniform mesh has been used in FEM, contrary to the regular lattice applied in LBM. An obvious consequence is approximate representation of the cylinder boundary as well as inadequate resolution of steep temperature gradients near the cylinder wall. In my opinion, a fair comparison of the Nu error level would need a similar length scale of the FE at the wall and of the LB lattice, obviously at the expense of degraded computational efficiency of LBM (**Question 3**: how do the CPU times of FEM and LBM compare for the same accuracy of results?). Second, the disparity of time scales for momentum and heat transfer, raised as an argument about high Pr flows, although true in general, seems inadequate for the low-Re flow past a heated body considered here, as such a flow is a steady one. Instead, one should rather refer to the disparity of length scales.

Chapter 10 is again a very short one (7 pages) and sketchy in style. In my opinion, it will be difficult to be understood by a reader not familiar with the phase field method for segregated two-phase systems. Also, it is not clear what are (if any) the original achievements of the Candidate? Finally, I cannot really agree with the statement about the *tanh* function as being used to smooth the interface. Rather, it represents the equilibrium solution of the phase field equation.

However, these remarks do not undermine my generally very positive opinion on the achievements reported in the present work.

4.2 Minor remarks, some misprints, etc.

These remarks refer to the points where more explanation is suggested for the sake of a better clarity, or misprints/mistakes have been spotted.

a) when introducing the WSIR equation system (p.5), the acronym is not immediately clear and its origin should be explained;

b) as a more general remark: notwithstanding the presence of the List of Symbols (which is never complete), for a streamlined reading it would be good to define the symbols, operators etc., at their first occurrence in the text (p.5, p.15ff);

c) several occurrences: “thorough” is used instead of “through”;

d) several occurrences: “refereed” (to) is used instead of “referred”;

e) Tab. 8.8: what are “narrow geometries”? – please be more precise;

f) p. 107: the second-line expression for *(abc)’* seems to be incorrect;

g) eq.11.30: what are the subscripts T there?

h) for the sake of completeness and for the Candidate’s convenience, some language slips (and misfortunate translations) in the scientific Polish need to be mentioned as well: “*solidyfikacja*” (*krzepnięcie*, p.6), “*ruch dystrybucji cząstek*” (p.6), “*prace porównawcze*” (*przeglądowe* - review papers, p.7), “*transfer momentu*” (!, p.8), “*kernele kolizyjne*” (*jądra zderzeń* – p.8), “*kolizja funkcji dystrybucji*” (p.10).

5. Final conclusion

The doctoral dissertation presented by Mr. Grzegorz Gruszczyński provides a proof of his good command of fluid thermomechanics in its theoretical aspects, creativity related to advanced lattice Boltzmann approach, the use of computational fluid dynamics tools, and applications to several flow problems including those of practical relevance. The thesis contains original analyses and novel findings beyond the state of the art. Given all the above, **my final conclusion about Mr. Grzegorz Gruszczyński being a doctoral candidate is positive and I recommend that he orally defends the PhD dissertation** with no reserve at all. Moreover, despite some concerns about the structure of the thesis, given (i) the degree of difficulty of the subject, (ii) the quality findings reported in the PhD work, listed in this review and published in renowned research journals, **I propose that the PhD thesis of Mr. Grzegorz Gruszczyński be awarded distinction** (*summa cum laude*).