Karlsruhe Institute of Technology

Institute for Applied and Numerical Mathematics 2
Mechanical Process Engineering and Mechanics
Lattice Boltzmann Research Group

PD Dr. Mathias J. Krause

Visiting Address:
Englerstr. 2, Bldg. 20.30
76131 Karlsruhe, Germany

Phone: +49 721-608-44191
Fax: +49 721-608-46679
Email: mathias.krause@kit.edu
Web: www.lbrg.kit.edu
www.openlb.net

Date: 2023-08-01

KIT-CS | IANM2 | Postfach 6980 | 76049 Karlsruhe, Germany

Warsaw University of Technology
Scientific Council of Mechanical Engineering
Prof. Robert Sinik, PhD, DSc.
ul. sw. A. Boboli 8
02-525 Warszawa
Poland

Report (review) for the doctoral dissertation of MSc. Grzegorz Marcin Gruszczynski with the title *Applications of the Lattice Boltzmann Method to solving advection-diffusion-reaction problems coupled with Navier-Stokes equations*

Personal Background

I know **M.Sc. Grzegorz Marcin Gruszczynski** form several talks at conferences on Lattice Boltzmann Methods (LBM), e.g. ICMMES 2022 in La Rochelle/France where I met him in person. In 2022 he was my guest in Karlsruhe at KIT for scientific exchange for a week, where he discussed various LBM related topics with my Master and PhD students. He also gave a talk on the analysis of LBM for solving an Advection Diffusion Reaction Equation (ADRE). Mr. Gruszczynski has started his PhD studies in 2017 at Warsaw University of Technology. He also worked for a private company during that time.

Scientific Background and Research Question

The pronounced aim of the thesis is to study the application of LBM to discretize and also simulate ADRE. It is aimed to be considered for various multi-physics fluid flow engineering problems whose governing equations are systems of Partial Differential Equations (PDE), coupling a Navier-Stokes Equation (NSE) with a particular ADRE. It is also started that by this thesis improvements of different existing LBM models are provided and that their numerical properties are compared. In particular, improvements for ADRE are aimed for the source term realization within LBM such that is leads to a second-order converging scheme in time and space. Mr. Gruszczynski also searches for stable and accurate LBM-based solutions for heat transfer problems at high Prandtl numbers. He aims at finding schemes which avoid numerical artefacts as dispersion errors known as wiggles. Finally, Mr. Gruszczynski researches ASRE in the context of phase field methods for the simulations of incompressible

Karlsruhe Institute of Technology

immiscible multi-component fluid flows with high density ratios, aiming at stable and Galilean-invariant schemes.

Scientific Content and Results Presented in the Thesis

Mr. Gruszczynski structures his thesis in 12 chapters, including an introduction (Chapter 1) and a summary (Chapter 12). Finally, references are given. An appendix is not provided. Altogether, his thesis has 238 pages. The doctoral dissertation is based on three publications where Mr. Gruszczynski is the first author. Their content is included in this thesis.

- Chapter 2 introduces LBM as general tool to discretize NSE and ADRE deriving it bottom up starting with the Boltzmann equation.
- Chapter 3 provides an overview of in the literature available LBM collision kernels.
- In **Chapter 4**, a novel second-order source term approach for LBM approaching the ADRE is introduced, analyzed for diffusive and acoustic scaling and tested for linear and non-linear test problems with source terms which dependent of the transported fields themselves. Illustrations of L2-norm errors are provided by isolines in a 2D map with special and temporal resolutions as axes. Although, the state-of-the-art is discussed in detail, a research gap is not stated explicitly. The key of Mr. Gruszczynski's approach is a closed form formulation and several approaches to solve the implicit source term formulation numerically. He applied it to a variety of common source terms, ranging from simple linear terms to Gompertz model and the Allen-Cahn equation. Using this implicit formulation in combination with an SRT and TRT LBM for ADRE second-order convergence is found by numerical experiments on both linear and non-linear source terms.
- The content of **Chapter 5** consists of the application of a particular ADRE to model epidemic population processes based on dividing a given population into three groups: susceptible (S), who may become ill; infected (I); and recovered (R). Again, in the beginning of the chapter an overview of the literature is provided not explicitly providing the research gap faced by Mr. Gruszczynski. He then introduces different kinds of SIR models, realizes them by an LBM for ADRE, applies them and discusses pros and cons.
- Chapter 6 introduces balance laws for conserving energy and entropy resulting in ADRE. It states the equations and introduces the notation used in the chapters following.
- Also the next chapter, Chapter 7, is of introducible charter. Here LBM schemes for ADRE are derived and different state-of-the-art approaches are reproduced.

