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Elements of the Lattice Boltzmann Method I: Linear Advection Equation

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Abstract. This paper opens a series of papers aimed at finalizing the development of the lattice Boltzmann method for complex hydrodynamic systems. The lattice Boltzmann method is introduced at the elementary level of the linear advection equation. Details are provided on lifting the target macroscopic equations to a kinetic equation, and, after that, to the fully discrete lattice Boltzmann scheme. The over-relaxation method is put forward as a cornerstone of the second-order temporal discretization, and its enhancement with the use of the entropy estimate is explained in detail. A new asymptotic expansion of the entropy estimate is derived, and implemented in the sample code. It is shown that the lattice Boltzmann method provides a computationally efficient way of numerically solving the advection equation with a controlled amount of numerical dissipation, while retaining positivity.

Key words: Lattice Boltzmann method; implicit schemes; advection; entropy; invariant manifold; kinetic theory.

1 Introduction

One of the most important achievements in the physical sciences is that many phenomena become understandable if one succeeds to recognize a particles' picture behind it. Particles (point masses) are the gift of Newton's classical mechanics. The corpuscular picture of light enabled Planck and Einstein to pioneer quantum mechanics. Some particle-based

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programs established links between different fields of science, and explained phenomenology on a simpler (particle-based) level. Such are the achievements of Gibbs, Boltzmann, Hilbert and Enskog who linked thermodynamics and fluid dynamics to the particles' dynamics. Some others programs still require further effort as, for example, eddy viscosity models of fluid turbulence dating back to Prandtl.

Computational physics is a large 'laboratory' where particles are used as an ingredient for the creation of numerical methods. Computational physics is led by efficiency and accuracy of computations; thus, in many situations 'good' computational particles are only remote relatives of the 'true' physical particles. These notes are about the lattice Boltzmann method (LBM) for solving partial differential equations. LBM evolved from a particles' picture of lattice gas automata, something which only barely resembles physical particles. For the history of the lattice Boltzmann the reader is directed to the book [1]. We believe that many of the readers of this paper have either heard of the keyword 'lattice Boltzmann method' or have their own experience about using a lattice Boltzmann scheme in some problem. This paper intends to shed some light on the lattice Boltzmann method for a newcomer.

The best way to explain a method or idea is to address a small understandable problem, and to consider in full detail how the method works to solve it. Certainly, one should not forget that once things are cleaned up on the level of a toy problem, different new ideas might be (and usually are) required when stepping into a 'real' problem. Yet, intuition gained from solving small problems can be of substantial help.

We have chosen the simplest possible equation - the linear advection equation in one spatial direction. While this is indeed a simple equation, it is often used to discuss numerical methods for solving partial differential equations. The problem of creating accurate and efficient numerical schemes for solving the linear advection equation is not simple at all. In this paper we systematically introduce the lattice Boltzmann scheme for the advection equation.

The linear advection equation is used as a showcase in order to highlight some elements of the lattice Boltzmann schemes, especially those which contribute to certain, probably unique, features of these schemes. The presentation therefore differs significantly from other expositions of LBM. After introducing the lifting of the advection equation to a kinetic system with three velocities (Section 2), and explaining how to tune the equilibrium in order to recover the advection equation from it (Section 3), we proceed directly to the heart of the lattice Boltzmann schemes, the over-relaxation mechanism of temporal discretization (Section 4). We discuss this in detail, and explain how entropy enters the game in order to control positivity of the particle's populations (Section 6). We derive a new asymptotic expansion of the entropy estimate. A sample code is provided in order to illustrate how a lattice Boltzmann code looks in practice, and how to incorporate the entropy estimate into it.

In the first place, we tried to make a 'demo-tour' over the lattice Boltzmann terrain without making it too technical. We also tried to make it possible for a reader to compile a concise glossary of notions used in kinetic theory; all of these notions are illustrated