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The Lattice Boltzmann Method

Principles and Practice

Springer

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Preface

Interest in the lattice Boltzmann method has been steadily increasing since it grew out of lattice gas models in the late 1980s. While both of these methods simulate the flow of liquids and gases by imitating the basic behaviour of a gas—molecules move forwards and are scattered as they collide with each other—the lattice Boltzmann method shed the major disadvantages of its predecessor while retaining its strengths. Furthermore, it gained a stronger theoretical grounding in the physical theory of gases. These days, researchers throughout the world are attracted to the lattice Boltzmann method for reasons such as its simplicity, its scalability on parallel computers, its extensibility, and the ease with which it can handle complex geometries.

We, the authors, are all young researchers who did our doctoral studies on the lattice Boltzmann method recently enough that we remember well how it was to learn about the method. We remember particularly well the aspects that were a little difficult to learn; some were not explained in the literature in as clear and straightforward a manner as they could have been, and some were not explained in sufficient detail. Some topics were not possible to find in a single place: as the lattice Boltzmann method is a young but rapidly growing field of research, most of the information on the method is spread across many, many articles that may follow different approaches and different conventions. Therefore, we have sought to write the book that the younger versions of ourselves would have loved to have had during our doctoral studies: an easily readable, practically oriented, theoretically solid, and thorough introduction to the lattice Boltzmann method.

As the title of this book says, we have attempted here to cover both the lattice Boltzmann method's *principles*, namely, its fundamental theory, and its *practice*, namely, how to apply it in practical simulations. We have made an effort to make the book as readable to beginners as possible: it does not expect much previous knowledge except university calculus, linear algebra, and basic physics, ensuring that it can be used by graduate students, PhD students, and researchers from a wide variety of scientific backgrounds. Of course, one textbook cannot cover everything, and for the lattice Boltzmann topics beyond the scope of this book, we refer to the literature.

The lattice Boltzmann method has become a vast research field in the past 25 years. We cannot possibly cover all important applications in this book. Examples of systems that are often simulated with the method but are not covered here in detail are turbulent flows, phase separation, flows in porous media, transonic and supersonic flows, non-Newtonian rheology, rarefied gas flows, micro- and nanofluidics, relativistic flows, magnetohydrodynamics, and electromagnetic wave propagation.

We believe that our book can teach you, the reader, the basics necessary to read and understand scientific articles on the lattice Boltzmann method, the ability to run practical and efficient lattice Boltzmann simulations, and the insights necessary to start contributing to research on the method.

How to Read This Book

Every textbook has its own style and idiosyncrasies, and we would like to make you aware of ours ahead of time.

The main text of this book is divided into four parts. First, Chaps. 1 and 2 provide background for the rest of the book. Second, Chaps. 3–7 cover the fundamentals of the lattice Boltzmann method for fluid flow simulations. Third, Chaps. 8–12 cover lattice Boltzmann extensions, improvements, and details. Fourth, Chap. 13 focuses on how the lattice Boltzmann method can be optimised and implemented efficiently on a variety of hardware platforms. Complete code examples accompany this book and can be found at https://github.com/lbm-principles-practice.

For those chapters where it is possible, we have concentrated the basic practical results of the chapter into an “in a nutshell” summary early in the chapter instead of giving a summary at the end. Together, the “in a nutshell” sections can be used as a crash course in the lattice Boltzmann method, allowing you to learn the basics necessary to get up and running with a basic LB code in very little time. Additionally, a special section before the first chapter answers questions frequently asked by beginners learning the lattice Boltzmann method.

Our book extensively uses index notation for vectors (e.g. u_α) and tensors (e.g. $\sigma_{\alpha\beta}$), where a Greek index represents any Cartesian coordinate (x, y, or z) and repetition of a Greek index in a term implies summation of that term for all possible values of that index. For readers with little background in fluid or solid mechanics, this notation is fully explained, with examples, in Appendix A.1.

The most important paragraphs in each chapter are highlighted, with a few keywords in bold. The purpose of this is twofold. First, it makes it easier to know which results are the most important. Second, it allows readers to quickly and easily pick out the most central concepts and results when skimming through a chapter by reading the highlighted paragraphs in more detail.