Karlsruhe Institute of Technology

- State-of-the-art LBM boundary conditions are introduced in Chapter 8. Pros and cons are discussed.
- **Chapter 9** is another chapter, were Mr. Gruszczynski presents his own published work. Thermal flows are to be simulated at high Prandtl numbers. After a detailed review of the available literature, Mr. Gruszczynski states that the novelty of his approach lies in the application of a cumulant collision kernel to simulate the ADRE using a D3Q27 instead the usual D3Q7 stencil. By conducting numerical experiments, he analyses pros and cons. In particular, he concludes that to alleviate numerical artefacts raised by low conductivity, a D3Q27 stencil should be used and that for cumulant collision kernel require “proper treatment” of the higher moments “play a more important role than the application of second-order boundary conditions to represent a curved geometry.”
- In Chapter 10 the author introduces a phase field approach with Allen-Cahn equation as governing equation for multi-component incompressible immiscible fluid flows. It release on an approach of Geier et al. [229]. So this chapter is of introductory character.
- **Chapter 11** is dedicated to propose and evaluate a phase field approach with Allen-Cahn equation (see Chapter 11) solved by a cascaded collision operator. The approach is based on Fakhari et al. [230] and is claim to be novel by the employed cascaded collision operator. After a detailed literature review, Mr. Gruszczynski derives the central moments of the continuous equilibrium function such that the Galilean invariance is insured. The approach and its realization are first verified by considering the layered Poiseuille flow benchmark case for those an analytical solution exists and other benchmark cases with numerical results from the literature which were obtained by a highly resolving finite difference approach as well as other LBM approaches using MRT for example. Besides stability and Galilean invariance, occurring spurious are discussed as well as the obtained performances.

Evaluation of the Thesis

Mr. Gruszczynski clearly shows by his thesis that he is capable of working on a scientific task in depth and independently.

He presents a structured dissertation in which three major peer-reviewed publications are imbedded, surrounded by state-of-the-art summaries of physical models and numerical schemes. Sometimes, his own contributions are not clearly deviated from the state-of-the-art. Explicit statements are partly missing which would make his own work much easy to be followed.

Karlsruhe Institute of Technology

His scientific approach is application-oriented which discusses pros and cons of different solution approaches by means of many numerical experiments. He uses L2-errror norms and EOC studies to analyze them quantitatively. This is one of the strengths of his work, since in many other publications and theses that is often missing but crucially needed for scientific assessments – it is still not standard in engineering disciplines. Another strength is his particular choice of the considered benchmark problems which systematically increase in complexity.

From his findings, I particularly liked his innovative idea for keeping LBM for non-linear ADRE second-order accurate by an implicate formulation via a forcing term. Here, also the result presentation is nicely done -- the error presentation as isolines in Chapter 4 is very intuitive and insightful.

Overall, I see his scientific contributions to the field of LBM for solving ADRE for real problems as valuable and likely to motivate further new insights.

In Conclusion, the candidate MSc. Grzegorz Marcin Gruszczynski clearly showed his ability of critical analysis, synthesis, scientific maturity as well as his ability to put the results into perspective. The thesis manuscript is also of high scientific standard. I see his overall performances, evidenced by his thesis, to be of good quality.

I recommend a continuation of the doctoral procedure.

M. J. K

PD Dr. Mathias J. Krause