Instead of gathering exercises at the end of each chapter, we have integrated them throughout the text. This allows you to occasionally test your understanding as you read through the book and allows us to quite literally leave certain proofs as "an exercise to the reader".

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Part I Background

Part II Lattice Boltzmann Fundamentals

Part III Lattice Boltzmann Extensions, Improvements, and Details

Part IV Numerical Implementation of the Lattice Boltzmann Method

Acronyms

ADE	Advection-diffusion equation
BB	Bounce-back
BC	Boundary condition
BGK	Bhatnagar-Gross-Krook (see also SRT)
CBC	Characteristic boundary condition
CFD	Computational fluid dynamics
CPU	Central processing unit
DdQq	d-dimensional set of q velocities
DPD	Dissipative particle dynamics
DSMC	Direct simulation Monte Carlo
ECC	Error-correcting code
FD(M)	Finite difference (method)
FE(M)	Finite element (method)
FV(M)	Finite volume (method)
GPU	Graphics processing unit
HP	Hermite polynomial
HPC	High-performance computing
IBB	Interpolated bounce-back
IBM	Immersed boundary method
LB(M/E)	Lattice Boltzmann (method/equation)
LBGK	Lattice BGK (i.e. LBM with BGK collisions)
LG(M/A)	Lattice gas (model/automaton)
MD	Molecular dynamics
MEA	Momentum exchange algorithm
Mlups	Million lattice updates per second
MPC	Multiparticle collision
MPI	Message-passing interface
MRT	Multiple relaxation time
NEBB	Non-equilibrium bounce-back (also called Zou-He)
NRBC	Nonreflecting boundary condition
NS(E)	Navier-Stokes (equations)

ODE	Ordinary differential equation
PDE	Partial differential equation
PML	Perfectly matched layer
PSM	Partially saturated method
RAM	Random access memory
SBB	Simple bounce-back
SPH	Smoothed-particle hydrodynamics
SRD	Stochastic rotation dynamics
SRT	Single relaxation time (see also BGK)
TRT	Two relaxation time
WSS	Wall shear stress

Frequently Asked Questions

Certain questions come up particularly frequently from people who are learning the lattice Boltzmann method. We have listed and answered many of these questions here, with references to the relevant book sections.

Getting Started

Q: How do I learn the basics of the LBM as quickly as possible?
A: We suggest referring to our summary sections, namely Sects. 3.2 and 3.3 for a general intro, Sect. 5.1 for an intro to boundary conditions, and Sect. 6.1 for an intro to forces.

Q: Why write vector quantities as, e.g. u_α instead of $\boldsymbol{u}$?
A: This index notation style is common in fluid mechanics due to its expressiveness; see Appendix A.1.

Q: How do I implement the LBM?
A: We cover this briefly and simply in Sect. 3.3 and cover it in more depth in Chap. 13.

Q: What is a “lattice”, and how do I choose a good one?
A: Lattices, or velocity sets, are discussed in Sect. 3.4.7.

Q: Do you have some simple example code to help me get started?
A: We do, in Chap. 13 and at https://github.com/lbm-principles-practice.

Q: How do we convert between physical units and simulation “lattice” units?
A: This is explained in Sect. 7.1.

Q: How do I choose the simulation parameters?
A: Section 7.2 deals with this question.

Q: How do I implement a body force (density)?
A: We cover this in Chap. 6.

Q: How can I use the LBM to simulate steady incompressible flow?
A: You need to ensure that Ma^2 is small, or you can use the incompressible equilibrium covered in Sect. 4.3.2.

Q: How do I simulate heat diffusion and thermal flows?
A: LBM for heat flow is covered in Sect. 8.4.

Q: How can I model multiphase or multicomponent flows?
A: Chapter 9 covers multiphase and multicomponent flows.

Capabilities of the LBM

Q: When is LBM a good choice to solve the Navier-Stokes equation?
A: See Sect. 2.4 for a discussion.

Q: Is mass conserved in the LBM?
A: Mass is exactly conserved in the bulk fluid, but various types of boundary conditions may still not conserve mass (cf. Sect. 5.4.2).

Q: Since the Boltzmann equation describes gas dynamics, why can the LBM also be used to simulate liquids?
A: As shown in Sect. 4.1.4, the LBM behaves macroscopically like the Navier-Stokes equations, which describe the motion of both gases and liquids.

Q: What is Galilean invariance, and is it obeyed by the LBM?
A: Galilean invariance states that physical laws are the same in any inertial reference frame. An $O(u^3)$ error term (cf. Sect. 4.1) in the standard LBM, due to the minimal discretisation of velocity space (cf. Sect. 3.4), means that it is not obeyed in the LBM. However, with a good choice of the simulation's inertial frame, this is seldom an issue except for simulations with large flow velocity variations.

Boundary Conditions

Q: Where in the LBM algorithm are boundary conditions applied?
A: See Sect. 5.1.

Q: What is the difference between "fullway" and "halfway" bounce-back?
A: This is explained in Sect. 5.3.3. In this book, we almost exclusively consider halfway bounce-back due to its additional benefits.

Q: When using a no-slip boundary condition, where exactly in the system is no-slip enforced?
A: The location depends on the type of no-slip boundary condition employed: see Fig. 5.7 and Sect. 5.2.4.

Q: How can an open inflow or outflow boundary be simulated?
A: This is explained in Sect. 5.3.5.

Q: How are boundary conditions handled at 2D or 3D corners?
A: See Sects. 5.3.6 and 5.4.4.

Q: How can I implement curved boundaries instead of "staircase" boundaries?
A: This is covered in Chap. 11.

Q: What kind of boundary conditions is used for advection-diffusion LBM?
A: See Sect. 8.5.

Q: How do I compute the momentum exchange between fluid and walls?
A: See Sect. 5.4.3 for straight boundaries and Sect. 11.2.1 for more complex cases.

Pressure and Compressibility

Q: Why do I have sound waves in my simulations?
A: The LBM solves the *compressible* Navier-Stokes equations, which allow sound waves; see Sects. 12.1 and 12.3.

Q: Why is my pressure field not as accurate as the velocity field?
A: Sound waves generated in your system (cf. Sect. 12.3) may be reflected back into the system by its velocity or density boundary conditions. See Sect. 12.4 for more on this.

Q: Why is the speed of sound not exactly $1/\sqrt{3}$ in my simulation?
A: $1/\sqrt{3}$ is the "ideal" speed of sound in LB simulations. The actual sound speed in simulations is affected by viscosity and discretisation error. See Sect. 12.2.

Q: Assuming the simulated fluid is an ideal gas, what is its heat capacity ratio γ?
A: We explain in Sect. 1.1.3 that $\gamma = 1$ in the simulated isothermal fluid and that γ is rarely relevant in nonthermal simulations.

Advanced Questions

Q: How is the lattice Boltzmann equation derived?
A: We show the derivation in Sects. 3.4 and 3.5.

Q: What is the basis of the Boltzmann equation?
A: We explain this in Sect. 1.3.

Q: How can we prove that the lattice Boltzmann equation can be used to simulate the Navier-Stokes equations?
A: This can be shown through the Chapman-Enskog analysis covered in Sect. 4.1, and can furthermore be validated by simulations of concrete cases.

Q: How can I evaluate the stress tensor locally?
A: You can compute it from f_i^{neq} as shown in (3.6).

Q: What is the Hermite expansion?
A: We answer this in Sect. 3.4.

Q: What is the advantage of advanced collision operators?
A: We explain their benefits in Chap. 10.

Q: What other collision operators are available?
A: Other than the BGK operator covered in Chap. 3 and the MRT and TRT operators covered in Chap. 10, we have a short overview with references at the end of Sect. 10.1.

Q: My code seems to be slow. How can I accelerate it?
A: See Chap. 13 for advice on implementation and efficiency.

Q: How do I implement a parallelised code?
A: See Chap. 13 for implementation advice.

Q: There are many forcing schemes around. Which one should I take?
A: We compare different forcing schemes in Sect. 6.4.

Q: How can I increase the accuracy or stability of my simulations without significantly increasing the simulation time?
A: We have guidelines for increasing stability in Sect. 4.4.4 and for accuracy in Sect. 4.5.6. You can also use TRT or MRT collision operators instead of BGK; see Chap. 10.

Q: Why is the LBM equilibrium truncated to $O(u^2)$?
A: This is explained in Sect. 3.4.

Q: How can I get in touch with the book authors, e.g. to ask a question or to point out a mistake I found?
A: You can send an email to authors@lbmbook.com.